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Optizelle v1.2.0

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Introduction

Optizelle [op-tuh-zel] is an open source software library designed to solve general purpose nonlinear optimization problems of the form

Unconstrained		Equali	ty Constrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
		st	g(x) = 0
Inequa	ality Constrained	C	onstrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
st	$h(x) \succeq 0$	st	$g(x) = 0$ $h(x) \succ 0$
			$h(x) \succeq 0$

It features

• State of the art algorithms

- Unconstrained steepest descent, preconditioned nonlinear-CG (Fletcher-Reeves, Polak-Ribiere, Hestenes-Stiefel), BFGS, Newton-CG, SR1, trust-region Newton, Barzilai-Borwein two-point approximation
- Equality constrained inexact composite-step SQP.
- Inequality constrained primal-dual interior point method for cone constraints (linear, secondorder cone, and semidefinite), log-barrier method for cone constraints
- Constrained any combination of the above

• Open source

- Released under the 2-Clause BSD License
- Free and ready to use with both open and closed sourced commercial codes
- Multilanguage support
 - Interfaces to C++, MATLAB/Octave, and Python
- Robust computations and repeatability
 - Can stop, archive, and restart the computation from any optimization iteration
 - Combined with the multilanguage support, the optimization can be started in one language and migrated to another. For example, archived optimization runs that started in Python can be migrated and completed in C++.
- User-defined parallelism
 - Fully compatible with OpenMP, MPI, or GPUs

• Extensible linear algebra

- Supports user-defined vector algebra and preconditioners
- Enables sparse, dense, and matrix-free computations
- Ability to define custom inner products and compatibility with preconditioners such as algebraic multigrid make Optizelle well-suited for PDE constrained optimization

• Sophisticated Control of the Optimization Algorithms

 Allows the user to insert arbitrary code into the optimization algorithm, which enables custom heuristics to be embedded without modifying the source. For example, in signal processing applications, the optimization iterates could be run through a band-pass filter at the end of each optimization iteration.

1.1 Licensing

Optizelle is copyrighted by OptimoJoe and licensed under the 2-Clause BSD License:

BSD 2-Clause License Copyright 2013-2016 OptimoJoe. Copyright 2012-2013 Sandia Corporation. Under the terms of Contract DE-AC04-94AL85000 with Sandia Corporation, the U.S. Government retains certain rights in this software. All rights reserved. Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met: 1. Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer. 2. Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution. THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT HOLDER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

In short, Optizelle is free to use in both open and closed sourced codes. If you do so, we ask that you provide a citation or link to http://www.optimojoe.com.

1.2 Support

News, updates, and download information for Optizelle can be found at

http://www.optimojoe.com/products/optizelle

Our user forum can be found at

http://forum.optimojoe.com

Finally, if you are interested in paid support and consulting, please contact us at contact@optimojoe.com.

1.3 Brief example

In order to see a short example of Optizelle in action, consider the unconstrained minimization of the Rosenbrock function

$$\min_{x \in \mathbb{R}^2} \quad (1 - x_1)^2 + 100(x_2 - x_1^2)^2.$$

In order to optimize this function, we use the following code and parameters, which generates the subsequent output.

```
Language
               C++
Code
               // In this example, we setup and minimize the Rosenbrock function.
               #include <vector>
               #include <iostream>
               #include <string>
               #include <cstdlib>
               #include "optizelle/optizelle.h"
               #include "optizelle/vspaces.h"
               #include "optizelle/json.h"
               //---Objective0---
               // Squares its input
               template <typename Real>
               Real sq(Real x){
                   return x*x;
               }
               // Define the Rosenbrock function where
               11
               // f(x,y)=(1-x)^2+100(y-x^2)^2
               //
               struct Rosenbrock
                   : public Optizelle::ScalarValuedFunction <double,Optizelle::Rm>
               ſ
                   typedef Optizelle::Rm <double> X;
                   // Evaluation of the Rosenbrock function
                   double eval(X::Vector const & x) const {
                       return sq(1.-x[0])+100.*sq(x[1]-sq(x[0]));
                   }
                   // Gradient
                   void grad(
                       X::Vector const & x,
                       X::Vector & grad
                   ) const {
                       grad[0] = -400.*x[0]*(x[1]-sq(x[0]))-2.*(1.-x[0]);
                       grad[1]=200.*(x[1]-sq(x[0]));
                   }
                   // Hessian-vector product
                   void hessvec(
                       X::Vector const & x,
                       X::Vector const & dx,
                       X::Vector & H_dx
                   ) const {
                       H_dx[0] = (1200.*sq(x[0])-400.*x[1]+2)*dx[0]-400.*x[0]*dx[1];
```

```
H_dx[1] = -400.*x[0]*dx[0]+200.*dx[1];
   }
}:
//---Objective1---
//---Preconditioner0---
// Define a perfect preconditioner for the Hessian
struct RosenHInv :
   public Optizelle::Operator <double,Optizelle::Rm,Optizelle::Rm>
ſ
public:
   typedef Optizelle::Rm <double> X;
   typedef X::Vector X_Vector;
private:
   X_Vector& x;
public:
   RosenHInv(X::Vector& x_) : x(x_) {}
   void eval(X_Vector const & dx,X_Vector & result) const {
       auto one_over_det=1./(80000.*sq(x[0])-80000.*x[1]+400.);
       result[0]=one_over_det*(200.*dx[0]+400.*x[0]*dx[1]);
       result[1]=one_over_det*
           (400.*x[0]*dx[0]+(1200.*x[0]*x[0]-400.*x[1]+2.)*dx[1]);
   }
};
//---Preconditioner1---
int main(int argc, char* argv[]){
   // Read in the name for the input file
   if(argc!=2) {
       std::cerr << "rosenbrock <parameters>" << std::endl;</pre>
       exit(EXIT_FAILURE);
   }
   auto fname = argv[1];
   //---State0---
   // Generate an initial guess for Rosenbrock
   auto x = std::vector <double> {-1.2, 1.};
   // Create an unconstrained state based on this vector
   Optizelle::Unconstrained <double,Optizelle::Rm>::State::t state(x);
   //---State1---
   //---Parameters0---
   // Read the parameters from file
   Optizelle::json::Unconstrained <double,Optizelle::Rm>::read(fname,state);
   //---Parameters1---
   //---Functions0---
   // Create the bundle of functions
   Optizelle::Unconstrained <double,Optizelle::Rm>::Functions::t fns;
   fns.f.reset(new Rosenbrock);
   fns.PH.reset(new RosenHInv(state.x));
   //---Functions1---
   //---Solver0---
   // Solve the optimization problem
   Optizelle::Unconstrained <double,Optizelle::Rm>::Algorithms
```

```
::getMin(Optizelle::Messaging::stdout,fns,state);
    //---Solver1---
   //---ExtractO---
   // Print out the reason for convergence
   std::cout << "The algorithm converged due to: " <<</pre>
       Optizelle::OptimizationStop::to_string(state.opt_stop) <<</pre>
       std::endl;
    // Print out the final answer
   std::cout << "The optimal point is: (" << state.x[0] << ','</pre>
       << state.x[1] << ')' << std::endl;
    //---Extract1---
    // Write out the final answer to file
   Optizelle::json::Unconstrained <double,Optizelle::Rm>::write_restart(
       "solution.json",state);
    // Successful termination
   return EXIT_SUCCESS;
}
```

```
Language
                Python
Code
                # In this example, we setup and minimize the Rosenbrock function.
                import Optizelle
                import numpy
                import sys
                #---Objective0---
                # Squares its input
                sq = lambda x:x*x
                # Define the Rosenbrock function where
                #
                # f(x,y)=(1-x)^{2}+100(y-x^{2})^{2}
                #
                class Rosenbrock(Optizelle.ScalarValuedFunction):
                   # Evaluation of the Rosenbrock function
                   def eval(self,x):
                       return sq(1.-x[0])+100.*sq(x[1]-sq(x[0]))
                    # Gradient
                    def grad(self,x,grad):
                       grad[0] = -400 * x[0] * (x[1] - sq(x[0])) - 2*(1-x[0])
                       grad[1]=200*(x[1]-sq(x[0]))
                    # Hessian-vector product
                    def hessvec(self,x,dx,H_dx):
                       H_dx[0] = (1200*sq(x[0])-400*x[1]+2)*dx[0]-400*x[0]*dx[1]
                       H_dx[1] = -400 * x[0] * dx[0] + 200 * dx[1]
                #---Objective1---
                #---Preconditioner0---
                # Define a perfect preconditioner for the Hessian
```

```
class RosenHInv(Optizelle.Operator):
                   def eval(self,state,dx,result):
                       x = state.x
                       one_over_det=1./(80000.*sq(x[0])-80000.*x[1]+400.)
                       result[0]=one_over_det*(200.*dx[0]+400.*x[0]*dx[1])
                       result[1]=(one_over_det*
                          (400.*x[0]*dx[0]+(1200.*x[0]*x[0]-400.*x[1]+2.)*dx[1]))
               #---Preconditioner1---
               # Read in the name for the input file
               if len(sys.argv)!=2:
                   sys.exit("python rosenbrock.py <parameters>")
               fname = sys.argv[1]
               #---State0---
               # Generate an initial guess for Rosenbrock
               x = numpy.array([-1.2, 1.0])
               # Create an unconstrained state based on this vector
               state=Optizelle.Unconstrained.State.t(Optizelle.Rm,x)
               #---State1---
               #---Parameters0---
               # Read the parameters from file
               Optizelle.json.Unconstrained.read(Optizelle.Rm,fname,state)
               #---Parameters1---
               #---Functions0---
               # Create the bundle of functions
               fns=Optizelle.Unconstrained.Functions.t()
               fns.f=Rosenbrock()
               fns.PH=RosenHInv()
               #---Functions1---
               #---Solver0---
               # Solve the optimization problem
               Optizelle.Unconstrained.Algorithms.getMin(
                   Optizelle.Rm,Optizelle.Messaging.stdout,fns,state)
               #---Solver1---
               #---Extract0---
               # Print out the reason for convergence
               print "The algorithm converged due to: %s" \% (
                   Optizelle.OptimizationStop.to_string(state.opt_stop))
               # Print out the final answer
               print "The optimal point is: (%e,%e)" % (state.x[0],state.x[1])
               #---Extract1---
               # Write out the final answer to file
               Optizelle.json.Unconstrained.write_restart(Optizelle.Rm, "solution.json", state)
Language
               MATLAB/Octave
               \% In this example, we setup and minimize the Rosenbrock function.
```

```
8
```

function rosenbrock(fname)

Code

```
% Read in the name for the input file
   if nargin ~=1
       error('rosenbrock <parameters>');
   end
   % Execute the optimization
   main(fname);
end
%---Objective0---
% Squares its input
function z = sq(x)
   z=x*x;
end
\% Define the Rosenbrock function where
%
% f(x,y)=(1-x)^2+100(y-x^2)^2
%
function self = Rosenbrock()
   % Evaluation of the Rosenbrock function
   self.eval = @(x) sq(1.-x(1))+100.*sq(x(2)-sq(x(1)));
   % Gradient
   self.grad = @(x) [
       -400.*x(1)*(x(2)-sq(x(1)))-2.*(1.-x(1));
       200.*(x(2)-sq(x(1)))];
   % Hessian-vector product
   self.hessvec = @(x,dx) [
       (1200.*sq(x(1))-400.*x(2)+2)*dx(1)-400.*x(1)*dx(2);
       -400.*x(1)*dx(1)+200.*dx(2)];
end
%---Objective1---
%---Preconditioner0---
\% Define a perfect preconditioner for the Hessian
function self = RosenHInv()
   self.eval = @(state,dx) eval(state,dx);
end
function result = eval(state,dx)
   x = state.x;
   one_over_det=1./(80000.*sq(x(1))-80000.*x(2)+400.);
   result = [
       one_over_det*(200.*dx(1)+400.*x(1)*dx(2));
       one_over_det*...
           (400.*x(1)*dx(1)+(1200.*x(1)*x(1)-400.*x(2)+2.)*dx(2))];
end
%---Preconditioner1---
% Actually runs the program
function main(fname)
   % Grab the Optizelle library
   global Optizelle;
   setupOptizelle();
```

```
%----State0----
   % Generate an initial guess for Rosenbrock
   x = [-1.2;1.];
   % Create an unconstrained state based on this vector
   state=Optizelle.Unconstrained.State.t(Optizelle.Rm,x);
   %---State1---
   %---Parameters0---
   % Read the parameters from file
   state=Optizelle.json.Unconstrained.read(Optizelle.Rm,fname,state);
   %---Parameters1---
   %---Functions0---
   % Create the bundle of functions
   fns=Optizelle.Unconstrained.Functions.t;
   fns.f=Rosenbrock();
   fns.PH=RosenHInv();
   %---Functions1---
   %---Solver0---
   % Solve the optimization problem
   state = Optizelle.Unconstrained.Algorithms.getMin( ...
       Optizelle.Rm,Optizelle.Messaging.stdout,fns,state);
   %---Solver1---
   %---Extract0---
   % Print out the reason for convergence
   fprintf('The algorithm converged due to: %s\n', ...
       Optizelle.OptimizationStop.to_string(state.opt_stop));
   % Print out the final answer
   fprintf('The optimal point is: (%e,%e)\n',state.x(1),state.x(2));
   %---Extract1---
   % Write out the final answer to file
   Optizelle.json.Unconstrained.write_restart( ...
       Optizelle.Rm, 'solution.json',state);
and
```

	end			
Language	Optizelle Pa	rameters		
Code	"iter	lle" :{ level" :1, c_max" :50, trunc" :1e-	-12	
Language	Optizelle Ou	ıtput		
Code	iter 1	f(x) 2.42e+01	<mark>grad</mark> 2.33e+02	dx

2

4.73e+00 4.64e+00 3.81e-01

	4.73e+00	4.64e+00	1.00e+00
3	4.00e+00	1.74e+01	5.00e-01
4	3.34e+00	2.33e+01	5.00e-01
5	2.58e+00	8.77e+00	2.04e-01
	2.58e+00	8.77e+00	4.91e-01
6	2.09e+00	8.48e+00	2.45e-01
7	1.65e+00	9.60e+00	2.45e-01
8	1.22e+00	5.00e+00	1.46e-01
9	9.64e-01	9.06e+00	2.13e-01
10	6.22e-01	1.77e+00	1.10e-01
	6.22e-01	1.77e+00	3.44e-01
11	4.40e-01	4.42e+00	1.72e-01
12	2.81e-01	3.72e+00	1.68e-01
13	1.71e-01	3.60e+00	1.72e-01
14	9.43e-02	3.58e+00	1.80e-01
15	4.49e-02	2.47e+00	1.60e-01
16	1.82e-02	2.40e+00	1.58e-01
17	5.16e-03	1.02e+00	1.11e-01
18	8.94e-04	7.81e-01	9.41e-02
19	4.86e-05	1.17e-01	3.89e-02
20	2.49e-07	1.55e-02	1.36e-02
21	7.47e-12	4.80e-05	7.98e-04
22	7.06e-21	2.62e-09	5.63e-06
The	algorithm converg	ed due to:	${\tt GradientSmall}$
The	optimal point is:	(1,1)	

1.4 History

Optizelle originated in 2010 as a code called PEOpt (Parameter Estimation Using Optimization) written by Joseph Young at Sandia National Laboratories. There, it was used as the computational driver for a variety of both internal and external customers. Due to the scale of the problems involved and the nuances of high-performance computing environments, PEOpt was designed specifically to integrate with large, existing code bases as quickly and unobtrusively as possible. Later, Sandia approved the open source release of PEOpt on two separate occasions in 2012 and 2013 under the 2-Clause BSD License. It was from this released code that Joseph continued work on Optizelle through a new company called OptimoJoe.

In the following chapter, we discuss how to download, build, and incorporate Optizelle into a new project.

2.1 Downloading

Optizelle can be downloaded from

http://www.optimojoe.com/products/optizelle

in a variety of precompiled packages. Here, we also provide direct access to our source code repository.

2.2 Installing and Uninstalling

The installation method depends on the platform, but generally involves opening the installer and following the specified instructions

WINDOWS Open the installer	Windows	Open the installer
-----------------------------------	---------	--------------------

- macOS 1. Open the installer
 - 2. Drag the Optizelle folder to Applications
 - 3. Copy the file

/Applications/Optizelle/share/optizelle/com.optimojoe.optizelle.plist to

/Library/LaunchAgents/

4. Close the Terminal application if open and reboot

Note, we summarize these steps and provide additional information in the ReadMe.txt file provided after opening the installer.

- Linux/Unix 1. Unzip the tar.gz file to a local directory or use the appropriate package manager to install the rpm or deb package directly
 - 2. Add /some/path/share/optizelle/matlab to the MATLABPATH
 - 3. Add /some/path/share/optizelle/octave to the OCTAVE_PATH
 - 4. Add /some/path/share/optizelle/python to the PYTHONPATH

where /some/path denotes the Optizelle install location. By default, the deb and rpm files install Optizelle to /usr/local/. Note, on most Linux distributions, we add a variable to the path by adding

export SOMEVARIABLE=\$SOMEVARIABLE:NEWPATH

to the file ~/.bashrc. In other words, if we install Optizelle to /usr/local, we add the following to text ~/.bashrc

export MATLABPATH=\$MATLABPATH:/usr/local/share/optizelle/matlab export OCTAVE_PATH=\$OCTAVE_PATH:/usr/local/share/optizelle/octave export PYTHONPATH=\$PYTHONPATH:/usr/local/share/optizelle/python

Remember to execute **source** ~/.bashrc on all active shells, log out and back in, or reboot for the changes to take affect.

Similar to installation, how we uninstall Optizelle depends on the platform

Windows	Click the menus Start \rightarrow Settings \rightarrow System \rightarrow Apps & features \rightarrow Optizelle \rightarrow Uninstall
macOS	 Drag the folder /Applications/Optizelle to the trash Drag the file /Library/LaunchAgents/com.optimojoe.optizelle.plist to the trash
Linux/Unix	 When installed locally using the tar.gz package, delete the installation folder When installed using the rpm or deb packages, use the package manager to remove Optizelle Delete any modifications to the path made in the file ~/.bashrc or other similar configuration file

2.3 Dependencies

Depending on its configuration, Optizelle uses the following software packages

Package	Version	License	C++	Python	MATLAB	Octave	Docs	Windows
Optizelle	1.2.0	BSD	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
JsonCpp	0.10.6	Public	\checkmark	\checkmark	\checkmark	\checkmark		\checkmark
BLAS/LAPACK	3.5.0	BSD	\checkmark	\checkmark	\checkmark	\checkmark		\checkmark
CMake	3.1	BSD	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
WiX	3.10	MS-RL						\checkmark
GCC	4.9	GPL	\checkmark	\checkmark	\checkmark	\checkmark		\checkmark
TeX Live	2014	Various					\checkmark	
Python	2.7	Python		\checkmark				
NumPy	1.10	BSD		\checkmark				
MATLAB	R2016a	Custom			\checkmark			
JSONlab	1.0-RC1	BSD			\checkmark	\checkmark		
Octave	4.0	GPL				\checkmark		

Note, we generally depend on GCC for both its C++ and Fortran compiler, but an alternative compiler such as Clang works as well. Since we do not modify GCC, the GCC Runtime Library Exception applies. In addition, Optizelle remains compatible with most high-performance varieties of BLAS and LAPACK.

2.4 Building

Optizelle uses CMake as its build system. On Linux, Unix, macOS, Cygwin, or MSYS, execute the following commands from the base Optizelle directory:

- 1. mkdir build
- $2. \ {\rm cd} \ {\rm build}$
- 3. ccmake ..
- 4. Configure the build.

 $5. \ {\tt make}$

On Windows, if not using Cygwin or MSYS, execute the following commands:

- 1. Using Windows Explorer, create a directory called build in the base Optizelle directory.
- 2. Run cmake-gui.exe
- 3. Set the source directory to the base Optizelle directory.
- 4. Set the build directory to the build folder created above.
- 5. Configure the build.
- 6. Build the code (make with Cygwin or MSYS.)

Rather than using ccmake, we can also run cmake directly in order to configure the build. This allows us to skip the CMake menu system and configure Optizelle directly, which can be advantageous when compiling Optizelle on multiple, but similar systems. In order to accomplish this, we execute a command such as

cmake \

```
-DENABLE_OPENMP:BOOL=ON \
-DENABLE_BUILD_JSONCPP:BOOL=ON \
-DJSONCPP_ARCHIVE:FILEPATH=/path/to/jsoncpp.zip \
-DENABLE_BUILD_BLAS_AND_LAPACK:BOOL=ON \
-DLAPACK_ARCHIVE:FILEPATH=/path/to/lapack.tgz \
-DENABLE_CPP_EXAMPLES:BOOL=ON \
-DENABLE_CPP_UNIT:BOOL=ON \
-DENABLE_PYTHON:BOOL=ON \
-DENABLE_PYTHON_EXAMPLES:BOOL=ON \
-DENABLE_PYTHON_UNIT:BOOL=ON \
-DENABLE_MATLAB:BOOL=ON \
-DMATLAB_EXECUTABLE:FILEPATH=/path/to/matlab \
-DMATLAB_INCLUDE_DIR:PATH=/path/to/extern/include \
-DMATLAB_LIBRARY:FILEPATH=/path/to/bin/glnxa64/libmex.so \
-DMATLAB_MEX_EXTENSION:STRING=mexa64 \
-DENABLE_MATLAB_EXAMPLES:BOOL=ON \
-DENABLE_MATLAB_UNIT:BOOL=ON \
-DENABLE_OCTAVE:BOOL=ON \
-DOCTAVE_EXECUTABLE:FILEPATH=/path/to/octave \
-DOCTAVE_INCLUDE_DIR:PATH=/path/to/octave \
-DOCTAVE_LIBRARY:FILEPATH=/path/to/liboctinterp.so \
-DENABLE_OCTAVE_EXAMPLES:BOOL=ON \
-DENABLE_OCTAVE_UNIT:BOOL=ON \
-DENABLE_BUILD_JSONLAB:BOOL=ON \
-DJSONLAB_ARCHIVE:FILEPATH=/path/to/jsonlab.zip \
```

where the actual paths, libraries, and archives depend on the individual system. Generally, we put this command inside a shell script or batch file in order to make it easier to edit. As far as the available options, we list them in the next section.

After building Optizelle, installation is as simple as executing

make install

from the CMake build directory using GNU Make, MSYS, or Cygwin. If using a different Make utility, call it on the install target. For a complete list of installed files, see

install_manifest.txt

located in the CMake build directory. After installation via make install, we must also

- 1. Add /some/path/share/optizelle/matlab to the MATLABPATH
- 2. Add /some/path/share/optizelle/octave to the <code>OCTAVE_PATH</code>
- 3. Add /some/path/share/optizelle/python to the PYTHONPATH

where <code>/some/path</code> denotes the path found in the <code>CMAKE_INSTALL_PREFIX</code> configuration variable described below. How we set environment variables depends on the platform

Windows	Modify each environment variable via the sequence
	1. Open File Explorer
	2. Right click This PC
	 Click the menus Advanced System Settings → System Properties → Environment Variables → New (if the variable doesn't exist) or Edit (if the variable does exist)
	4. Modify PATH with C:\some\path\lib and C:\some\path\share\optizelle\thirdparty\lib
	5. Modify MATLABPATH with C:\some\path\share\optizelle\matlab
	6. Modify OCTAVE_PATH with C:\some\path\share\optizelle\octave
	7. Modify PYTHONPATH with C:\some\path\share\optizelle\python
	where C:\some\path denotes the installation path found in the CMake variable CMAKE_INSTALL_PREFI
macOS	Add a plist file to /Library/LaunchAgents or ~/Library/LaunchAgents. For exam-
	<pre>ple</pre>
Linux/Unix	When using the Bash shell, we add
	export MATLABPATH=\$MATLABPATH:/some/path/share/optizelle/matlab export OCTAVE_PATH=\$OCTAVE_PATH:/some/path/share/optizelle/octave export PYTHONPATH=\$PYTHONPATH:/some/path/share/optizelle/python

to ~/.bashrc where /some/path denotes the installation path found in the CMake variable CMAKE_INSTALL_PREFIX. Note, we must also execute the command source ~/.bashrc on all active shells, log out and back in, or reboot for the changes to take affect.

As a final note, CMake does not provide a native uninstallation process when installing Optizelle in this manner. Nevertheless, on Linux, Unix, macOS, MSYS, or Cygwin, the command

xargs rm < install_manifest.txt</pre>

will remove the installation. Also, don't forget to remove each of the environment variables added in the above installation process.

2.5 Configuring

Optizelle provides several different options within CMake in order to customize the build. We describe these flags in the table below:

Flag	CMAKE_INSTALL_PREFIX
Type	РАТН
Default	Varies
Dependency	None
Enables	None
Autodetect?	No
Description	Install location of Optizelle.
Flag	ENABLE_DOCUMENTATION
Туре	BOOL
Default	OFF
Dependency	None
Enables	PDFLATEX_COMPILER, ENABLE_A4_PAPER
Autodetect?	No
Description	Enables the build of the Optizelle manual from the LaTeX source. It builds a pdf file of the manual.
Flag	PDFLATEX_COMPILER
Type	FILEPATH
Default	None
Dependency	ENABLE_DOCUMENTATION
Enables	None
Autodetect?	Yes
Description	Complete path and executable for pdflatex.

Flag	ENABLE_A4_PAPER
Туре	BOOL
Default	OFF
Dependency	ENABLE_DOCUMENTATION
Enables	None
Autodetect?	No
Description	When ON, the manual uses A4 paper. Otherwise, the manual uses Letter paper.
Description	When on, the manual uses 114 paper. Otherwise, the manual asso herer paper.
Flag	ENABLE_CPP
Туре	BOOL
Default	OFF
Dependency	None
Enables	CMAKE_CXX_FLAGS, CMAKE_BUILD_TYPE, ENABLE_OPENMP, ENABLE_BUILD_BLAS_AND_LAPACK, ENABLE_BUILD_JSONCPP, BLAS_LIBRARY, LAPACK_LIBRARY, JSONCPP_INCLUDE_DIR, JSONCPP_LIBRARY, ENABLE_CPP_EXAMPLES, ENABLE_CPP_UNIT, ENABLE_PYTHON, ENABLE_MATLAB, ENABLE_OCTAVE
Autodetect?	No
Description	Enables the Optizelle C++ library.
Flag	CMAKE_CXX_FLAGS
Flag Type	CMAKE_CXX_FLAGS STRING
-	
Туре	STRING
Type Default	STRING None
Type Default Dependency	STRING None ENABLE_CPP
Type Default Dependency Enables	STRING None ENABLE_CPP None
Type Default Dependency Enables Autodetect?	STRING None None No
Type Default Dependency Enables Autodetect?	STRING None None No
Type Default Dependency Enables Autodetect? Description	STRING None No C++ compiler specific flags.
Type Default Dependency Enables Autodetect? Description	STRING None ENABLE_CPP None CH++ compiler specific flags. CMAKE_BUILD_TYPE
Type Default Dependency Enables Autodetect? Description Flag Type	STRING None None No CMAKE_BUILD_TYPE STRING
Type Default Dependency Enables Autodetect? Description Flag Type Default	STRING None None No CMAKE_BUILD_TYPE STRING None
Type Default Dependency Enables Autodetect? Description Flag Type Default Dependency	STRING None ENABLE_CPP None C++ compiler specific flags. STRING None STRING None ENABLE_CPP
Type Default Dependency Enables Autodetect? Description Flag Type Default Dependency Enables	STRING None ENABLE_CPP No C++ compiler specific flags. CMAKE_BUILD_TYPE STRING None ENABLE_CPP None
Type Default Dependency Enables Autodetect? Description Flag Type Default Dependency Enables Autodetect?	STRING None ENABLE_CPP None C++ compiler specific flags. CMAKE_BUILD_TYPE STRING None ENABLE_CPP None String None CHARE_CPP String Stri

Туре	BOOL
Default	OFF
Dependency	ENABLE_CPP
Enables	None
Autodetect?	No
Description	Enable OpenMP/threaded support for the default, dense vector spaces. Note, many BLAS and LAPACK libraries such as those from ATLAS benefit from OpenMP directives.
Flag	ENABLE_BUILD_BLAS_AND_LAPACK
Type	BOOL
Default	OFF
Dependency	ENABLE_CPP
Enables	LAPACK_ARCHIVE
Autodetect?	No
Description	Builds BLAS and LAPACK from source in case an optimized version is not available.
Flag	LAPACK_ARCHIVE
Туре	FILEPATH
Default	None
Dependency	ENABLE_BUILD_BLAS_AND_LAPACK
Enables	None
Autodetect?	No
Description	Location of the LAPACK archive downloaded from Netlib.
Flag	ENABLE_BUILD_JSONCPP
\mathbf{Type}	BOOL
Default	OFF
Dependency	ENABLE_CPP
Enables	JSONCPP_ARCHIVE
Autodetect?	
11400400000	No
Description	
	No
	No
Description	No Builds JsonCpp from source.

Dependency	ENABLE_BUILD_JSONCPP	
Enables	None	
Autodetect?	No	
Description	Location of the JsonCpp archive downloaded from GitHub.	
Flag	BLAS_LIBRARY	
Type	FILEPATH	
Default	None	
Dependency	ENABLE_CPP	
Enables	None	
Autodetect?	Yes	
Description	A semicolon separated list of the complete path and library used to provide BLAS. This must include all required libraries in order to successfully compile a BLAS dependent application. For example, using ATLAS BLAS, one possible entry is:	

/usr/lib/libf77blas.a;/usr/lib/libatlas.a

Flag	LAPACK_LIBRARY	
Type	FILEPATH	
Default	None	
Dependency	ENABLE_CPP	
Enables	None	
Autodetect?	Yes	
Description	A semicolon separated list of the complete path and library used to provide LA-PACK. This must include all required libraries, except for BLAS libraries specified in BLAS_LIBRARY , in order to successfully compile a LAPACK dependent application. For example, using ATLAS LAPACK, one possible entry is:	
	/usr/lib/liblapack.a;/usr/lib/libgfortran.a	
	Note, this example assumes that we include libatlas.a in our BLAS_LIBRARY filepath.	
Flag	JSONCPP_INCLUDE_DIR	
Type	РАТН	
Default	None	

Delault	None
Dependency	ENABLE_CPP
Enables	None
Autodetect?	Yes
Description	A path that indicates where the jsoncpp headers have been installed. The actual headers must be found in <code>\$JSONCPP_INCLUDE_DIR/json/</code>

Flag	JSONCPP_LIBRARY		
Туре	FILEPATH		
Default	None		
Dependency	ENABLE_CPP		
Enables	None		
Autodetect?	Yes		
Description	Complete path and library for JsonCpp.		
Flag	ENABLE_CPP_EXAMPLES		
Type	BOOL		
Default	OFF		
Dependency	ENABLE_CPP		
Enables	None		
Autodetect?	No		
Description	Enables the build and installation of simple examples that demonstrate the use of Optizelle.		
Flag	ENABLE_CPP_UNIT		
Flag Type	ENABLE_CPP_UNIT BOOL		
_			
Туре	BOOL		
Type Default	BOOL OFF		
Type Default Dependency	BOOL OFF ENABLE_CPP		
Type Default Dependency Enables	BOOL OFF ENABLE_CPP None		
Type Default Dependency Enables Autodetect?	BOOL OFF ENABLE_CPP None No Enables the build of unit tests that help validate the Optizelle code. Execute these		
Type Default Dependency Enables Autodetect?	BOOL OFF ENABLE_CPP None No Enables the build of unit tests that help validate the Optizelle code. Execute these		
Type Default Dependency Enables Autodetect? Description	BOOL OFF ENABLE_CPP None No Enables the build of unit tests that help validate the Optizelle code. Execute these unit tests by running ctest in the CMake build directory.		
Type Default Dependency Enables Autodetect? Description	BOOL OFF ENABLE_CPP None No Enables the build of unit tests that help validate the Optizelle code. Execute these unit tests by running ctest in the CMake build directory.		
Type Default Dependency Enables Autodetect? Description	BOOL OFF ENABLE_CPP None No Enables the build of unit tests that help validate the Optizelle code. Execute these unit tests by running ctest in the CMake build directory.		
Type Default Dependency Enables Autodetect? Description Flag Type Default	BOOL OFF ENABLE_CPP None No Enables the build of unit tests that help validate the Optizelle code. Execute these unit tests by running ctest in the CMake build directory. ENABLE_PYTHON BOOL OFF		
Type Default Dependency Enables Autodetect? Description Flag Type Default Dependency	BOOL OFF ENABLE_CPP None No Enables the build of unit tests that help validate the Optizelle code. Execute these unit tests by running ctest in the CMake build directory. ENABLE_PYTHON BOOL OFF ENABLE_CPP PYTHON_INCLUDE_DIR, PYTHON_LIBRARY, PYTHON_EXECUTABLE, ENABLE_PYTHON_EXAMPLES,		
Type Default Dependency Enables Autodetect? Description Flag Type Default Dependency Enables	BODL OFF ENABLE_CPP None No Enables the build of unit tests that help validate the Optizelle code. Execute these unit tests by running ctest in the CMake build directory. ENABLE_PYTHON BOOL OFF BOOL PYTHON_LIBERARY, PYTHON_EXECUTABLE, ENABLE_PYTHON_EXAMPLES, ENABLE_PYTHON_UNIT		

.

TypeFILEPATHDefaultNoneDependencyENABLE_PYTHONAutodetect?NoneAutodetect?YesDescriptionApath that indicates where the Python 2.7 headers have been installed. We do not be prevenee of the python 2.1 headers and the
DependencyENABLE_PYTHONEnablesNoneAutodetect?YesDescriptionA path that indicates where the Python 2.7 headers have been installed. We do not
EnablesNoneAutodetect?YesDescriptionA path that indicates where the Python 2.7 headers have been installed. We do not
Autodetect?YesDescriptionA path that indicates where the Python 2.7 headers have been installed. We do not
Description A path that indicates where the Python 2.7 headers have been installed. We do not
Flag PYTHON_LIBRARY
Type FILEPATH
Default None
Dependency ENABLE_PYTHON
Enables None
Autodetect? Yes
Description Complete path and library for Python 2.7.
Flag PYTHON_EXECUTABLE
Type FILEPATH
Default None
Dependency ENABLE_PYTHON
Enables None
Autodetect? Yes
Description Complete path and executable for Python 2.7.
Flag ENABLE_PYTHON_EXAMPLES
Type BOOL
Default OFF
Dependency ENABLE_PYTHON
Enables None
Autodetect? No
Description Enables the build and installation of simple examples that demonstrate the use of the Python wrappers for Optizelle.
Flag ENABLE_PYTHON_UNIT
Type BOOL

Default	OFF		
Dependency	ENABLE_PYTHON		
Enables	None		
Autodetect?	No		
Description	Enables the build of unit tests that help validate the Python wrappers for the Optizelle code. Execute these unit tests by running ctest in the CMake build directory.		
Flag	ENABLE_MATLAB		
Type	BOOL		
Default	OFF		
Dependency	ENABLE_CPP		
Enables	MATLAB_MEX_EXTENSION, MATLAB_INCLUDE_DIR, MATLAB_LIBRARY, MATLAB_EXECUTABLE, ENABLE_BUILD_JSONLAB, JSONLAB_DIR, ENABLE_MATLAB_EXAMPLES, ENABLE_MATLAB_UNIT		
Autodetect?	No		
Description	Enables the build of the MATLAB wrappers for Optizelle.		
Flag	MATLAB_MEX_EXTENSION		
\mathbf{Type}	STRING		
Default	None		
Dependency	ENABLE_MATLAB		
Enables	None		
Autodetect?	No		
Description	Extension of mex files on the system. This can be found by typing in the command 'mexext' inside of MATLAB.		
Flag	MATLAB_INCLUDE_DIR		
Туре	FILEPATH		
Default	None		
Dependency	ENABLE_MATLAB		
Enables	None		
Autodetect?	Yes		
Description	Path that indicates where the MATLAB header mex.h has been installed. We do not prefix these headers, so we look directly in the directory provided here. Generally, this is generally the extern/include directory inside the primary MATLAB directory.		
Flag	ΜΑΤΊ ΔΕ Ι ΤΒΡΑΡΥ		

Flag MATLAB_LIBRARY

Туре	FILEPATH	
Default	None	
Dependency	ENABLE_MATLAB	
Enables	None	
Autodetect?	Yes	
Description	Complete path and library for MATLAB, mex. Sometimes, we have to include the mx library as well. If compilation fails and there are several undefined symbols with prefixed with mx, then add the mx library and separate it from mex with a semicolon. Generally, these libraries are generally found nested within the bin directory in the primary MATLAB folder.	
Flag	MATLAB_EXECUTABLE	
Туре	FILEPATH	
Default	None	
Dependency	ENABLE_MATLAB	
Enables	None	
Autodetect?	No	
Description	Complete path and executable for MATLAB.	
Flag	ENABLE_MATLAB_EXAMPLES	
Type	BOOL	
Default	OFF	
Dependency	ENABLE_MATLAB	
Enables	None	
Autodetect?	No	
Description	Enables the build and installation of simple examples that demonstrate the use of the MATLAB wrappers for Optizelle.	
Flag	ENABLE_MATLAB_UNIT	
Туре	BOOL	
Default	OFF	
Dependency	ENABLE_MATLAB	
Enables	None	
Autodetect?	No	
Description	Enables the build of unit tests that help validate the MATLAB wrappers for the Optizelle code. Execute these unit tests by running ctest in the CMake build directory.	

TypeBOOLDefaultOFFDependencyENABLE_CPPEnablesOCTAVE_INCLUDE_DIR, OCTAVE_LIBRARY, OCTAVE_EXECUTABLE ENABLE_BUILD_JSONLAB, ENABLE_OCTAVE_UNITAutodetect?No		
Dependency ENABLE_CPP Enables OCTAVE_INCLUDE_DIR, OCTAVE_LIBRARY, ENABLE_BUILD_JSONLAB, SONLAB_DIR OCTAVE_EXECUTABLE ENABLE_OCTAVE_EXAMPLES, ENABLE_OCTAVE_UNIT JSONLAB_DIR		
Enables OCTAVE_INCLUDE_DIR, ENABLE_BUILD_JSONLAB, ENABLE_OCTAVE_EXAMPLES, ENABLE_OCTAVE_UNIT OCTAVE_EXECUTABLE JSONLAB_DIF		
ENABLE_BUILD_JSONLAB, JSONLAB_DIF ENABLE_OCTAVE_EXAMPLES, ENABLE_OCTAVE_UNIT		
Autodetect? No		
Description Enables the build of the Octave wrappers for Optizelle.		
Flag OCTAVE_INCLUDE_DIR		
Type FILEPATH		
Default None		
Dependency ENABLE_OCTAVE		
Enables None		
Autodetect? Yes		
Description Path that indicates where the Octave header mex.h has been installed. We do not prefix these headers, so we look directly in the directory provided here. Generally, this is the folder called octave-x.x.x/octave inside the system include directory where x.x.x denotes the version number.	\mathbf{s}	
Flag OCTAVE_LIBRARY		
Type FILEPATH		
Default None		
Dependency ENABLE_OCTAVE		
Enables None		
Autodetect? Yes		
Description Complete path and library for Octave, octinterp. Generally, this library is found nested within the octave directory inside the system lib directory.	Complete path and library for Octave, octinterp. Generally, this library is found	
Flag OCTAVE_EXECUTABLE		
FlagOCTAVE_EXECUTABLETypeFILEPATH		
Type FILEPATH		
TypeFILEPATHDefaultNone		
TypeFILEPATHDefaultNoneDependencyENABLE_OCTAVE		

Flag	ENABLE_OCTAVE_EXAMPLES		
Туре	BOOL		
Default	OFF		
Dependency	ENABLE_OCTAVE		
Enables	None		
Autodetect?	No		
Description	Enables the build and installation of simple examples that demonstrate the use of the		
-	Octave wrappers for Optizelle.		
Flag	ENABLE_OCTAVE_UNIT		
Type	BOOL		
Default	OFF		
Dependency	ENABLE_OCTAVE		
Enables	None		
Autodetect?	No		
Description	Enables the build of unit tests that help validate the Octave wrappers for the Optizelle		
	code. Execute these unit tests by running ctest in the CMake build directory.		
Flag	ENABLE BUILD_JSONLAB		
Flag Type	ENABLE_BUILD_JSONLAB		
Туре	BOOL		
Type Default			
Туре	BOOL OFF		
Type Default Dependency	BOOL OFF ENABLE_MATLAB or ENABLE_OCTAVE		
Type Default Dependency Enables	BOOL OFF ENABLE_MATLAB OF ENABLE_OCTAVE JSONLAB_ARCHIVE		
Type Default Dependency Enables Autodetect?	BOOL OFF ENABLE_MATLAB OF ENABLE_OCTAVE JSONLAB_ARCHIVE No		
Type Default Dependency Enables Autodetect?	BOOL OFF ENABLE_MATLAB OF ENABLE_OCTAVE JSONLAB_ARCHIVE No		
Type Default Dependency Enables Autodetect? Description	BOOL OFF ENABLE_MATLAB OF ENABLE_OCTAVE JSONLAB_ARCHIVE No Builds jsonlab from source.		
Type Default Dependency Enables Autodetect? Description	BOOL OFF ENABLE_MATLAB OR ENABLE_OCTAVE JSONLAB_ARCHIVE No Builds jsonlab from source.		
Type Default Dependency Enables Autodetect? Description Flag Type	BOOL OFF ENABLE_MATLAB OR ENABLE_OCTAVE JSONLAB_ARCHIVE Builds jsonlab from source. JSONLAB_ARCHIVE FILEPATH		
Type Default Dependency Enables Autodetect? Description Flag Type Default	BOOL OFF ENABLE_MATLAB or ENABLE_OCTAVE JSONLAB_ARCHIVE No Builds jsonlab from source. JSONLAB_ARCHIVE FILEPATH None		
Type Default Dependency Enables Autodetect? Description Flag Type Default Dependency	BOOL OFF ENABLE_MATLAB OF ENABLE_OCTAVE JSONLAB_ARCHIVE No JSONLAB_ARCHIVE JSONLAB_ARCHIVE FILEPATH None ENABLE_BUILD_JSONLAB		
Type Default Dependency Enables Autodetect? Description Flag Type Default Dependency Enables	BOOL OFF ENABLE_MATLAB OF ENABLE_OCTAVE ISONLAB_ARCHIVE No Builds jsonlab from source. JSONLAB_ARCHIVE FILEPATH None ENABLE_BUILD_JSONLAB		
Type Default Dependency Enables Autodetect? Description Flag Type Default Dependency Enables Autodetect?	BOOL OFF ENABLE_MATLAB OR ENABLE_OCTAVE SONLAB_ARCHIVE No Builds jsonlab from source. JSONLAB_ARCHIVE FILEPATH None ENABLE_BUILD_JSONLAB None		

Type	PATH
Default	None
Dependency	ENABLE_MATLAB or ENABLE_OCTAVE
Enables	None
Autodetect?	Yes
Description	A path that indicates where the jsonlab library has been installed. This is automatically set when ENABLE_BUILD_JSONLAB is enabled.

2.6 Platform Specific Configuration

Due to a variety of platform specific quirks, some additional compilation flags may be necessary. In order to use these flags, place them in the CMAKE_CXX_FLAGS variable, separated by spaces, in the CMake configuration.

Flag	-include math.h		
Platform	Windows		
Interface	Python		
Indication	During compilation, error: '::hypot' has not been declared		
Description	Fixes a bug inside of Python where hypot has been renamed		
Flag	-DMS_WIN64		
Platform	Windows		
Interface	Python		
	During compilation, undefined reference to 'imp_Py_InitModule4'		
Indication	$\label{eq:completion} During \ compilation, \ \texttt{undefined reference to `\imp_Py_InitModule4'}$		

Basic API

We organize Optizelle's algorithms into four different categories:

Unconstrained	Equality Constrained
$\min_{x \in X} f(x)$	$\min_{x \in X} f(x)$
	st $g(x) = 0$
Inequality Constrained	Constrained
$\min_{x \in X} f(x)$	$\min_{x \in X} f(x)$
st $h(x) \succeq 0$	st $g(x) = 0$
	$h(x) \succeq 0$

Since these formulations necessitate different algorithms, we segregate the overall structure of Optizelle and the algorithms themselves into these categories. In order to optimize these formulations, we follow the general procedure:

- 1. Import Optizelle
- 2. Import or define the appropriate vector spaces
- 3. Define the objective function
- 4. (Optional) Define the constraints
- 5. (Optional) Define the preconditioners
- 6. Create the optimization state
- 7. Set the optimization parameters
- 8. Accumulate the functions
- 9. Call the optimization solver
- 10. Extract the solution
- 11. Compile/run the program

We discuss how to implement each of the above steps below.

3.1 Import Optizelle

Each interface uses its own method to import Optizelle:

Language C++

Code	<pre>#include "optizelle/optizelle.h" #include "optizelle/vspaces.h" #include "optizelle/json.h"</pre>
Language	Python
Code	<pre>import Optizelle</pre>

Language	MATLAB/Octave
Code	global Optizelle
	<pre>setupOptizelle();</pre>

In C++, we always require optizelle/optizelle.h, but only require optizelle/json.h when working with JSON and optizelle/vspaces.h when using our default vector spaces such as Optizelle::Rm and Optizelle::SQL. In Python, we simply need to include the Optizelle module and everything else is automatically imported. Finally, in MATLAB/Octave, we encapsulate all of the required functions in the global variable Optizelle.

3.2 Import or define the appropriate vector spaces

In the optimization problems

U	nconstrained	Equali	ty Constrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
$x \in \Lambda$		$x \in X$ st	g(x) = 0
Inequa	lity Constrained	С	onstrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
st	$h(x) \succeq 0$	st	g(x) = 0
			$h(x) \succeq 0$

we require that

$$f: X \to \mathbb{R}$$
$$g: X \to Y$$
$$h: X \to Z.$$

Here, the spaces X, Y, and Z denote vector spaces, more specifically, Hilbert spaces. For most problems, these vector spaces just denote \mathbb{R}^m , but we also allow these vector spaces to be spaces of functions such as $L^2(\Omega)$ or matrices such as $\mathbb{R}^{m \times n}$ as long as they contain the necessary operations that we describe in the section Customized vector spaces. A vector space consists of two separate pieces: the actual vector and the operations required to compute on this vector. In Optizelle, we maintain this separation. For \mathbb{R}^m , we provide a reasonable implementation of the vector space with the following:

Language	C++
Vector	std::vector
Operations	Optizelle::Rm
Language	C++

Vector	numpy.array
Operations	Optizelle.Rm
Language	MATLAB/Octave
Vector	[] (column vector)
Operations	Optizelle.Rm

To be precise, each of these vector spaces uses the inner product $\langle x, y \rangle = x^T y$ and defines inequalities pointwise, $x \succeq y \iff x_i \ge y_i$ for all $1 \le i \le m$. Note, we don't require users to use these vector operations in their code. Simply, if we're happy using the above vectors, we can use these operations exclusively in Optizelle and forget their details.

3.3 Define the objective function

In the optimization problems

Unconstrained		Equali	ty Constrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
		st	g(x) = 0
Inequa	ality Constrained	C	onstrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
st	$h(x) \succeq 0$	st	g(x) = 0
			$h(x) \succeq 0$

the function $f: X \to \mathbb{R}$ denotes the *objective function*. Note, we restrict ourselves to scalar-valued functions and do not consider multi-objective optimization problems. In order to optimize with this function, we require information about its evaluation and derivatives. Specifically, we require its evaluation, f(x), and gradient, $\nabla f(x)$. In order to use second-order algorithms, we also require the Hessian-vector product, $\nabla^2 f(x) \delta x$. In the case that $f: \mathbb{R}^m \to \mathbb{R}$, we can obtain each of these quantities from its partial derivatives. Specifically, we write

$$f(x) = f(x_1, \ldots, x_m).$$

Then, we have that

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x) \\ \vdots \\ \frac{\partial f}{\partial x_m}(x) \end{bmatrix},$$
$$\nabla^2 f(x) \delta x = \begin{bmatrix} \frac{\partial f}{\partial x_{11}}(x) & \dots & \frac{\partial f}{\partial x_{1m}}(x) \\ \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial x_{m1}}(x) & \dots & \frac{\partial f}{\partial x_{mm}}(x) \end{bmatrix} \delta x.$$

In code, we specify this function as:

Language	C++
Structure	Optizelle::ScalarValuedFunction
Interface	Inheritance
Code	<pre>namespace Optizelle{ // A scalar valued function interface, f : X -> R template < typename Real, template <typename> class XX</typename></pre>

	<pre>> struct ScalarValuedFunction { // Create some type shortcuts typedef XX <real> X; typedef typename X::Vector Vector; // <- f(x) virtual Real eval(Vector const & x) const = 0; // grad = grad f(x) virtual void grad(Vector const & x,Vector & grad) const = 0; // H_dx = hess f(x) dx</real></pre>	
	<pre>virtual void hessvec(Vector const & x,Vector const & dx,Vector & H_dx)</pre>	
Language	Python	
Structure	Optizelle.ScalarValuedFunction	
Interface	Inheritance	
Code	<pre>class ScalarValuedFunction(object): """A simple scalar valued function interface, f : X -> R""" def _err(self,fn): """Produces an error message for an undefined function""" raise Exception.t("%s function is not defined in a " % (fn) + "ScalarValuedFunction")</pre>	
	<pre>def eval(self,x): """<- f(x)""" _err(self,"eval") def grad(self,x,grad): """<- grad f(x)""" _err(self,"grad") def hessvec(self,x,dx,H_dx): """<- hess f(x) dx""" _err(self,"grad")</pre>	
Language	MATLAB/Octave	

Interface Members present

Note, we require that the Hessian-vector product always be present. If one is not available, we simply return zero. As an example, in our Rosenbrock example, we minimize the function $f : \mathbb{R}^2 \to \mathbb{R}$ where

$$f(x) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2.$$

This function has a gradient of

$$\nabla f(x) = \begin{bmatrix} -400x_1(x_2 - x_1^2) - 2(1 - x_1) \\ 200(x_2 - x_1^2) \end{bmatrix}$$

and Hessian-vector product of

$$\nabla^2 f(x)\delta x = \begin{bmatrix} 1200x_1^2 - 400x_2 + 2 & -400x_1 \\ -400x_1 & 200 \end{bmatrix} \delta x.$$

Using Optizelle's internal vector spaces, we implement these functions as:

```
Language
               C++
Code
               // Squares its input
               template <typename Real>
               Real sq(Real x){
                   return x*x;
               }
               // Define the Rosenbrock function where
               11
               // f(x,y)=(1-x)^2+100(y-x^2)^2
               11
               struct Rosenbrock
                   : public Optizelle::ScalarValuedFunction <double,Optizelle::Rm>
               {
                   typedef Optizelle::Rm <double> X;
                   // Evaluation of the Rosenbrock function
                   double eval(X::Vector const & x) const {
                       return sq(1.-x[0])+100.*sq(x[1]-sq(x[0]));
                   }
                   // Gradient
                   void grad(
                       X::Vector const & x,
                       X::Vector & grad
                   ) const {
                       grad[0] = -400.*x[0]*(x[1]-sq(x[0]))-2.*(1.-x[0]);
                       grad[1]=200.*(x[1]-sq(x[0]));
                   }
                   // Hessian-vector product
                   void hessvec(
                       X::Vector const & x,
```

```
X::Vector const & dx,
X::Vector & H_dx
) const {
    H_dx[0]=(1200.*sq(x[0])-400.*x[1]+2)*dx[0]-400.*x[0]*dx[1];
    H_dx[1]=-400.*x[0]*dx[0]+200.*dx[1];
};
```

```
Language
               Python
Code
               # Squares its input
               sq = lambda x:x*x
               # Define the Rosenbrock function where
               #
               # f(x,y)=(1-x)^2+100(y-x^2)^2
               #
               class Rosenbrock(Optizelle.ScalarValuedFunction):
                   # Evaluation of the Rosenbrock function
                   def eval(self,x):
                       return sq(1.-x[0])+100.*sq(x[1]-sq(x[0]))
                   # Gradient
                   def grad(self,x,grad):
                       grad[0] = -400 * x[0] * (x[1] - sq(x[0])) - 2*(1-x[0])
                       grad[1]=200*(x[1]-sq(x[0]))
                   # Hessian-vector product
                   def hessvec(self,x,dx,H_dx):
                       H_dx[0] = (1200*sq(x[0])-400*x[1]+2)*dx[0]-400*x[0]*dx[1]
                       H_dx[1] = -400*x[0]*dx[0] + 200*dx[1]
Language
               MATLAB/Octave
Code
               % Squares its input
               function z = sq(x)
                   z=x*x;
               end
               % Define the Rosenbrock function where
               %
               % f(x,y)=(1-x)^2+100(y-x^2)^2
               %
               function self = Rosenbrock()
                   % Evaluation of the Rosenbrock function
                   self.eval = @(x) sq(1.-x(1))+100.*sq(x(2)-sq(x(1)));
                   % Gradient
                   self.grad = @(x) [
                       -400.*x(1)*(x(2)-sq(x(1)))-2.*(1.-x(1));
                       200.*(x(2)-sq(x(1)))];
                   % Hessian-vector product
```

```
self.hessvec = @(x,dx) [
    (1200.*sq(x(1))-400.*x(2)+2)*dx(1)-400.*x(1)*dx(2);
    -400.*x(1)*dx(1)+200.*dx(2)];
```

end

In our Simple equality constrained example, we have an objective $f: \mathbb{R}^2 \to \mathbb{R}$ where

$$f(x) = x_1^2 + x_2^2$$

This function has a gradient of

$$\nabla f(x) = \begin{bmatrix} 2x_1\\2x_2 \end{bmatrix}$$

and Hessian-vector product of

$$\nabla^2 f(x)\delta x = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \delta x.$$

We implement this function with the code:

```
C++
Language
Code
               // Squares its input
               template <typename Real>
               Real sq(Real const & x){
                   return x*x;
               }
               // Define a simple objective where
               11
               // f(x,y)=x^{2}+y^{2}
               11
               struct MyObj
                   : public Optizelle::ScalarValuedFunction <double,Optizelle::Rm>
                {
                   typedef Optizelle::Rm <double> X;
                   // Evaluation
                   double eval(X::Vector const & x) const {
                       return sq(x[0])+sq(x[1]);
                   }
                   // Gradient
                   void grad(
                       X::Vector const & x,
                       X::Vector & grad
                   ) const {
                       grad[0]=2.*x[0];
                       grad[1]=2.*x[1];
                   }
                   // Hessian-vector product
                   void hessvec(
                       X::Vector const & x,
                       X::Vector const & dx,
                       X::Vector & H_dx
                   ) const {
                       H_dx[0]=2.*dx[0];
                       H_dx[1]=2.*dx[1];
                   }
               };
```

```
Language
                Python
Code
                # Squares its input
                sq = lambda x:x*x
                # Define a simple objective where
                #
                # f(x,y)=x^{2}+y^{2}
                #
                class MyObj(Optizelle.ScalarValuedFunction):
                   # Evaluation
                   def eval(self,x):
                       return sq(x[0])+sq(x[1])
                   # Gradient
                   def grad(self,x,grad):
                       grad[0]=2.*x[0]
                       grad[1]=2.*x[1]
                   # Hessian-vector product
                   def hessvec(self,x,dx,H_dx):
                       H_dx[0]=2.*dx[0]
                       H_dx[1]=2.*dx[1]
                MATLAB/Octave
Language
Code
                % Squares its input
                function z = sq(x)
                   z=x*x;
                end
                \% Define a simple objective where
                %
                % f(x,y)=x^2+y^2
                %
                function self = MyObj()
                   % Evaluation
                   self.eval = @(x) sq(x(1))+sq(x(2));
                   % Gradient
                   self.grad = @(x) [ ...
                       2.*x(1); ...
                       2.*x(2)];
                   % Hessian-vector product
                   self.hessvec = @(x,dx) [ ...
                       2.*dx(1); \ldots
                       2.*dx(2)];
                end
```

3.4 (Optional) Define the constraints

In the optimization problems

U	Unconstrained		ty Constrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
$x \in A$		$x \in X$ st	g(x) = 0
Inequa	ality Constrained	C	onstrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
st	$h(x) \succeq 0$	st	g(x) = 0
			$h(x) \succeq 0$

the vector-valued functions $g: X \to Y$ and $h: X \to Z$ denote the equality and inequality constraints, respectfully. Here, we allow the equality constraints to be nonlinear, but require that the inequality constraints be affine. Recall, an affine function is one where $h(\alpha x + (1 - \alpha)x) = \alpha h(x) + (1 - \alpha)h(y)$ for all $\alpha \in \mathbb{R}$ or equivalently where h''(x) = 0. We require affine inequality constraints in order to simplify the line search that maintains the nonnegativity of the inequality constraints. In case we have a nonlinear inequality constraint, we must reformulate the problem in order to make it affine. The easiest method for doing so is through the reformulations

$$\begin{array}{cc} \min_{x \in X} & f(x) \\ \mathrm{st} & h(x) \succeq 0 \end{array} \right\} \rightsquigarrow \begin{cases} \min_{x \in X, z \in Z} & f(x) \\ \mathrm{st} & h(x) - z = 0 \\ & z \succeq 0 \end{cases}$$

and

$$\begin{array}{ccc} \min_{\substack{x \in X \\ \text{st} \\ n(x) \succeq 0 \end{array}} & f(x) \\ \text{st} & g(x) = 0 \\ h(x) \succeq 0 \end{array} \right\} \rightsquigarrow \begin{cases} \min_{\substack{x \in X, z \in Z \\ x \in X, z \in Z \end{array}} & f(x) \\ \text{st} & \begin{bmatrix} g(x) \\ h(x) - z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\ z \succeq 0. \end{cases}$$

Similar to the objective function, we require derivative information in order optimize effectively. Specifically, we require the evaluation, g(x), Fréchet (total) derivative applied to a vector, $g'(x)\delta x$, and the adjoint of the Fréchet derivative applied to a vector, $g'(x)^*\delta y$. In order to use second order algorithms, we also require the second derivative operation $(g''(x)\delta x)^*\delta y$. Note, we require the same operations from h, but since h is affine, $(h''(x)\delta x)^*\delta z = 0$. In the case that $g: \mathbb{R}^m \to \mathbb{R}^n$ and we use the inner product $\langle x, y \rangle = x^T y$ for both \mathbb{R}^m and \mathbb{R}^n , the derivation of these derivatives is quite simple. Here, we write g as

$$g(x) = \begin{bmatrix} g_1(x) \\ \vdots \\ g_n(x) \end{bmatrix}.$$

This means that we have

$$g'(x)\delta x = \begin{bmatrix} \nabla g_1(x)^T \\ \vdots \\ \nabla g_n(x)^T \end{bmatrix} \delta x$$
$$g'(x)^* \delta y = \begin{bmatrix} \nabla g_1(x) & \dots & \nabla g_n(x) \end{bmatrix} \delta y$$
$$(g''(x)\delta x)^* \delta y = \sum_{i=1}^n \delta y_i \nabla^2 g_i(x) \delta x.$$

In code, these derivatives become:

Language	C++
Structure	Optizelle::VectorValuedFunction
Interface	Inheritance

```
Code
               namespace Optizelle{
                   // A vector valued function interface, f : X -> Y
                   template <</pre>
                       typename Real,
                       template <typename> class XX,
                       template <typename> class YY
                   >
                   struct VectorValuedFunction {
                       // Create some type shortcuts
                       typedef XX <Real> X;
                       typedef typename X::Vector X_Vector;
                       typedef YY <Real> Y;
                       typedef typename Y::Vector Y_Vector;
                       // y=f(x)
                       virtual void eval(X_Vector const & x,Y_Vector & y) const = 0;
                        // y=f'(x)dx
                        virtual void p(
                           X_Vector const & x,
                           X_Vector const & dx,
                           Y_Vector & y
                        ) const = 0;
                        // z=f'(x)*dy
                        virtual void ps(
                           X_Vector const & x,
                           Y_Vector const & dy,
                           X_Vector & z
                        ) const= 0;
                        // z=(f','(x)dx)*dy
                        virtual void pps(
                           X_Vector const & x,
                           X_Vector const & dx,
                           Y_Vector const & dy,
                           X_Vector & z
                        ) const = 0;
                        // Allow a derived class to deallocate memory
                        virtual ~VectorValuedFunction() {}
                   };
               }
Language
               Python
Structure
               Optizelle.VectorValuedFunction
Interface
               Inheritance
Code
               class VectorValuedFunction(object):
                   """A vector valued function interface, f : X -> Y"""
                   def _err(self,fn):
                       """Produces an error message for an undefined function"""
                       raise Exception.t("%s function is not defined in a " % (fn) +
```

"VectorValuedFunction")

```
def eval(self,x,y):
    """y <- f(x)"""
    _err(self,"eval")

def p(self,x,dx,y):
    """y <- f'(x)dx"""
    _err(self,"p")

def ps(self,x,dx,z):
    """z <- f'(x)dx"""
    _err(self,"ps")

def pps(self,x,dx,dy,z):
    """z <- (f''(x)dx)*dy"""
    _err(self,"pps")</pre>
```

Language	MATLAB/Octave
Structure	Optizelle.VectorValuedFunction
Interface	Members present
Code	<pre>% A vector valued function interface, f : X -> Y err_vvf=@(x)error(sprintf(</pre>

Note, we require that the second derivative always be present. If one is not available, we simply return zero. For example, in our Simple equality constrained example, we define a simple equality constraint as

$$g(x) = [(x_1 - 2)^2 + (x_2 - 2)^2 - 1].$$

Then, we have that

$$g'(x)\delta x = \begin{bmatrix} 2(x_1 - 2) & 2(x_2 - 2) \end{bmatrix} \delta x$$
$$g'(x)^* \delta y = \begin{bmatrix} 2(x_1 - 2) \\ 2(x_2 - 2) \end{bmatrix} \delta y$$
$$(g''(x)\delta x)^* \delta y = \delta y \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \delta x$$

Using Optizelle's internal vector spaces, we implement these functions as:

```
typedef Optizelle::Rm <double> X;
    typedef Optizelle::Rm <double> Y;
   // y=g(x)
   void eval(
       X::Vector const & x,
       Y::Vector & y
   ) const {
       y[0] = sq(x[0]-2.)+sq(x[1]-2.)-1.;
   }
   // y=g'(x)dx
   void p(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector & y
   ) const {
       y[0] = 2.*(x[0]-2.)*dx[0]+2.*(x[1]-2.)*dx[1];
   }
   // xhat=g'(x)*dy
   void ps(
       X::Vector const & x,
       Y::Vector const & dy,
       X::Vector & xhat
   ) const {
       xhat[0] = 2.*(x[0]-2.)*dy[0];
       xhat[1] = 2.*(x[1]-2.)*dy[0];
   }
   // xhat=(g''(x)dx)*dy
   void pps(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector const & dy,
       X::Vector & xhat
   ) const {
       xhat[0] = 2.*dx[0]*dy[0];
       xhat[1] = 2.*dx[1]*dy[0];
   }
};
```

```
y[0] = 2.*(x[0]-2.)*dx[0]+2.*(x[1]-2.)*dx[1]
                   # xhat=g'(x)*dy
                   def ps(self,x,dy,xhat):
                       xhat[0] = 2.*(x[0]-2.)*dy[0]
                       xhat[1] = 2.*(x[1]-2.)*dy[0]
                   # xhat=(g''(x)dx)*dy
                   def pps(self,x,dx,dy,xhat):
                       xhat[0] = 2.*dx[0]*dy[0]
                       xhat[1] = 2.*dx[1]*dy[0]
Language
               MATLAB/Octave
Code
               % Define a simple equality constraint
                %
                % g(x,y) = [(x-2)^2 + (y-2)^2 = 1]
                %
                function self = MyEq()
                   % y=g(x)
                   self.eval = @(x) [ ... ]
                       sq(x(1)-2.)+sq(x(2)-2.)-1.];
                   % y=g'(x)dx
                   self.p = @(x,dx) [ \dots
                       2.*(x(1)-2.)*dx(1)+2.*(x(2)-2.)*dx(2)];
                   % xhat=g'(x)*dy
                   self.ps = @(x,dy) [ ...
                       2.*(x(1)-2.)*dy(1); ...
                       2.*(x(2)-2.)*dy(1)];
                   % xhat=(g''(x)dx)*dy
                   self.pps = @(x,dx,dy) [ ...
                       2.*dx(1)*dy(1); ...
                       2.*dx(2)*dy(1) ];
                end
```

3.5 (Optional) Define the preconditioners

Since Optizelle is fully matrix-free, its performance depends highly on the quality of the preconditioners provided to it by the user. To that end, there are two places where preconditioning matters: the Hessian of the objective function and a KKT system that relates to the equality constraints. Specifically, we benefit when we can define $P_H: X \to X$ such that

$$P_H \approx \nabla^2 f(x)^{-1}$$

and $P_l: Y \to Y$ along with $P_r: Y \to Y$ such that

$$P_l(g'(x)g'(x)^*)P_r \approx I.$$

Before we discuss these operators in detail, let us emphasize two points. First, as we describe below, we require only the action of this preconditioner on a vector. This enables Optizelle to continue to be matrix-free. Second, even though we use matrix-free abstractions, most of the time, we're better off just using matrices.

At this point in time, both dense and sparse linear algebra libraries are extremely fast. Unless we have a large PDE constrained optimization problem, just form a matrix of the operator, factor it, and move on.

In the objective function, we use a preconditioner for the Hessian in several different places. Foremost, we use it to precondition linear systems related to second-order algorithms such as Newton's method. In addition, we use it within first-order algorithms such as nonlinear-CG and steepest descent. Certainly, $\nabla^2 f(x)^{-1}$ represents the best such preconditioner, but the Hessian may become singular during the course of optimization, so we must take care in how we generate this preconditioner. As such, even though $\nabla^2 f(x)$ is self-adjoint, the LU factorization provides a simple, effective manner to factorize the Hessian. In other words, we find operators L and U such that

$$LU = \nabla^2 f(x).$$

Then, our preconditioner $P_H: X \to X$ approximates

$$P_H \delta x \approx U^{-1} L^{-1} \delta x.$$

We say approximate because either U^{-1} or L^{-1} may not exist. In this case, we note that the action of U^{-1} and L^{-1} on a vector denotes a back and forward solve, respectively. When the inverse does not exist, we can simply modify these solves to ignore any variables that cause problems. As a note, we only benefit from a Hessian preconditioner in unconstrained and inequality constrained problems. For problems with equality constraints, we use a composite-step SQP method. Here, the tangential subproblem requires a null-space projection that replaces the Hessian preconditioner. If preconditioning the quantities in the objective is important to the performance of the problem, then we need to reformulate the problem, so that these quantities appear as equality constraints and then use an appropriate Schur preconditioner below. For example, we can reformulate the problem

$$\min_{x \in X} \{f(x) : g(x) = 0\}$$

as

$$\min_{x \in X, x_0 \in \mathbb{R}} \{ x_0 : x_0 = f(x), g(x) = 0 \}.$$

Note, this transformation may destroy convexity of the problem, so a different transformation may be more appropriate. For the equality constraints, our algorithms require the repeated solution of a system whose operator is

$$\begin{bmatrix} I & g'(x)^* \\ g'(x) & 0 \end{bmatrix}$$

As it happens, if g'(x) is full-rank, the preconditioner

$$\begin{bmatrix} I & 0 \\ 0 & (g'(x)g'(x)^*)^{-1} \end{bmatrix}$$

allows a Krylov method to solve the above system in three iterations. As such, Optizelle focuses on preconditioning the operator

$$g'(x)g'(x)^*.$$

Note, unlike the Hessian, we allow both left and right preconditioners for this operator. In addition, this operator depends on the inner product used by the vector space because it involves an adjoint. If we're working in \mathbb{R}^m with the inner product $\langle x, y \rangle = x^T y$, we can ignore this nuance. Otherwise, we must modify our factorizations to correctly account for the change in inner product. Outside of this difficulty, we note the operator is always symmetric and positive-semidefinite. However, like the Hessian, it can and likely will become singular during the course of optimization. As such, we propose two ways of dealing with this. In one case, we use a QR factorization of $g'(x)^*$,

$$QR = g'(x)^*,$$

then form the preconditioners $P_l: Y \to Y$ and $P_r: Y \to Y$ where

$$P_l \delta x \approx R^{-1} R^{-*} \delta x$$
$$P_r \delta x = \delta x.$$

Again, we must take care in case R is singular. Alternatively, we can just form $g'(x)g'(x)^*$ and find its LU factorization like we do with the Hessian,

$$LU = g'(x)g'(x)^*.$$

This gives us the preconditioners

 $P_l \delta x \approx U^{-1} L^{-1} \delta x,$ $P_r \delta x = \delta x.$

In theory, we can use a Choleski factorization to solve this system. The problem with this approach is that the Choleski factorization will fail when g'(x) is not full rank. Generally, we find it easier to fix a failing forward or back solve, as is the case with a QR or LU factorization, than to fix a failing factorization. In code, we represent preconditioners as a generic linear operator:

Language	C++
Structure	Optizelle::Operator
Interface	Inheritance
Code	<pre>namespace Optizelle { // A linear operator specification, A : X->Y template < typename Real, template <typename> class X, template <typename> class Y struct Operator { // Create some type shortcuts typedef typename X <real>::Vector X_Vector; typedef typename Y <real>::Vector Y_Vector; // y = A(x) virtual void eval(X_Vector const & x,Y_Vector &y) const = 0; // Allow a derived class to deallocate memory virtual ~Operator() {} }; };</real></real></typename></typename></pre>
Language	Python
Structure	Optizelle.Operator
Interface	Inheritance
Code	<pre>class Operator(object): """A linear operator specification, A : X->Y""" def _err(self,fn): """Produces an error message for an undefined function""" raise Exception.t("%s function is not defined in an " % (fn) + "Operator") def eval(self,state,x,y): """y <- A(x)""" _err(self,"eval")</pre>

Language MATLAB/Octave

Structure	Optizelle.Operator
Interface	Members present
Code	<pre>% A linear operator specification, A : X->Y err_op=@(x)error(sprintf('The %s function is not defined in an Operator.',x)); Optizelle.Operator = struct('eval',@(state,x)err_op('eval'));</pre>

As we can see, there is a slight difference when we compare C++ to Python and MATLAB/Octave. In Python and MATLAB/Octave, we provide the preconditioner with the variable state that we describe in the section Create the optimization state. We omit this variable in C++. If we need access to the state in C++, we can simply pass in a reference to it during the operator's construction. In Python and MATLAB/Octave, this is not an option, so we must pass the state directly. To be clear, access to the variable state is important for most preconditioners. Recall, we must either evaluate an approximation to $\nabla^2 f(x)^{-1} \delta x$ or $(g'(x)g'(x)^*)^{-1} \delta y$. When Optizelle calls the preconditioner, it provides δx and δy and expects $P_H \delta x$, $P_l \delta y$, and $P_r \delta y$ as its return. Optizelle does not call the preconditioner on the variables x and y. If we want access to these variables, we must find them in the state. As another important note, Optizelle can not optimize user defined factorizations. Meaning, during the course of an optimization iteration, we call these preconditioners several different times at the same optimization iterate, x. As such, if we factorize $\nabla^2 f(x)$ or $g'(x)g'(x)^*$, it is critical to our performance that we cache these factorizations. The easiest way to tell when a new factorization is needed is to monitor the variable \mathbf{x} inside of state. This variable represents the current optimization iterate and it does not change until we take a new step in the optimization algorithms. Recall, in our Rosenbrock example, we have a Hessian-vector product of

$$\nabla^2 f(x)\delta x = \begin{bmatrix} 1200x_1^2 - 400x_2 + 2 & -400x_1 \\ -400x_1 & 200 \end{bmatrix} \delta x.$$

This allows us to find the inverse using Cramer's rule

$$\nabla^2 f(x)^{-1} \delta x = \frac{1}{80000x_1^2 - 80000x_2 + 400} \begin{bmatrix} 200 & 400x_1 \\ 400x_1 & 1200x_1^2 - 400x_2 + 2 \end{bmatrix} \delta x.$$

Generally, we claim using Cramer's rule is a bad idea when compared to an LU factorization, but it works fine on this small example. Using this formulation, we define our preconditioner to the Hessian with the code:

Language	Python
Code	<pre># Define a perfect preconditioner for the Hessian class RosenHInv(Optizelle.Operator): def eval(self,state,dx,result): x = state.x one_over_det=1./(80000.*sq(x[0])-80000.*x[1]+400.) result[0]=one_over_det*(200.*dx[0]+400.*x[0]*dx[1]) result[1]=(one_over_det*</pre>
Language	MATLAB/Octave
Code	<pre>% Define a perfect preconditioner for the Hessian function self = RosenHInv() self.eval = @(state,dx) eval(state,dx); end function result = eval(state,dx) x = state.x; one_over_det=1./(80000.*sq(x(1))-80000.*x(2)+400.); result = [one_over_det*(200.*dx(1)+400.*x(1)*dx(2)); one_over_det* (400.*x(1)*dx(1)+(1200.*x(1)*x(1)-400.*x(2)+2.)*dx(2))]; end</pre>

For our simple equality constraint

$$g(x) = [(x_1 - 2)^2 + (x_2 - 2)^2 - 1].$$

We have that

$$g'(x)\delta x = \begin{bmatrix} 2(x_1 - 2) & 2(x_2 - 2) \end{bmatrix} \delta x$$
$$g'(x)^* \delta y = \begin{bmatrix} 2(x_1 - 2) \\ 2(x_2 - 2) \end{bmatrix} \delta y.$$

This means that

$$g'(x)g'(x)^*\delta y = (4(x_1-2)^2 + 4(x_2-2)^2)\delta y$$

and we have a perfect preconditioner

$$(g'(x)g'(x)^*)^{-1}\delta y = \frac{1}{4(x_1-2)^2 + 4(x_2-2)^2}\delta y.$$

We implement this in our Simple equality constrained example with the code:

Language	C++
Code	<pre>// Define a Schur preconditioner for the equality constraints struct MyPrecon: public Optizelle::Operator <double,optizelle::rm,optizelle::rm> { public: typedef Optizelle::Rm <double> X; typedef X::Vector X_Vector; typedef Optizelle::Rm <double> Y; typedef Y::Vector Y_Vector; private:</double></double></double,optizelle::rm,optizelle::rm></pre>

```
X_Vector& x;
               public:
                   MyPrecon(X::Vector& x_) : x(x_) {}
                   void eval(Y_Vector const & dy,Y_Vector & result) const {
                       result[0]=dy[0]/sq(4.*(x[0]-2.)+4.*sq(x[1]-2.));
                   }
               };
Language
               Python
Code
               # Define a Schur preconditioner for the equality constraints
               class MyPrecon(Optizelle.Operator):
                   def eval(self,state,dy,result):
                       result[0]=dy[0]/sq(4.*(x[0]-2.)+4.*sq(x[1]-2.))
Language
               MATLAB/Octave
Code
               % Define a Schur preconditioner for the equality constraints
               function self = MyPrecon()
                   self.eval=@(state,dy)dy(1)/sq(4.*(state.x(1)-2.)+4.*sq(state.x(2)-2.));
               end
```

3.6 Create the optimization state

In Optizelle, the optimization state contains an entire description of the current state of the optimization algorithm. This is unique to the particular optimization formulation, but all algorithms in a particular formulations share the same state. Most algorithms do not require information about all of these pieces, but they are present to make it easier to switch from one algorithm to another. For example, trust-region and line-search algorithms share several components, but the trust-region radius is unique to trust-region algorithms and the line-search step length is unique to line-search algorithms. Nevertheless, we may want to switch from one algorithm to another, so they share the same components. In order to define an optimization state, we instantiate the state class within the particular class of formulation we require. The syntax is:

Language	C++
Code	<pre>Optizelle::Unconstrained <real,xx>::State::t state(x);</real,xx></pre>
	<pre>Optizelle::EqualityConstrained <real,xx,yy>::State::t state(x,y);</real,xx,yy></pre>
	<pre>Optizelle::InequalityConstrained <real,xx,zz>::State::t state(x,z);</real,xx,zz></pre>
	<pre>Optizelle::Constrained <real,xx,yy,zz>::State::t state(x,y,z);</real,xx,yy,zz></pre>
Language	Python
Code	<pre>state = Optizelle.Unconstrained.State.t(XX,x)</pre>
	<pre>state = Optizelle.EqualityConstrained.State.t(XX,YY,x,y)</pre>
	<pre>state = Optizelle.InequalityConstrained.State.t(XX,ZZ,x,z)</pre>
	<pre>state = Optizelle.Constrained.State.t(XX,YY,ZZ,x,y,z)</pre>

Language	MATLAB/Octave	
Code	<pre>state = Optizelle.Unconstrained.State.t(XX,x);</pre>	
	<pre>state = Optizelle.EqualityConstrained.State.t(XX,YY,x,y);</pre>	
	<pre>state = Optizelle.InequalityConstrained.State.t(XX,ZZ,x,z);</pre>	
	<pre>state = Optizelle.Constrained.State.t(XX,YY,ZZ,x,y,z);</pre>	

Here, XX, YY, and ZZ correspond to the vector spaces X, Y, and Z described in the section Import or define the appropriate vector spaces. Likely, they are just Optizelle::Rm or Optizelle.Rm. Next, the variable x denotes an initial guess for the optimization problem. This guess is very important to the performance of the algorithms, so choose wisely. The variables y and z represent arbitrary elements in the codomain of g and h, respectively. We do not use the values of these variables, so any properly allocated vector works fine. As an example, we create the optimization state in the Rosenbrock example with the following code:

Language	C++
Code	<pre>// Generate an initial guess for Rosenbrock auto x = std::vector <double> {-1.2, 1.};</double></pre>
	<pre>// Create an unconstrained state based on this vector Optizelle::Unconstrained <double,optizelle::rm>::State::t state(x);</double,optizelle::rm></pre>
Language	Python
Code	<pre># Generate an initial guess for Rosenbrock x = numpy.array([-1.2,1.0])</pre>
	<pre># Create an unconstrained state based on this vector state=Optizelle.Unconstrained.State.t(Optizelle.Rm,x)</pre>
Language	MATLAB/Octave
Code	<pre>% Generate an initial guess for Rosenbrock x = [-1.2;1.];</pre>
	% Create an unconstrained state based on this vector state=Optizelle.Unconstrained.State.t(Optizelle.Rm,x);
In our Simple equalit	y constrained example, we have:
Language	C++
Code	<pre>// Generate an initial guess auto x = std::vector <double> {2.1, 1.1};</double></pre>
	<pre>// Allocate memory for the equality multiplier auto y = std::vector <double> (1);</double></pre>

// Create an optimization state
Optizelle::EqualityConstrained <double,Rm,Rm>::State::t state(x,y);

Language Python

Code	<pre># Generate an initial guess x = numpy.array([2.1,1.1])</pre>
	<pre># Allocate memory for the equality multiplier y = numpy.array([0.])</pre>
	<pre># Create an optimization state state=Optizelle.EqualityConstrained.State.t(Optizelle.Rm,Optizelle.Rm,x,y)</pre>
Language	MATLAB/Octave
Code	% Generate an initial guess x = [2.1;1.1];
	<pre>% Allocate memory for the equality multiplier y = [0.];</pre>
	% Create an optimization state state= Optizelle.EqualityConstrained.State.t(Optizelle.Rm,Optizelle.Rm,x,y);

3.7 Set the optimization parameters

For each optimization problem, the parameters required for an efficient optimization solve can vary wildly. Nevertheless, the parameters that guide this process reside within the state object. There are two mechanisms for modifying these entries. First, the state object created in the section Create the optimization state is simply an object with a variety of elements that can be modified directly. Alternatively, and preferably, we can use the JSON reader. The syntax for reading a parameter file in JSON format from file is:

Language	C++
Code	<pre>Optizelle::json::Unconstrained <real,xx>::read(fname,state);</real,xx></pre>
	<pre>Optizelle::json::EqualityConstrained <real,xx,yy>::read(fname,state);</real,xx,yy></pre>
	<pre>Optizelle::json::InequalityConstrained <real,xx,zz>::read(fname,state);</real,xx,zz></pre>
	<pre>Optizelle::json::Constrained <real,xx,yy,zz>::read(fname,state);</real,xx,yy,zz></pre>
Language	Python
Code	<pre>Optizelle.json.Unconstrained.read(XX,fname,state)</pre>
	<pre>Optizelle.json.EqualityConstrained.read(XX,YY,fname,state)</pre>
	<pre>Optizelle.json.InequalityConstrained.read(XX,ZZ,fname,state)</pre>
	<pre>Optizelle.json.Constrained.read(XX,YY,ZZ,fname,state)</pre>
Language	MATLAB/Octave

Code	<pre>state = Optizelle.json.Unconstrained.read(XX,fname,state);</pre>
	<pre>state = Optizelle.json.EqualityConstrained.read(XX,YY,fname,state);</pre>
	<pre>state = Optizelle.json.InequalityConstrained.read(XX,ZZ,fname,state);</pre>
	<pre>state = Optizelle.json.Constrained.read(XX,YY,ZZ,fname,state);</pre>

Here, most of the parameters required are identical to those required in the section Create the optimization state. The lone, new parameter is fname, which corresponds to a string of the file name where we read the JSON formatted parameters. As to what these parameters are, we discuss that in the chapter Optimization parameters. In our Rosenbrock example, we use the following code to read the optimization parameters:

	Language	C++
	Code	<pre>// Read the parameters from file Optizelle::json::Unconstrained <double,optizelle::rm>::read(fname,state);</double,optizelle::rm></pre>
	Language	Python
	Code	<pre># Read the parameters from file Optizelle.json.Unconstrained.read(Optizelle.Rm,fname,state)</pre>
	Language	MATLAB/Octave
	Code	% Read the parameters from file state=Optizelle.json.Unconstrained.read(Optizelle.Rm,fname,state);
Th	is becomes the foll	owing in our Simple equality constrained example:

Language	C++
Code	<pre>// Read the parameters from file Optizelle::json::EqualityConstrained <double,optizelle::rm,optizelle::rm> ::read(fname,state);</double,optizelle::rm,optizelle::rm></pre>
Language	Python
Code	<pre># Read the parameters from file Optizelle.json.EqualityConstrained.read(Optizelle.Rm,Optizelle.Rm,fname,state)</pre>
Language	MATLAB/Octave
Code	<pre>% Read the parameters from file state = Optizelle.json.EqualityConstrained.read(Optizelle.Rm,Optizelle.Rm,fname,state);</pre>

3.8 Accumulate the functions

In order to pass the functions used in the optimization to Optizelle, we accumulate each of them into a bundle of functions. These bundles are simple structures that contain the appropriate function. The syntax for creating these objects is:

Language C++

Code	<pre>Optizelle::Unconstrained <real,xx>::Functions::t fns;</real,xx></pre>
	<pre>Optizelle::EqualityConstrained <real,xx,yy>::Functions::t fns;</real,xx,yy></pre>
	<pre>Optizelle::InequalityConstrained <real,xx,zz>::Functions::t fns;</real,xx,zz></pre>
	<pre>Optizelle::Constrained <real,xx,yy,zz>::Functions::t fns;</real,xx,yy,zz></pre>
_	
Language	Python
Code	<pre>fns = Optizelle.Unconstrained.Functions.t()</pre>
	<pre>fns = Optizelle.EqualityConstrained.Functions.t()</pre>
	<pre>fns = Optizelle.InequalityConstrained.Functions.t()</pre>
	<pre>fns = Optizelle.Constrained.Functions.t()</pre>
Language	MATLAB/Octave
Code	<pre>fns = Optizelle.Unconstrained.Functions.t;</pre>
	<pre>fns = Optizelle.EqualityConstrained.Functions.t;</pre>
	<pre>fns = Optizelle.InequalityConstrained.Functions.t;</pre>
	<pre>fns = Optizelle.Constrained.Functions.t;</pre>

As was the case in the section Create the optimization state, XX, YY, and ZZ correspond to the vector spaces X, Y, and Z described in the section Import or define the appropriate vector spaces. Likely, they are just Optizelle::Rm or Optizelle.Rm. Now, each of structures contains a number of required and optional elements. We summarize these elements as follows:

Element	f
Type	ScalarValuedFunction
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Required	Yes
Description	Objective function.
Element	РН
Type	Operator
	Operator Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Problem Class Required	Unconstrained, Equality Constrained, Inequality Constrained, Constrained No
Problem Class Required	Unconstrained, Equality Constrained, Inequality Constrained, Constrained No

Problem Class	Equality Constrained, Constrained
Required	Yes
Description	Equality constraint.
Element	PSchur_left
\mathbf{Type}	Operator
Problem Class	Equality Constrained, Constrained
Required	No
Description	Left Schur preconditioner for derivative of the equality constraint, $g'(x)g'(x)^*$.
Element	PSchur_right
Element Type	PSchur_right Operator
	Operator
Туре	Operator
Type Problem Class	Operator Equality Constrained, Constrained
Type Problem Class Required	Operator Equality Constrained, Constrained No
Type Problem Class Required	Operator Equality Constrained, Constrained No
Type Problem Class Required Description	Operator Equality Constrained, Constrained No Right Schur preconditioner for derivative of the equality constraint, $g'(x)g'(x)^*$.
Type Problem Class Required Description Element Type	OperatorEquality Constrained, ConstrainedNoRight Schur preconditioner for derivative of the equality constraint, $g'(x)g'(x)^*$.h

Description Inequality constraint.

In C++, we represent each of the these elements as a std::unique_ptr using the type specified above. In Python, we use simple class elements. In MATLAB/Octave, we use a structure array. As a final note, since they are optional, we do **not** utilize PH, PSchur_left, or PSchur_right by default even when they are defined. In order to active these functions, we must modify the PH_type, PSchur_left_type, and PSchur_right_type elements in the state, respectively. We describe these variables in the chapter Optimization parameters. In our Rosenbrock example, we accumulate our functions with the following code:

Language	C++
Code	<pre>// Create the bundle of functions Optizelle::Unconstrained <double,optizelle::rm>::Functions::t fns; fns.f.reset(new Rosenbrock); fns.PH.reset(new RosenHInv(state.x));</double,optizelle::rm></pre>
Language	Python
Code	<pre># Create the bundle of functions fns=Optizelle.Unconstrained.Functions.t() fns.f=Rosenbrock() fns.PH=RosenHInv()</pre>

Language	MATLAB/Octave
Code	% Create the bundle of functions fns=Optizelle.Unconstrained.Functions.t;
	<pre>fns.f=Rosenbrock();</pre>
	<pre>fns.PH=RosenHInv();</pre>

As another example, we accomplish the same task in our Simple equality constrained example with the code:

Language	C++
Code	<pre>// Create a bundle of functions Optizelle::EqualityConstrained <double,rm,rm>::Functions::t fns; fns.f.reset(new MyObj); fns.g.reset(new MyEq); fns.PSchur_left.reset(new MyPrecon(state.x));</double,rm,rm></pre>
Language	Python
Code	<pre># Create a bundle of functions fns=Optizelle.EqualityConstrained.Functions.t() fns.f=MyObj() fns.g=MyEq() fns.PSchur_left=MyPrecon()</pre>
Language	MATLAB/Octave
Code	<pre>% Create a bundle of functions fns=Optizelle.EqualityConstrained.Functions.t; fns.f=MyObj(); fns.g=MyEq(); fns.PSchur_left=MyPrecon();</pre>

3.9 Call the optimization solver

Once the state, parameters, and functions are set, calling the optimization solver is straightforward. Simply, we call one of the four commands:

Language	C++
Code	<pre>Optizelle::Unconstrained<real,xx>::Algorithms::getMin(msg,fns,state);</real,xx></pre>
	<pre>Optizelle::EqualityConstrained<real,xx,yy>::Algorithms::getMin(msg,fns,state);</real,xx,yy></pre>
	<pre>Optizelle::InequalityConstrained<real,xx,zz>::Algorithms::getMin(msg,fns,state);</real,xx,zz></pre>
	<pre>Optizelle::Constrained<real,xx,yy,zz>::Algorithms::getMin(msg,fns,state);</real,xx,yy,zz></pre>
Language	Python

Code	<pre>Optizelle.Unconstrained.Algorithms.getMin(XX,msg,fns,state)</pre>
	<pre>Optizelle.EqualityConstrained.Algorithms.getMin(XX,YY,msg,fns,state)</pre>
	<pre>Optizelle.InequalityConstrained.Algorithms.getMin(XX,ZZ,msg,fns,state)</pre>
	<pre>Optizelle.Constrained.Algorithms.getMin(XX,YY,ZZ,msg,fns,state)</pre>
Language	MATLAB/Octave
Code	<pre>state = Optizelle.Unconstrained.Algorithms.getMin(XX,msg,fns,state);</pre>
	<pre>state = Optizelle.EqualityConstrained.Algorithms.getMin(XX,YY,msg,fns,state);</pre>
	<pre>state = Optizelle.InequalityConstrained.Algorithms.getMin(XX,ZZ,msg,fns,state);</pre>
	<pre>state = Optizelle.Constrained.Algorithms.getMin(XX,YY,ZZ,msg,fns,state);</pre>

As was the case in the section Create the optimization state, XX, YY, and ZZ correspond to the vector spaces X, Y, and Z described in the section Import or define the appropriate vector spaces. Likely, they are just Optizelle::Rm or Optizelle.Rm. Next, we call the function with a Messaging object, msg. In the simple case, we can simply use Optizelle::Messaging::stdout in C++, Optizelle.Messaging.stdout in Python, and Optizelle.Messaging.stdout in MATLAB/Octave. For more complicated cases, see the section User-defined messaging. Finally, we pass in the state and bundle of functions that we discussed in the sections Create the optimization state and Accumulate the functions, respectively.

In our Rosenbrock example, we call Optizelle's solver with the code:

Language	C++
Code	<pre>// Solve the optimization problem Optizelle::Unconstrained <double,optizelle::rm>::Algorithms ::getMin(Optizelle::Messaging::stdout,fns,state);</double,optizelle::rm></pre>
Language	Python
Code	<pre># Solve the optimization problem Optizelle.Unconstrained.Algorithms.getMin(</pre>
Language	MATLAB/Octave
Code	<pre>% Solve the optimization problem state = Optizelle.Unconstrained.Algorithms.getMin(Optizelle.Rm,Optizelle.Messaging.stdout,fns,state);</pre>

With the Simple equality constrained example, this becomes:

Language	C++
Code	<pre>// Solve the optimization problem Optizelle::EqualityConstrained <double,rm,rm>::Algorithms::getMin(</double,rm,rm></pre>

Language Python

Code	<pre># Solve the optimization problem Optizelle.EqualityConstrained.Algorithms.getMin(</pre>
Language	MATLAB/Octave
Code	<pre>% Solve the optimization problem state = Optizelle.EqualityConstrained.Algorithms.getMin(Optizelle.Rm,Optizelle.Rm,Optizelle.Messaging.stdout,fns,state);</pre>

3.10 Extract the solution

After the optimization routine concludes, the solution resides inside of the optimization state in a variable called x and the reason we stopped the optimization resides in a variable called opt_stop. At this point, we can examine our solution and run any post optimization diagnostics we require. In our Rosenbrock example, we print out the final solution with the code:

Language	C++		
Code	<pre>// Print out the reason for convergence std::cout << "The algorithm converged due to: " << Optizelle::OptimizationStop::to_string(state.opt_stop) << std::endl;</pre>		
	<pre>// Print out the final answer std::cout << "The optimal point is: (" << state.x[0] << ','</pre>		
Language	Python		
Code	<pre># Print out the reason for convergence print "The algorithm converged due to: %s" % (</pre>		
	<pre># Print out the final answer print "The optimal point is: (%e,%e)" % (state.x[0],state.x[1])</pre>		
Language	MATLAB/Octave		
Code	<pre>% Print out the reason for convergence fprintf('The algorithm converged due to: %s\n', Optizelle.OptimizationStop.to_string(state.opt_stop));</pre>		
	<pre>% Print out the final answer fprintf('The optimal point is: (%e,%e)\n',state.x(1),state.x(2));</pre>		
our Simple equali	try constrained example this becomes		

In our Simple equality constrained example, this becomes:

Language C++

Code	<pre>// Print out the reason for convergence std::cout << "The algorithm converged due to: " << Optizelle::OptimizationStop::to_string(state.opt_stop) << std::endl;</pre>		
	<pre>// Print out the final answer std::cout << std::scientific << std::setprecision(16)</pre>		
Language	Python		
Code	<pre># Print out the reason for convergence print "The algorithm converged due to: %s" % (</pre>		
	<pre># Print out the final answer print "The optimal point is: (%e,%e)" % (state.x[0],state.x[1])</pre>		
Language	MATLAB/Octave		
Code	<pre>% Print out the reason for convergence fprintf('The algorithm converged due to: %s\n', Optizelle.OptimizationStop.to_string(state.opt_stop));</pre>		
	<pre>% Print out the final answer fprintf('The optimal point is: (%e,%e)\n',state.x(1),state.x(2));</pre>		

3.11 Compile/run the program

As a final step, we need to either compile or run the program. Each language has its own nuances that we describe below.

3.11.1 C++

By default, we install the C++ relevant headers and libraries to

```
/some/path

lib

liboptizelle.a

optizelle.lib

liboptizelle.so

liboptizelle.dylib

optizelle.dll

include

optizelle

yson.h

yspaces.h
```

where <code>/some/path</code> denotes the installation directory. Therefore, in order to compile an Optizelle program, we must add the directory

/some/path/include

to the list of include directories and

/some/path/lib

to the list of library directories. For the static library, we link either liboptizelle.a or optizelle.lib. For the dynamic library, we link either liboptizelle.so, liboptizelle.dylib, or optizelle.dll. Note, Optizelle depends on JsonCpp, BLAS, and LAPACK as well. Therefore, these headers and libraries must be included in any compilation command as well. For example, in GCC, we may have the following set of build flags

-I/usr/include -L/usr/lib -L/usr/share/optizelle/thirdparty/lib -loptizelle -ljson -lblas -llapack

where we assume CMAKE_INSTALL_PREFIX=/usr.

3.11.2 Python/MATLAB/Octave

We require no compilation.

Optimization parameters

4

The parameters that guide the optimization solver have a dramatic effect its performance. To that end, we find each of these parameters within the optimization state that we initially discussed in the section Create the optimization state. These parameters are based on the canonical formulations

Unconstrained			ty Constrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
		st	g(x) = 0
Inequality Constrained		C	onstrained
$\min_{x \in X}$	f(x)	$\min_{x \in X}$	f(x)
st	$h(x) \succeq 0$	st	$g(x) = 0$ $h(x) \succeq 0$
			$h(x) \succeq 0$

and come in one of nine types:

Type	Real	
Description	Floating point numbers. In C++, this may be a type such as double or float as long as it matches the template parameters used in items such as state and fns. In Python and Matlab/Octave, we use the default floating point representation.	
Туре	Natural	
Description	Nonnegative integer. In C++, we use the type Optizelle::Natural, which we set to be size_t. In Python, we use the default integer representation. In MATLAB/Octave, we use the default floating point representation.	
Type	Enumerated	
Description	Enumerated type. In C++, we use an enum type called t wrapped inside a namespace that we type explicitly to Natural. For example, we refer to the algorithm class as AlgorithmClass and define its type as AlgorithmClass::t. Then, we refer to the enumerated values as:	

- AlgorithmClass::TrustRegion
- AlgorithmClass::LineSearch
- AlgorithmClass::UserDefined

In Python, we use integers, which we wrap inside of a class. For example, the class AlgorithmClass contains three integer values that we access with:

- AlgorithmClass.TrustRegion
- AlgorithmClass.LineSearch
- AlgorithmClass.UserDefined

In MATLAB/Octave, we use floating point numbers, which we wrap inside of a structured array. For example, the structure array AlgorithmClass contains three floating point values that we designate as:

- AlgorithmClass.TrustRegion
- AlgorithmClass.LineSearch
- AlgorithmClass.UserDefined

In all cases, we also provide a function called to_string in the class or namespace that converts the enumerated type to a string with the name of the enumerated element. Using our previous example of AlgorithmClass, in C++ we use

AlgorithmClass::to_string

whereas in Python and MATLAB/Octave we use

AlgorithmClass.to_string.

As to our specific enumerated types, we elaborate on them below.

Type	X_Vector		
Description	User defined vector within the vector space X, the domain of our objective function, $f: X \to \mathbb{R}$.		
Type	Y_Vector		
Description	User defined vector within the vector space Y, the codomain of our equality constraint, $g: X \to Y$ with $g(x) = 0$.		
Type	Z_Vector		
Description	User defined vector within the vector space Z, the codomain of our inequality constraint, $h: X \to Z$ with $h(x) \succeq 0$.		
Type	List		
Description	List of a specified kind of vectors. In C++, this denotes a std::list. In Python, this becomes a list. Finally, in MATLAB/Octave, we use a cell array.		
Type	Function		
Description	Function of a specified kind of variable. This type represents a function inside the state structure that we use to set a number of similar parameters. However, in the JSON parameter files, we set it like it was just another parameter.		

We further classify our enumerated types into the following:

Type AlgorithmClass

Values	TrustRegion, // Trust-Region algorithms LineSearch, // Line-search algorithms UserDefined // User provides the iterate	
Type Values	OptimizationStop NotConverged, // Algorithm did not converge GradientSmall, // Gradient was sufficiently small StepSmall, // Change in the step is small MaxItersExceeded, // Maximum number of iterations exceeded InteriorPointInstability,// Instability in the interior point method GlobalizationFailure, // Too many failed globalization iterations UserDefined // Some user defined stopping condition	
Туре	Operators	
Values	<pre>Identity, // Identity approximation Zero, // Zero approximation ScaledIdentity, // Scaled identity approximation //</pre>	
Type	LineSearchDirection	
Values	<pre>// Note, all methods here, save BFGS, are preconditioned. This // includes steepest descent, where dx = -PH grad. This is a good // way to implement a user-defined search direction. For example, // when we define PH to be the inverse of the Hessian, we get // a globalized Newton method. SteepestDescent, // SteepestDescent FletcherReeves, // Fletcher-Reeves CG PolakRibiere, // Polak-Ribiere CG HestenesStiefel, // HestenesStiefel CG BFGS, // Limited-memory BFGS NewtonCG // Newton-CG</pre>	
Туре	LineSearchKind	
Values	GoldenSection, // Golden-section search BackTracking, // BackTracking search TwoPointA, // Barzilai and Borwein's method A TwoPointB // Barzilai and Borwein's method B	

Туре	OptimizationLocation
Values	<pre>// Occurs at the start of the optimization function BeginningOfOptimization,</pre>
	<pre>// Occurs before the initial function and gradient evaluation BeforeInitialFuncAndGrad,</pre>
	<pre>// Occurs after the initial function and gradient evaluation AfterInitialFuncAndGrad,</pre>
	<pre>// Occurs just before the main optimization loop BeforeOptimizationLoop,</pre>
	<pre>// Occurs at the beginning of the optimization loop BeginningOfOptimizationLoop,</pre>
	<pre>// Occurs just before we take the optimization step x+dx BeforeSaveOld,</pre>
	<pre>// Occurs just before we take the optimization step x+dx BeforeStep,</pre>
	// Occurs before we calculate our new step. BeforeGetStep,
	<pre>// Occurs during a user defined get step calculation. GetStep,</pre>
	<pre>// Occurs after we take the optimization step x+dx, but before // we calculate the gradient based on this new step. In addition, // after this point we set the objective value, f_x, to be // f_xpdx. AfterStepBeforeGradient,</pre>
	<pre>// Occurs just after the gradient computation with the new // trial step AfterGradient,</pre>
	<pre>// Occurs before we update our quasi-Newton information. BeforeQuasi,</pre>

	// Occurs after we update our quasi-Newton information. AfterQuasi,	
	<pre>// This occurs after we check our stopping condition. This is // where the equality and inequality algorithms adjust the // stopping conditions. AfterCheckStop,</pre>	
	<pre>// This occurs last in the optimization loop. At this point, // we have already incremented our optimization iteration and // checked our stopping condition EndOfOptimizationIteration,</pre>	
	<pre>// This occurs prior to the computation of the line search BeforeLineSearch,</pre>	
	<pre>// This occurs after a rejected trust-region step AfterRejectedTrustRegion,</pre>	
	<pre>// This occurs after a rejected line-search step AfterRejectedLineSearch,</pre>	
	<pre>// This occurs prior to checking the predicted versus actual // reduction in a trust-region method. BeforeActualVersusPredicted,</pre>	
	<pre>// This occurs at the end of all optimization EndOfOptimization</pre>	
Type	ProblemClass	
Values	Unconstrained, // Unconstrained optimization EqualityConstrained, // Equality constrained optimization InequalityConstrained, // Inequality constrained optimization Constrained // Fully constrained optimization	
Type	DiagnosticScheme	
Values	<pre>Never, // Never compute our diagnostic checks DiagnosticsOnly, // No optimization. Only diagnostics. EveryIteration // Every iteration at the start of the iteration</pre>	
Type	FunctionDiagnostics	
Values	NoDiagnostics, // No diagnostic checks FirstOrder, // First-order function checks SecondOrder // Second-order function checks	
Type	VectorSpaceDiagnostics	
Values	NoDiagnostics, // No diagnostic checks Basic, // Test our basic vector space operations EuclideanJordan // Test our Euclidean-jordan algebraic	

\mathbf{Type}	ToleranceKind
Values	Relative,// Relative stopping tolerancesAbsolute,// Absolute stopping tolerances
Туре	QuasinormalStop
Values	<pre>Newton, // Obtained the full Newton point CauchyTrustRegion, // Cauchy point truncated by the TR CauchySafeguard, // Cauchy point truncated by the safeguard DoglegTrustRegion, // Dogleg point truncated by the TR DoglegSafeguard, // Dogleg point truncated by the safeguard NewtonTrustRegion, // Newton point truncated by the TR NewtonSafeguard, // Newton point truncated by the safeguard Feasible, // Skipped due to feasibility CauchySolved, // Cauchy point solved g'(x)dx_cp+g(x)=0 LocalMin, // Skipped due to a local min in the // least-squares formulation, min 0.5 // g'(x)dx + g(x) ^2, or g'(x)*g(x)=0 NewtonFailed // Augmented system solve for the Newton</pre>
	<pre>// point failed, so we regressed to the // Cauchy point</pre>
\mathbf{Type}	TruncatedStop
Values	NotConverged, // Algorithm has not converged NegativeCurvature, // Negative curvature detected RelativeErrorSmall, // Relative error is small MaxItersExceeded, // Relative error is small MaxItersExceeded, // Maximum number of iterations exceeded TrustRegionViolated, // Trust-region radius violated NanOperator, // NaN detected in the operator NanPreconditioner, // NaN detected in the preconditioner NonProjectorPreconditioner,// Detected a nonprojecting // preconditioner when one is required. // Too much inexactness in the // composite-step SQP method can trigger // this.
	NonSymmetricPreconditioner,// Detected a nonsymmetric preconditioner NonSymmetricOperator, // Detected a nonsymmetric operator LossOfOrthogonality, // Loss of orthogonality between the // Krylov vectors detected
	OffsetViolatesTrustRegion, // Offset is chosen such that // x_offset > delta where // delta is the trust-region radius
	OffsetViolatesSafeguard, // Offset violates the safeguard TooManyFailedSafeguard, // Too many safeguarded steps have failed ObjectiveIncrease // CG objective, 0.5 <abx,bx> - b,Bx> // increased between iterations, which // shouldn't happen.</abx,bx>

Type

Cone

Values	Linear,	// Nonnegative orthant
	Quadratic,	// Second order cone
	Semidefinite	<pre>// Cone of positive semidefinite matrices</pre>

Based on these types, we catalog the precise meaning of our parameters below. As a note, the field **JSON Param** denotes whether or not we allow the parameter to be set in the JSON file described in the section Set the optimization parameters. Generally, these settable parameters correspond to parameters that tune the behavior the algorithms. The other parameters correspond to internal quantities that assist in diagnostics or advanced heuristics.

Name	eps_grad
Type	Real
Valid Value	<pre>state.eps_grad > Real(0.)</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	1e-8
Description	Tolerance for the gradient stopping criteria reported in opt_stop . We satisfy this stopping criteria when
	$\mathbf{Unconstrained} \hspace{0.2cm} \ \nabla f(\mathbf{x}))\ \leq \texttt{eps_grad} \cdot \texttt{norm_gradtyp},$
	$\begin{aligned} \mathbf{Inequality} \qquad \ \nabla f(\mathbf{x}) - h'(\mathbf{x})^* \mathbf{z}\ \leq \mathtt{eps_grad} \cdot \mathtt{norm_gradtyp}, \end{aligned}$
	$\textbf{Constrained} \qquad \ \nabla f(\textbf{x}) + g'(\textbf{x})^*\textbf{y} - h'(\textbf{x})^*\textbf{z}\ \leq \texttt{eps_grad} \cdot \texttt{norm_gradtyp}.$
	At each iteration, we output the norm on the left of the inequality under the label <code> grad </code> .
Name	ens dx
Name	eps_dx
Туре	Real
	-
Туре	Real
Type Valid Value	Real state.eps_dx > Real(0.)
Type Valid Value Problem Class	Real state.eps_dx > Real(0.) Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Type Valid Value Problem Class JSON Param	<pre>Real state.eps_dx > Real(0.) Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes 1e-16 Tolerance for the step length stopping criteria reported in opt_stop. We satisfy this stopping criteria when</pre>
Type Valid Value Problem Class JSON Param Default	<pre>Real state.eps_dx > Real(0.) Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes 1e-16 Tolerance for the step length stopping criteria reported in opt_stop. We satisfy this</pre>
Type Valid Value Problem Class JSON Param Default	<pre>Real state.eps_dx > Real(0.) Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes le-16 Tolerance for the step length stopping criteria reported in opt_stop. We satisfy this stopping criteria when</pre>
Type Valid Value Problem Class JSON Param Default Description	<pre>Real state.eps_dx > Real(0.) Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes 1e-16 Tolerance for the step length stopping criteria reported in opt_stop. We satisfy this stopping criteria when</pre>

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param	Yes
Default	0
Description	Number of vectors stored for use with quasi-Newton methods such as SR1 and BFGS.
Name	iter
Туре	Natural
Valid Value	<pre>state.iter > 0</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	1
Description	Current optimization iteration. We output iter at each iteration under the label iter .
Name	iter_max
Туре	Natural
Valid Value	<pre>state.iter_max > 0</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	<pre>std::numeric_limits <integer>::max()</integer></pre>
Description	Maximum number of optimization iterations for the stopping criteria reported in opt_stop . We satisfy this stopping criteria when
	$iter \geq iter_max$
Name	glob_iter
Туре	Natural
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	0
Description	Current globalization iteration. Here, globalization means the current iteration of the trust-region or line-search method and involves operations such as checking the actual versus predicted reduction or the sufficient decrease condition.
Name	glob_iter_max
Туре	Natural

Valid Value	<pre>state.glob_iter_max > 0</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	10
Delauit	
Description	Maximum number of globalization iterations that we take before we exit the opti- mization. In other words, we only allow this many failed trust-region or line-search iterations before we exit the algorithm.
Name	glob_iter_total
Туре	Natural
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of globalization iterations taken across all iterations. This information is helpful when determining the overall expense of the algorithm. When we properly setup an equality constrained problem, we generally do one factorization of $g'(x)g'(x)^*$ every globalization iteration. In addition, evaluating the globalization routines for trust-region methods requires one Hessian-vector product every globalization iteration. We output glob_iter_total at each iteration under the label glb_itr_tot.
Name	opt_stop
Type	OptimizationStop
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	OptimizationStop::NotConverged
Description	Why we've stopping the optimization. We use the following logic when determining when to stop
	 If the optimization iteration exceeds the maximum number of iterations, stop. We control this with the parameter iter_max.
	2. If size of the optimization step becomes too small, stop. We control this with the parameter eps_dx.
	 If we have inequality constraints and the estimated interior point parameter mu_est becomes negative, stop.
	4. If the size of the gradient becomes too small and we satisfy the following additional conditions, stop. We control this with the parameter eps_grad .
	(a) For problems with equality constraints, we require that the norm of the equal- ity constraint be small. We control this with the parameter eps_constr .

(b) For problems with inequality constraints, we require that estimated interior point parameter be small. We control this with the parameter **eps_mu**.

Name	trunc_iter
Type	Natural
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	0
Description	Current number of iterations taken by truncated CG when solving the optimality conditions. We output trunc_iter at each iteration under the label trunc_iter.
Name	trunc_iter_max
Type	Natural
Valid Value	<pre>state.trunc_iter_max > 0</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	10
Description	Maximum number of iterations taken by truncated CG when solving the optimality conditions.
Name	trunc_iter_total
Type	Natural
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of iterations ever taken by the truncated CG when solving the optimality conditions. This gives information about the total amount computational effort taken by Optizelle as we evaluate one Hessian-vector product each iteration. We output
	trunc_iter_total at each iteration under the label trc_itr_tot.
Name	trunc_iter_total at each iteration under the label trc_itr_tot.
Name Туре	

Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	1
Description	Number of vectors stored and used in the orthogonalization of truncated CG. In theory, we only need 1 for unconstrained and inequality constrained problems, but this leads to numerical instabilities. In practice, if memory is available, it may be worthwhile to over orthogonalize.
Name	trunc_orthog_iter_max
Туре	Natural
Valid Value	<pre>state.trunc_orthog_iter_max > 0</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	1
Description	Maximum number of orthogonalization iterations that we use in truncated-CG. In theory, 1 should be enough, which means that we orghogonalize against all the stored previous directions once. In practice, we'll eventually lose orthogonality, so using 2 may help at the cost of additional computation.
Name	trunc_stop
Name Type	trunc_stop TruncatedStop
Type Valid Value	TruncatedStop
Type Valid Value	TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Type Valid Value Problem Class	TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Type Valid Value Problem Class JSON Param	TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No
Type Valid Value Problem Class JSON Param Default	TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No TruncatedStop::RelativeErrorSmall Reason why truncated CG exited when solving the optimality system. We output
Type Valid Value Problem Class JSON Param Default Description	TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No TruncatedStop::RelativeErrorSmall Reason why truncated CG exited when solving the optimality system. We output trunc_stop at each iteration under the label trunc_stop.
Type Valid Value Problem Class JSON Param Default Description	TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No TruncatedStop::RelativeErrorSmall Reason why truncated CG exited when solving the optimality system. We output trunc_stop at each iteration under the label trunc_stop. trunc_err
Type Valid Value Problem Class JSON Param Default Description Name Type Valid Value	TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No TruncatedStop::RelativeErrorSmall Reason why truncated CG exited when solving the optimality system. We output trunc_stop at each iteration under the label trunc_stop. trunc_err Real
Type Valid Value Problem Class JSON Param Default Description Name Type Valid Value	TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No TruncatedStop::RelativeErrorSmall Reason why truncated CG exited when solving the optimality system. We output trunc_stop at each iteration under the label trunc_stop. trunc_err Real // Any
Type Valid Value Problem Class JSON Param Default Description Name Type Valid Value Problem Class	<pre>TruncatedStop // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No TruncatedStop::RelativeErrorSmall Reason why truncated CG exited when solving the optimality system. We output trunc_stop at each iteration under the label trunc_stop. trunc_err Real // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained</pre>

Name	eps_trunc
Туре	Real
Valid Value	<pre>state.eps_trunc > Real(0.)</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	1e-2
Description	Relative stopping criteria for truncated CG. In truncated CG, when solving the system $Ax = b$ with preconditioner B , we use the stopping criteria $ B(Ax_k - b) \leq eps_trunc B(Ax_0 - b) $.
Name	algorithm_class
Type	AlgorithmClass
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	AlgorithmClass::TrustRegion
Description	Class of algorithm used in optimization.
Name	PH_type
Type	Operators
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	Operators::Identity
Description	Preconditioner used when solving the optimality conditions. Note, in order to accom- modate the null space projection, we currently ignore this quantity if problems with equality constraints.
Name	H_type
\mathbf{Type}	Operators
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes

Default	Operators::UserDefined
Description	Hessian approximation for the objective function.
Name	norm_gradtyp
Type	Real
Valid Value	<pre>state.norm_gradtyp >= Real(0.) (state.iter==1 && state.norm_gradtyp!=state.norm_gradtyp)</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>
Description	Norm of a typical gradient defined as
	Unconstrained $\ \nabla f(\mathbf{x}_0)\ ,$
	Equality $\ \nabla f(\mathbf{x}_0) + g'(\mathbf{x}_0)^* \mathbf{y}_0\ ,$
	Inequality $\ \nabla f(\mathbf{x}_0) - h'(\mathbf{x}_0)^* \mathbf{z}_0\ ,$
	$\textbf{Constrained} \qquad \ \nabla f(\mathbf{x}_0) + g'(\mathbf{x}_0)^* \mathbf{y}_0 - h'(\mathbf{x}_0)^* \mathbf{z}_0\ ,$
	where \mathbf{x}_0 , \mathbf{y}_0 , and \mathbf{z}_0 denote our variables at the first iteration. Sometimes, we use norm_gradtyp with the stopping criteria described in eps_grad . Specifically, we only refer to this quantity when eps_kind is set to Relative. When eps_kind is set to Absolute, we ignore this value and instead use 1.0.
Name	norm_dxtyp
Type	Real
Valid Value	<pre>state.norm_dxtyp >= Real(0.) (state.iter==1 && state.norm_dxtyp!=state.norm_dxtyp)</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	
	No
Default	No std::numeric_limits <real>::quiet_NaN()</real>
Default Description	
	<pre>std::numeric_limits<real>::quiet_NaN() Norm of a typical optimization step. Similar to norm_gradtyp, we set this to be the gradient found at the initial guess and use it in the stopping criteria described in eps_dx. Since an optimization algorithm may have numerical issues on the first optimization iteration, we do not use the first optimization step generated. By using the norm of the gradient, we approximate the norm of a step taken by the steepest descent algorithm. As a note, we only refer to this quantity when eps_kind is set to</real></pre>
Description	<pre>std::numeric_limits<real>::quiet_NaN() Norm of a typical optimization step. Similar to norm_gradtyp, we set this to be the gradient found at the initial guess and use it in the stopping criteria described in eps_dx. Since an optimization algorithm may have numerical issues on the first optimization iteration, we do not use the first optimization step generated. By using the norm of the gradient, we approximate the norm of a step taken by the steepest descent algorithm. As a note, we only refer to this quantity when eps_kind is set to Relative. When eps_kind is set to Absolute, we ignore this value and instead use 1.0.</real></pre>

Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	X::copy(x_user,x);
Description	Optimization variable.
Name	grad
Туре	X_Vector
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Gradient of the objective, $\nabla f(\mathbf{x})$.
Name	dx
\mathbf{Type}	X_Vector
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
IGON D	N
JSON Param	No
JSON Param Default	No X::init(x_user)
Default	X::init(x_user) Step taken during the optimization iteration. Every iteration we set $x=x+dx$. In
Default Description	X::init(x_user) Step taken during the optimization iteration. Every iteration we set $x=x+dx$. In addition, we output the norm of this vector at each iteration under the label $ dx $.
Default Description Name	<pre>X::init(x_user) Step taken during the optimization iteration. Every iteration we set $x=x+dx$. In addition, we output the norm of this vector at each iteration under the label dx . x_old</pre>
Default Description Name Type	<pre>X::init(x_user) Step taken during the optimization iteration. Every iteration we set x=x+dx. In addition, we output the norm of this vector at each iteration under the label dx . x_old X_Vector // Any</pre>
Default Description Name Type Valid Value	<pre>X::init(x_user) Step taken during the optimization iteration. Every iteration we set x=x+dx. In addition, we output the norm of this vector at each iteration under the label dx . x_old X_Vector // Any</pre>
Default Description Name Type Valid Value Problem Class	<pre>X::init(x_user) Step taken during the optimization iteration. Every iteration we set x=x+dx. In addition, we output the norm of this vector at each iteration under the label dx . x_old X_Vector // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained</pre>
Default Description Name Type Valid Value Problem Class JSON Param	<pre>X::init(x_user) Step taken during the optimization iteration. Every iteration we set x=x+dx. In addition, we output the norm of this vector at each iteration under the label dx . x_old X_Vector // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No</pre>
Default Description Name Type Valid Value Problem Class JSON Param Default Description	<pre>X::init(x_user) Step taken during the optimization iteration. Every iteration we set x=x+dx. In addition, we output the norm of this vector at each iteration under the label dx . x_old X_Vector // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No X::init(x_user) Optimization variable from the last iteration.</pre>
Default Description Name Name Valid Value Problem Class JSON Param Default Description	<pre>X::init(x_user) Step taken during the optimization iteration. Every iteration we set x=x+dx. In addition, we output the norm of this vector at each iteration under the label dx . x_old X_Vector // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No X::init(x_user) Optimization variable from the last iteration. grad_old</pre>
Default Description Name Type Valid Value Problem Class JSON Param Default Description	<pre>X::init(x_user) Step taken during the optimization iteration. Every iteration we set x=x+dx. In addition, we output the norm of this vector at each iteration under the label dx . x_old X_Vector // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No X::init(x_user) Optimization variable from the last iteration.</pre>

Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Gradient of the objective from the last iteration.
Name	dx_old
Туре	X_Vector
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Optimization step from the last iteration.
Name	oldY
Type	List(X_Vector)
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Problem Class JSON Param	Unconstrained, Equality Constrained, Inequality Constrained, Constrained No
JSON Param	No
JSON Param Default	No // Empty
JSON Param Default	No // Empty Difference in prior gradients,
JSON Param Default Description	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x_{iter}}) - \nabla f(\mathbf{x_{iter-1}}), \dots, \nabla f(\mathbf{x_{iter-stored history}}) - \nabla f(\mathbf{x_{iter-stored history-1}})].$ We use this list in our quasi-Newton methods.
JSON Param Default Description Name	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x_{iter}}) - \nabla f(\mathbf{x_{iter-1}}), \dots, \nabla f(\mathbf{x_{iter-stored history}}) - \nabla f(\mathbf{x_{iter-stored history-1}})].$ We use this list in our quasi-Newton methods. oldS
JSON Param Default Description Name Type	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x_{iter}}) - \nabla f(\mathbf{x_{iter-1}}), \dots, \nabla f(\mathbf{x_{iter-stored history}}) - \nabla f(\mathbf{x_{iter-stored history-1}})].$ We use this list in our quasi-Newton methods. oldS List(X_Vector)
JSON Param Default Description Name	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x_{iter}}) - \nabla f(\mathbf{x_{iter-1}}), \dots, \nabla f(\mathbf{x_{iter-stored history}}) - \nabla f(\mathbf{x_{iter-stored history-1}})].$ We use this list in our quasi-Newton methods. oldS
JSON Param Default Description Name Type	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x_{iter}}) - \nabla f(\mathbf{x_{iter-1}}), \dots, \nabla f(\mathbf{x_{iter-stored history}}) - \nabla f(\mathbf{x_{iter-stored history-1}})].$ We use this list in our quasi-Newton methods. oldS List(X_Vector)
JSON Param Default Description Name Type Valid Value	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x_{iter}}) - \nabla f(\mathbf{x_{iter-1}}), \dots, \nabla f(\mathbf{x_{iter-stored.history}}) - \nabla f(\mathbf{x_{iter-stored.history-1}})].$ We use this list in our quasi-Newton methods. oldS List(X_Vector) // Any
JSON Param Default Description Name Type Valid Value Problem Class	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x}_{iter}) - \nabla f(\mathbf{x}_{iter-1}), \dots, \nabla f(\mathbf{x}_{iter-stored\ history}) - \nabla f(\mathbf{x}_{iter-stored\ history-1})].$ We use this list in our quasi-Newton methods. oldS List(X_Vector) // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param Default Description Name Name Valid Value Problem Class JSON Param	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x}_{iter}) - \nabla f(\mathbf{x}_{iter-1}), \dots, \nabla f(\mathbf{x}_{iter-stored history}) - \nabla f(\mathbf{x}_{iter-stored history-1})].$ We use this list in our quasi-Newton methods. oldS List(X_Vector) // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No
JSON Param Default Description Name Type Valid Value Problem Class JSON Param Default	No // Empty Difference in prior gradients, $[\nabla f(\mathbf{x_{iter}}) - \nabla f(\mathbf{x_{iter-1}}), \dots, \nabla f(\mathbf{x_{iter-stored.history}}) - \nabla f(\mathbf{x_{iter-stored.history-1}})].$ We use this list in our quasi-Newton methods. oldS List(X_Vector) // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained No // Empty

We use this list in our quasi-Newton methods.

Name	f_x
Type	Real
Valid Value	<pre>state.f_x == state.f_x state.iter==1</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>
Description	Current value of the objective function, $f(\mathbf{x})$. We output $\mathbf{f}_{\mathbf{x}}$ at each iteration under the label $\mathbf{f}(\mathbf{x})$.
Name	f_xpdx
Type	Real
Valid Value	<pre>state.f_xpdx == state.f_xpdx state.iter==1</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>
Description	Value of the objective function at the trial step, $f(\mathbf{x} + \mathbf{dx})$.
Name	msg_level
Name Type	msg_level Natural
Type Valid Value	Natural
Type Valid Value	Natural // Any
Type Valid Value Problem Class	Natural // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Type Valid Value Problem Class JSON Param	Natural // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes
Type Valid Value Problem Class JSON Param Default	 Natural // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes 1 Messaging level. To turn messages off, use 0. For normal messaging, set to 1. For more detailed information, set to 2. For linear solver information, set to 3. To see precise information about what information we display, refer to the chapter entitled
Type Valid Value Problem Class JSON Param Default Description	 Natural // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes 1 Messaging level. To turn messages off, use 0. For normal messaging, set to 1. For more detailed information, set to 2. For linear solver information, set to 3. To see precise information about what information we display, refer to the chapter entitled Output.
Type Valid Value Problem Class JSON Param Default Description	Natural // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes 1 Messaging level. To turn messages off, use 0. For normal messaging, set to 1. For more detailed information, set to 2. For linear solver information, set to 3. To see precise information about what information we display, refer to the chapter entitled Output. safeguard_failed_max
Type Valid Value Problem Class JSON Param Default Description	Natural // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes 1 Messaging level. To turn messages off, use 0. For normal messaging, set to 1. For more detailed information, set to 2. For linear solver information, set to 3. To see precise information about what information we display, refer to the chapter entitled Output. safeguard_failed_max Natural
Type Valid Value Problem Class JSON Param Default Description	<pre>Natural // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes 1 Messaging level. To turn messages off, use 0. For normal messaging, set to 1. For more detailed information, set to 2. For linear solver information, set to 3. To see precise information about what information we display, refer to the chapter entitled Output. safeguard_failed_max Natural state.safeguard_failed_max >=1</pre>

Description	Number of failed safe-guard steps before exiting truncated CG. We use this exclusively for our inequality constraints.
Name	safeguard_failed
Type	Natural
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	0
Description	Number of failed safe-guard steps during the last iteration. We output safeguard_failed at each iteration under the label safe_fail .
Name	safeguard_failed_total
Type	Natural
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of failed safe-guard steps.
Name	alpha_x
Туре	Real
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits <real>::quiet_NaN()</real></pre>
Description	How much we truncate dx in an interior point method in order to maintain strict feasibility. When 1.0, we do not truncate and take a full step. We output alpha_x at each iteration under the label alpha_x.
Name	alpha_x_qn
Type	Real
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No

<pre>std::numeric_limits <real>::quiet_NaN()</real></pre>
How much we truncate dx_n in an interior point method in order to maintain strict feasibility. When 1.0, we do not truncate and take a full step.
We output alpha_x_qn at each iteration under the label alpha_x_qn .
eps_kind
ToleranceKind
// Any
Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Yes
ToleranceKind::Absolute
Kind of stopping tolerance used by the algorithms.
delta
Real
<pre>state.delta >= Real(0.)</pre>
Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Yes
1.
Trust region radius. We use this as a starting value. Later, we adjust the radius depending on the behavior of the algorithms. As a note, we output delta at each iteration under the label delta .
eta1
Real
<pre>state.eta1 > Real(0.) && state.eta1 < Real(1.)</pre>
Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Yes
.1
When the actual versus predicted reduction for a trust-region method is below this threshold, we reject the step. Otherwise, we accept it.
eta2
Real
<pre>state.eta2 > state.eta1 && state.eta2 < Real(1.)</pre>

Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained	
JSON Param	Yes	
Default	.9	
Description	When the actual versus predicted reduction for a trust-region method is above this threshold and the size of the trial step equals the trust-region radius, we increase the size of the trust-region radius.	
Name	ared	
Туре	Real	
Valid Value	// Any	
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained	
JSON Param	No	
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>	
Description	Actual reduction in the merit function between the current iterate and the iterate after taking the trial step, $ared \equiv merit(x) - merit(x + dx).$	
	We use the following merit functions, $merit : X_Vector \rightarrow Real$,	
	Unconstrained $f(\mathbf{x})$,	
	Equality $f(\mathbf{x}) + \langle \mathbf{y}, g(\mathbf{x}) \rangle + \mathbf{rho} g(\mathbf{x}) ^2$,	
	Inequality $f(\mathbf{x}) - \mathbf{mu} \cdot \mathbf{barr}(h(\mathbf{x})),$	
	$\textbf{Constrained} \qquad f(\textbf{x}) + \langle \textbf{y}, g(\textbf{x}) \rangle + \textbf{rho} g(\textbf{x}) ^2 - \textbf{mu} \cdot \textbf{barr}(h(\textbf{x})).$	
	Here, barr refers to the barrier function, which we describe in the section Customized vector spaces. As a note, we output the value of the merit function at each iteration under the label merit(x) and ared under the label ared.	
Name	pred	
Type	Real	
Valid Value	// Any	
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained	
JSON Param	No	
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>	
Description	Predicted reduction in the merit function between the current iterate and the iterate after taking the trial step,	
	$\mathbf{pred} \equiv \mathtt{model}(0) - \mathtt{model}(\mathtt{dx}).$	
	We use the following model functions, $model : X_Vector \rightarrow Real$,	

Unconstrained

$$f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), d\mathbf{x} \rangle + \frac{1}{2} \langle H(\mathbf{x}) d\mathbf{x}, d\mathbf{x} \rangle,$$

Equality

$f(\mathbf{x}) + \langle \mathbf{y}, g(\mathbf{x}) \rangle + \mathbf{rho} g(\mathbf{x}) ^2$
$+\langle abla f(\mathbf{x}) + g'(\mathbf{x})^* \mathbf{y}, \mathbf{dx} angle$
$+ \tfrac{1}{2} \langle H(\mathbf{x}) d\mathbf{x} + (g''(\mathbf{x}) d\mathbf{x})^* \mathbf{y}, d\mathbf{x} \rangle,$

Inequality

$f(\mathtt{x}) - \mathtt{mu} \cdot \mathtt{barr}(h(\mathtt{x}))$
$+\langle \nabla f(\mathbf{x}) - \mathbf{mu} \cdot h'(\mathbf{x})^* L(h(\mathbf{x}))^{-1} e, \mathbf{dx} \rangle$
$+\frac{1}{2}\langle H(\mathbf{x})d\mathbf{x}+h'(\mathbf{x})^*L(h(\mathbf{x}))^{-1}(h'(\mathbf{x})d\mathbf{x}\circ\mathbf{z}),d\mathbf{x}\rangle,$

Constrained

$$\begin{split} &f(\mathbf{x}) + \langle \mathbf{y}, g(\mathbf{x}) \rangle + \mathbf{rho} ||g(\mathbf{x})||^2 - \mathbf{mu} \cdot \mathbf{barr}(h(\mathbf{x})) \\ &+ \langle \nabla f(\mathbf{x}) + g'(\mathbf{x})^* \mathbf{y} - \mathbf{mu} \cdot h'(\mathbf{x})^* L(h(\mathbf{x}))^{-1} e, \mathbf{dx} \rangle \\ &+ \frac{1}{2} \langle H(\mathbf{x}) \mathbf{dx} + (g''(\mathbf{x}) \mathbf{dx})^* \mathbf{y} + h'(\mathbf{x})^* L(h(\mathbf{x}))^{-1} (h'(\mathbf{x}) \mathbf{dx} \circ \mathbf{z}), \mathbf{dx} \rangle. \end{split}$$

Here, \circ denotes the Jordan product, **prod**; $L(h(x))^{-1}$ denotes the inverse of the linear operator induced by the Jordan product, **linv**; *e* denotes the identity element in the pseudo-Euclidean-Jordan algebra, **id**; and **barr** denotes the barrier function. We describe each of these operations further in the section Customized vector spaces. As a note, we output **pred** at each iteration under the label **pred**.

Name	alpha0
Туре	Real
Valid Value	<pre>state.alpha0 >= Real(0.)</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	1.
Description	Base line-search step length. Generally, our line-search methods search for a scaling $alpha \in [0, 2 \cdot alpha0]$. Once we find $alpha$, we increase $alpha0$ when our search always brackets to the right and decrease it when our search always brackets to the left. As a note, we output $alpha0$ at each iteration under the label $alpha0$.
Name	alpha
Type	Real
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits <real>::quiet_NaN()</real></pre>
Description	Actual line-search step length. After our line-search process completes, we modify our step $dx \leftarrow alpha \cdot dx$. As a note, we output alpha at each iteration under the label alpha.
Name	c1
Туре	Real

Valid Value	<pre>state.c1 > Real(0.) && state.c1 < Real(1.)</pre>	
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained	
JSON Param	Yes	
Default	1e-4	
Description		ameter. When we set algorithm_class to LineSearch, we only $c(x + alpha \cdot dx) < merit(x) + c1 \cdot alpha \langle \tilde{x}, dx \rangle$ where we define
	Unconstrained	$ abla f(\mathbf{x}),$
		$ abla f(\mathbf{x}) + g'(\mathbf{x})^* \mathbf{y},$
		$\nabla f(\mathbf{x}) - \mathbf{m} \cdot h'(\mathbf{x})^* L(h(\mathbf{x}))^{-1} e,$
	Constrained	$\nabla f(\mathbf{x}) + g'(\mathbf{x})^* \mathbf{y} - \mathbf{m} \mathbf{u} \cdot h'(\mathbf{x})^* L(h(\mathbf{x}))^{-1} e.$
	product, $linv$; and e	tes the inverse of the linear operator induced by the Jordan denotes the identity element in the pseudo-Euclidean-Jordan be each of these operations further in the section Customized
Name	ls_iter	
Type	Natural	
Valid Value	// Any	
Problem Class	Unconstrained, Equalit	y Constrained, Inequality Constrained, Constrained
JSON Param	No	
Default	0	
Description	amount of computation	rations used in the line search. We use this to determine the nal effort used by Optizelle during the last iteration. As a note, each iteration under the label <code>ls_iter</code> .
Name	ls_iter_max	
Type	Natural	
Valid Value	<pre>state.ls_iter_max ></pre>	0
Problem Class	Unconstrained, Equalit	y Constrained, Inequality Constrained, Constrained
JSON Param	Yes	
Default	5	
Description		terations used in the line search before checking the sufficient e use this to tune the amount of work done by the line search.
Name	ls_iter_total	
Type	Natural	

Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of iterations ever taken by the line search. We use this to determine the amount of computational effort used by Optizelle.
Name	eps_ls
Type	Real
Valid Value	<pre>state.eps_ls > Real(0.)</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	1e-2
Description	Relative stopping tolerance used by the line search. At the moment, we do not use this parameter.
Name	dir
Type	LineSearchDirection
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	LineSearchDirection::SteepestDescent
Description	Line-search direction taken by the line-search algorithm.
Name	kind
Type	LineSearchKind
Valid Value	<pre>(state.kind!=LineSearchKind::GoldenSection state.ls_iter_max >= 2) && (state.kind!=LineSearchKind::TwoPointA state.kind!=LineSearchKind::TwoPointB state.dir==LineSearchDirection::SteepestDescent)</pre>
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	LineSearchKind::GoldenSection
Description	Kind of line-search used in the line-search algorithm.

Name	f_diag
Type	FunctionDiagnostics
Valid Value	// Any
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	FunctionDiagnostics::NoDiagnostics
Description	Function diagnostics on f .
Name	L_diag
Туре	FunctionDiagnostics
Valid Value	// Any
	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
JSON Param	Yes
Default	FunctionDiagnostics::NoDiagnostics
Description	Function diagnostics on the Lagrangian.
Name	x_diag
	x_diag VectorSpaceDiagnostics
Name Type Valid Value	<pre>x_diag VectorSpaceDiagnostics // Any</pre>
Type Valid Value	VectorSpaceDiagnostics
Type Valid Value	VectorSpaceDiagnostics // Any
Type Valid Value Problem Class	VectorSpaceDiagnostics // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Type Valid Value Problem Class JSON Param	VectorSpaceDiagnostics // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes
Type Valid Value Problem Class JSON Param Default Description	VectorSpaceDiagnostics // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes VectorSpaceDiagnostics::NoDiagnostics Vector space diagnostics on X.
Type Valid Value Problem Class JSON Param Default Description	VectorSpaceDiagnostics // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes VectorSpaceDiagnostics::NoDiagnostics Vector space diagnostics on X. dscheme
Type Valid Value Problem Class JSON Param Default Description	VectorSpaceDiagnostics // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes VectorSpaceDiagnostics::NoDiagnostics Vector space diagnostics on X.
Type Valid Value Problem Class JSON Param Default Description Name Type Valid Value	<pre>VectorSpaceDiagnostics // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes VectorSpaceDiagnostics::NoDiagnostics Vector space diagnostics on X. dscheme DiagnosticScheme // Any</pre>
Type Valid Value Problem Class JSON Param Default Description	VectorSpaceDiagnostics // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes VectorSpaceDiagnostics::NoDiagnostics Vector space diagnostics on X. dscheme DiagnosticScheme
Type Valid Value Problem Class JSON Param Default Description Name Type Valid Value Problem Class	<pre>VectorSpaceDiagnostics // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained Yes VectorSpaceDiagnostics::NoDiagnostics Vector space diagnostics on X. dscheme DiagnosticScheme // Any Unconstrained, Equality Constrained, Inequality Constrained, Constrained</pre>

Name	У
Type	Y_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	<pre>// Equality constrained // argmin_y grad f(x) + g'(x)*y // // Constrained</pre>
	// argmin_y grad f(x) + g'(x)*y - h'(x)*z
Description	Equality multiplier (dual variable or Lagrange multiplier.)
Name	dy
Туре	Y_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	Y::init(y_user)
Description	Step in the equality multiplier. Every iteration we set $y=y+dy$.
Name	zeta
Type	Real
Valid Value	<pre>state.zeta > Real(0.) && state.zeta < Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	0.8
Description	Fraction of the total trust region used in the quasi-normal step.
Name	eta0
Туре	Real
Valid Value	<pre>state.eta0 > Real(0.) && state.eta0 < Real(1.)-state.eta1</pre>
Duchlam Class	
Problem Class	Equality Constrained, Constrained
JSON Param	Equality Constrained, Constrained Yes

Description Trust-region parameter that bounds the error in the predicted-reduction.

Name	rho
Туре	Real
Valid Value	<pre>state.rho >= Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	1.0
Description	Penalty parameter for the augmented-Lagrangian. In problems with equality con- straints, this term appears in the merit functions
	$ \begin{split} \mathbf{Equality} & f(\mathbf{x}) + \langle \mathbf{y}, g(\mathbf{x}) \rangle + \mathtt{rho} g(\mathbf{x}) ^2, \\ \mathbf{Constrained} & f(\mathbf{x}) + \langle \mathbf{y}, g(\mathbf{x}) \rangle + \mathtt{rho} g(\mathbf{x}) ^2 - \mathtt{mu} \cdot \mathtt{barr}(h(\mathbf{x})). \end{split} $
	Have been referre to the harming function, which we describe in the section Customined

Here, **barr** refers to the barrier function, which we describe in the section Customized vector spaces.

Name	rho_old
Type	Real
Valid Value	<pre>state.rho_old >= Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	rho
Description	Penalty parameter from the last iteration.
Name	rho_bar
Type	Real
Valid Value	<pre>state.rho_bar > Real(0.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	1e-8
Description	Fixed increase in the penalty parameter in the augmented Lagrangian merit function.
Name	eps_constr
Type	Real
Valid Value	<pre>state.eps_constr > Real(0.)</pre>

Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	1e-8
Description	Relative stopping tolerance for feasibility with respect to the equality constraint reported in opt_stop. We satisfy this stopping criteria when
	$\ g(\mathtt{x})\ < \mathtt{eps_constr} \cdot \mathtt{norm_gxtyp}.$
	At each iteration, we output the norm on the left of the inequality under the label $ g(x) $. Note, since this value tunes a <i>relative</i> stopping criteria, if we start with a feasible solution, we need to adjust this value to be something like 1.0. This states that we do not seek relative improvement in the infeasibility.
Name	xi_qn
Type	Real
Valid Value	<pre>state.xi_qn > Real(0.) && state.xi_qn < Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	1e-4
Description	Relative stopping tolerance for the augmented system solve associated with the quasi- Newton step.
Name	xi_pg
Type	Real
Valid Value	<pre>state.xi_pg > Real(0.) && state.xi_pg < Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	1e-4
Description	Relative stopping tolerance for the augmented system solve associated with the pro- jection of the gradient prior to solving the tangential subproblem.
Name	xi_proj
Type	Real
Valid Value	<pre>state.xi_proj > Real(0.) && state.xi_proj < Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	1e-4

Description	Relative stopping tolerance for the augmented system solve associated with the null-space projection of the iterate in the tangential subproblem.
Name	xi_tang
Type	Real
Valid Value	<pre>state.xi_tang > Real(0.) && state.xi_tang < Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	1e-4
Description	Relative stopping tolerance for the augmented system solve associated with the tan- gential step computation after solving the tangential subproblem.
Name	xi_lmh
Type	Real
Valid Value	<pre>state.xi_lmh > Real(0.) && state.xi_lmh < Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	1e-4
Description	Relative stopping tolerance for the augmented system solve associated with the equality multiplier computation.
Name	xi_all
Type	Function(Real)
Valid Value	<pre>// state.xi_all > Real(0.) && state.xi_all < Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	// None
Description	Relative stopping tolerance for all of the augmented system solves, xi_qn, xi_pg, xi_proj, xi_proj, xi_tang, and xi_lmh.
Name	xi_lmg
Type	Real
Valid Value	<pre>state.xi_lmg > Real(0.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes

Default	1e4
Description	Absolute tolerance on the residual of the equality multiplier solve.
Name	xi_4
Type	Real
Valid Value	<pre>state.xi_4 > Real(1.)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	2.
Description	Tolerance for how much error is acceptable after computing the tangential step given the result from the tangential subproblem.
Name	rpred
Туре	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>
Description	Residual term in the predicted reduction. We use this quantity to determine if we computed a tangential step that is accurate enough.
Name	PSchur_left_type
Type	Operators
Valid Value	<pre>state.PSchur_left_type == Operators::Identity state.PSchur_left_type == Operators::UserDefined</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	Operators::Identity
Description	Left preconditioner for the augmented system. For a full discussion of this precondi- tioner, see the section (Optional) Define the preconditioners.
Name	PSchur_right_type
Type	Operators
Valid Value	<pre>state.PSchur_right_type == Operators::Identity state.PSchur_right_type == Operators::UserDefined</pre>

Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	Operators::Identity
Description	Right preconditioner for the augmented system. For a full discussion of this precondi- tioner, see the section (Optional) Define the preconditioners.
Name	augsys_iter_max
Type	Natural
Valid Value	<pre>state.augsys_iter_max > 0</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	100
Description	Maximum number of GMRES iterations allowed when solving an augmented system.
Name	augsys_rst_freq
Type	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	0
Description	How often we restart the augmented system solve. We restart GMRES every specified number of iterations in order to save memory. When 0, we do not restart.
Name	augsys_qn_iter
Туре	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Number of iterations taken during the last iterate by the augmented system solve for the quasi-normal step.
Name	augsys_pg_iter
Туре	Natural

Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Number of iterations taken during the last iterate by the augmented system solve when projecting the gradient prior to the tangential subproblem.
Name	augsys_proj_iter
Туре	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Number of iterations taken during the last iterate by the augmented system solve during the nullspace projection in the tangential subproblem. Since there are likely many projections, this is the total number of iterations over all projections.
Name	augsys_tang_iter
Туре	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Number of iterations taken during the last iterate by the augmented system solve during the tangential step.
Name	augsys_lmh_iter
Type	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	
	0

Name	augsys_qn_iter_total
Туре	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of iterations taken by the augmented system solve for the quasi-normal step.
Name	augsys_pg_iter_total
Type	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of iterations taken by the augmented system solve when projecting the gradient prior to the tangential subproblem.
Name	augsys_proj_iter_total
Type	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of iterations taken by the augmented system solve during the nullspace projection in the tangential subproblem.
Name	augsys_tang_iter_total
Туре	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0

Description	Total number of iterations taken by the augmented system solve during the tangential step.
Name	augsys_lmh_iter_total
Type	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of iterations taken by the augmented system solve during the equality multiplier solve.
Name	augsys_iter_total
Туре	Natural
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0
Description	Total number of iterations taken by all augmented system solves.
Name	augsys_qn_err
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Error in the last augmented system solve for the quasi-normal step.
Name	augsys_pg_err
Туре	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.

Description	Error in the last augmented system solve when projecting the gradient prior to the tangential subproblem.
Name	augsys_proj_err
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Error in the last augmented system solve during the nullspace projection in the tan- gential subproblem. Note, since there are likely many projections during a single tangential subproblem, this represents the error from the last such solve.
Name	augsys_tang_err
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Error in the last augmented system solve during the tangential step.
Name	augsys_lmh_err
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Error in the last augmented system solve during the equality multiplier solve.
Name	augsys_qn_err_target
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No

Default	0.
Description	Target error in the last augmented system solve for the quasi-normal step.
Name	augsys_pg_err_target
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem.
Name	augsys_proj_err_target
Туре	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Target error in the last augmented system solve during the nullspace projection in the tangential subproblem. Note, since there are likely many projections during a single tangential subproblem, this represents the target error from the last such solve.
Name	augsys_tang_err_target
Туре	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Target error in the last augmented system solve during the tangential step.
Name	augsys_lmh_err_target
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained

Problem Class Equality Constrained, Constrained

JSON Param	No
Default	0.
Description	Target error in the last augmented system solve during the equality multiplier solve.
Name	augsys_qn_failed
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Number of failed quasinormal augmented system solves.
Name	augsys_pg_failed
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Number of failed projected gradient augmented system solves.
Name	augsys_proj_failed
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Number of failed nullspace projection augmented system solves.
Name	augsys_tang_failed
Type	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No

Default	0.
Description	Number of tangential step augmented system solves.
Name	augsys_lmh_failed
Туре	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Number of equality multiplier augmented system solves.
Name	augsys_failed_total
Туре	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	0.
Description	Total number of failed augmented system solves. In short, the theory for convergence to a local minima requires that augmented system solves meet their specified tolerance. Sometimes, a lower tolerance can be used and these tolerances are controlled by xi_all, xi_qn, xi_pg, xi_proj, xi_tang, and xi_lmh. However, even with a lower specified tolerance, the inexact composite step SQP method can still require a tighter tolerance in order to guarantee convergence. Generally, the algorithms are tolerant to a few failed solves. However, if there are failed solves at every iteration, then there's a problem with the given preconditioner or no preconditioner was specified. See the section (Optional) Define the preconditioners for more information on how to implement an appropriate preconditioner.
Name	g_x
Туре	Y_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	Y::init(y_user)
Description	Equality constraint evaluated a \mathbf{x} , $g(\mathbf{x})$. We use this in the quasi-normal step as well as in the computation of the linear Taylor series at \mathbf{x} in the direction $d\mathbf{x}_n$. As a note, we output the norm of this vector each iteration under the label $ g(\mathbf{x}) $.

Name	norm_gxtyp
Type	Real
Valid Value	<pre>state.norm_gxtyp >= Real(0.) (state.iter==1 && state.norm_gxtyp!=state.norm_gxtyp)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>
Description	Norm of a typical equality constraint, which we define to be the norm of the equality constraint at the first iteration. Sometimes, we use norm_gxtyp with the stopping criteria described in eps_constr. Specifically, we only refer to this quantity when eps_kind is set to Relative. When eps_kind is set to Absolute, we ignore this value and instead use 1.0.
Name	norm_gpsgxtyp
Type	Real
Valid Value	<pre>state.norm_gpsgxtyp >= Real(0.) (state.iter==1 && state.norm_gpsgxtyp!=state.norm_gpsgxtyp)</pre>
Problem Class	Equality Constrained, Constrained
JSON Param	No
JSON Param Default	No std::numeric_limits <real>::quiet_NaN()</real>
Default	std::numeric_limits <real>::quiet_NaN() Norm of a typical value of $g'(\mathbf{x})^* g(\mathbf{x})$, which we define to be the value of this quan- tity at the first iteration. When we compute the quasinormal step, we compute the Cauchy point by finding the least-squares solution to the linearized equality constraint, $\min_{\partial x} \frac{1}{2} g'(x)\partial x + g(x) ^2$. Here, the gradient is $g'(x)^* g'(x)\partial x + g'(x)^* g(x)$. Now, for the Cauchy point, we start with $\partial x = 0$, so the steepest descent direction be- comes $\partial x = -g'(x)^* g(x)$. We find the Cauchy point, by doing an exact line-search along this direction in the objective for the least-squares problem above. Now, when $g'(x)^* g(x) = 0$, we sit at a local minima to the least-squares problem above. Gen- erally, this is bad since we're not feasible and we don't have good information as to where to move to improve our infeasibility. Nevertheless, the tangential step will likely move us off that point unless we've already achieved optimality with respect to the Lagrangian. In any case, we require norm_gpsgxtyp to determine when the relative</real>
Default Description	std::numeric_limits <real>::quiet_NaN() Norm of a typical value of $g'(\mathbf{x})^*g(\mathbf{x})$, which we define to be the value of this quan- tity at the first iteration. When we compute the quasinormal step, we compute the Cauchy point by finding the least-squares solution to the linearized equality constraint, $\min_{\partial x} \frac{1}{2} g'(x)\partial x + g(x) ^2$. Here, the gradient is $g'(x)^*g'(x)\partial x + g'(x)^*g(x)$. Now, for the Cauchy point, we start with $\partial x = 0$, so the steepest descent direction be- comes $\partial x = -g'(x)^*g(x)$. We find the Cauchy point, by doing an exact line-search along this direction in the objective for the least-squares problem above. Now, when $g'(x)^*g(x) = 0$, we sit at a local minima to the least-squares problem above. Gen- erally, this is bad since we're not feasible and we don't have good information as to where to move to improve our infeasibility. Nevertheless, the tangential step will likely move us off that point unless we've already achieved optimality with respect to the Lagrangian. In any case, we require norm_gpsgxtyp to determine when the relative norm of $g'(x)^*g(x)$ is small and hence fall into this local minima.</real>
Default Description	std::numeric_limits <real>::quiet_NaN() Norm of a typical value of $g'(\mathbf{x})^*g(\mathbf{x})$, which we define to be the value of this quan- tity at the first iteration. When we compute the quasinormal step, we compute the Cauchy point by finding the least-squares solution to the linearized equality constraint, $\min_{\partial x} \frac{1}{2} g'(x)\partial x + g(x) ^2$. Here, the gradient is $g'(x)^*g'(x)\partial x + g'(x)^*g(x)$. Now, for the Cauchy point, we start with $\partial x = 0$, so the steepest descent direction be- comes $\partial x = -g'(x)^*g(x)$. We find the Cauchy point, by doing an exact line-search along this direction in the objective for the least-squares problem above. Now, when $g'(x)^*g(x) = 0$, we sit at a local minima to the least-squares problem above. Gen- erally, this is bad since we're not feasible and we don't have good information as to where to move to improve our infeasibility. Nevertheless, the tangential step will likely move us off that point unless we've already achieved optimality with respect to the Lagrangian. In any case, we require norm_gpsgxtyp to determine when the relative norm of $g'(x)^*g(x)$ is small and hence fall into this local minima.</real>
Default Description Name Type Valid Value	std::numeric_limits <real>::quiet_NaN() Norm of a typical value of $g'(\mathbf{x})^*g(\mathbf{x})$, which we define to be the value of this quan- tity at the first iteration. When we compute the quasinormal step, we compute the Cauchy point by finding the least-squares solution to the linearized equality constraint, $\min_{\partial x} \frac{1}{2} g'(x)\partial x + g(x) ^2$. Here, the gradient is $g'(x)^*g'(x)\partial x + g'(x)^*g(x)$. Now, for the Cauchy point, we start with $\partial x = 0$, so the steepest descent direction be- comes $\partial x = -g'(x)^*g(x)$. We find the Cauchy point, by doing an exact line-search along this direction in the objective for the least-squares problem above. Now, when $g'(x)^*g(x) = 0$, we sit at a local minima to the least-squares problem above. Gen- erally, this is bad since we're not feasible and we don't have good information as to where to move to improve our infeasibility. Nevertheless, the tangential step will likely move us off that point unless we've already achieved optimality with respect to the Lagrangian. In any case, we require norm_gpsgxtyp to determine when the relative norm of $g'(x)^*g(x)$ is small and hence fall into this local minima. gpxdxn_p-gx Y_Vector</real>

Default	Y::init(y_user)
---------	-----------------

Description Linear Taylor series at **x** in the direction dx_n. We use this both in the predicted reduction as well as the residual predicted reduction.

Name	gpxdxt
Туре	Y_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	Y::init(y_user)
Description	Derivative of the constraint applied to the tangential step this is used in the residual predicted reduction.
Name	norm_gpxdxnpgx
Туре	Real
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>
Description	Norm of gpxdxn_p_gx. We use this in the penalty parameter computation and pre- dicted reduction.
Name	dx_n
Type	X_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Normal step. We output the norm of this vector at each iteration under the label $ dx_n $.
Name	dx_ncp
Type	X_Vector
Valid Value	// Any

Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Cauchy point for normal step.
Name	dx_t
Туре	X_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	(Corrected) tangential step. We output the norm of this vector at each iteration under the label $ dx_t $.
Name	dx_t_uncorrected
Туре	X_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Tangential step prior to correction.
Name	dx_tcp_uncorrected
Туре	X_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Cauchy point for tangential step prior to correction.
Name	H_dxn
Туре	X_Vector
Type Valid Value	// Any
vallu value	// нцу

Problem Class JSON Param	Equality Constrained, Constrained No
Default	X::init(x_user)
Description	Hessian applied to the normal step. We require this in ${\tt W_gradpHdxn}$ as well as the predicted reduction.
Name	W_gradpHdxn
Type	X_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Quantity grad $f(\mathbf{x}) + g'(\mathbf{x}) * \mathbf{y} + H d\mathbf{x}$ n projected into the null-space of the constraints. We require this in the tangential subproblem and the predicted reduction.
Name	H_dxtuncorrected
Type	X_Vector
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	X::init(x_user)
Description	Hessian applied to the uncorrected tangential step. We require this in the predicted reduction.
Name	g_diag
Type	FunctionDiagnostics
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	FunctionDiagnostics::NoDiagnostics
Description	Function diagnostics on g .
Name	y_diag
Туре	VectorSpaceDiagnostics

Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	Yes
Default	VectorSpaceDiagnostics::NoDiagnostics
Description	Vector space diagnostics on Y.
Name	qn_stop
Type	QuasinormalStop
Valid Value	// Any
Problem Class	Equality Constrained, Constrained
JSON Param	No
Default	QuasinormalStop::Feasible
Description	Reason why the quasinormal problem exited.
Name	z
Type	Z_Vector
Valid Value	// Any
Problem Class	Inequality Constrained, Constrained
JSON Param	No
Default	// mu inv(L(h(x))) e
Default	// mu inv(L(h(x))) e
Default	// mu inv(L(h(x))) e
Default Description	// mu inv(L(h(x))) e Inequality multiplier (dual variable or Lagrange multiplier.)
Default Description Name	<pre>// mu inv(L(h(x))) e Inequality multiplier (dual variable or Lagrange multiplier.) dz</pre>
Default Description Name Type Valid Value	<pre>// mu inv(L(h(x))) e Inequality multiplier (dual variable or Lagrange multiplier.) dz Z_Vector</pre>
Default Description Name Type Valid Value	<pre>// mu inv(L(h(x))) e Inequality multiplier (dual variable or Lagrange multiplier.) dz Z_Vector // Any</pre>
Default Description Name Type Valid Value Problem Class	<pre>// mu inv(L(h(x))) e Inequality multiplier (dual variable or Lagrange multiplier.) dz Z_Vector // Any Inequality Constrained, Constrained</pre>
Default Description Name Type Valid Value Problem Class JSON Param	<pre>// mu inv(L(h(x))) e Inequality multiplier (dual variable or Lagrange multiplier.) dz Z_Vector // Any Inequality Constrained, Constrained No</pre>
Default Description Name Type Valid Value Problem Class JSON Param Default	<pre>// mu inv(L(h(x))) e Inequality multiplier (dual variable or Lagrange multiplier.) dz Z_Vector // Any Inequality Constrained, Constrained No Z::init(z_user)</pre>
Default Description Name Type Valid Value Problem Class JSON Param Default	<pre>// mu inv(L(h(x))) e Inequality multiplier (dual variable or Lagrange multiplier.) dz Z_Vector // Any Inequality Constrained, Constrained No Z::init(z_user)</pre>

Valid Value	// Any
Problem Class	Inequality Constrained, Constrained
JSON Param	No
Default	Z::init(z_user)
Description	The inequality constraint evaluated at x. In theory, we can always just evaluate this when we need it. However, we require its computation both in the gradient as well as Hessian calculations. More specifically, when computing with SDP constraints, we require a factorization of this quantity. By caching it, we have the ability to cache the factorization.
Name	mu
Type	Real
Valid Value	<pre>state.mu > Real(0.)</pre>
Problem Class	Inequality Constrained, Constrained
JSON Param	Yes
Default	1.0
Description	Interior point parameter. We use this as the target for the interior-point parameter estimate mu_est. As the interior point method progresses, we drive this value toward zero. As a note, we output mu at each iteration under the label mu.
Name	mu_est
Name Type	
	mu_est
Type Valid Value	mu_est Real
Type Valid Value	<pre>mu_est Real state.mu_est == state.mu_est state.iter == 1</pre>
Type Valid Value Problem Class	<pre>mu_est Real state.mu_est == state.mu_est state.iter == 1 Inequality Constrained, Constrained</pre>
Type Valid Value Problem Class JSON Param	<pre>mu_est Real state.mu_est == state.mu_est state.iter == 1 Inequality Constrained, Constrained No</pre>
Type Valid Value Problem Class JSON Param Default	<pre>mu_est Real state.mu_est == state.mu_est state.iter == 1 Inequality Constrained, Constrained No std::numeric_limits<real>::quiet_NaN()</real></pre>
Type Valid Value Problem Class JSON Param Default	<pre>mu_est Real state.mu_est == state.mu_est state.iter == 1 Inequality Constrained, Constrained No std::numeric_limits<real>::quiet_NaN() Current interior-point estimate. We define this as</real></pre>
Type Valid Value Problem Class JSON Param Default	<pre>mu_est Real state.mu_est == state.mu_est state.iter == 1 Inequality Constrained, Constrained No std::numeric_limits<real>::quiet_NaN() Current interior-point estimate. We define this as $mu_est \equiv \frac{\langle z, h x \rangle}{\langle e, e \rangle}.$ As a note, we output mu_est at each iteration under the label mu_est. Also note, we require this value to be small relative to mu_typ for convergence and control the</real></pre>
Type Valid Value Problem Class JSON Param Default Description	<pre>mu_est Real state.mu_est == state.mu_est state.iter == 1 Inequality Constrained, Constrained No std::numeric_limits<real>::quiet_NaN() Current interior-point estimate. We define this as $mu_est \equiv \frac{\langle z, h.x \rangle}{\langle e, e \rangle}$. As a note, we output mu_est at each iteration under the label mu_est. Also note, we require this value to be small relative to mu_typ for convergence and control the relative decrease required with the parameter eps_mu.</real></pre>

Problem Class	Inequality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits<real>::quiet_NaN()</real></pre>
Description	Typical value for mu, which we define as the value of mu_est at the first iteration. Sometimes, we use mu_typ with the stopping criteria described in eps_mu. Specifically, we only refer to this quantity when eps_kind is set to Relative. When eps_kind is set to Absolute, we ignore this value and instead use 1.0.
Name	eps_mu
Type	Real
Valid Value	<pre>state.eps_mu > Real(0.)</pre>
Problem Class	Inequality Constrained, Constrained
JSON Param	Yes
Default	1e-8
Description	Relative stopping tolerance for satisfying the complementary slackness condition for the inequality constraint. We satisfy this stopping criteria when 1. $ mu - mu_typ \cdot eps_mu \le mu_typ \cdot eps_mu$
	2. $ mu - mu_est \le mu$
Name	sigma
Type	Real
Valid Value	<pre>state.sigma > Real(0.) && state.sigma < Real(1.)</pre>
Problem Class	Inequality Constrained, Constrained
JSON Param	Yes
Default	0.1

JSON Param	Yes
Default	0.1
Description	Rate that we decrease the interior point parameter.
Name	gamma
\mathbf{Type}	Real
Valid Value	<pre>state.gamma > Real(0.) && state.gamma < Real(1.)</pre>
Problem Class	Inequality Constrained, Constrained
JSON Param	Yes
Default	0.99
Description	How close we move to the boundary during a single step. A step of 1.0 allows a step to touch the boundary of the inequality constraint in a single step, which is disallowed by the interior point algorithm.

Name	alpha_z
Type	Real
Valid Value	// Any
Problem Class	Inequality Constrained, Constrained
JSON Param	No
Default	<pre>std::numeric_limits <real>::quiet_NaN()</real></pre>
Description	How much we truncate dz in an interior point method in order to maintain strict feasibility. When 1.0, we do not truncate and take a full step. We output alpha_z at each iteration under the label alpha_z.
Name	h_diag
Type	FunctionDiagnostics
Valid Value	// Any
Problem Class	Inequality Constrained, Constrained
JSON Param	Yes
Default	FunctionDiagnostics::NoDiagnostics
Description	Function diagnostics on h .
N	
Name	z_diag
Туре	VectorSpaceDiagnostics
Valid Value	// Any
Problem Class	Inequality Constrained, Constrained
JSON Param	Yes
Default	VectorSpaceDiagnostics::NoDiagnostics
Description	Vector space diagnostics on Z.

Output

Optizelle generates a series of diagnostics while running that give information about the behavior and performance of the underlying algorithm. This information is organized into columns that are exactly 12 characters wide. When no information is available, we print a single dot, .. In this way, each column always has some sort of information, which makes the output easy to parse using standard Unix utilities such as cut or awk. For example, to only print the iteration, objective value, and norm of the step on the Rosenbrock example, we use the following commands on POSIX compliant systems:

./rosenbrock tr_newton.json | awk '{printf "%-12s%-12s%-12s\n", \$1,\$2,\$4}'

and

```
./rosenbrock tr_newton.json | cut -c1-12,13-24,37-48
```

As far as the information in the columns themselves, we detail their meaning below. In terms of convergence, we require the values ||grad||, ||g(x)||, and mu_est be small relative to their starting value and control the relative decrease required with the parameters eps_grad, eps_constr, and eps_mu, respectively. In addition, if the value ||dx|| becomes too small relative to its starting value, we terminate the optimization. We control the amount of relative decrease allowed in ||dx|| with the parameter eps_dx.

Name	iter
State Param	iter
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
$\mathbf{Min} \; \mathtt{msg_level}$	1
Description	Current optimization iteration. If the value of this entry is *, then either a trust-region algorithm has rejected a step due to an unfavorable actual versus predicted reduction or a line-search algorithm has rejected a step due to a lack of sufficient decrease. In a trust-region method, we tune the rejection of steps with the parameter eta1 . In a line-search method, we tune the rejection of steps with the parameter c1 .
Name	f(x)
State Param	f_x
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
$\mathbf{Min} \; \texttt{msg_level}$	1
Description	Value of the objective function at the start of the specified iteration.

Name	grad
State Param	None
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
${f Min}$ msg_level	1
Description	Norm of the gradient of either the objective function or the Lagrangian, which we describe in the description of eps_grad. We use this value within our gradient stopping condition described by the parameter eps_grad. In general, we need this value to be small relative to the starting value for convergence.
Name	dx
State Param	None
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
${f Min}$ msg_level	1
Description	Norm of the step taken during the last iteration. We calculate this value by taking the norm of the value found in dx and use this within our stopping condition controlled by eps_dx. As a safeguard, we exit the optimization if this value becomes too small relative to the starting value.
Name	g(x)
State Param	None
Problem Class	Equality Constrained, Constrained
${f Min}$ msg_level	1
Description	Norm of the equality constraint at the start of the optimization iteration, which we calculate in g_x. We use this value within our equality constraint feasibility stopping condition described by the parameter eps_constr. In short, we need this value to be small relative to the starting value for convergence. If the starting value is already acceptably small, then we have started with a feasible solution. In this case, we may need to adjust eps_constr to something like 1.0, which states that we do not seek relative improvement in the infeasibility.
Name	mu_est
State Param	mu_est
Problem Class	Inequality Constrained, Constrained
${f Min}$ msg_level	1
Description	Current interior-point estimate. We use this value within our complementary slackness stopping condition described by the parameter <code>eps_mu</code> . In short, we need this value to be small relative to its starting value for convergence. We control the relative decrease required with the parameter <code>eps_mu</code> .
Name	merit(x)
State Param	None

Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
$\mathbf{Min} \; \texttt{msg_level}$	2
Description	Value of the merit function at the start of the specified iteration. We specify the various merit functions in the description of the parameter ared .
Name	trunc_iter
State Param	trunc_iter
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
$\mathbf{Min} \; \mathtt{msg_level}$	2
Description	Number of iterations used by truncated CG when solving the optimality system. We tune the maximum number of truncated CG iterations with the parameter trunc_iter_max.
Name	trunc_err
State Param	trunc_err
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Min msg_level	2
Description	Error in truncated CG when solving the optimality system. We control this error with the parameter <code>eps_trunc</code> and indirectly affect it with the parameters <code>trunc_orthog_storage_max</code> and <code>trunc_orthog_iter_max</code> .
Name	trunc_stop
Name State Param	trunc_stop trunc_stop
State Param	
State Param	trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained
State Param Problem Class	trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained
State Param Problem Class Min msg_level	trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Why truncated CG terminated. Although we shorten the strings, we describe each
State Param Problem Class Min msg_level Description	 trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Why truncated CG terminated. Although we shorten the strings, we describe each possible outcome in the enumerated type TruncatedStop.
State Param Problem Class Min msg_level Description	trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Why truncated CG terminated. Although we shorten the strings, we describe each possible outcome in the enumerated type TruncatedStop. ared
State Param Problem Class Min msg_level Description Name State Param	<pre>trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Why truncated CG terminated. Although we shorten the strings, we describe each possible outcome in the enumerated type TruncatedStop. ared ared</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class	<pre>trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Why truncated CG terminated. Although we shorten the strings, we describe each possible outcome in the enumerated type TruncatedStop. ared ared Unconstrained, Equality Constrained, Inequality Constrained, Constrained</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level	<pre>trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Why truncated CG terminated. Although we shorten the strings, we describe each possible outcome in the enumerated type TruncatedStop. ared ared Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Actual reduction in the merit function between the current iterate and the iterate after</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level Description	<pre>trunc_stop Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Why truncated CG terminated. Although we shorten the strings, we describe each possible outcome in the enumerated type TruncatedStop. ared ared Unconstrained, Equality Constrained, Inequality Constrained, Constrained 2 Actual reduction in the merit function between the current iterate and the iterate after taking the trial step.</pre>

 $\label{eq:problem Class} {\bf Problem \ Class} \ \ {\rm Unconstrained, \ Equality \ Constrained, \ Inequality \ Constrained, \ Constrained}$

Min msg_level	2
Description	Predicted reduction in the merit function between the current iterate and the iterate after taking the trial step.
Name	ared/pred
State Param	None
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
$Min \ \tt msg_level$	2
Description	Actual versus predicted reduction. Simply, we divide the outputs ared and pred . For a perfect model, this ratio is 1.0.
Name	delta
State Param	delta
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
${\bf Min} \; {\tt msg_level}$	2
Description	Trust-region radius.
Name	ls_iter
State Param	ls_iter
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
$\mathbf{Min} \; \texttt{msg_level}$	2
Description	Number of iterations taken by the line search. We tune the maximum number of line- search iterations with the parameter <code>ls_iter_max</code> and indirectly control the number of iterations with the parameter <code>eps_ls</code> .
Name	alpha
State Param	alpha
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
$\mathbf{Min} \; \texttt{msg_level}$	2
Description	Actual line-search step length.
Name	alpha0
State Param	alpha0
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
$Min \ \tt msg_level$	2
Description	Base line-search step length.

Name	qn_stop
State Param	qn_stop
Problem Class	Equality Constrained, Constrained
$\mathbf{Min} \; \mathtt{msg_level}$	2
Description	Reason why the quasinormal problem exited.

Name	aug_fail
State Param	augsys_failed_total
Problem Class	Equality Constrained, Constrained
Min msg_level	2
Description	Total number of failed augmented system solves.

Name	mu
State Param	mu
Problem Class	Inequality Constrained, Constrained
$\mathbf{Min} \; \texttt{msg_level}$	2
Description	Interior point parameter.
Name	alpha_x
Name State Param	alpha_x alpha_x
State Param	
State Param	alpha_x Inequality Constrained, Constrained

Name	alpha_z
State Param	alpha_z
Problem Class	Inequality Constrained, Constrained
$\mathbf{Min} \; \texttt{msg_level}$	2
Description	Amount we truncate dz in order to maintain feasibility with respect to the inequality multiplier. Note, we only reference this when we are using a primal-dual interior point method.

Name safe_fail

State Param safeguard_failed

Problem Class	Inequality Constrained, Constrained
Min msg_level	2
Description	Number of failed safe-guard steps during the last iteration. Note, we only reference this when using a trust-region method.
Name	alpha_x_qn
State Param	alpha_x_qn
Problem Class	Constrained
${\rm Min} \ {\tt msg_level}$	2
Description	Amount we truncate dx_n in order to maintain feasibility with respect to the inequality constraint.
Name	glb_itr_tot
State Param	glob_iter_total
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
${f Min}$ msg_level	3
Description	Total number of globalization iterations taken across all iterations.
Name	trc_itr_tot
Name State Param	trc_itr_tot trunc_iter_total
State Param	trunc_iter_total
State Param Problem Class	trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained
State Param Problem Class Min msg_level Description	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run.</pre>
State Param Problem Class Min msg_level Description	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. dx_n </pre>
State Param Problem Class Min msg_level Description Name State Param	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. IIdx_n[] Equality Constrained, Constrained</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. IIdx_n[] Equality Constrained, Constrained None</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. IIdx_n[] Equality Constrained, Constrained None 3</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. IIdx_n[] Equality Constrained, Constrained None</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. IIdx_n[] Equality Constrained, Constrained None 3</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level Description	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. //dx_n// Equality Constrained, Constrained None 3 Norm of the quasinormal step, dx_n, taken during the last iteration.</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level Description	<pre>trunc_iter_total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. dx_n Equality Constrained, Constrained None 3 Norm of the quasinormal step, dx_n, taken during the last iteration. dx_t </pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level Description	<pre>trunc.iter.total Unconstrained, Equality Constrained, Inequality Constrained, Constrained 3 Total number of iterations used by truncated CG when solving the optimality system. We typically use this to determine how many Hessian-vector products we've computed over the entire optimization run. [[dx.n]] Equality Constrained, Constrained None 3 Norm of the quasinormal step, dx.n, taken during the last iteration. [[dx.t]] Equality Constrained, Constrained</pre>

Description Norm of the tangential step, dx_t, taken during the last iteration.

Name	qn_iter
	augsys_qn_iter
	Equality Constrained, Constrained
	3
_	Number of iterations taken during the last iterate by the augmented system solve for the quasi-normal step.
Name	qn_iter_tot
State Param	augsys_qn_iter_total
Problem Class	Equality Constrained, Constrained
$\mathbf{Min} \; \texttt{msg_level}$	3
	Total number of iterations taken by the augmented system solve for the quasi-normal step.
Name	qn_err
State Param	augsys_qn_err
Problem Class	Equality Constrained, Constrained
Min msg_level	3
Description	Error in the last augmented system solve for the quasi-normal step.
Name	qn_err_trg
State Param	augsys_qn_err_target
Problem Class	Equality Constrained, Constrained
Min msg_level	3
Description	Target error in the last augmented system solve for the quasi-normal step.
D.T.	
	qn_fail
	augsys_qn_failed
	Equality Constrained, Constrained 3
U	
Description	
	Number of failed quasinormal augmented system solves.
Name	

Problem Class	Equality Constrained, Constrained
Min msg_level	3
Description	Number of iterations taken during the last iterate by the augmented system solve when projecting the gradient prior to the tangential subproblem.
Name	pg_iter_tot
State Param	augsys_pg_iter_total
Problem Class	Equality Constrained, Constrained
${f Min}$ msg_level	3
Description	Total number of iterations taken by the augmented system solve when projecting the gradient prior to the tangential subproblem.
Name	pg_err
State Param	augsys_pg_err
Problem Class	Equality Constrained, Constrained
$\mathbf{Min} \; \texttt{msg_level}$	3
Description	Error in the last augmented system solve when projecting the gradient prior to the tangential subproblem.
Name	pg_err_trg
Name State Param	pg_err_trg augsys_pg_err_target
State Param	augsys_pg_err_target
State Param Problem Class	augsys_pg_err_target Equality Constrained, Constrained
State Param Problem Class Min msg_level	<pre>augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to</pre>
State Param Problem Class Min msg_level Description	<pre>augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem.</pre>
State Param Problem Class Min msg_level Description Name	<pre>augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem. pg_fail</pre>
State Param Problem Class Min msg_level Description Name State Param	<pre>augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem. pg_fail augsys_pg_failed</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class	<pre>augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem. pg_fail augsys_pg_failed Equality Constrained, Constrained</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level Description	<pre>augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem. pg_fail augsys_pg_failed Equality Constrained, Constrained 3 Number of failed projected gradient augmented system solves.</pre>
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level Description	augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem. pg_fail augsys_pg_failed Equality Constrained, Constrained 3 Number of failed projected gradient augmented system solves.
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level Description Name State Param	augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem. pg_fail augsys_pg_failed Equality Constrained, Constrained 3 Number of failed projected gradient augmented system solves. pr_iter augsys_proj_iter
State Param Problem Class Min msg_level Description Name State Param Problem Class Min msg_level Description	augsys_pg_err_target Equality Constrained, Constrained 3 Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem. pg_fail augsys_pg_failed Equality Constrained, Constrained 3 Number of failed projected gradient augmented system solves.

Description	Number of iterations taken during the last iterate by the augmented system solve during the nullspace projection in the tangential subproblem. Since there are likely many projections, this is the total number of iterations over all projections.		
Name	pr_iter_tot		
State Param	augsys_proj_iter_total		
Problem Class	Equality Constrained, Constrained		
${f Min}\ {\tt msg_level}$	3		
Description	Total number of iterations taken by the augmented system solve during the nullspace projection in the tangential subproblem.		
Name	pr_err		
State Param	augsys_proj_err		
Problem Class	Equality Constrained, Constrained		
${\bf Min} \ {\tt msg_level}$	3		
Description	Error in the last augmented system solve during the nullspace projection in the tan- gential subproblem. Note, since there are likely many projections during a single tangential subproblem, this represents the error from the last such solve.		
Name	pr_err_trg		
State Param	augsys_proj_err_target		
Problem Class	Equality Constrained, Constrained		
${\bf Min} \ {\tt msg_level}$	3		
Description	Target error in the last augmented system solve during the tangential step.		
Name	pr_fail		
State Param	augsys_proj_failed		
Problem Class	Equality Constrained, Constrained		
Min msg_level	3		
Description	Number of failed nullspace projection augmented system solves.		
Name	tg_iter		
State Param	augsys_tang_iter		
Problem Class	Equality Constrained, Constrained		
$\mathbf{Min} \; \mathtt{msg_level}$	3		
Description	Number of iterations taken during the last iterate by the augmented system solve during the tangential step.		

Name	tg_iter_tot		
State Param	augsys_tang_iter_total		
Problem Class	Equality Constrained, Constrained		
${f Min}$ msg_level	3		
Description	Total number of iterations taken by the augmented system solve during the tangential step.		
Name	tg_err		
State Param	augsys_tang_err		
Problem Class	Equality Constrained, Constrained		
$\mathbf{Min} \; \texttt{msg_level}$	3		
Description	Error in the last augmented system solve during the tangential step.		
Name	tg_err_trg		
State Param	augsys_tang_err_target		
Problem Class	Equality Constrained, Constrained		
$\mathbf{Min} \; \texttt{msg_level}$	3		
Description	Target error in the last augmented system solve during the tangential step.		
Name	tg_fail		
State Param	augsys_tang_failed		

Problem Class	Equality Constrained, Constrained
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 ${\bf Min \ msg_level} \quad 3$

Description Number of failed tangential step augmented system solves.

Name	lm_iter	
State Param	augsys_lmh_iter	
Problem Class	Equality Constrained, Constrained	
$\mathbf{Min} \; \texttt{msg_level}$	3	
Description	Number of iterations taken during the last iterate by the augmented system solve during the equality multiplier solve.	
Name	lm_iter_tot	

State Param augsys_lmh_iter_total

Problem Class Equality Constrained, Constrained

$\mathbf{Min} \; \underline{\texttt{msg}}_{\texttt{level}}$	3		
Description	Total number of iterations taken by the augmented system solve during the equality multiplier solve.		
Name	lm_err		
State Param	augsys_lmh_err		
Problem Class	Equality Constrained, Constrained		
$\mathbf{Min} \; \texttt{msg_level}$	3		
Description	Error in the last augmented system solve during the equality multiplier solve.		
Name	lm_err_trg		
State Param	augsys_lmh_err_target		
Problem Class	Equality Constrained, Constrained		
$\mathbf{Min} \; \texttt{msg_level}$	3		
Description	Target error in the last augmented system solve during the equality multiplier solve.		
Name	lm_fail		
State Param	augsys_lmh_failed		
Problem Class	Equality Constrained, Constrained		
$\mathbf{Min} \; \texttt{msg_level}$	3		
Description	Number of failed equality multiplier augmented system solves.		
Name	aug_itr_tot		
State Param	augsys_iter_total		
Problem Class	Equality Constrained, Constrained		
$\mathbf{Min} \; \mathtt{msg_level}$	3		
Description	Total number of iterations taken by all augmented system solves. We use this to help determine the overall expense of the augmented system solver and its precondition.		

Advanced API

Optizelle contains many additional features such as customizing the output and defining custom vector spaces. We detail these features below.

6.1 User-defined messaging

By default, we output messages from Optizelle to **stdout**. However, in some environments, we require different behavior. For example,

- When we use Optizelle in a program with a GUI, we may not to display the output to a separate window.
- When using MPI in a distributed, parallel environment we likely want to restrict our output to only the rank 0 processor.

In these cases, we want to define a new messaging object. Messaging objects are simply functions that accept a string and print it accordingly. In code, we specify this object as:

Language	C++		
Structure	Optizelle::Messaging::t		
Interface	Function matches type		
Code	<pre>namespace Optizelle{ // Defines how we output messages to the user namespace Messaging { // At its core, we take in a string and then write it somewhere typedef std::function<void(std::string &="" const="" msg)=""> t; } }</void(std::string></pre>		
Language	Python		
Structure	Optizelle.Messaging.t		
Interface	Function matches type		
Code	<pre>def t(msg): """At its core, we take in a string and then write it somewhere""" raise Optizelle.Exception.t("Undefined messaging function")</pre>		

Language	MATLAB/Octave		
Structure	Optizelle.Messaging.t		
Interface	Function matches type		
Code	% At its core, we take in a string and then write it somewhere Optizelle.Messaging.t = @(x)error('Undefined messaging function');		

Once we define a custom messaging object, we are free to pass it to Optizelle, which occurs when we call the function getMin. We describe this process in the section Call the optimization solver. As an example, we modify the messaging object in our Rosenbrock advanced API example:

Language	C++
Code	<pre>// Define a custom messaging object void mymessaging(std::string const & msg) { std::cout << "PRINT: " << msg << std::endl; }</pre>
Language	Python
Code	<pre># Define a custom messaging object def mymessaging(msg): """Prints out normal diagnostic information""" sys.stdout.write("PRINT: %s\n" %(msg))</pre>
Language	MATLAB/Octave
Code	<pre>% Define a custom messaging object function MyMessaging(msg) fprintf('PRINT: %s\n',msg); end</pre>

6.2 Handling errors

In general, Optizelle handles algorithmic errors gracefully and will exit the optimization with the current best solution. However, errors in the problem setup or functions provided by the user cause Optizelle to exit its routines immediately.

The mechanism for handling errors depends on the type and interface. For errors that originate with Optizelle, we use the following scheme

Language	C++		
Structure	Optizelle::Exception::t		
Interface	Exception handling		
Code	<pre>namespace Optizelle {namespace Exception { struct t : public std::runtime_error { using std::runtime_error::runtime_error; }; }}</pre>		

Language	Python	
Structure	Optizelle.Exception.t	
Interface	Exception handling	
Code	<pre>class t(Exception): """Type for Optizell's exceptions""" pass</pre>	
Language	MATLAB/Octave	
Structure	error	

Interface Native error function

For errors that originate within the user code, we exit Optizelle and propagate the original error back to parent code. Typically, the best way to throw an error in the user code is by exceptions in C++ and Python and the error function in MATLAB/Octave. As an example, reading an invalid parameter from file raises an Optizelle error. We catch this error with the following code

-	č
Language	C++
Code	<pre>// Read parameters from file try { Optizelle::json::Unconstrained <real,xx>::read(fname,state); } catch(Optizelle::Exception::t const & e) { // Convert the error message to a string msg = Optizelle::Exception::to_string(e); // Print the error message directly</real,xx></pre>
T	<pre>Optizelle::Exception::to_stderr(e); }</pre>
Language	Python
Code	<pre># Read parameters from file try: Optizelle.json.Unconstrained.read(XX,fname,state); except Optizelle.Exception.t as e: # Convert the error message to a string msg = e.message # Print the error message directly print e</pre>
Language	MATLAB/Octave
Code	<pre>try state = Optizelle.json.Unconstrained.read(XX,fname,state); catch e % Convert the error message into a string msg = e.message; % Print the message directly disp(e.message); end</pre>

6.3 Customized vector spaces

In continuous optimization, we most often optimize over a simple vector of numbers in \mathbb{R}^m . If that's the case, we provide a reasonable implementation of this vector space and describe it in section Import or define the appropriate vector spaces. However, in some situations we want to use a different space. For example:

- In PDE constrained optimization, we may want to optimize over a space of functions such as $L^2(\Omega)$.
- In certain relaxations to discrete optimization problems, we must optimize over the space of symmetric, positive definite matrices.
- When the variables in \mathbb{R}^m have radically different scalings, we may need to alter the inner product to normalize our variables.
- On large-scale problems with billions of variables, we must store the vectors in parallel and compute operations using a messaging system such as MPI.

In each of these cases, we need to define a custom vector space for our problem. Each custom vector space requires us to define the following operations:

Name	init	
Definition	C++ init(x)	
		$init \leftarrow \xi(W)$ where $x \in W$
	Python	init(x)
		$init \leftarrow \xi(W)$ where $x \in W$
	MATLAB/Octave	<pre>init(x)</pre>
		$init \leftarrow \xi(W)$ where $x \in W$
Description	Initializes memory for a new vector. Here, the function $\xi : \{X, Y, Z\} \to X \cup Y \cup Z$ denotes a choice function that selects an arbitrary element from the appropriate set. Essentially, this states that we want a valid element in the vector space, but we don't care what the element is.	
Name	сору	
Definition	C++	copy(x,y)
		$y \leftarrow x$
	Python	copy(x,y)
		$y \leftarrow x$
	MATLAB/Octave	copy(x)
		$copy \leftarrow x$
Description	In C++ and Python, a shallow copy of the vector x into the vector $y.$ In MAT-LAB/Octave, return the vector x	
Name	scal	
Definition	C++	<pre>scal(alpha,x)</pre>
		$x \leftarrow \alpha x$
	Python	<pre>scal(alpha,x)</pre>
		$x \leftarrow \alpha x$
	MATLAB/Octave	-
		$scal \leftarrow \alpha x$

Description In C++ and Python, overwrite x with αx . In MATLAB/Octave, return αx .

Name	axpy	
Definition	C++	axpy(alpha,x,y)
		$y \leftarrow \alpha x + y$
	Python	axpy(alpha,x,y)
		$y \leftarrow \alpha x + y$
	MATLAB/Octave	axpy(alpha,x,y)
		$axpy \leftarrow \alpha x + y$
Description	In C++ and Python, over	rwrite y with $\alpha x + y$. In MATLAB/Octave, return $\alpha x + y$.
Name	innr	
Definition	C++	<pre>innr(x,y)</pre>
		$innr \leftarrow \langle x, y angle$
	Python	<pre>innr(x,y)</pre>
		$innr \leftarrow \langle x, y \rangle$
	MATLAB/Octave	<pre>innr(x,y)</pre>
		$innr \leftarrow \langle x, y \rangle$
Description	Return the inner product	between x and y .
Name	zero	
Definition	C++	zero(x)
		$x \leftarrow 0$
	Python	zero(x)
		$x \leftarrow 0$
	MATLAB/Octave	zero(x)
		$zero \leftarrow 0$
Description	In C++ and Python, overwrite x with 0. In MATLAB/Octave, return 0. Note, this is not necessarily the same as scal(0.,x) since, in practice, x may contain NaNs and Infs. As such, we consider zero to be a safe operation that returns 0. whereas scal may be an unsafe operation.	
Name	rand	
Definition	C++	rand(x)
		$x \leftarrow \psi(W)$ where $x \in W$
	Python	rand(x)
		$x \leftarrow \psi(W)$ where $x \in W$
	MATLAB/Octave	rand(x)
		$rand \leftarrow \psi(W)$ where $x \in W$

Description In C++ and Python, overwrite x with a random vector. In MATLAB/Octave, return a random vector. Here, the function $\psi : \{X, Y, Z\} \to X \cup Y \cup Z$ denotes a stochastic choice function that randomly selects an element from the appropriate set. Essentially, this states that we want a valid, random element in the vector space. Primarily, we use these vectors for our diagnostic tests controlled by the parameters f_diag, g_diag, and h_diag.

In addition, the vector space associated with the codomain of the inequality constraints, Z, requires the following operations:

```
NameprodDefinitionC++prod(x,y,z)z \leftarrow x \circ yprod(x,y,z)z \leftarrow x \circ yprod(x,y,z)z \leftarrow x \circ yprod(x,y)prod(x,y)prod(x,y)prod \leftarrow x \circ y
```

DescriptionIn C++ and Python, overwrite z with $x \circ y$. In MATLAB/Octave, return $x \circ y$. Here,
 \circ denotes a pseudo-Jordan product between two elements. We say pseudo-Jordan in
the sense that we do not require a full Euclidean-Jordan algebra. Instead, we drop the
requirement for commutativity. Hence, for linear bound constraints, we define that

$$[x \circ y]_i = x_i y_i.$$

Hence, the product denotes the pointwise or Hadamard product. For second-order cone constraints, we define that

$$\begin{bmatrix} x_0\\ \bar{x} \end{bmatrix} \circ \begin{bmatrix} y_0\\ \bar{y} \end{bmatrix} = \begin{bmatrix} x_0y_0 + \bar{x}^T\bar{y}\\ x_0\bar{y} + y_0\bar{x} \end{bmatrix}$$

For semidefinite programming, we have that

 $X \circ Y = XY.$

Alternatively, we can define that

$$X \circ Y = \frac{XY + YX}{2},$$

but the inverse operation linv below becomes far less efficient.

Ivame	Ιū		
Definition		C++	id(x)
			$x \leftarrow e$
		Python	id(x)
			$x \leftarrow e$
		MATLAB/Octave	id(x)
			$id \leftarrow e$

id

Namo

Description In C++ and Python, overwrite x with e. In MATLAB/Octave, return e. In this function, e denotes the identity element for the Jordan algebra. Hence, this function creates element e so that $x \circ e = x$. For linear bound constraints, e denotes the vector of all ones. For second-order cone constraints, $e = \begin{bmatrix} 1 & 0 & \dots & 0 \end{bmatrix}^T$. For semidefinite constraints, e = I

Name linv

Definition C++ linv(x,y,z)

- $\begin{aligned} z \leftarrow L(x)^{-1}y \\ \text{Python} & \text{linv}(x,y,z) \\ z \leftarrow L(x)^{-1}y \\ \text{MATLAB/Octave} & \text{linv}(x,y) \\ & \text{linv} \leftarrow L(x)^{-1}y \end{aligned}$
- **Description** In C++ and Python, overwrite z with $L(x)^{-1}y$. In MATLAB/Octave, return $L(x)^{-1}y$. Here, the function linv denotes the inverse operation to prod. Note, prod defines a bilinear operation so that there exists a linear operator L(x) such that $x \circ y = L(x)y$. The function linv computes the action of the *inverse* of L(x) on a vector. For linear bound constraints, L(x) = Diag(x), where Diag(x) denotes the diagonal matrix with x on the diagonal. For second-order cone constraints, L(x) = Arw(x) where we define Arw(x) as

$$\operatorname{Arw}\left(\begin{bmatrix} x_0\\ \bar{x} \end{bmatrix}\right) = \begin{bmatrix} x_0 & \bar{x}^T\\ \bar{x} & x_0 I \end{bmatrix}$$

For semidefinite constraints, we can either define that L(X) = X or that $L(X) = \frac{X \cdot + \cdot X}{2}$. Generally, it is preferable to use the first definition since $L(X)^{-1} = X^{-1}$. In the second case, we require the solution of the Sylvester equations.

Name	barr	
Definition	C++	barr(x)
		$barr \leftarrow \phi(x)$ where $x \circ \nabla \phi(x) = e$
	Python	barr(x)
		$barr \leftarrow \phi(x)$ where $x \circ \nabla \phi(x) = e$
	MATLAB/Octave	barr(x)
		$barr \leftarrow \phi(x)$ where $x \circ \nabla \phi(x) = e$
Description		barrier function applied to a vector. Here, the function rrier function, which we require to satisfy

$$x \circ \nabla \phi(x) = e.$$

For linear bound constraints, this is simply the log-barrier function

$$\phi(x) = \sum_{i=1}^{m} \log(x_i).$$

For second-order cone constraints, we define this as

$$\phi\left(\begin{bmatrix}x_0\\\bar{x}\end{bmatrix}\right) = \frac{1}{2}\log(x_0^2 - \langle \bar{x}, \bar{x} \rangle).$$

For semidefinite constraints, we define this as

 $\phi(X) = \log(\det(X))$

where det(X) denotes the determinant of X.

Name	srch	
Definition	C++	<pre>srch(x,y)</pre>
		$srch \leftarrow \arg \max\{\alpha \in \mathbb{R} : \alpha x + y \succeq 0, \alpha \ge 0\}$
	Python	<pre>srch(x,y)</pre>
		$srch \leftarrow \arg \max\{\alpha \in \mathbb{R} : \alpha x + y \succeq 0, \alpha \ge 0\}$
	MATLAB/Octave	<pre>srch(x,y)</pre>
		$srch \leftarrow \arg \max\{\alpha \in \mathbb{R} : \alpha x + y \succeq 0, \alpha \ge 0\}$
Description	nonnegativity. In other w	move in the direction x from the point y before violating ords, the function srch denotes the search function used to with respect to the inequality constraint. We define this as
	а	$\arg\max\{\alpha\in\mathbb{R}:\alpha x+y\succeq 0,\alpha\geq 0\}$
	ũ	Hence, α denotes the maximum distance we can move in the t $\alpha x + y$ remains feasible. Note, sometimes this number is , we must return Inf.
Name	symm	
Definition	C++	symm(x)
		$x \leftarrow \pi(x)$ where $\pi(x \circ y) = \pi(y \circ x)$
	Python	symm(x)
		$x \leftarrow \pi(x)$ where $\pi(x \circ y) = \pi(y \circ x)$
	MATLAB/Octave	-
		$symm \leftarrow \pi(x)$ where $\pi(x \circ y) = \pi(y \circ x)$
Description	turn the symmetrization of tion operator. We require from the Euclidean-Jorda cone constraints, this oper where $X \circ Y = \frac{XY+YX}{2}$,	rwrite x with its symmetrization. In MATLAB/Octave, re- of x. Here, the function $\pi: Z \to Z$ denotes the symmetriza- this operator since we relax the commutativity requirement an algebra. For linear bound constraints and second-order ration does nothing. In addition, for semidefinite constraints this operation does nothing. However, for semidefinite con- Y, we may use symmetrization,
		$\pi(X) = \frac{X + X^T}{2},$
	or more generally the sim	ilar symmetrization operator,
		$\pi_P(X) = \frac{(PXP^{-1} + (PXP^{-1})^T)}{2},$
	where we require P to be	nonsingular.
ext, we require these	e vector-space functions be	encapsulated in the following structures:
Language	C++	

Interface	Templated struct with static members and a single type def called ${\tt Vector}$
Description	A vector space in $C++$ must be declared as a templated struct with static members. As far as the template parameter, we template on our real scalar type and require that each of the functions that accept or return a scalar use this type. This template parameter allows us to insure that each of the vector spaces uses the same real type, which is important for consistency. Next, each of the above functions must be included

and declared static. This allows us to access the functions without instantiating the struct. We also require a single typedef called Vector. This defines the vector type used by each of the vector-space functions. In addition to the typedef, we require that this vector type implement move semantics, which includes both the move constructor as well as move semantics for the assignment operator. Note, items in the standard library all properly implement move semantics. As such, as long as we use std::vector, std::unique_ptr, or std::shared_ptr, we satisfy this requirement.

Language	Python
Interface	Class with static methods
Description	A vector space in Python must be declared as a class consisting entirely of static meth- ods. In other words, we require a class that implements all of the above vector-space functions where we decorate each function definition with the decorator <code>@staticmethod</code> .
Language	MATLAB/Octave

Interface	Structure array
Description	A vector space in MATLAB/Octave must be declared as a structure array with all of the above methods present.

As an example, we define and use a custom vector space for \mathbb{R}^m in our Rosenbrock advanced API example:

Language	C++
Code	<pre>// Defines the vector space used for optimization. template <typename real=""> struct MyVS { typedef std::vector <real> Vector; // Memory allocation and size setting static Vector init(Vector const & x) { return std::move(Vector(x.size())); } }</real></typename></pre>
	<pre>// y <- x (Shallow. No memory allocation.) static void copy(Vector const & x, Vector & y) { for(Natural i=0;i<x.size();i++){ pre="" y[i]="x[i];" }="" }<=""></x.size();i++){></pre>
	<pre>// x <- alpha * x static void scal(const Real& alpha, Vector & x) { for(Natural i=0;i<x.size();i++){ pre="" x[i]="alpha*x[i];" }="" }<=""></x.size();i++){></pre>
	<pre>// x <- 0 static void zero(Vector & x) { for(Natural i=0;i<x.size();i++){ pre="" x[i]="0.;" }="" }<=""></x.size();i++){></pre>

```
// y <- alpha * x + y
static void axpy(const Real& alpha, Vector const & x, Vector & y) {
   for(Natural i=0;i<x.size();i++){</pre>
       y[i]=alpha*x[i]+y[i];
   }
}
// innr <- <x,y>
static Real innr(Vector const & x,Vector const & y) {
   Real z=0;
   for(Natural i=0;i<x.size();i++)</pre>
       z+=x[i]*y[i];
   return z;
}
// x <- random
static void rand(Vector & x){
   std::mt19937 gen(1);
   std::uniform_real_distribution<Real> dis(Real(0.),Real(1.));
   for(Natural i=0;i<x.size();i++)</pre>
       x[i]=Real(dis(gen));
}
// Jordan product, z <- x o y.</pre>
static void prod(Vector const & x, Vector const & y, Vector & z) {
   for(Natural i=0;i<x.size();i++)</pre>
       z[i]=x[i]*y[i];
}
// Identity element, x \leftarrow e such that x \circ e = x.
static void id(Vector & x) {
   for(Natural i=0;i<x.size();i++)</pre>
       x[i]=Real(1.);
}
// Jordan product inverse, z \le inv(L(x)) y where L(x) y = x \circ y.
static void linv(Vector const & x,Vector const & y,Vector & z) {
   for(Natural i=0;i<x.size();i++)</pre>
       z[i]=y[i]/x[i];
}
// Barrier function, barr <- barr(x) where x o grad barr(x) = e.
static Real barr(Vector const & x) {
   Real z=Real(0.);
   for(Natural i=0;i<x.size();i++)</pre>
       z+=log(x[i]);
   return z;
}
// Line search, srch <- argmax {alpha i \in 0 : alpha x + y >= 0}
// where y > 0.
static Real srch(Vector const & x, Vector const & y) {
   // Line search parameter
   Real alpha=std::numeric_limits <Real>::infinity();
   // Search for the optimal linesearch parameter.
   for(Natural i=0;i<x.size();i++) {</pre>
```

```
if(x[i] < Real(0.)) {</pre>
                               Real alpha0 = -y[i]/x[i];
                               alpha = alpha0 < alpha ? alpha0 : alpha;</pre>
                           }
                       }
                       return alpha;
                    }
                    // Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric</pre>
                    // operator.
                    static void symm(Vector & x) { }
                };
Language
                Python
Code
                # Defines the vector space used for optimization.
                class MyVS(object):
                    @staticmethod
                    def init(x):
                        """Memory allocation and size setting"""
                       return copy.deepcopy(x)
                    @staticmethod
                    def copy(x,y):
                       """y <- x (Shallow. No memory allocation.)"""
                       y[:]=x[:]
                    @staticmethod
                    def scal(alpha,x):
                       """x <- alpha * x"""
                       for i in xrange(0,len(x)):
                           x[i]=alpha*x[i]
                    @staticmethod
                    def zero(x):
                       """x <- 0"""
                       for i in xrange(0,len(x)):
                           x[i]=0.
                    @staticmethod
                    def axpy(alpha,x,y):
                       """y <- alpha * x + y"""
                       for i in xrange(0,len(x)):
                           y[i]=alpha*x[i]+y[i]
                    @staticmethod
                    def innr(x,y):
                       """<- <x,y>"""
                       return reduce(lambda z,xy:xy[0]*xy[1]+z,zip(x,y),0.)
                    @staticmethod
                    def rand(x):
                        """"x <- random"""
                       for i in xrange(0,len(x)):
                           x[i]=random.uniform(0.,1.)
```

```
@staticmethod
                   def prod(x,y,z):
                       """Jordan product, z <- x o y"""
                       for i in xrange(0,len(x)):
                          z[i]=x[i]*y[i]
                   @staticmethod
                   def id(x):
                       """Identity element, x <- e such that x o e = x"""
                       for i in xrange(0,len(x)):
                          x[i]=1.
                   @staticmethod
                   def linv(x,y,z):
                       ""Jordan product inverse, z \leftarrow inv(L(x)) y where L(x) y = x \circ y""
                       for i in xrange(0,len(x)):
                          z[i]=y[i]/x[i]
                   @staticmethod
                   def barr(x):
                       """Barrier function, <- barr(x) where x o grad barr(x) = e"""
                       return reduce(lambda x,y:x+math.log(y),x,0.)
                   @staticmethod
                   def srch(x,y):
                       """Line search, <- argmax {alpha i \in 0 : alpha x + y >= 0} where y >
                       alpha = float("inf")
                       for i in xrange(0,len(x)):
                          if x[i] < 0:
                              alpha0 = -y[i]/x[i]
                              if alpha0 < alpha:</pre>
                                  alpha=alpha0
                       return alpha
                   @staticmethod
                   def symm(x):
                       """Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric operator
                       pass
Language
               MATLAB/Octave
Code
               % Convert a vector to structure
               function y = tostruct(x)
                   y = struct('data',x);
               end
               % Defines the vector space used for optimization.
               function self = MyVS()
                   % Memory allocation and size setting
                   self.init = @(x) x;
```

```
% <- x (Shallow. No memory allocation.)
self.copy = @(x) x;</pre>
```

```
% <- alpha * x
   self.scal = @(alpha,x) tostruct(alpha*x.data);
   % <- 0
   self.zero = @(x) tostruct(zeros(size(x.data)));
   % <- alpha * x + y
   self.axpy = @(alpha,x,y) tostruct(alpha * x.data + y.data);
   %<- <x,y>
   self.innr = @(x,y)x.data'*y.data;
   % <- random
   self.rand = @(x)tostruct(randn(size(x.data)));
   % Jordan product, z <- x o y.
   self.prod = @(x,y)tostruct(x.data .* y.data);
   % Identity element, x < -e such that x \circ e = x.
   self.id = @(x)tostruct(ones(size(x.data)));
   % Jordan product inverse, z \leftarrow inv(L(x)) y where L(x) y = x \circ y.
   self.linv = @(x,y)tostruct(y.data ./ x.data);
   % Barrier function, barr <- barr(x) where x o grad barr(x) = e.
   self.barr = @(x)sum(log(x.data));
   % Line search, srch <- argmax {alpha i >= 0 : alpha x + y >= 0}
   % where y > 0.
   self.srch = @(x,y) feval(@(z)min([min(z(find(z>0)));inf]),-y.data ./x.data);
   \% Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric
   % operator.
   self.symm = @(x)x;
end
```

6.4 Symmetric cone programming

In the case of C++ and MATLAB/Octave, we provide a built-in vector space for semidefinite, second-order cone, and linear (SQL) programs:

C++
Optizelle::SQL::Vector
Optizelle::SQL
MATLAB/Octave
Optizelle.SQL.create (produces a structure array)
Optizelle.SQL

In order to create a C++ SQL::Vector, we use the following constructor

```
namespace Optizelle {
   template <typename Real>
   struct SQL {
      struct Vector {
          // We require a vector of cone types and their sizes.
          Vector (
            std::vector <Cone::t> const & types_,
            std::vector <Natural> const & sizes_
          )
      };
   };
}
```

Here, **Cone::t** corresponds to the enumerated type **Cone** and **Natural** refers to the architecture specific unsigned integer defined in **Optizelle::Natural**. The constructor creates an SQL variable with the specified types and sizes of cones. Specifically, a linear cone of size m denotes a vector in \mathbb{R}^m that lies in the nonnegative orthant. A quadratic cone of size m denotes a vector in \mathbb{R}^m that lies in the quadratic cone. Finally, a semidefinite cone of size m denotes a matrix in $\mathbb{R}^{m \times m}$ that lies in the quadratic cone. Finally, a semidefinite cone of size m denotes a matrix in $\mathbb{R}^{m \times m}$ that lies in the cone of positive semidefinite matrices. Note, even though we ultimately find a symmetric matrix, we compute with a full $m \times m$ matrix and not just the upper or lower half. Using a full matrix affects how we define the derivatives of our inequality constraint h, so take care. Specifically, h'(x) and $h'(x)^*$ need to assume that their arguments are not symmetric, so consider both upper and lower triangular parts of the matrices. In order to create a MATLAB/Octave SQL vector, we use the function

z = Optizelle.SQL.create(types,sizes);

where types is a vector containing elements from the enumerated type Cone and sizes is a vector denoting the size of the cones. For example, in order to define a SQL vector with a semidefinite, quadratic, and linear cone with sizes 2, 2, and 1, we use the syntax

```
types = ...
[Optizelle.Cone.Semidefinite, ...
Optizelle.Cone.Quadratic, ...
Optizelle.Cone.Linear];
sizes = [2,2,1];
```

Otherwise, we define the meaning of each of these cones to be the same as the C++ case above. In order to access the elements of a C++ SQL vector, \mathbf{x} , we use the following indexing functions

Number of cones	Type of cone	Type of Indexing	Use
Single	Quadratic/Linear	Specific element	x(i)
Multiple	Quadratic/Linear	Specific element	x(k,i)
Multiple	Semidefinite	Specific element	x(k,i,j)
Multiple	Semidefinite/Quadratic/Linear	First element	x.front(k)
Multiple	Quadratic	First element	x.naught(k)
Multiple	Quadratic	Second element	x.bar(k)

Finally, we have a couple of query functions

Purpose	Use
Size of block	x.blkSize(k)
Type of block	<pre>x.blkType(k)</pre>
Number of blocks	<pre>x.numblocks()</pre>

In order to access the elements of a MATLAB/Octave SQL vector, \mathbf{x} , we note that the cones are stored in the cell array \mathbf{x} .data where each element in the cell array denotes a different cone. We store quadratic and linear elements as column vectors and semidefinite elements as matrices. For example, to access the *i*th element of the *k*th block when this block is quadratic or linear, we use the syntax \mathbf{x} .data{k}(i). To access the (*i*, *j*)th element of the *k*th block when the block is semidefinite, we use the syntax \mathbf{x} .data{k}(i,j). As an example, we setup and solve a simple second-order cone program in our simple quadratic cone example:

```
Language
               C++
Code
               // Optimize a simple problem with an optimal solution of (2.5, 2.5)
               #include <iostream>
               #include <iomanip>
               #include "optizelle/optizelle.h"
               #include "optizelle/vspaces.h"
               #include "optizelle/json.h"
               // Create some type shortcuts
               using Optizelle::Rm;
               using Optizelle::SQL;
               typedef double Real;
               // Squares its input
               template <typename Real>
               Real sq(Real x){
                   return x*x;
               }
               // Define a simple objective where
               11
               // f(x,y)=(x-3)^2+(y-2)^2
               11
               struct MyObj : public Optizelle::ScalarValuedFunction <Real,Rm> {
                   typedef Rm <Real> X;
                   // Evaluation
                   double eval(X::Vector const & x) const {
                       return sq(x[0]-Real(3.))+sq(x[1]-Real(2.));
                   }
                   // Gradient
                   void grad(
                       X::Vector const & x,
                       X::Vector & grad
                   ) const {
                       grad[0]=2*x[0]-6;
                       grad[1]=2*x[1]-4;
                   }
                   // Hessian-vector product
                   void hessvec(
                       X::Vector const & x,
                       X::Vector const & dx,
                       X::Vector & H_dx
                   ) const {
                       H_dx[0] = Real(2.)*dx[0];
                       H_dx[1] = Real(2.)*dx[1];
                   }
               };
               // Define a simple SOCP inequality
               11
               // h(x,y) = [y >= |x|]
               // h(x,y) = (y,x) >=_Q 0
```

```
11
struct MyIneq : public Optizelle::VectorValuedFunction <Real,Rm,SQL> {
    typedef Rm <Real> X;
    typedef SQL <Real> Z;
    // z=h(x)
    void eval(
        X::Vector const & x,
        Z::Vector & z
    ) const {
        z(1,1)=x[1];
        z(1,2)=x[0];
    }
    // z=h'(x)dx
    void p(
        X::Vector const & x,
        X::Vector const & dx,
        Z::Vector & z
    ) const {
        z(1,1) = dx[1];
        z(1,2) = dx[0];
    }
    // xhat=h'(x)*dz
    void ps(
        X::Vector const & x,
        Z::Vector const & dz,
        X::Vector & xhat
    ) const {
        xhat[0] = dz(1,2);
        xhat[1] = dz(1,1);
    }
    // xhat=(h''(x)dx)*dz
    void pps(
        X::Vector const & x,
        X::Vector const & dx,
        Y::Vector const & dz,
        X::Vector & xhat
    ) const {
        X::zero(xhat);
    }
};
int main(int argc, char* argv[]){
    // Create some type shortcuts
    typedef Rm <Real>::Vector Rm_Vector;
    typedef SQL <Real>::Vector SQL_Vector;
    // Read in the name for the input file % \left( {{\left( {{{\left( {{{\left( {{{c}}} \right)}} \right)}_{i}}} \right)}_{i}}} \right)
    if(argc!=2) {
        std::cerr << "simple_quadratic_cone <parameters>" << std::endl;</pre>
        exit(EXIT_FAILURE);
    }
    auto fname = argv[1];
```

```
// Generate an initial guess for the primal
                   auto x = Rm_Vector(\{1.2, 3.1\});
                   // Allocate memory for the dual
                   auto z = SQL_Vector ({Optizelle::Cone::Quadratic},{2});
                   // Create an optimization state
                   Optizelle::InequalityConstrained <Real,Rm,SQL>::State::t state(x,z);
                   // Read the parameters from file
                   Optizelle::json::InequalityConstrained <Real,Rm,SQL>::read(fname,state);
                   // Create a bundle of functions
                   Optizelle::InequalityConstrained <Real,Rm,SQL>::Functions::t fns;
                   fns.f.reset(new MyObj);
                   fns.h.reset(new MyIneq);
                   // Solve the optimization problem
                   Optizelle::InequalityConstrained <Real,Rm,SQL>
                       ::Algorithms::getMin(Optizelle::Messaging::stdout,fns,state);
                   // Print out the reason for convergence
                   std::cout << "The algorithm converged due to: " <<</pre>
                       Optizelle::OptimizationStop::to_string(state.opt_stop) << std::endl;</pre>
                   // Print out the final answer
                   std::cout << std::setprecision(16) << std::scientific</pre>
                       << "The optimal point is: (" << state.x[0] << ','
                   << state.x[1] << ')' << std::endl;
                   // Write out the final answer to file
                   Optizelle::json::InequalityConstrained <Real,Rm,SQL>
                       ::write_restart("solution.json",state);
                   // Successful termination
                   return EXIT_SUCCESS;
               }
Language
               MATLAB/Octave
Code
               \% Optimize a simple problem with an optimal solution of (2.5,2.5)
               function simple_quadratic_cone(fname)
                   % Read in the name for the input file
                   if nargin ~=1
                       error('simple_quadratic_cone <parameters>');
                   end
                   % Execute the optimization
                   main(fname);
               end
               % Squares its input
               function z = sq(x)
                   z=x*x;
               end
```

```
% Define a simple objective where
%
% f(x,y)=(x-3)^2+(y-2)^2
%
function self = MyObj()
   % Evaluation
   self.eval = @(x) sq(x(1)-3.)+sq(x(2)-2.);
   % Gradient
   self.grad = @(x) [
       2.*x(1)-6;
       2.*x(2)-4];
   % Hessian-vector product
   self.hessvec = @(x,dx) [
       2.*dx(1);
       2.*dx(2)];
end
% Define a simple SOCP inequality
%
h(x,y) = [y >= |x|]
\[ \] h(x,y) = (y,x) >= Q \] 0
%
function self = MyIneq()
   % y=h(x)
   self.eval = @(x)MyIneq_eval(x);
   % z=h'(x)dx
   self.p = @(x,dx)MyIneq_p(x,dx);
   % xhat=h'(x)*dz
   self.ps = @(x,dz) [
       dz.data{1}(2);
       dz.data{1}(1)];
   % xhat=(h''(x)dx)*dz
   self.pps = @(x,dx,dz) [
       0;
       0];
end
% z=h(x)
function z=MyIneq_eval(x)
   global Optizelle;
   z = Optizelle.SQL.create([Optizelle.Cone.Quadratic],[2]);
   z.data{1} = [
       x(2);
       x(1)];
end
% z=h'(x)dx
function z=MyIneq_p(x,dx)
   global Optizelle;
   z = Optizelle.SQL.create([Optizelle.Cone.Quadratic],[2]);
```

```
z.data{1} = [
                           dx(2);
                           dx(1)];
                   end
                   % Actually runs the program
                   function main(fname)
                       % Grab the Optizelle library
                       global Optizelle;
                       setupOptizelle();
                       % Generate an initial guess for the primal
                       x = [1.2; 3.1];
                       \% Generate an initial guess for the dual
                       z = Optizelle.SQL.create([Optizelle.Cone.Quadratic],[2]);
                       % Create an optimization state
                       state=Optizelle.InequalityConstrained.State.t( ...
                           Optizelle.Rm,Optizelle.SQL,x,z);
                       % Read the parameters from file
                       state=Optizelle.json.InequalityConstrained.read( ...
                           Optizelle.Rm,Optizelle.SQL,fname,state);
                       % Create a bundle of functions
                       fns=Optizelle.InequalityConstrained.Functions.t;
                       fns.f=MyObj();
                       fns.h=MyIneq();
                       % Solve the optimization problem
                       state=Optizelle.InequalityConstrained.Algorithms.getMin( ...
                           Optizelle.Rm,Optizelle.SQL,Optizelle.Messaging.stdout,fns,state);
                       % Print out the reason for convergence
                       fprintf('The algorithm converged due to: %s\n', ...
                           Optizelle.OptimizationStop.to_string(state.opt_stop));
                       % Print out the final answer
                       fprintf('The optimal point is: (%e,%e)\n',state.x(1),state.x(2));
                       % Write out the final answer to file
                       Optizelle.json.InequalityConstrained.write_restart( ...
                           Optizelle.Rm,Optizelle.SQL,'solution.json',state);
                   end
Similarly, we setup and solve a simple semidefinite program in our simple SDP cone example:
                   C++
   Language
```

Code // Optimize a simple problem with an optimal solution of (0.5,.25) #include <iostream> #include <iomanip> #include "optizelle/optizelle.h" #include "optizelle/vspaces.h" #include "optizelle/json.h"

```
// Create some type shortcuts
using Optizelle::Rm;
using Optizelle::SQL;
typedef double Real;
// Define a simple objective where
11
// f(x,y)=-x+y
11
struct MyObj : public Optizelle::ScalarValuedFunction <Real,Rm> {
   typedef Rm <Real> X;
   // Evaluation
   double eval(X::Vector const & x) const {
       return -x[0]+x[1];
   }
   // Gradient
   void grad(
       X::Vector const & x,
       X::Vector & grad
   ) const {
       grad[0]=Real(-1.);
       grad[1]=Real(1.);
   }
   // Hessian-vector product
   void hessvec(
       X::Vector const & x,
       X::Vector const & dx,
       X::Vector & H_dx
   ) const {
       H_dx[0] = Real(0.);
       H_dx[1] = Real(0.);
   }
};
// Define a simple SDP inequality
11
// h(x,y) = [y x] >= 0
11
          [x1]
11
struct MyIneq : public Optizelle::VectorValuedFunction <Real,Rm,SQL> {
   typedef Rm <Real> X;
   typedef SQL <Real> Z;
   // z=h(x)
   void eval(
       X::Vector const & x,
       Z::Vector & z
   ) const {
       z(1,1,1)=x[1];
       z(1,1,2)=x[0];
       z(1,2,1)=x[0];
       z(1,2,2)=Real(1.);
   }
```

```
// z=h'(x)dx
   void p(
       X::Vector const & x,
       X::Vector const & dx,
       Z::Vector & z
    ) const {
       z(1,1,1)=dx[1];
       z(1,1,2)=dx[0];
       z(1,2,1)=dx[0];
       z(1,2,2)=Real(0.);
   }
   // xhat=h'(x)*dz
   void ps(
       X::Vector const & x,
       Z::Vector const & dz,
       X::Vector & xhat
   ) const {
       xhat[0] = dz(1,1,2)+dz(1,2,1);
       xhat[1] = dz(1,1,1);
   }
   // xhat=(h''(x)dx)*dz
   void pps(
       X::Vector const & x,
       X::Vector const & dx,
       Z::Vector const & dz,
       X::Vector & xhat
    ) const {
       X::zero(xhat);
    3
};
int main(int argc, char* argv[]){
   // Create some type shortcuts
   typedef Rm <Real>::Vector Rm_Vector;
   typedef SQL <Real>::Vector SQL_Vector;
   // Read in the name for the input file
   if(argc!=2) {
       std::cerr << "simple_sdp_cone <parameters>" << std::endl;</pre>
       exit(EXIT_FAILURE);
   }
   auto fname = argv[1];
   // Generate an initial guess for the primal
    auto x = Rm_Vector(\{1.2, 3.1\});
    // Allocate memory for the dual
    auto z = SQL_Vector ({Optizelle::Cone::Semidefinite},{2});
    // Create an optimization state
   Optizelle::InequalityConstrained <Real,Rm,SQL>::State::t state(x,z);
    // Read the parameters from file
   Optizelle::json::InequalityConstrained <Real,Rm,SQL>::read(fname,state);
```

	<pre>// Create a bundle of functions Optizelle::InequalityConstrained <real,rm,sql>::Functions::t fns; fns.f.reset(new MyObj); fns.h.reset(new MyIneq);</real,rm,sql></pre>
	<pre>// Solve the optimization problem Optizelle::InequalityConstrained <real,rm,sql></real,rm,sql></pre>
	<pre>// Print out the reason for convergence std::cout << "The algorithm converged due to: " <<</pre>
	<pre>// Print out the final answer std::cout << std::setprecision(16) << std::scientific</pre>
	<pre>// Write out the final answer to file Optizelle::json::InequalityConstrained <real,rm,sql> ::write_restart("solution.json",state);</real,rm,sql></pre>
	<pre>// Successful termination return EXIT_SUCCESS; }</pre>
Language	MATLAB/Octave
Code	% Optimize a simple problem with an optimal solution of (0.5,.25)
	<pre>function simple_sdp_cone(fname) % Read in the name for the input file if nargin ~=1 error('simple_sdp_cone <parameters>'); end</parameters></pre>
	<pre>% Execute the optimization main(fname); end</pre>
	<pre>% Define a simple objective where % % f(x,y)=-x+y % function self = MyObj()</pre>
	% Evaluation self.eval = $Q(x) - x(1) + x(2);$
	<pre>% Gradient self.grad = @(x) [-1.; 1.];</pre>
	% Hessian-vector product

```
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```

```
self.hessvec = @(x,dx) [
       0;
       0];
end
% Define a simple SDP inequality
%
% h(x,y) = [y x] >= 0
%
         [x1]
%
function self = MyIneq()
   % z=h(x)
   self.eval = @(x)MyIneq_eval(x);
   % z=h'(x)dx
   self.p = @(x,dx)MyIneq_p(x,dx);
   % xhat=h'(x)*dz
   self.ps = Q(x,dz) [
       dz.data{1}(2,1)+dz.data{1}(1,2);
       dz.data{1}(1,1)];
   % xhat=(h''(x)dx)*dz
   self.pps = @(x,dx,dz) [
       0;
       0];
end
% z=h(x)
function z=MyIneq_eval(x)
   global Optizelle;
   z = Optizelle.SQL.create([Optizelle.Cone.Semidefinite],[2]);
   z.data{1} = [
       x(2) x(1);
       x(1) 1. ];
end
% z=h'(x)dx
function z=MyIneq_p(x,dx)
   global Optizelle;
   z = Optizelle.SQL.create([Optizelle.Cone.Semidefinite],[2]);
   z.data{1} = [
       dx(2) dx(1);
       dx(1) 0. ];
end
% Actually runs the program
function main(fname)
   % Grab the Optizelle library
   global Optizelle;
   setupOptizelle();
   % Generate an initial guess for the primal
   x = [1.2; 3.1];
```

```
% Generate an initial guess for the dual
   z = Optizelle.SQL.create([Optizelle.Cone.Semidefinite],[2]);
   % Create an optimization state
   state=Optizelle.InequalityConstrained.State.t( ...
       Optizelle.Rm,Optizelle.SQL,x,z);
   % Read the parameters from file
   state=Optizelle.json.InequalityConstrained.read( ...
       Optizelle.Rm,Optizelle.SQL,fname,state);
   % Create a bundle of functions
   fns=Optizelle.InequalityConstrained.Functions.t;
   fns.f=MyObj();
   fns.h=MyIneq();
   % Solve the optimization problem
   state=Optizelle.InequalityConstrained.Algorithms.getMin( ...
       Optizelle.Rm,Optizelle.SQL,Optizelle.Messaging.stdout,fns,state);
   % Print out the reason for convergence
   fprintf('The algorithm converged due to: %s\n', ...
       Optizelle.OptimizationStop.to_string(state.opt_stop));
   % Print out the final answer
   fprintf('The optimal point is: (%e,%e)\n',state.x(1),state.x(2));
   % Write out the final answer to file
   Optizelle.json.InequalityConstrained.write_restart( ...
       Optizelle.Rm,Optizelle.SQL,'solution.json',state);
end
```

6.5 State manipulation

State manipulation is a process that allows us to insert arbitrary code into the optimization algorithms. We use this to add new features such as the following:

- Real-time optimal control systems require hard computational time limit. After this time, we must exit the optimization cleanly and return our most current solution.
- For a particular application, we may want to use a custom line-search, but not recode the rest of the optimization algorithms.
- In signal processing, we may know our optimal solution does not have any frequencies above a certain threshold. When this is difficult to formulate as a constraint, we can simply run a high-pass filter on the optimization variable at the end of each iteration.
- When our algorithms perform poorly, we may want to run some custom diagnostics at the end of each optimization iteration.
- In order to replicate our optimization runs, we need to write a restart file at the end of each optimization iteration. We describe this process in the section Restarts.
- Internally, we use state manipulation to add algorithms such as the interior point method to the composite-step SQP method.

In each of these situations, we make use of the **StateManipulator**. In order to manipulate the state, we use an object called the **StateManipulator**. During the optimization computation, we repeatedly call this object with the **bundle of functions**, optimization state, and the location. At this point, we may do any computation and modify the state as desired. In C++ and Python, we implicitly return these changes to the state. In MATLAB/Octave, we must return the state explicitly. In code, we specify the **StateManipulator** as:

, , ,	
Language	C++
Structure	Optizelle::StateManipulator
Interface	Inheritance
Code	<pre>namespace Optizelle{ // A function that has free reign to manipulate or analyze the state. template <typename problemclass=""> struct StateManipulator { // Disallow constructors NO_COPY_ASSIGNMENT(StateManipulator) // Give an empty default constructor StateManipulator() {} // Application virtual void eval(typename ProblemClass::Functions::t const & fns, typename ProblemClass::State::t & state, OptimizationLocation::t const & loc) const = 0; // Allow the derived class to deallocate memory virtual ~StateManipulator() {} }; } </typename></pre>
Language	Python
Structure	Optizelle.StateManipulator
Interface	Inheritance
Code	<pre>class StateManipulator(object): """A function that has free reign to manipulate or analyze the state""" def eval(self,fns,state,loc): """Application""" pass</pre>
Language	MATLAB/Octave

Structure	Optizelle.StateManipulator
Interface	Members present
Code	% A function that has free reign to manipulate or analyze the state. Optizelle.StateManipulator = struct('eval',@(fns,state,loc)state);

Once we define the **StateManipulator**, we call the optimization solver with one of the following four commands, which differs slightly from those defined in the section **Call the optimization solver**. In essence, we add the **StateManipulator** as the last argument to getMin:

Language C++

Code	<pre>Optizelle::Unconstrained<real,xx>::Algorithms::getMin(msg,fns,state,smanip);</real,xx></pre>
	<pre>Optizelle::EqualityConstrained<real,xx,yy>::Algorithms::getMin(msg,fns,state,smanip);</real,xx,yy></pre>
	<pre>Optizelle::InequalityConstrained<real,xx,zz>::Algorithms::getMin(msg,fns,state,smanip);</real,xx,zz></pre>
	<pre>Optizelle::Constrained<real,xx,yy,zz>::Algorithms::getMin(msg,fns,state,smanip);</real,xx,yy,zz></pre>
Language	Python
Code	<pre>Optizelle.Unconstrained.Algorithms.getMin(XX,msg,fns,state,smanip)</pre>
	<pre>Optizelle.EqualityConstrained.Algorithms.getMin(XX,YY,msg,fns,state,smanip)</pre>
	<pre>Optizelle.InequalityConstrained.Algorithms.getMin(XX,ZZ,msg,fns,state,smanip)</pre>
	<pre>Optizelle.Constrained.Algorithms.getMin(XX,YY,ZZ,msg,fns,state,smanip)</pre>
Language	MATLAB/Octave
Code	<pre>state = Optizelle.Unconstrained.Algorithms.getMin(XX,msg,fns,state,smanip);</pre>
	<pre>state = Optizelle.EqualityConstrained.Algorithms.getMin(XX,YY,msg,fns,state,smanip);</pre>
	<pre>state = Optizelle.InequalityConstrained.Algorithms.getMin(XX,ZZ,msg,fns,state,smanip);</pre>
	<pre>state = Optizelle.Constrained.Algorithms.getMin(XX,YY,ZZ,msg,fns,state,smanip);</pre>
an arampla was	use the StateManipulator to add restarts to our Resembred Advanced API example. We

As an example, we use the **StateManipulator** to add restarts to our **Rosenbrock** advanced API example. We discuss restarts in the section entitled **Restarts**.

Language	C++
Code	<pre>// Define a state manipulator that writes out the optimization state at // each iteration. struct MyRestartManipulator : Optizelle::StateManipulator <optizelle::unconstrained <double,myvs=""> > { void eval(typename Optizelle::Unconstrained <double,myvs></double,myvs></optizelle::unconstrained></pre>
	<pre>case Optizelle::OptimizationLocation::EndOfOptimizationIteration: {</pre>

```
std::stringstream ss;
                           ss << "rosenbrock_advanced_api_";</pre>
                           ss << std::setw(4) << std::setfill('0') << state.iter;</pre>
                           ss << ".json";</pre>
                           // Write the restart file
                           Optizelle::json::Unconstrained <double,MyVS>::write_restart(
                              ss.str(),state);
                           break;
                       } default:
                           break;
                       }
                   }
               };
               Python
Language
Code
               # Define a state manipulator that writes out the optimization state at
                # each iteration.
                class MyRestartManipulator(Optizelle.StateManipulator):
                   def eval(self,fns,state,loc):
                       # At the end of the optimization iteration, write the restart file
                       if loc == Optizelle.OptimizationLocation.EndOfOptimizationIteration:
                           # Create a reasonable file name
                           ss = "rosenbrock_advanced_api_%04d.json" % (state.iter)
                           # Write the restart file
                           Optizelle.json.Unconstrained.write_restart(MyVS,ss,state)
Language
               MATLAB/Octave
Code
               \% Define a state manipulator that writes out the optimization state at
               % each iteration.
                function smanip=MyRestartManipulator()
                   smanip=struct('eval',@(fns,state,loc)MyRestartManipulator_(fns,state,loc));
                end
               function state=MyRestartManipulator_(fns,state,loc)
                   global Optizelle;
                   \% At the end of the optimization iteration, write the restart file
                   if(loc == Optizelle.OptimizationLocation.EndOfOptimizationIteration)
                       % Create a reasonable file name
                       ss = sprintf('rosenbrock_advanced_api_%04d.json',state.iter);
                       % Write the restart file
                       Optizelle.json.Unconstrained.write_restart(MyVS(),ss,state);
                   end
               end
```

In order to use this **StateManipulator**, we call Optizelle's solver with the code:

Language C++

Code	<pre>// Solve the optimization problem Optizelle::Unconstrained <double,myvs>::Algorithms ::getMin(mymessaging,fns,state,MyRestartManipulator());</double,myvs></pre>
Language	Python
Code	<pre># Solve the optimization problem Optizelle.Unconstrained.Algorithms.getMin(MyVS,mymessaging,fns,state,MyRestartManipulator())</pre>
Language	MATLAB/Octave
Code	<pre>% Solve the optimization problem state=Optizelle.Unconstrained.Algorithms.getMin(MyVS(),@MyMessaging,fns,state,MyRestartManipulator());</pre>

6.6 Restarts

Restarts are a mechanism to read, write, and archive the progress and solution of an optimization algorithm. In other words, restarts allow us to save the state of an optimization algorithm before it finishes computing. We do this for several reasons:

- In scientific or engineering tasks, we may need to replicate or reproduce our work.
- Large, computationally expensive problems typically require parallel computing clusters. With thousands of computers working in concert, the chance that a hardware failure occurs increases. One way to recover from these failures it to restart the computation after a crash.
- Parallel computing clusters generally share their computing resources between several users. In order to fairly divide use, batch jobs require us to specify the amount of time required to run a job. If we guess this number poorly, restarts allow us to complete the computation later.
- For many problems, it's unclear what algorithm we should use. Second-order methods such as Newton's method are only guaranteed to converge quadratically near the solution. As such, we may be well served to start the computation with a first-order method and then switch to a second-order method as we approach optimality. We can accomplish this by writing a restart file, modifying the specified algorithm, and then resuming the computation.
- Often an algorithm makes progress toward a solution, but then stagnates. In order to diagnose why the algorithm stagnated, we may examine the restart file at the iteration of stagnation. Furthermore, if we have insight into the underlying problem structure, we could modify the solution by hand or with an outside tool and then restart the computation.

Each of these situations requires restarts. As long as we use our built-in vector spaces such as Rm and SQL, we can easily read and write the state to a JSON formatted file with the commands:

Language C++

Code	<pre>Optizelle::json::Unconstrained <real,xx>::write_restart(fname,state);</real,xx></pre>
	<pre>Optizelle::json::Unconstrained <real,xx>::read_restart(fname,x,state);</real,xx></pre>
	<pre>Optizelle::json::EqualityConstrained <real,xx,yy>::write_restart(fname,state);</real,xx,yy></pre>
	<pre>Optizelle::json::EqualityConstrained <real,xx,yy>::read_restart(fname,x,y,state);</real,xx,yy></pre>
	<pre>Optizelle::json::InequalityConstrained <real,xx,zz>::write_restart(fname,state);</real,xx,zz></pre>
	<pre>Optizelle::json::InequalityConstrained <real,xx,zz>::read_restart(fname,x,z,state);</real,xx,zz></pre>
	<pre>Optizelle::json::Constrained <real,xx,yy,zz>::write_restart(fname,state);</real,xx,yy,zz></pre>
	<pre>Optizelle::json::Constrained <real,xx,yy,zz>::read_restart(fname,x,y,z,state);</real,xx,yy,zz></pre>
Language	Python
Code	<pre>Optizelle.json.Unconstrained.write_restart(XX,fname,state); Optizelle.json.Unconstrained.read_restart(XX,fname,x,state);</pre>
	<pre>Optizelle.json.EqualityConstrained.write_restart(XX,YY,fname,state); Optizelle.json.EqualityConstrained.read_restart(XX,YY,fname,x,y,state);</pre>
	<pre>Optizelle.json.InequalityConstrained.write_restart(XX,ZZ,fname,state); Optizelle.json.InequalityConstrained.read_restart(XX,ZZ,fname,x,z,state);</pre>
	<pre>Optizelle.json.Constrained.write_restart(XX,YY,ZZ,fname,state); Optizelle.json.Constrained.read_restart(XX,YY,ZZ,fname,x,y,z,state);</pre>
Language	MATLAB/Octave
Code	<pre>Optizelle.json.Unconstrained.write_restart(XX,fname,state); state = Optizelle.json.Unconstrained.read_restart(XX,fname,x);</pre>
	<pre>Optizelle.json.EqualityConstrained.write_restart(XX,YY,fname,state); state = Optizelle.json.EqualityConstrained.read_restart(XX,YY,fname,x,y);</pre>
	<pre>Optizelle.json.InequalityConstrained.write_restart(XX,ZZ,fname,state); state = Optizelle.json.InequalityConstrained.read_restart(XX,ZZ,fname,x,z);</pre>
	<pre>Optizelle.json.Constrained.write_restart(XX,YY,ZZ,fname,state); state = Optizelle.json.Constrained.read_restart(XX,YY,ZZ,fname,x,y,z);</pre>

As was the case before, XX, YY, and ZZ correspond to the vector spaces X, Y, and Z described in the section Import or define the appropriate vector spaces. Likely, they are just Rm or SQL. Next, we call the function with a Messaging object, msg. Third, the string fname denotes the file name that we read or write the restart. Next, the variable state denotes a State object. During a write, we write the provided state to file. During a read, we read the restart file into the specified state. Finally, the variables x, y, and z denote variables in the spaces XX, YY, and ZZ, respectively. We only use them to initialize memory, so any valid vector works. As an example, we return to our Rosenbrock advanced API example. We already showed how to write a restart file at the end of each optimization iteration in our discussion of StateManipulators. Specifically, we used the write_restart command in our StateManipulator example. To compliment that code, we read an optional restart file prior to optimization with the code:

Language	C++
Code	<pre>// If we have a restart file, read in the parameters if(argc==3) Optizelle::json::Unconstrained <double,myvs>::read_restart(rname,x,state); // Read additional parameters from file Optizelle::json::Unconstrained <double,myvs>::read(pname,state);</double,myvs></double,myvs></pre>
Language	Python
Code	<pre># If we have a restart file, read in the parameters if len(sys.argv)==3: Optizelle.json.Unconstrained.read_restart(MyVS,rname,x,state)</pre>
	<pre># Read additional parameters from file Optizelle.json.Unconstrained.read(MyVS,pname,state)</pre>
Language	MATLAB/Octave
Code	<pre>% If we have a restart file, read in the parameters if(nargin==2) state = Optizelle.json.Unconstrained.read_restart(MyVS(),rname,x); end</pre>
	<pre>% Read additional parameters from file state=Optizelle.json.Unconstrained.read(MyVS(),pname,state);</pre>

As a note, we call the JSON reader after we read the restart file. If we do this in the reverse order, the restart read process overwrites all of our parameters. For Rm and SQL, the above process works seamlessly. In fact, C++, Python, and MATLAB/Octave all use the same format for Rm, which means we can write a restart file in one language and then read the same restart file in a different language. However, for customized vector spaces, we must provide Optizelle information on how to translate a vector to a JSON formatted file using the following commands:

Language	C++
Code	<pre>namespace Optizelle { namespace json { template <> struct Serialization <real,ww> { static std::string serialize(typename WW <real>::Vector const & x, std::string const & name, Natural const & iter) { throw; } static typename WW <real>::Vector deserialize(typename WW <real>::Vector const & x, std::string const & x_json) { throw; } }; }; }</real></real></real></real,ww></pre>

Language	Python
Code	<pre>Optizelle.json.Serialization.serialize.register(serialize,vector_type) Optizelle.json.Serialization.deserialize.register(deserialize,vector_type)</pre>
Language	MATLAB/Octave
Code	<pre>Optizelle.json.Serialization.serialize('register',serialize,check); Optizelle.json.Serialization.deserialize('register',deserialize,check);</pre>

In each command, the serialize and deserialize functions work in a similar manner. The serialize function accepts a vector, the vector's name, and the current iteration. Then, serialize returns a valid JSON structure corresponding to this vector. For Rm, we use simple JSON vector notation such as [1.2, 2.3, 3.4], but this can be significantly more complicated. In fact, for large-scale optimization problems, we suggest storing the vector in a separate binary file and returning a JSON structure that denotes the name of the file. In order to make process of defining these file names easier, we provide access to the variable name and iteration number as the second and third arguments, respectively. Next, the deserialize function accepts two arguments and returns a vector. The first argument denotes a vector in the same vector space as the vector we need translated. The second argument denotes a JSON formatted string of the vector we need to translate. Generally, we use the first argument to initialize memory for the vector we eventually return. Then, we use the JSON formatted string to fill in the appropriate information. In C++, we accomplish this process through template specialization. In Python, we call the serialize and deserialize functions in the Optizelle. json. Serialization module with the "registration" string. Then, we provide our custom serialize and deserialize routines along with the type of the vector that we want to serialize in the variable vector_type. We obtain this information with the type command and require it in order to disambiguate multiple serialization routines. In MATLAB/Octave, we call the serialize and deserialize functions in the Optizelle.json.Serialization structure with the 'registration' string. Then, similar to Python, we provide our custom serialize and deserialize routines along with a function check. The function check accepts a single argument and returns 1 when called with the kind of vector we want to serialize and 0 otherwise. We require the check function to disambiguate the different serialization functions, so we try to make it as specific as possible. As an example, we return to our Rosenbrock advanced API example. There, we define custom serialization routines with the code:

Language	C++
Language Code	<pre>C++ // Define serialization routines for MyVS namespace Optizelle { namespace json { template <> struct Serialization <double,myvs> { static std::string serialize(typename MyVS <double>::Vector const & x, std::string const & name, Natural const & iter) { // Create a string with the format </double></double,myvs></pre>
	<pre>// Greate a string with the format // [x1, x2,, xm]. std::stringstream x_json; x_json.setf(std::ios::scientific); x_json.precision(16); x_json << "["; for(Natural i=0;i<x.size()-1;i++) "="" ",="" ";="" <<=""]";="" pre="" return="" string<="" the="" x.back()="" x[i]="" x_json=""></x.size()-1;i++)></pre>

```
return x_json.str();
                           }
                           static MyVS <double>::Vector deserialize(
                              typename MyVS <double>::Vector const & x_,
                              std::string const & x_json_
                           ) {
                              // Make a copy of x_json_
                              auto x_json = x_json_;
                              // Filter out the commas and brackets from the string
                              char formatting[] = "[],";
                              for(Natural i=0;i<3;i++)</pre>
                                  x_json.erase(
                                      std::remove(x_json.begin(),x_json.end(),formatting[i]),
                                      x_json.end());
                              // Create a new vector that we eventually return
                              auto x = std::vector <double>(x_.size());
                              // Create a stream out of x_json
                              std::stringstream ss(x_json);
                              // Read in each of the elements
                              for(auto i=0;i<x.size();i++)</pre>
                                  ss >> x[i];
                              // Return the result
                              return std::move(x);
                           }
                       };
                   }
               }
Language
               Python
               def serialize_MyVS(x,name,iter):
                   """Serializes an array for the vector space MyVS"""
                   # Create the json representation
                   x_json="[ "
                   for i in xrange(0,len(x)):
                       x_json += str(x[i]) + ", "
                   x_json=x_json[0:-2]
                   x_json +=" ]"
                   return x_json
               def deserialize_MyVS(x,x_json):
                   """Deserializes an array for the vector space MyVS"""
                   # Eliminate all whitespace
                   x_json="".join(x_json.split())
                   # Check if we're a vector
```

```
if x_json[0:1]!="[" or x_json[-1:]!="]":
   raise TypeError("Attempted to deserialize a non-array vector.")
```

Code

```
# Eliminate the initial and final delimiters
                   x_json=x_json[1:-1]
                   # Create a list of the numbers involved
                   x_json=x_json.split(",")
                   # Convert the strings to numbers
                   x_json=map(lambda x:float(x),x_json)
                   # Create a MyVS vector
                   return array.array('d',x_json)
               # Register the serialization routines for arrays
               def MySerialization():
                   Optizelle.json.Serialization.serialize.register(
                       serialize_MyVS,array.array)
                   Optizelle.json.Serialization.deserialize.register(
                       deserialize_MyVS,array.array)
Language
               MATLAB/Octave
Code
               \% Define serialization routines for MyVS
               function MySerialization()
                   global Optizelle;
                   Optizelle.json.Serialization.serialize( ...
                       'register', ...
                       @(x,name,iter)strrep(mat2str(x.data'),' ',', '), ...
                       @(x)isstruct(x) && isfield(x,'data') && isvector(x.data));
                   Optizelle.json.Serialization.deserialize( ...
                       'register', ...
                       @(x,x_json)tostruct(str2num(x_json)'), ...
                       @(x)isstruct(x) && isfield(x,'data') && isvector(x.data));
               end
```

As another example, we refer to our Simple constrained advanced API example. This differs from the previous example since we write our vectors to a separate file. In order to accomplish this, we define custom serialization routines with the code:

Language	C++
Code	<pre>// Define serialization routines for MyVS namespace Optizelle { namespace json { template <> struct Serialization <double,myvs> {</double,myvs></pre>
	static std::string serialize(
	<pre>typename MyVS <double>::Vector const & x,</double></pre>
	<pre>std::string const & name,</pre>
	Natural const & iter
) {
	<pre>// Create the filename where we put our vector</pre>
	<pre>std::stringstream fname;</pre>
	<pre>fname << "./restart/";</pre>
	<pre>fname << name << ".";</pre>
	<pre>fname << std::setw(4) << std::setfill('0') << iter;</pre>

```
fname << ".txt";</pre>
   // Actually write the vector there
   std::ofstream fout(fname.str());
   if(fout.fail()) {
       std::stringstream msg;
       msg << "While writing the variable " << name</pre>
           << " to file on iteration " << iter
           << ", unable to open the file: "
           << fname.str() << ".";
       throw Optizelle::Exception::t(msg.str());
   }
   fout.setf(std::ios::scientific);
   fout.precision(16);
   for(Natural i=0;i<x.size();i++)</pre>
       fout << x[i] << std::endl;</pre>
   // Close out the file
   fout.close();
   // Use this filename as the json string
   std::stringstream x_json;
   x_json << "\"" << fname.str() << "\"";</pre>
   return x_json.str();
}
static MyVS <double>::Vector deserialize(
   typename MyVS <double>::Vector const & x_,
   std::string const & x_json_
) {
   // Make a copy of x_json_
   auto x_json = x_json_;
   // Filter out the quotes and newlines from the string
   auto formatting = "\"\n";
   for(auto i=0;i<2;i++)</pre>
       x_json.erase(
           std::remove(x_json.begin(),x_json.end(),formatting[i]),
           x_json.end());
   // Open the file for reading
   std::ifstream fin(x_json.c_str());
   if(!fin.is_open())
       throw Optizelle::Exception::t(
           "Error while opening the file " + x_json + ": " +
           strerror(errno));
   // Create a new vector that we eventually return
   auto x = std::vector <double> (x_.size());
   // Read in each of the elements
   for(auto i=0;i<x.size();i++)</pre>
       fin >> x[i];
   // Return the result
   return std::move(x);
}
```

};

```
}
Language
               Python
Code
               def serialize_MyVS(x,name,iter):
                   """Serializes an array for the vector space MyVS"""
                   # Create the filename where we put our vector
                   fname = "./restart/%s.%04d.txt" % (name,iter)
                   # Actually write the vector there
                   fout = open(fname, "w");
                   for i in xrange(0,len(x)):
                       fout.write("%1.16e\n" % x[i])
                   # Close out the file
                   fout.close()
                   # Use this filename as the json string
                   x_json = "\"%s\"" % fname
                   return x_json
               def deserialize_MyVS(x_,x_json):
                   """Deserializes an array for the vector space MyVS"""
                   # Eliminate all whitespace
                   x_json="".join(x_json.split())
                   # Eliminate the initial and final delimiters
                   x_json=x_json[1:-1]
                   # Open the file for reading
                   fin = open(x_json,"r")
                   # Allocate a new vector to return
                   x = copy.deepcopy(x_)
                   # Read in each of the elements
                   for i in xrange(0,len(x)):
                       x[i] = float(fin.readline())
                   # Close out the file
                   fin.close()
                   # Return the result
                   return x
               # Register the serialization routines for arrays
               def MySerialization():
                   Optizelle.json.Serialization.serialize.register(
                       serialize_MyVS,array.array)
                   Optizelle.json.Serialization.deserialize.register(
                       deserialize_MyVS,array.array)
```

}

```
MATLAB/Octave
Language
Code
               % Define the serialize routine for MyVS
               function x_json=serialize_MyVS(x,name,iter)
                   % Create the filename where we put our vector
                   fname=sprintf('./restart/%s.%04d.txt',name,iter);
                   % Actually write the vector there
                   dlmwrite(fname,x.data);
                   % Use this filename as the json string
                   x_json = sprintf('\"%s\"',fname);
               end
               % Define the deserialize routine for MyVS
               function x=deserialize_MyVS(x_,x_json)
                   \% Filter out the quotes and newlines from the string
                   x_json = strrep(x_json,'"',');
                   x_json = strrep(x_json, sprintf('\n'), ');
                   % Read the data into x
                   x=tostruct(dlmread(x_json));
               end
               % Define serialization routines for MyVS
               function MySerialization()
                   global Optizelle;
                   Optizelle.json.Serialization.serialize( ...
                       'register', ...
                      @(x,name,iter)serialize_MyVS(x,name,iter), ...
                      @(x)isstruct(x) && isfield(x,'data') && isvector(x.data));
                   Optizelle.json.Serialization.deserialize( ...
                       'register', ...
                      @(x,x_json)deserialize_MyVS(x,x_json), ...
                      @(x)isstruct(x) && isfield(x,'data') && isvector(x.data));
               end
```

In some situations, we want to avoid using JSON all together. Generally, this occurs when integrating Optizelle into an existing application with rigid I/O requirements. In this case, we provide an alternative mechanism to generate restarts.

At its core, restarts consist of two mechanisms: release and capture. Release transforms the state into a collection of lists that contain all of the optimization information. Capture reverses this process. Generally, we do a release, write these lists containing the state information to file, and then capture the state. The idea behind this process is that we don't expect ourselves to remember all of the optimization variables. Certainly, this collection of variables changes whenever we update the code or add new algorithms. However, if we know how to write a list of variables to file, we can simply iterate over the list and take the appropriate action. More specifically, the capture and release functions operate on lists of tuples. As far as the type used for the lists, we have:

Language	C++
Туре	std::list
Language	Python
\mathbf{Type}	list

Language MATLAB/Octave

Type cell

For the type used by the tuples, we have

Language	C++
Type	std::pair
Language	Python
Type	tuple
Language	MATLAB/Octave
Type	cell

In these tuples, we always use a string for the first element. This represents the unique label for the item. The second items depends on the type involved and we enumerate these possibilities below:

\mathbf{Type}	Reals
Description	List of Real numbers and labels.
\mathbf{Type}	Naturals
Description	List of Natural numbers and labels.
\mathbf{Type}	Params
Description	List of strings and labels. These strings correspond to the various Enumerated types that have been converted to strings using the to_string function, which we also describe in the Enumerated type documentation.
Туре	X_Vectors
Description	List of X_Vector vectors and labels.
2 occurption	
Type	Y_Vectors
Description	List of Y_Vector vectors and labels.
\mathbf{Type}	Z_Vectors
Description	List of Z_Vector vectors and labels.
Based on the above types, we release and capture the state with the following code:	

Language C++

```
Code
```

```
Optizelle::Unconstrained <Real,XX>::Restart::X_Vectors xs;
Optizelle::Unconstrained <Real,XX>::Restart::Reals reals;
Optizelle::Unconstrained <Real,XX>::Restart::Naturals nats;
Optizelle::Unconstrained <Real,XX>::Restart::Params params;
Optizelle::Unconstrained <Real,XX>::Restart
    ::release(state,xs,reals,nats,params);
Optizelle::Unconstrained <Real,XX>::Restart
   ::capture(state,xs,reals,nats,params);
Optizelle::EqualityConstrained <Real,XX,YY>::Restart::X_Vectors xs;
Optizelle::EqualityConstrained <Real,XX,YY>::Restart::Y_Vectors ys;
Optizelle::EqualityConstrained <Real,XX,YY>::Restart::Reals reals;
Optizelle::EqualityConstrained <Real,XX,YY>::Restart::Naturals nats;
Optizelle::EqualityConstrained <Real,XX,YY>::Restart::Params params;
Optizelle::EqualityConstrained <Real,XX,YY>::Restart
    ::release(state,xs,ys,reals,nats,params);
Optizelle::EqualityConstrained <Real,XX,YY>::Restart
   ::capture(state,xs,ys,reals,nats,params);
Optizelle::InequalityConstrained <Real,XX,ZZ>::Restart::X_Vectors xs;
Optizelle::InequalityConstrained <Real,XX,ZZ>::Restart::Z_Vectors zs;
Optizelle::InequalityConstrained <Real,XX,ZZ>::Restart::Reals reals;
Optizelle::InequalityConstrained <Real,XX,ZZ>::Restart::Naturals nats;
Optizelle::InequalityConstrained <Real,XX,ZZ>::Restart::Params params;
Optizelle::InequalityConstrained <Real,XX,ZZ>::Restart
   ::release(state,xs,zs,reals,nats,params);
Optizelle::InequalityConstrained <Real,XX,ZZ>::Restart
   ::capture(state,xs,zs,reals,nats,params);
Optizelle::Constrained <Real,XX,YY,ZZ>::Restart::X_Vectors xs;
Optizelle::Constrained <Real,XX,YY,ZZ>::Restart::Y_Vectors ys;
Optizelle::Constrained <Real,XX,YY,ZZ>::Restart::Z_Vectors zs;
Optizelle::Constrained <Real,XX,YY,ZZ>::Restart::Reals reals;
Optizelle::Constrained <Real,XX,YY,ZZ>::Restart::Naturals nats;
Optizelle::Constrained <Real,XX,YY,ZZ>::Restart::Params params;
Optizelle::Constrained <Real,XX,YY,ZZ>::Restart
   ::release(state,xs,ys,zs,reals,nats,params);
Optizelle::Constrained <Real,XX,YY,ZZ>::Restart
   ::capture(state,xs,ys,zs,reals,nats,params);
```

Language	Python
Code	<pre>xs = Optizelle.Unconstrained.Restart.X_Vectors() reals = Optizelle.Unconstrained.Restart.Reals() nats = Optizelle.Unconstrained.Restart.Naturals() params = Optizelle.Unconstrained.Restart.Params() Optizelle.Unconstrained.Restart.release(XX,state,xs,reals,nats,params) Optizelle.Unconstrained.Restart.capture(XX,state,xs,reals,nats,params) xs = Optizelle.EqualityConstrained.Restart.Y_Vectors() ys = Optizelle.EqualityConstrained.Restart.Reals() nats = Optizelle.EqualityConstrained.Restart.Naturals() params = Optizelle.EqualityConstrained.Restart.Naturals() Optizelle.EqualityConstrained.Restart.Params() Optizelle.EqualityConstrained.Restart.Params() Optizelle.EqualityConstrained.Restart.release(XX,YY,state,xs,ys,reals,nats,params) Optizelle.EqualityConstrained.Restart.capture(</pre>
	XX,YY,state,xs,ys,reals,nats,params)

	<pre>xs = Optizelle.InequalityConstrained.Restart.X_Vectors() zs = Optizelle.InequalityConstrained.Restart.Z_Vectors() reals = Optizelle.InequalityConstrained.Restart.Reals() nats = Optizelle.InequalityConstrained.Restart.Naturals() params = Optizelle.InequalityConstrained.Restart.Params() Optizelle.InequalityConstrained.Restart.Params() Optizelle.InequalityConstrained.Restart.release(XX,ZZ,state,xs,zs,reals,nats,params) Optizelle.InequalityConstrained.Restart.capture(XX,ZZ,state,xs,zs,reals,nats,params) xs = Optizelle.Constrained.Restart.X_Vectors() ys = Optizelle.Constrained.Restart.Z_Vectors() reals = Optizelle.Constrained.Restart.Reals() nats = Optizelle.Constrained.Restart.Naturals() params = Optizelle.Constrained.Restart.Params() Optizelle.Constrained.Restart.Params() Optizelle.Constrained.Restart.release(XX,YY,ZZ,state,xs,ys,zs,reals,nats,params) Optizelle.Constrained.Restart.release(XX,YY,ZZ,state,xs,ys,zs,reals,nats,params)</pre>
Language	MATLAB/Octave
Code	<pre>xs = Optizelle.Unconstrained.Restart.X_Vectors; reals = Optizelle.Unconstrained.Restart.Reals; nats = Optizelle.Unconstrained.Restart.Naturals; params = Optizelle.Unconstrained.Restart.Params; [xs reals nats params] = Optizelle.Unconstrained.Restart.release(XX,state); state = Optizelle.Unconstrained.Restart.capture(XX,state,xs,reals,nats,params); xs = Optizelle.EqualityConstrained.Restart.X_Vectors; reals = Optizelle.EqualityConstrained.Restart.Y_Vectors; reals = Optizelle.EqualityConstrained.Restart.Naturals; params = Optizelle.EqualityConstrained.Restart.Naturals; state = Optizelle.EqualityConstrained.Restart.Params; [xs ys reals nats params] = Optizelle.EqualityConstrained.Restart.release(XX,YY,state); state = Optizelle.EqualityConstrained.Restart.capture(XX,YY,state); state = Optizelle.EqualityConstrained.Restart.Z_Vectors; zs = Optizelle.InequalityConstrained.Restart.X_Vectors; zs = Optizelle.InequalityConstrained.Restart.Z_Vectors; reals = Optizelle.InequalityConstrained.Restart.Reals; nats = Optizelle.InequalityConstrained.Restart.Reals; state = Optizelle.InequalityConstrained.Restart.Reals; nats = Optizelle.InequalityConstrained.Restart.Params; [xs zs reals nats params] = Optizelle.InequalityConstrained.Restart.capture(XX,ZZ,state); state = Optizelle.InequalityConstrained.Restart.capture(XX,ZZ,state,xs,zs,reals,nats,params);</pre>

```
xs = Optizelle.Constrained.Restart.X_Vectors;
ys = Optizelle.Constrained.Restart.Y_Vectors;
zs = Optizelle.Constrained.Restart.Z_Vectors;
reals = Optizelle.Constrained.Restart.Reals;
nats = Optizelle.Constrained.Restart.Naturals;
params = Optizelle.Constrained.Restart.Params;
[xs ys zs reals nats params] = Optizelle.Constrained.Restart.release( ...
XX,YY,ZZ,state);
state = Optizelle.Constrained.Restart.capture( ...
XX,YY,ZZ,state,xs,ys,zs,reals,nats,params);
```

As with read_restart and write_restart, we most likely use this functions within a StateManipulator. However, when possible, we are likely better off just using the JSON formatted restart mechanisms within read_restart and write_restart.

6.7 Caching Computations

Internally, Optizelle caches many operations in order to reduce unnecessary computation. This includes computations such as the objective or gradient evaluations. Nevertheless, there are operations that should be cached that Optizelle does not control due to its matrix-free nature. These operations must be cached by the user's code. In the following section, we detail what these operations are and how they should be cached. The following table summarizes the different pieces of the code that can be cached, the number of items that should be stored, and the priority of caching this particular element.

Computation	Objective evaluation during the first gradient solve
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Priority	Low
Number Stored	11
Description	During initialization, Optizelle evaluates the gradient before the objective function. Depending on the problem, it may be possible to evaluate and cache the objective function at the same time as this computation. Specifically, when the objective function has the form $J(x) = f(g(x))$, we calculate the gradient as
	$ abla J(x) = g'(x)^* abla f(g(x)).$
	When the evaluation of $g(x)$ is expensive, such as solving a PDE or computing an inverse, we can use this calculation for both the gradient and the objective function by simultaneously computing both $f(g(x))$ and $\nabla f(g(x))$.
	Despite this utility, we do not typically prioritize this optimization. We only benefit from saving this computation on the first iteration since Optizelle automatically caches the appropriate objective evaluations from the globalization, be that from line-search or trust-region algorithms, for the rest of the algorithm. Therefore, subsequent gradient evaluations don't need to cache information about the objective since it's already been cached. Nevertheless, when we repeatedly run the first iteration of an optimization problem in order to check the problem setup, this caching can save in the overall computation.
Computation	Nested computations and state solves
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Priority	High
Number Stored	1 1

Description During the discussion of caching the objective, we spoke of objective functions of the form J(x) = f(g(x)). As we noted before, we have that

$$\nabla J(x) = g'(x)^* \nabla f(g(x)),$$

but we also note that

 $\nabla^2 J(x)\partial x = (g''(x)\partial x)^* \nabla f(g(x)) + g'(x)^* \nabla^2 f(g(x))g'(x)\partial x.$

Here, we see that we repeatedly use the quantity g(x). When the evaluation of g(x) is expensive, such as solving a PDE or computing an inverse, then caching this element allows us to save significantly on the computational cost. When the evaluation of g(x) corresponds to a PDE solve, we refer to its evaluation as a state solve.

Computation Hessian

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

Priority Low

- Number Stored 1
- **Description** Although Optizelle implements matrix-free algorithms, we can still use a precomputed Hessian when one is available. Since calculating a Hessian can be expensive, we should only calculate it once per iteration and use it both in computing in the Hessian-vector product as well as the Hessian preconditioner.

Overall, we do not prioritize computing the Hessian explicitly as it tends to require a lot of memory. In addition, we rely on Newton's method in order to obtain quadratic convergence, but this fast convergence only occurs when close to the optimal solution. When far away from the optimal solution, we waste computational effort when fully computing second-order information. Generally, truncated-CG does a good job at determining how many Hessian-vector products are required and this does not require a fully computed Hessian.

- Computation Factorization, inverse, or approximate inverse of the Hessian
- Problem Class Unconstrained, Inequality Constrained
- **Priority** Low

Number Stored 1

Description For problems without equality constraints, Optizelle allows the user to define a preconditioner for the Hessian. Recall, the null space projection inherent to the compositestep SQP method precludes a Hessian preconditioner from being used on problems with equality constraints. For more details see the section (Optional) Define the preconditioners. In any case, barring some kind of problem specific preconditioner, we can always compute and then factorize the Hessian to be used as a preconditioner. If we do this, we should also cache the Hessian computation itself.

Overall, we do not prioritize caching this information. Similar to the discussion of caching the Hessian, far from the optimal solution, Newton's method does not guarantee quadratic convergence. Therefore, we waste computational effort when computing the Hessian and factorizing it every iteration in order to force a pure Newton step.

Computation Total derivative (Jacobian) of the equality constraints

Problem Class Equality Constrained, Constrained

Priority High

Number Stored 2

Description Although Optizelle only requires the action of the derivative of the equality constraints on a vector, $g'(x)\partial x$, we benefit greatly from computing the total derivative g'(x) and caching the result. First, depending on the inner product, when g'(x) or $g'(x)^*$ is explicitly available, we can quickly compute its adjoint. For example, when using the inner product $\langle x, y \rangle = x^T y$, we simply have to transpose the matrix. Second, each augmented system solve requires the repeated application of $g'(x)\partial x$ and $g'(x)^*\partial y$. Combined with the first point, we can compute these operations by simply multiplying the cached result by a vector. Third, when solving a problem with more than tens of variables, we require a preconditioner for the augmented system, which can be accomplished by finding a preconditioner for the operator $g'(x)g'(x)^*$. When these derivatives are explicitly available, we can easily form and factorize this matrix. As we discuss below, we should also cache this factorization.

Note, unlike most of the other caching, we require two cached elements for an efficient code. During globalization, we compute a new equality multiplier, which requires an augmented system solve at the trial point. If we accept the point, we can reuse the new cached derivative. However, if we reject the point, we will continue to require the current cached derivative. As a final note, it's often easier to cache and store $g'(x)^*$ as opposed to g'(x). For example, given the inner product $\langle x, y \rangle = x^T y$ and a function of the form

$$g(x) = \begin{bmatrix} g_1(x) \\ \vdots \\ g_m(x) \end{bmatrix},$$

we can compute $g'(x)^*$ as

$$g'(x)^* = \begin{bmatrix} \nabla g_1(x) & \dots & \nabla g_m(x) \end{bmatrix}.$$

Especially with tools like automatic differentiation, this form becomes somewhat more natural to compute since we don't have to compute an extra transpose, which we undo later. Further, if we decide to compute the Schur preconditioner using a QR factorization, we actually factorize $g'(x)^*$ and not g'(x). Though, as we stated above, we can quickly compute one form from the other, so we always use what's easiest to compute and calculate. For more information on preconditioning, see the section (Optional) Define the preconditioners.

Computation Factorization, inverse, or approximate inverse for the Schur preconditioner

- Problem Class Equality Constrained, Constrained
- **Priority** High
- Number Stored 2
- **Description** As we discuss in the section (Optional) Define the preconditioners, we require a Schur preconditioner for equality constrained problems that contain more than tens of variables. To accomplish this, we generally factorize $g'(x)g'(x)^*$, but we can use a problem specific preconditioner as well. In either case, it's important that we cache this computation since we repeatedly require it and it's likely expensive to compute. Similar to our discussion of caching the total derivative of the equality constraints, we require two cached factorizations for an efficient code.

Computation Adjoint of the second derivative of the equality constraints applied to a vector

Problem Class Equality Constrained, Constrained

Priority Low

Number Stored 1

Description During the tangential subproblem, which solves the optimality conditions, we require the repeated computation of $(g''(x)\partial x)^*y$. Sometimes, we can precompute part of this computation, which can accelerate this application. For example, when we use the inner product $\langle x, y \rangle = x^T y$ and have a function of the form

$$g(x) = \begin{bmatrix} g_1(x) \\ \vdots \\ g_m(x) \end{bmatrix},$$

we have that

$$(g''(x)\partial x)^* y = \left(\sum_{i=1}^m y_i \nabla^2 g_i(x)\right) \partial x.$$

In this case, we can cache the quantity

$$\sum_{i=1}^m y_i \nabla^2 g_i(x)$$

to accelerate the computation.

Most of the time, we do not prioritize caching this operator. This operator has the same size as the Hessian, which tends to require a lot of memory. Further, when far from the optimal solution, we may only require the action of this operator on a vector a few times each iteration. Therefore, computing the entire operator can be wasteful.

In order to illustrate these caching techniques, let us setup and solve a simple parameter estimation problem. In parameter estimation, we seek an unknown parameter, k, that characterizes a model, which is often a PDE describing some kind of physical system. In order to find these parameters, we run a series of experiments on the physical system and collect the measurable data, d. Then, we match this data to the output of the model, u. For example, we can model a parameter estimation problem governed by the steady-state convection-diffusion equations in 1-D as

$$\min_{\substack{k \in \mathbb{R}^2, u \in C^2([0,1])}} \frac{\frac{1}{2} \|u - d\|^2}{\text{st}}$$
$$k_1 \nabla \cdot (\nabla u) + k_2 \nabla \cdot u = f$$
$$u(0) = a$$
$$u(1) = b.$$

To be sure, we give the simplest possible case here. Really, there should be a time component and k should represent material properties that vary spatially like u. Nevertheless, this problem will demonstrate that even a problem with only two variables can be very expensive to solve and that intermediate quantities should be cached appropriately. To that end, our strategy for this example will be to

- 1. Discretize the differential equation using a finite-difference method
- 2. Implement caching on the reduced-space (unconstrained) formulation
- 3. Implement caching on the full-space (equality constrained) formulation

This includes code written in MATLAB/Octave demonstrating the caching called computation_caching in the examples directory. We explain the terms *reduced-space* and *full-space* below.

Discretization

In order to discretize the diffusion operator, $\nabla \cdot \nabla$, we use the second-order accurate finite-difference operator

$$A = \frac{1}{\partial x^2} \begin{bmatrix} -2 & -1 & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}.$$

In order to accommodate the Dirichlet boundary conditions, we also define a vector that we use to modify the right hand side with information about the boundary conditions,

$$\hat{A} = \frac{1}{\partial x^2} \begin{bmatrix} -a \\ 0 \\ \vdots \\ 0 \\ -b \end{bmatrix}.$$

Normally, we just subtract this quantity from the discretized f, but since we have unknown material properties k, we represent it explicitly. Next, we discretize the convection operator, $\nabla \cdot$, using the first-order accurate finite difference operator

$$B = \frac{1}{\partial x} \begin{bmatrix} 1 & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}$$

As before, we accommodate the Dirichlet boundary condition with a vector to modify the right hand side with information about the boundary conditions,

$$\hat{B} = \frac{1}{\partial x} \begin{bmatrix} -a \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

This allows us to specify the discretized parameter estimation problem as

$$\min_{\substack{k \in \mathbb{R}^2, u \in \mathbb{R}^m \\ \text{st}}} \frac{\frac{1}{2} \|u - d\|^2}{(k_1 A + k_2 B)u} = f - k_1 \hat{A} - k_2 \hat{B}.$$

For brevity, we specify that

$$C(k) = k_1 A + k_2 B$$
$$g(k) = f - k_1 \hat{A} - k_2 \hat{B}$$

which allows us to reformulate the discretized parameter estimation problem as

$$\min_{\substack{k \in \mathbb{R}^2, u \in \mathbb{R}^m \\ \text{st}}} \frac{\frac{1}{2} \|u - d\|^2}{\text{st}} = G(k).$$

We call the above formulation the *full-space formulation*. Alternatively, we can solve for u in the constraints and instead solve $\min_{k=1}^{n} \frac{||C(k)|^{-1}c(k) - d||^2}{||C(k)|^{-1}c(k) - d||^2}$

$$\min_{k \in \mathbb{R}^2} \quad \frac{1}{2} \| C(k)^{-1} g(k) - d \|$$

which we call the *reduced-space formulation*.

Caching the reduced-space (unconstrained) formulation

In the reduced-space formulation, let us set

$$J(k) = \frac{1}{2} \|C(k)^{-1}g(k) - d\|^2$$

In order to optimize with this function, we require the gradient and the Hessian-vector product. In order to derive the gradient, we calculate the partial derivative with respect to k_i as

$$\begin{aligned} J_i'(k) = & \langle C(k)^{-1}g(k) - d, -C(k)^{-1}C_i'(k)C(k)^{-1}g(k) + C(k)^{-1}g_i'(k) \rangle \\ = & \langle C(k)^{-1}g(k) - d, -C(k)^{-1}(C_i'(k)C(k)^{-1}g(k) - g_i'(k)) \rangle \end{aligned}$$

where

$$C'_1(k) = A, \quad C'_2(k) = B,$$

 $g'_1(k) = -\hat{A}, \quad g'_2(k) = -\hat{B}.$

Then,

$$abla J(k) = \begin{bmatrix} J_1'(k) \\ J_2'(k) \end{bmatrix}.$$

In order to calculate the Hessian-vector product, we continue this process and compute the full Hessian. We see that the second partial derivative of J with respect to k_i and k_j is

$$\begin{split} J_{ij}''(k) = & \langle -C(k)^{-1}(C_j'(k)C(k)^{-1}g(k) - g_j'(k)), -C(k)^{-1}(C_i'(k)C(k)^{-1}g(k) - g_i'(k)) \rangle \\ & + \langle C(k)^{-1}g(k) - d, C(k)^{-1}C_j'(k)C(k)^{-1}(C_i'(k)C(k)^{-1}g(k) - g_i'(k)) \rangle \\ & + \langle C(k)^{-1}g(k) - d, C(k)^{-1}(C_i'(k)C(k)^{-1}C_j'(k)C(k)^{-1}g(k)) \rangle \\ & + \langle C(k)^{-1}g(k) - d, -C(k)^{-1}(C_i'(k)C(k)^{-1}g_j'(k)) \rangle. \end{split}$$

Certainly, we could group terms more optimally, but this formulation is good enough for our purposes. Then, we have that

$$\nabla^2 J(k) = \begin{bmatrix} J_{11}''(k) & J_{12}''(k) \\ J_{21}''(k) & J_{22}''(k) \end{bmatrix}.$$

At this point, we can implement the necessary optimization functions and cache effectively. We begin with caching the initial objective function solve in the code

```
% Evaluates the objective
function z = obj_eval(params,x)
   % Cached objective evaluation. Really, this only saves us the first
   % objective evaluation as the subsequent evaluations are cached by
   % Optizelle
   global ocache
   % Performance diagnostis
   global diagnostics
   \% Grab the cached objective evaluation when possible
   if ~isempty(ocache) && isequal(x,ocache.x)
       z = ocache.eval;
       diagnostics.used_cached_objective = diagnostics.used_cached_objective+1;
   else
       % We don't use the caching state solve here because the objective
       % may be evaluated at multiple points during a single optimization
       \% iteration, primarily for globalization. This differs from the
       \% gradient and Hessian-vector product, which are both evalated at a
       % fixed point each iteration.
       u = state_uncached(params,x,rhs(params,x));
       % Evaluate the objective
       z = 0.5 * norm(u-params.d)^2;
```

```
end
end
% Evaluates the gradient
function grad = obj_grad(params,x)
   % Cached objective evaluation
   global ocache
   % Solve for the current solution
   u = state(params,x,rhs(params,x));
   % Cached the state solution globally for the objective
   if isempty(ocache) || ~isequal(x,ocache.x)
       ocache.x = x;
       ocache.eval = 0.5 * norm(u-params.d)^2;
   end
   % Set each element of the gradient
   grad = zeros(2,1);
   for i=1:2
       grad(i) = innr( ...
           u-params.d, ...
           -state(params,x,op_p(i,params,x)*u - rhs_p(i,params,x)));
   end
end
```

In the function obj_grad, we compute the objective during the gradient solve and store it in the global variable ocache. Then, the function obj_eval uses this cached value when possible. Note, it's possible to accomplish the same effect without global variables by using an intermediate function with persistent variables, but this method works well enough. Next, we cache the state solves with the code

```
% Solves the discretized PDE with caching
function z = state(params,x,rhs)
   % Keep track of where the solve occurs
   persistent cache
   % Performance diagnostics
   global diagnostics
   \% Cache the factorization when required
   if isempty(cache) || ~isequal(x,cache.x)
       % Save the point we're factorizing at
       cache.x = x;
       % Factorize the operator
       [cache.l cache.u cache.p cache.q cache.r] = ...
           lu(op(params,x),'vector');
       % Keep track that we did a new factorization
       diagnostics.state_factorization_cached = ...
           diagnostics.state_factorization_cached+1;
   end
   % Solve the linear system
   z = zeros(size(rhs));
   z(cache.q) = cache.u\(cache.l\(cache.r(:,cache.p)\rhs));
end
```

We greatly improve the code's performance with this routine because it insures that we only factorize the linear system associated with the discretized convection-diffusion equations once per iteration. It accomplishes this by storing the cached results in the persistent variable **cache**. As far as the second-order information, we see how to compute and cache the Hessian-vector product with the code

% Evaluates the Hessian-vector product

```
function hv = obj_hv(params,x,dx)
   hv = hessian(params,x)*dx;
end
% Finds the Hessian
function H = hessian(params,x)
   % Keep track of where the construction occurs
   persistent cache
   % Performance diagnostics
   global diagnostics
   % Cache the Hessian when required
   if isempty(cache) || ~isequal(x,cache.x)
       % Save the point we're evaluating the Hessian at
       cache.x = x;
       % Solve for the current solution
       u = state(params,x,rhs(params,x));
       % Calculate the Hessian
       cache.H = zeros(2);
       innr = @(x,y)x'*y;
       for j=1:2
           for i=1:j
               cache.H(i,j) = ...
                  innr( ...
                      -state(params, x, ...
                          op_p(j,params,x)*u - rhs_p(j,params,x)), ...
                      -state(params, x, ...
                          op_p(i,params,x)*u - rhs_p(i,params,x))) + ...
                  innr(u-params.d, ...
                      state(params, x, ...
                          op_p(j,params,x) * state(params,x, ...
                             op_p(i,params,x)*u-rhs_p(i,params,x))))+ ...
                  innr(u-params.d, ...
                      state(params, x, ...
                          op_p(i,params,x) * state(params,x, ...
                             op_p(j,params,x) * u))) + ...
                  innr(u-params.d, ...
                      -state(params, x, ...
                          op_p(i,params,x) * ...
                             state(params,x,rhs_p(j,params,x))));
           end
       end
       cache.H(2,1)=cache.H(1,2);
       % Keep track that we cache a Hessian
       diagnostics.hessian_cached = diagnostics.hessian_cached+1;
   end
```

```
% Evaluate the Hessian-vector product
H = cache.H;
end
```

Notice that we compute and cache the dense Hessian in the routine **hessian**, which makes the Hessian-vector product a simple multiplication. As before, we accomplish this caching with the persistent variable **cache**. Also note, this code relies on the cached state solves we describe above for fast performance. Finally, we implement and cache a Hessian preconditioner using the inverse of the Hessian computed with the code

```
\% Evaluates the inverse of the Hessian applied to a vector
function ihv = obj_hv_inv(params,x,dx)
   % Keep track of where the factorization occurs
   persistent cache
   % Performance diagnostics
   global diagnostics
   \% Cache the Hessian factorization when required
   if isempty(cache) || ~isequal(x,cache.x)
       \% Save the point we're factorizing the Hessian factorization at
       cache.x = x;
       % Grab the current Hessian
       H = hessian(params,x);
       % Factorize the Hessian
       [cache.l cache.u cache.p]=lu(H, 'vector');
       % Keep track that we cache a Hessian factorization
       diagnostics.hessian_factorization_cached = ...
           diagnostics.hessian_factorization_cached+1;
   end
   % Apply the inverse to the direction
   ihv = cache.u\(cache.l\dx(cache.p));
end
```

Similar to the other functions, we cache the intermediate results in the persistent variable cache. Also note that we rely on the cached Hessian in the code listed above.

Caching the full-space (equality constrained) formulation

If the full-space formulation, we focus on the constraint

$$G(k, u) = C(k)u - g(k)$$

In order to derive the total derivative, we note that

$$G'_{k_i}(k, u) = C'_i u - g'_i(k)$$
$$G'_u(k, u) = C(k).$$

This implies that the total derivative and its adjoint are

$$G'(k,u) = \begin{bmatrix} C'_1 u - g'_1(k) & C'_2 u - g'_2(k) & C(k) \end{bmatrix}$$
$$G'(k,u)^* = \begin{bmatrix} (C'_1 u - g'_1(k))^T \\ (C'_2 u - g'_2(k))^T \\ C(k)^T \end{bmatrix}.$$

We wrote out the adjoint explicitly because it makes it easier to derive the adjoint of the second-derivative in a more cacheable form

$$(G^{\prime\prime}(k,u)(\partial k,\partial u))^*\partial y = \begin{bmatrix} 0 & 0 & \partial y^T C_1^\prime(k) \\ 0 & 0 & \partial y^T C_2^\prime(k) \\ C_1^\prime(k)^T \partial y & C_2^\prime(k)^T \partial y & 0 \end{bmatrix} \begin{bmatrix} \partial k_1 \\ \partial k_2 \\ \partial u \end{bmatrix}$$

```
\% Evaluates the derivative of the equality constraint
function z = eq_p(params,x,dx)
   z = deriv(params,x)*dx;
end
\% Evaluates the adjoint of the derivative of the equality constraint
function z = eq_ps(params,x,dy)
   z = deriv(params,x)'*dy;
end
% Finds the total derivative of the equality constraints
function D = deriv(params,x)
   % Keep track of where the evaluation occurs
   persistent cache
   % Performance diagnostics
   global diagnostics
   % Figure out if we match a cached element
   [cache iscached]=cache_search(cache,x);
   % If we don't have a match, cache a new factorization
   if ~iscached
       % Save the current location
       cache{1}.x = x;
       % Find the total derivative
       cache{1}.D = [ ...
           op_p(1,params,x)*x(params.idx.u)-rhs_p(1,params,x) ...
           op_p(2,params,x)*x(params.idx.u)-rhs_p(2,params,x) ...
           op(params,x)];
       % Keep track that we cached a derivative
       diagnostics.first_derivative_cached = ...
           diagnostics.first_derivative_cached+1;
   end
   % Return the derivative
   D = cache{1}.D;
end
\% Prepares our cached element according to the following scheme
%
\% 1. Item not cached, copy first cached element to the second. Return that no
%
     cached item found.
%
% 2. Item found in first cached element. Return that cached item found.
%
% 3. Item found in second cached element. Exchange first and second cached
     elements. Return that cached item found.
%
function [cache iscached] = cache_search(cache,x)
   % Determine what cached item matches x
   which = 0;
```

Now, let us look at the code that caches these operations effectively. First, we start with the code that caches

```
if ~isempty(cache)
    for i=1:length(cache)
```

the total derivative of G

```
if isequal(x,cache{i}.x)
           which = i;
           break;
       end
   end
end
% No items match
if which==0
   iscached = 0;
   if ~isempty(cache)
       cache{2} = cache{1};
   end
% First item matches
elseif which==1
   iscached = 1;
% Second item matches
elseif which==2
   iscached = 1;
   cache(2:-1:1)=cache;
end
```

```
end
```

Here, we see that our reliance on computing an explicit representation for the total derivative of G simplifies the functions eq_p and eq_ps to simple multiplications. Next, as before, we store the cached information in a persistent variable called cache. However, unlike before, we store two separate cached items and manage them with the function cache_search. In this function, we keep the most recently used cached item as the first element in the cache. When we evaluate the derivative at a new point, we discard the the second item. Recall, we require two cached items due to an additional augmented system solve for the equality multiplier during globalization. In a similar manner, we define the code that implements and caches the Schur preconditioner as

```
% Evaluates the Schur preconditioner
function z = eq_schur(params,x,dx)
   % Keep track of where the evaluation occurs
   persistent cache
   % Performance diagnostics
   global diagnostics
   \% Here, we need to cache two elements due to the equality multiplier solve.
   \% Basically, the equality multiplier solve during globalization requires a
   \% solve at a new iterate. If globalization accepts this point, we can
   % reuse this factorization. However, if globalization rejects this point,
   % we want to use our old factorization.
   % Figure out if we match a cached element
   [cache iscached]=cache_search(cache,x);
   % If we don't have a match, cache a new factorization
   if ~iscached
       % Save the current location
       cache{1}.x = x;
       % Exact Schur preconditioner
       if params.approx_schur==0
```

```
% Factorize the total derivative of g'
       [q cache{1}.r] = qr(deriv(params,x)',0);
   % Approximate Schur preconditioner
   else
       % Factorize the differential operator
       [cache{1}.l cache{1}.u cache{1}.p cache{1}.q cache{1}.r] = ...
          lu(op(params,x),'vector');
   end
   \% Keep track that we did a new factorization
   diagnostics.factorization_cached = diagnostics.factorization_cached+1;
end
% Solve the linear system
if params.approx_schur==0
   z = cache{1}.r(cache{1}.r'dx);
else
   % Forward
   z=zeros(params.nx,1);
   z(cache{1},q) = cache{1}.u(cache{1}.l(cache{1}.r(:,cache{1}.p)dx));
   % Adjoint
   z = cache{1}.r(:,cache{1}.p)'\(cache{1}.l'\(cache{1}.u'\z(cache{1}.q)));
end
```

```
\operatorname{end}
```

Like the code that cached the total derivative of G, we cache two elements in the persistent variable **cache**. However, here, we store the factorization of the system $G'(k, u)G'(k, u)^*$. Note, caching the total derivative above helps accelerate this code as well. As a side note, we actually define two different preconditioners in this code. The true Schur preconditioner factorizes the system $G'(k, u)G'(k, u)^*$, which typically yields a dense factorization due to the derivatives with respect to k. Alternatively, we can define an approximate Schur preconditioner from the factorization of $G'_u(k, u)G'_u(k, u)^*$. Although we can no longer solve the augmented system in exactly three iterations, this preconditioner allows us to factorize $G'_u(k, u)$ directly, which yields a sparse decomposition. Finally, we cache the adjoint of the second derivative applied to the equality multiplier with the code

```
% Evaluates the adjoint of second derivative of the equality constraint
function z = eq_pps(params,x,dx,dy)
   z = deriv2(params,x,dy)*dx;
end
% Finds the second total derivative adjoint of the equality constraints applied
% to the equality multiplier
function D2 = deriv2(params,x,dy)
   % Keep track of where the evaluation occurs
   persistent cache
   global diagnostics
   % Cache the total derivative when possible
   if isempty(cache) || ~isequal(x,cache.x) || ~isequal(dy,cache.dy)
       % Save the current location
       cache.x = x;
       cache.dy = dy;
       % Find the adjoint of the second derivative applied to the equality
       % multiplier
       cache.D2 = sparse(params.nx+2,params.nx+2);
```

```
cache.D2(params.idx.k(1),params.idx.u) = dy'*op_p(1,params,x);
cache.D2(params.idx.k(2),params.idx.u) = dy'*op_p(2,params,x);
cache.D2(params.idx.u,params.idx.k(1)) = op_p(1,params,x)'*dy;
cache.D2(params.idx.u,params.idx.k(2)) = op_p(2,params,x)'*dy;
% Keep track that we cache a derivative
diagnostics.second_derivative_cached = ...
diagnostics.second_derivative_cached+1;
nd
```

```
end
```

```
% Return the derivative
D2 = cache.D2;
end
```

As before, we store the cached information in a persistent variable called **cache**. The nuance in this case is that we should check both x and dy when determining whether we've moved to a new point and need to recompute the second derivative.

Additional examples

During the configure process, we compile and install a variety of examples whenever the ENABLE_CPP_EXAMPLES, ENABLE_PYTHON_EXAMPLES, or ENABLE_MATLAB_EXAMPLES are turned to ON. For reference, we include some of these examples here.

7.1 Simple equality constrained

In our Simple equality constrained example, we optimize the formulation

$$\min_{\substack{x \in \mathbb{R}^2 \\ \text{st}}} \qquad x^2 + y^2 \left. x - 2 \right)^2 + (y - 2)^2 = 1$$

with the code:

```
Language
               C++
Code
               // Optimize a simple optimization problem with an optimal solution
               // of (2-sqrt(2)/2,2-sqrt(2)/2).
               #include "optizelle/optizelle.h"
               #include "optizelle/vspaces.h"
               #include "optizelle/json.h"
               #include <iostream>
               #include <iomanip>
               #include <cstdlib>
               //---Objective0---
               // Squares its input
               template <typename Real>
               Real sq(Real const & x){
                   return x*x;
               }
               // Define a simple objective where
               11
               // f(x,y)=x^2+y^2
               11
               struct MyObj
                   : public Optizelle::ScalarValuedFunction <double,Optizelle::Rm>
               {
                   typedef Optizelle::Rm <double> X;
```

```
// Evaluation
   double eval(X::Vector const & x) const {
       return sq(x[0])+sq(x[1]);
   }
   // Gradient
   void grad(
       X::Vector const & x,
       X::Vector & grad
   ) const {
       grad[0]=2.*x[0];
       grad[1]=2.*x[1];
   }
   // Hessian-vector product
   void hessvec(
       X::Vector const & x,
       X::Vector const & dx,
       X::Vector & H_dx
   ) const {
       H_dx[0]=2.*dx[0];
       H_dx[1]=2.*dx[1];
   }
};
//---Objective1---
//---EqualityConstraintO---
// Define a simple equality constraint
11
// g(x,y) = [ (x-2)^2 + (y-2)^2 = 1 ]
11
struct MyEq
   :public Optizelle::VectorValuedFunction<double,Optizelle::Rm,Optizelle::Rm>
ł
   typedef Optizelle::Rm <double> X;
   typedef Optizelle::Rm <double> Y;
   // y=g(x)
   void eval(
       X::Vector const & x,
       Y::Vector & y
   ) const {
       y[0] = sq(x[0]-2.)+sq(x[1]-2.)-1.;
   }
   // y=g'(x)dx
   void p(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector & y
   ) const {
       y[0] = 2.*(x[0]-2.)*dx[0]+2.*(x[1]-2.)*dx[1];
   }
   // xhat=g'(x)*dy
   void ps(
       X::Vector const & x,
```

```
Y::Vector const & dy,
       X::Vector & xhat
   ) const {
       xhat[0] = 2.*(x[0]-2.)*dy[0];
       xhat[1] = 2.*(x[1]-2.)*dy[0];
   }
   // xhat=(g''(x)dx)*dy
   void pps(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector const & dy,
       X::Vector & xhat
   ) const {
       xhat[0] = 2.*dx[0]*dy[0];
       xhat[1] = 2.*dx[1]*dy[0];
   }
};
//---EqualityConstraint1---
//---Preconditioner0---
// Define a Schur preconditioner for the equality constraints
struct MyPrecon:
   public Optizelle::Operator <double,Optizelle::Rm,Optizelle::Rm>
{
public:
   typedef Optizelle::Rm <double> X;
   typedef X::Vector X_Vector;
   typedef Optizelle::Rm <double> Y;
   typedef Y::Vector Y_Vector;
private:
   X_Vector& x;
public:
   MyPrecon(X::Vector& x_) : x(x_) {}
   void eval(Y_Vector const & dy,Y_Vector & result) const {
       result[0]=dy[0]/sq(4.*(x[0]-2.)+4.*sq(x[1]-2.));
   }
};
//---Preconditioner1---
int main(int argc, char* argv[]){
   // Read in the name for the input file
   if(argc!=2) {
       std::cerr << "simple_equalty <parameters>" << std::endl;</pre>
       exit(EXIT_FAILURE);
   }
   auto fname = argv[1];
   // Create a type shortcut
   using Optizelle::Rm;
   //---State0---
   // Generate an initial guess
   auto x = std::vector <double> {2.1, 1.1};
   // Allocate memory for the equality multiplier
   auto y = std::vector <double> (1);
```

```
// Create an optimization state
                   Optizelle::EqualityConstrained <double,Rm,Rm>::State::t state(x,y);
                   //---State1---
                   //---Parameters0---
                   // Read the parameters from file
                   Optizelle::json::EqualityConstrained <double,Optizelle::Rm,Optizelle::Rm>
                       ::read(fname,state);
                   //---Parameters1---
                   //---Functions0---
                   // Create a bundle of functions
                   Optizelle::EqualityConstrained <double,Rm,Rm>::Functions::t fns;
                   fns.f.reset(new MyObj);
                   fns.g.reset(new MyEq);
                   fns.PSchur_left.reset(new MyPrecon(state.x));
                   //---Functions1---
                   //---Solver0---
                   // Solve the optimization problem
                   Optizelle::EqualityConstrained <double,Rm,Rm>::Algorithms::getMin(
                       Optizelle::Messaging::stdout,fns,state);
                   //---Solver1---
                   //---ExtractO---
                   // Print out the reason for convergence
                   std::cout << "The algorithm converged due to: " <<</pre>
                       Optizelle::OptimizationStop::to_string(state.opt_stop) <<</pre>
                       std::endl;
                   // Print out the final answer
                   std::cout << std::scientific << std::setprecision(16)</pre>
                       << "The optimal point is: (" << state.x[0] << ','
                   << state.x[1] << ')' << std::endl;
                   //---Extract1---
                   // Write out the final answer to file
                   Optizelle::json::EqualityConstrained <double,Optizelle::Rm,Optizelle::Rm>
                       ::write_restart("solution.json",state);
                   // Return that we've exited successfuly
                   return EXIT_SUCCESS;
               }
Language
               Python
Code
               # Optimize a simple optimization problem with an optimal solution
               # of (2-sqrt(2)/2,2-sqrt(2)/2).
                import Optizelle
                import numpy
                import sys
                #---ObjectiveO---
                # Squares its input
```

```
sq = lambda x:x*x
# Define a simple objective where
#
# f(x,y)=x^2+y^2
#
class MyObj(Optizelle.ScalarValuedFunction):
   # Evaluation
   def eval(self,x):
       return sq(x[0])+sq(x[1])
   # Gradient
   def grad(self,x,grad):
       grad[0]=2.*x[0]
       grad[1]=2.*x[1]
   # Hessian-vector product
   def hessvec(self,x,dx,H_dx):
       H_dx[0]=2.*dx[0]
       H_dx[1]=2.*dx[1]
#---Objective1---
#---EqualityConstraintO---
# Define a simple equality constraint
#
# g(x,y) = [ (x-2)^2 + (y-2)^2 = 1 ]
#
class MyEq(Optizelle.VectorValuedFunction):
   \# y=g(x)
   def eval(self,x,y):
       y[0] = sq(x[0]-2.)+sq(x[1]-2.)-1.
   \# y=g'(x)dx
   def p(self,x,dx,y):
       y[0] = 2.*(x[0]-2.)*dx[0]+2.*(x[1]-2.)*dx[1]
   # xhat=g'(x)*dy
   def ps(self,x,dy,xhat):
       xhat[0] = 2.*(x[0]-2.)*dy[0]
       xhat[1] = 2.*(x[1]-2.)*dy[0]
   # xhat=(g''(x)dx)*dy
   def pps(self,x,dx,dy,xhat):
       xhat[0] = 2.*dx[0]*dy[0]
       xhat[1] = 2.*dx[1]*dy[0]
#---EqualityConstraint1---
#---Preconditioner0---
# Define a Schur preconditioner for the equality constraints
class MyPrecon(Optizelle.Operator):
   def eval(self,state,dy,result):
       result[0]=dy[0]/sq(4.*(x[0]-2.)+4.*sq(x[1]-2.))
#---Preconditioner1---
# Read in the name for the input file
```

```
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```

```
if len(sys.argv)!=2:
   sys.exit("simple_equality.py <parameters>")
fname=sys.argv[1]
#---State0---
# Generate an initial guess
x = numpy.array([2.1,1.1])
# Allocate memory for the equality multiplier
y = numpy.array([0.])
# Create an optimization state
state=Optizelle.EqualityConstrained.State.t(Optizelle.Rm,Optizelle.Rm,x,y)
#---State1---
#---Parameters0---
# Read the parameters from file
Optizelle.json.EqualityConstrained.read(Optizelle.Rm,Optizelle.Rm,fname,state)
#---Parameters1---
#---Functions0---
# Create a bundle of functions
fns=Optizelle.EqualityConstrained.Functions.t()
fns.f=MyObj()
fns.g=MyEq()
fns.PSchur_left=MyPrecon()
#---Functions1---
#---Solver0---
# Solve the optimization problem
Optizelle.EqualityConstrained.Algorithms.getMin(
   Optizelle.Rm, Optizelle.Rm, Optizelle.Messaging.stdout, fns, state)
#---Solver1---
#---ExtractO---
# Print out the reason for convergence
print "The algorithm converged due to: %s" % (
   Optizelle.OptimizationStop.to_string(state.opt_stop))
# Print out the final answer
print "The optimal point is: (%e,%e)" % (state.x[0],state.x[1])
#---Extract1---
# Write out the final answer to file
Optizelle.json.EqualityConstrained.write_restart(
   Optizelle.Rm,Optizelle.Rm,"solution.json",state)
MATLAB/Octave
% Optimize a simple optimization problem with an optimal solution
% of (2-sqrt(2)/2,2-sqrt(2)/2).
function simple_equality(fname)
   % Read in the name for the input file
   if nargin ~=1
       error('simple_equality <parameters>');
   end
```

Language

Code

```
% Execute the optimization
   main(fname);
end
%---Objective0---
% Squares its input
function z = sq(x)
   z=x*x;
end
\% Define a simple objective where
%
% f(x,y)=x^2+y^2
%
function self = MyObj()
   % Evaluation
   self.eval = @(x) sq(x(1))+sq(x(2));
   % Gradient
   self.grad = @(x) [ ...
       2.*x(1); ...
       2.*x(2)];
   \% Hessian-vector product
   self.hessvec = @(x,dx) [ ...
       2.*dx(1); ...
       2.*dx(2)];
end
%---Objective1---
%---EqualityConstraint0---
% Define a simple equality constraint
%
g(x,y) = [(x-2)^2 + (y-2)^2 = 1]
%
function self = MyEq()
   % y=g(x)
   self.eval = Q(x) [ ... ]
       sq(x(1)-2.)+sq(x(2)-2.)-1.];
   % y=g'(x)dx
   self.p = @(x,dx) [ ...
       2.*(x(1)-2.)*dx(1)+2.*(x(2)-2.)*dx(2)];
   % xhat=g'(x)*dy
   self.ps = @(x,dy) [ ...
       2.*(x(1)-2.)*dy(1); \ldots
       2.*(x(2)-2.)*dy(1)];
   % xhat=(g''(x)dx)*dy
   self.pps = @(x,dx,dy) [ ...
       2.*dx(1)*dy(1); ...
       2.*dx(2)*dy(1) ];
end
```

```
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```

```
%---EqualityConstraint1---
%---Preconditioner0---
\% Define a Schur preconditioner for the equality constraints
function self = MyPrecon()
   self.eval=@(state,dy)dy(1)/sq(4.*(state.x(1)-2.)+4.*sq(state.x(2)-2.));
end
%---Preconditioner1---
% Actually runs the program
function main(fname)
   % Grab the Optizelle library
   global Optizelle;
   setupOptizelle();
   %---State0---
   % Generate an initial guess
   x = [2.1; 1.1];
   % Allocate memory for the equality multiplier
   y = [0.];
   % Create an optimization state
   state= Optizelle.EqualityConstrained.State.t(Optizelle.Rm,Optizelle.Rm,x,y);
   %---State1---
   %---Parameters0---
   % Read the parameters from file
   state = Optizelle.json.EqualityConstrained.read( ...
       Optizelle.Rm,Optizelle.Rm,fname,state);
   %---Parameters1---
   %---Functions0---
   % Create a bundle of functions
   fns=Optizelle.EqualityConstrained.Functions.t;
   fns.f=MyObj();
   fns.g=MyEq();
   fns.PSchur_left=MyPrecon();
   %---Functions1---
   %---Solver0---
   % Solve the optimization problem
   state = Optizelle.EqualityConstrained.Algorithms.getMin( ...
       Optizelle.Rm,Optizelle.Rm,Optizelle.Messaging.stdout,fns,state);
   %---Solver1---
   %---Extract0---
   % Print out the reason for convergence
   fprintf('The algorithm converged due to: %s\n', ...
       Optizelle.OptimizationStop.to_string(state.opt_stop));
   % Print out the final answer
   fprintf('The optimal point is: (%e,%e)\n',state.x(1),state.x(2));
   %---Extract1---
   % Write out the final answer to file
```

```
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```

end

7.2 Simple inequality constrained

In our Simple inequality constrained example, we optimize the formulation

$\min_{x \in \mathbb{R}^2}$	$(x+1)^2 + (y+1)^2$
st	$x + 2y \ge 1$
	$2x + y \ge 1$

with the code:

Language	C++
Code	// Optimize a simple optimization problem with an optimal solution // of $(1/3, 1/3)$
	<pre>#include "optizelle/optizelle.h" #include "optizelle/vspaces.h" #include "optizelle/json.h" #include <iostream> #include <iostream> #include <cstdlib></cstdlib></iostream></iostream></pre>
	<pre>// Squares its input template <typename real=""> Real sq(Real const & x){ return x*x;</typename></pre>
	}
	<pre>// Define a simple objective where // // f(x,y)=(x+1)^2+(y+1)^2 //</pre>
	<pre>struct MyObj : public Optizelle::ScalarValuedFunction <double,optizelle::rm> { typedef Optizelle::Rm <double> X;</double></double,optizelle::rm></pre>
	<pre>// Evaluation double eval(const X::Vector& x) const { return sq(x[0]+1.)+sq(x[1]+1.); }</pre>
	<pre>// Gradient void grad(X::Vector const & x, X::Vector & grad) const { grad[0]=2.*x[0]+2.; grad[1]=2.*x[1]+2.;</pre>
	}
	<pre>// Hessian-vector product void hessvec(</pre>

```
X::Vector const & x,
       X::Vector const & dx,
       X::Vector & H_dx
   ) const {
       H_dx[0]=2.*dx[0];
       H_dx[1]=2.*dx[1];
   }
};
// Define simple inequalities
11
// h(x,y)= [ x + 2y >= 1 ]
         [ 2x + y >= 1 ]
11
11
struct MyIneq
   :public Optizelle::VectorValuedFunction<double,Optizelle::Rm,Optizelle::Rm>
{
   typedef Optizelle::Rm <double> X;
   typedef Optizelle::Rm <double> Y;
   // y=h(x)
   void eval(
       X::Vector const & x,
       Y::Vector & y
   ) const {
       y[0]=x[0]+2.*x[1]-1.;
       y[1]=2.*x[0]+x[1]-1.;
   }
   // y=h'(x)dx
   void p(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector & y
   ) const {
       y[0] = dx[0]+2.*dx[1];
       y[1] = 2.*dx[0]+dx[1];
   }
   // z=h'(x)*dy
   void ps(
       X::Vector const & x,
       Y::Vector const & dy,
       X::Vector & z
   ) const {
       z[0] = dy[0]+2.*dy[1];
       z[1] = 2.*dy[0]+dy[1];
   }
   // z=(h''(x)dx)*dy
   void pps(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector const & dy,
       X::Vector & z
   ) const {
       X::zero(z);
```

```
}
};
int main(int argc, char* argv[]){
    // Read in the name for the input file
   if(argc!=2) {
       std::cerr << "simple_inequality <pre>parameters>" << std::endl;</pre>
       exit(EXIT_FAILURE);
    }
    auto fname = argv[1];
    // Create a type shortcut
    using Optizelle::Rm;
    // Generate an initial guess
    auto x = std::vector <double> {2.1, 1.1};
    // Allocate memory for the inequality multipler
   auto z = std::vector <double>(2);
    // Create an optimization state
   Optizelle::InequalityConstrained <double,Rm,Rm>::State::t state(x,z);
    // Read the parameters from file
   Optizelle::json::InequalityConstrained <double,Optizelle::Rm,Optizelle::Rm>
       ::read(fname,state);
    // Create a bundle of functions
    Optizelle::InequalityConstrained <double,Rm,Rm>::Functions::t fns;
    fns.f.reset(new MyObj);
   fns.h.reset(new MyIneq);
    // Solve the optimization problem
   Optizelle::InequalityConstrained <double,Rm,Rm>::Algorithms
       ::getMin(Optizelle::Messaging::stdout,fns,state);
    // Print out the reason for convergence
   std::cout << "The algorithm converged due to: " <<</pre>
       Optizelle::OptimizationStop::to_string(state.opt_stop) <<</pre>
       std::endl;
    // Print out the final answer
   std::cout << std::scientific << std::setprecision(16)</pre>
       << "The optimal point is: (" << state.x[0] << ','
    << state.x[1] << ')' << std::endl;
    // Write out the final answer to file
   Optizelle::json::InequalityConstrained<double,Rm,Rm>
       ::write_restart("solution.json",state);
    // Return that the program exited properly
   return EXIT_SUCCESS;
}
```

Language Python

```
Code
                # Optimize a simple optimization problem with an optimal solution
                \# \text{ of } (1/3, 1/3)
                import Optizelle
                import numpy
                import sys
                # Squares its input
                sq = lambda x:x*x
                # Define a simple objective where
                #
                # f(x,y)=(x+1)^2+(y+1)^2
                #
                class MyObj(Optizelle.ScalarValuedFunction):
                    # Evaluation
                    def eval(self,x):
                       return sq(x[0]+1.)+sq(x[1]+1.)
                    # Gradient
                    def grad(self,x,grad):
                       grad[0]=2.*x[0]+2.
                       grad[1]=2.*x[1]+2.
                    # Hessian-vector product
                    def hessvec(self,x,dx,H_dx):
                       H_dx[0]=2.*dx[0]
                       H_dx[1]=2.*dx[1]
                # Define simple inequalities
                #
                # h(x,y)= [ x + 2y >= 1 ]
                         [2x + y >= 1]
                #
                #
                class MyIneq(Optizelle.VectorValuedFunction):
                   \# z=h(x)
                    def eval(self,x,z):
                       z[0] = x[0] + 2 \cdot x[1] - 1.
                       z[1]=2.*x[0]+x[1]-1.
                    # z=h'(x)dx
                    def p(self,x,dx,z):
                       z[0] = dx[0]+2.*dx[1]
                       z[1] = 2.*dx[0]+dx[1]
                    # xhat=h'(x)*dz
                    def ps(self,x,dz,xhat):
                       xhat[0] = dz[0]+2.*dz[1]
                       xhat[1] = 2.*dz[0]+dz[1]
                    # xhat=(h''(x)dx)*dz
                    def pps(self,x,dx,dz,xhat):
                       xhat.fill(0.)
```

```
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```

Read in the name for the input file

```
if len(sys.argv)!=2:
   sys.exit("simple_inequality.py <parameters>")
fname=sys.argv[1]
# Generate an initial guess
x = numpy.array([2.1,1.1])
# Allocate memory for the inequality multiplier
z = numpy.array([0.,0.])
# Create an optimization state
state=Optizelle.InequalityConstrained.State.t(Optizelle.Rm,Optizelle.Rm,x,z)
# Read the parameters from file
Optizelle.json.InequalityConstrained.read(Optizelle.Rm,Optizelle.Rm,fname,state)
# Create a bundle of functions
fns=Optizelle.InequalityConstrained.Functions.t()
fns.f=MyObj()
fns.h=MyIneq()
# Solve the optimization problem
Optizelle.InequalityConstrained.Algorithms.getMin(
   Optizelle.Rm,Optizelle.Rm,Optizelle.Messaging.stdout,fns,state)
# Print out the reason for convergence
print "The algorithm converged due to: %s" % (
   Optizelle.OptimizationStop.to_string(state.opt_stop))
# Print out the final answer
print "The optimal point is: (%e,%e)" % (state.x[0],state.x[1])
# Write out the final answer to file
Optizelle.json.InequalityConstrained.write_restart(
   Optizelle.Rm,Optizelle.Rm,"solution.json",state)
MATLAB/Octave
\% Optimize a simple optimization problem with an optimal solution
% of (1/3,1/3)
function simple_inequality(fname)
   % Read in the name for the input file
   if nargin ~=1
       error('simple_inequality parameters>');
   end
   % Execute the optimization
   main(fname);
end
% Squares its input
function z = sq(x)
   z=x*x;
end
% Define a simple objective where
```

Language

Code

```
%
% f(x,y)=(x+1)^2+(y+1)^2
%
function self = MyObj()
   % Evaluation
   self.eval = @(x) sq(x(1)+1.)+sq(x(2)+1.);
   % Gradient
   self.grad = O(x) [
       2.*x(1)+2.;
       2.*x(2)+2.];
   % Hessian-vector product
   self.hessvec = Q(x,dx) [
       2.*dx(1);
       2.*dx(2)];
end
% Define simple inequalities
%
% h(x,y)= [ x + 2y >= 1 ]
        [ 2x + y >= 1 ]
%
%
function self = MyIneq()
   % z=h(x)
   self.eval = @(x) [
       x(1)+2.*x(2)-1.;
       2.*x(1)+x(2)-1. ];
   % z=h'(x)dx
   self.p = @(x,dx) [
       dx(1)+2.*dx(2);
       2.*dx(1)+dx(2) ];
   % xhat=h'(x)*dz
   self.ps = @(x,dz) [
       dz(1)+2.*dz(2);
       2.*dz(1)+dz(2) ];
   % xhat=(h''(x)dx)*dz
   self.pps = @(x,dx,dz) zeros(2,1);
end
\% Actually runs the program
function main(fname)
   % Grab the Optizelle library
   global Optizelle;
   setupOptizelle();
   % Generate an initial guess
   x = [2.1; 1.1];
   % Allocate memory for the inequality multiplier
   z = [0.;0.];
```

```
% Create an optimization state
   state=Optizelle.InequalityConstrained.State.t( ...
       Optizelle.Rm,Optizelle.Rm,x,z);
   % Read the parameters from file
   state=Optizelle.json.InequalityConstrained.read( ...
       Optizelle.Rm,Optizelle.Rm,fname,state);
   % Create a bundle of functions
   fns=Optizelle.InequalityConstrained.Functions.t;
   fns.f=MyObj();
   fns.h=MyIneq();
   % Solve the optimization problem
   state=Optizelle.InequalityConstrained.Algorithms.getMin( ...
       Optizelle.Rm,Optizelle.Rm,Optizelle.Messaging.stdout,fns,state);
   % Print out the reason for convergence
   fprintf('The algorithm converged due to: %s\n', ...
       Optizelle.OptimizationStop.to_string(state.opt_stop));
   % Print out the final answer
   fprintf('The optimal point is: (%e,%e)\n',state.x(1),state.x(2));
   % Write out the final answer to file
   Optizelle.json.InequalityConstrained.write_restart( ...
       Optizelle.Rm,Optizelle.Rm,'solution.json',state);
end
```

7.3 Simple constrained

In our Simple constrained example, we optimize the formulation

$\min_{x \in \mathbb{R}^2}$	$(x+1)^2 + (y+1)^2$
st	x + 2y = 1
	$2x + y \ge 1$

with the code:

Language	C++
Code	// Optimize a simple optimization problem with an optimal // solution of $(1/3, 1/3)$
	<pre>#include "optizelle/optizelle.h" #include "optizelle/vspaces.h" #include "optizelle/json.h" #include <iostream> #include <iomanip> #include <cstdlib></cstdlib></iomanip></iostream></pre>
	<pre>// Squares its input template <typename real=""> Real sq(Real const & x){ return x*x; }</typename></pre>

```
// Define a simple objective where
11
// f(x,y)=(x+1)^2+(y+1)^2
11
struct MyObj
   : public Optizelle::ScalarValuedFunction <double,Optizelle::Rm>
{
   typedef Optizelle::Rm <double> X;
   // Evaluation
   double eval(X::Vector const & x) const {
       return sq(x[0]+1.)+sq(x[1]+1.);
   }
   // Gradient
   void grad(
       X::Vector const & x,
       X::Vector & grad
   ) const {
       grad[0]=2*x[0]+2;
       grad[1]=2*x[1]+2;
   }
   // Hessian-vector product
   void hessvec(
       X::Vector const & x,
       X::Vector const & dx,
       X::Vector & H_dx
   ) const {
       H_dx[0]=2.*dx[0];
       H_dx[1]=2.*dx[1];
   }
};
// Define a simple equality
11
// g(x,y)= [ x + 2y = 1 ]
11
struct MyEq
    :public Optizelle::VectorValuedFunction<double,Optizelle::Rm,Optizelle::Rm>
ſ
   typedef Optizelle::Rm <double> X;
   typedef Optizelle::Rm <double> Y;
   // y=g(x)
   void eval(
       X::Vector const & x,
       Y::Vector & y
   ) const {
       y[0] = x[0] + 2 \cdot x[1] - 1 \cdot;
   }
   // y=g'(x)dx
   void p(
       X::Vector const & x,
       X::Vector const & dx,
```

```
Y::Vector & y
   ) const {
       y[0] = dx[0]+2.*dx[1];
   }
   // xhat=g'(x)*dy
   void ps(
       X::Vector const & x,
       Y::Vector const & dy,
       X::Vector & xhat
   ) const {
       xhat[0] = dy[0];
       xhat[1] = 2.*dy[0];
   }
   // xhat=(g''(x)dx)*dy
   void pps(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector const & dy,
       X::Vector & xhat
   ) const {
       X::zero(xhat);
   }
};
// Define a simple inequality
11
// h(x,y)= [ 2x + y >= 1 ]
11
struct MyIneq
   :public Optizelle::VectorValuedFunction<double,Optizelle::Rm,Optizelle::Rm>
{
   typedef Optizelle::Rm <double> X;
   typedef Optizelle::Rm <double> Z;
   // z=h(x)
   void eval(
       X::Vector const & x,
       Z::Vector & z
   ) const {
       z[0]=2.*x[0]+x[1]-1.;
   }
   // z=h'(x)dx
   void p(
       X::Vector const & x,
       X::Vector const & dx,
       Z::Vector & z
   ) const {
       z[0] = 2.*dx[0]+dx[1];
   }
   // xhat=h'(x)*dz
   void ps(
       X::Vector const & x,
       Z::Vector const & dz,
```

```
X::Vector & xhat
   ) const {
       xhat[0] = 2.*dz[0];
       xhat[1] = dz[0];
   }
   // xhat=(h''(x)dx)*dz
   void pps(
       X::Vector const & x,
       X::Vector const & dx,
       Z::Vector const & dz,
       X::Vector & xhat
    ) const {
       X::zero(xhat);
    ľ
};
int main(int argc, char* argv[]){
   // Read in the name for the input file
   if(argc!=2) {
       std::cerr << "simple_constrained <parameters>" << std::endl;</pre>
       exit(EXIT_FAILURE);
   }
   auto fname = argv[1];
    // Create a type shortcut
   using Optizelle::Rm;
    // Generate an initial guess for the primal
   auto x = std::vector <double> {2.1, 1.1};
    // Allocate memory for equality multiplier
    auto y = std::vector <double> (1);
    // Allocate memory for the inequality multiplier
    auto z = std::vector <double> (1);
    // Create an optimization state
   Optizelle::Constrained <double,Rm,Rm,Rm>::State::t state(x,y,z);
    // Read the parameters from file
   Optizelle::json::Constrained <double,Rm,Rm,Rm>::read(fname,state);
    // Create a bundle of functions
    Optizelle::Constrained <double,Rm,Rm,Rm>::Functions::t fns;
   fns.f.reset(new MyObj);
   fns.g.reset(new MyEq);
   fns.h.reset(new MyIneq);
    // Solve the optimization problem
   Optizelle::Constrained <double,Rm,Rm,Rm>::Algorithms
       ::getMin(Optizelle::Messaging::stdout,fns,state);
    // Print out the reason for convergence
   std::cout << "The algorithm converged due to: " <<</pre>
       Optizelle::OptimizationStop::to_string(state.opt_stop) <<</pre>
       std::endl;
```

```
// Print out the final answer
                    std::cout << std::scientific << std::setprecision(16)</pre>
                       << "The optimal point is: (" << state.x[0] << ','
                       << state.x[1] << ')' << std::endl;
                    // Write out the final answer to file
                    Optizelle::json::Constrained <double,Rm,Rm,Rm>::write_restart(
                        "solution.json",state);
                    // Successful termination
                    return EXIT_SUCCESS;
                }
Language
                Python
Code
                # Optimize a simple optimization problem with an optimal solution
                \# \text{ of } (1/3, 1/3)
                import Optizelle
                import numpy
                import sys
                # Squares its input
                sq = lambda x:x*x
                # Define a simple objective where
                # f(x,y)=(x+1)^2+(y+1)^2
                #
                class MyObj(Optizelle.ScalarValuedFunction):
                    # Evaluation
                    def eval(self,x):
                       return sq(x[0]+1.)+sq(x[1]+1.)
                    # Gradient
                    def grad(self,x,grad):
                       grad[0]=2.*x[0]+2.
                       grad[1]=2.*x[1]+2.
                    # Hessian-vector product
                    def hessvec(self,x,dx,H_dx):
                       H_dx[0]=2.*dx[0]
                       H_dx[1]=2.*dx[1]
                # Define a simple equality
                #
                # g(x,y)= [ x + 2y = 1 ]
                #
                class MyEq(Optizelle.VectorValuedFunction):
                    # y=g(x)
                    def eval(self,x,y):
                       y[0] = x[0] + 2 \cdot x[1] - 1.
```

```
\# y=g'(x)dx
   def p(self,x,dx,y):
       y[0] = dx[0]+2.*dx[1]
   # xhat=g'(x)*dy
   def ps(self,x,dy,xhat):
       xhat[0] = dy[0]
       xhat[1]= 2.*dy[0]
   # xhat=(g''(x)dx)*dy
   def pps(self,x,dx,dy,xhat):
       xhat.fill(0.)
# Define simple inequalities
#
# h(x,y)= [ 2x + y >= 1 ]
#
class MyIneq(Optizelle.VectorValuedFunction):
   \# z=h(x)
   def eval(self,x,z):
       z[0]=2.*x[0]+x[1]-1.
   # z=h'(x)dx
   def p(self,x,dx,z):
       z[0] = 2.*dx[0]+dx[1]
   # xhat=h'(x)*dz
   def ps(self,x,dz,xhat):
       xhat[0] = 2.*dz[0]
       xhat[1] = dz[0]
   # xhat=(h''(x)dx)*dz
   def pps(self,x,dx,dz,xhat):
       xhat.fill(0.)
# Read in the name for the input file
if len(sys.argv)!=2:
   sys.exit("simple_constrained.py <parameters>")
fname=sys.argv[1]
# Generate an initial guess
x = numpy.array([2.1,1.1])
# Allocate memory for the equality multiplier
y = numpy.array([0.])
# Allocate memory for the inequality multiplier
z = numpy.array([0.])
# Create an optimization state
state=Optizelle.Constrained.State.t(
   Optizelle.Rm,Optizelle.Rm,Optizelle.Rm,x,y,z)
# Read the parameters from file
Optizelle.json.Constrained.read(
   Optizelle.Rm,Optizelle.Rm,Optizelle.Rm,fname,state)
```

```
# Create a bundle of functions
               fns=Optizelle.Constrained.Functions.t()
               fns.f=MyObj()
               fns.g=MyEq()
               fns.h=MyIneq()
               # Solve the optimization problem
               Optizelle.Constrained.Algorithms.getMin(
                   Optizelle.Rm,Optizelle.Rm,Optizelle.Rm,Optizelle.Messaging.stdout,fns,state)
               # Print out the reason for convergence
               print "The algorithm converged due to: %s" % (
                   Optizelle.OptimizationStop.to_string(state.opt_stop))
               # Print out the final answer
               print "The optimal point is: (%e,%e)" % (state.x[0],state.x[1])
               # Write out the final answer to file
               Optizelle.json.Constrained.write_restart(Optizelle.Rm,Optizelle.Rm,Optizelle.Rm,
                   "solution.json",state)
Language
               MATLAB/Octave
Code
               \% Optimize a simple optimization problem with an optimal solution
               % of (1/3,1/3)
               function simple_constrained(fname)
                   % Read in the name for the input file
                   if nargin ~=1
                       error('simple_constrained <parameters>');
                   end
                   % Execute the optimization
                   main(fname);
               end
               % Squares its input
               function z = sq(x)
                   z=x*x;
               end
               % Define a simple objective where
               %
               % f(x,y)=(x+1)^2+(y+1)^2
               %
               function self = MyObj()
                   % Evaluation
                   self.eval = @(x) sq(x(1)+1.)+sq(x(2)+1.);
                   % Gradient
                   self.grad = @(x) [
                       2.*x(1)+2.;
                       2.*x(2)+2.];
                   % Hessian-vector product
```

```
self.hessvec = @(x,dx) [
       2.*dx(1);
       2.*dx(2)];
end
% Define a simple equality
%
% g(x,y) = [x + 2y = 1]
%
function self = MyEq()
   % y=g(x)
   self.eval = @(x) [x(1)+2.*x(2)-1.];
   % y=g'(x)dx
   self.p = @(x,dx) [dx(1)+2.*dx(2)];
   % xhat=g'(x)*dy
   self.ps = Q(x,dy) [
       dy(1);
       2.*dy(1)];
   % xhat=(g''(x)dx)*dy
   self.pps = @(x,dx,dy) zeros(2,1);
end
\% Define simple inequalities
%
h(x,y) = [2x + y > = 1]
%
function self = MyIneq()
   % z=h(x)
   self.eval = O(x) [
       2.*x(1)+x(2)-1];
   % z=h'(x)dx
   self.p = @(x,dx) [
       2.*dx(1)+dx(2)];
   % xhat=h'(x)*dz
   self.ps = Q(x,dz) [
       2.*dz(1)
       dz(1)];
   % xhat=(h''(x)dx)*dz
   self.pps = @(x,dx,dz) [ 0. ];
end
\% Actually runs the program
function main(fname)
   % Grab the Optizelle library
   global Optizelle;
   setupOptizelle();
   % Generate an initial guess
```

```
x = [2.1; 1.1];
   % Allocate memory for the equality multiplier
   y = [0.];
   % Allocate memory for the inequality multiplier
   z = [0.];
   % Create an optimization state
   state = Optizelle.Constrained.State.t( ...
       Optizelle.Rm,Optizelle.Rm,Optizelle.Rm,x,y,z);
   % Read the parameters from file
   state = Optizelle.json.Constrained.read( ...
       Optizelle.Rm,Optizelle.Rm,Optizelle.Rm,fname,state);
   % Create a bundle of functions
   fns = Optizelle.Constrained.Functions.t;
   fns.f = MyObj();
   fns.g = MyEq();
   fns.h = MyIneq();
   % Solve the optimization problem
   state = Optizelle.Constrained.Algorithms.getMin( ...
       Optizelle.Rm,Optizelle.Rm,Optizelle.Rm,Optizelle.Messaging.stdout, ...
       fns,state);
   % Print out the reason for convergence
   fprintf('The algorithm converged due to: %s\n', ...
       Optizelle.OptimizationStop.to_string(state.opt_stop));
   % Print out the final answer
   fprintf('The optimal point is: (%e,%e)\n',state.x(1),state.x(2));
   % Write out the final answer to file
   Optizelle.json.Constrained.write_restart( ...
       Optizelle.Rm,Optizelle.Rm,Optizelle.Rm,'solution.json',state);
end
```

7.4 Rosenbrock advanced API

In our Rosenbrock advanced API example, we optimize the formulation

$$\min_{x \in \mathbb{R}^2} \quad (1 - x_1)^2 + 100(x_2 - x_1^2)^2.$$

using the features described in our chapter Advanced API. We accomplish this with the code:

Language C++

Code

// In this example, we duplicate the Rosenbrock example while demonstrating
// some of the more advanced API features such as custom vector spaces,
// messaging objects, and restarts.

#include <vector>
#include <iostream>
#include <iomanip>
#include <string>

```
#include <sstream>
#include <algorithm>
#include "optizelle/optizelle.h"
#include "optizelle/json.h"
// Grab Optizelle's Natural type
using Optizelle::Natural;
//---VectorSpace0---
// Defines the vector space used for optimization.
template <typename Real>
struct MyVS {
   typedef std::vector <Real> Vector;
   // Memory allocation and size setting
   static Vector init(Vector const & x) {
       return std::move(Vector(x.size()));
   }
   // y <- x (Shallow. No memory allocation.)</pre>
   static void copy(Vector const & x, Vector & y) {
       for(Natural i=0;i<x.size();i++){</pre>
           y[i]=x[i];
       }
   }
   // x <- alpha * x
   static void scal(const Real& alpha, Vector & x) {
       for(Natural i=0;i<x.size();i++){</pre>
           x[i]=alpha*x[i];
       }
   }
   // x <- 0
   static void zero(Vector & x) {
       for(Natural i=0;i<x.size();i++){</pre>
           x[i]=0.;
       }
   }
   // y <- alpha * x + y
   static void axpy(const Real& alpha, Vector const & x, Vector & y) {
       for(Natural i=0;i<x.size();i++){</pre>
           y[i]=alpha*x[i]+y[i];
       }
   }
   // innr <- <x,y>
   static Real innr(Vector const & x,Vector const & y) {
       Real z=0;
       for(Natural i=0;i<x.size();i++)</pre>
           z+=x[i]*y[i];
       return z;
   }
   // x <- random
   static void rand(Vector & x){
```

```
std::mt19937 gen(1);
       std::uniform_real_distribution<Real> dis(Real(0.),Real(1.));
       for(Natural i=0;i<x.size();i++)</pre>
           x[i]=Real(dis(gen));
    }
    // Jordan product, z <- x o y.</pre>
    static void prod(Vector const & x, Vector const & y, Vector & z) {
       for(Natural i=0;i<x.size();i++)</pre>
           z[i]=x[i]*y[i];
    }
    // Identity element, x \leftarrow e such that x \circ e = x.
    static void id(Vector & x) {
       for(Natural i=0;i<x.size();i++)</pre>
           x[i]=Real(1.);
    }
    // Jordan product inverse, z \le inv(L(x)) y where L(x) y = x \circ y.
    static void linv(Vector const & x,Vector const & y,Vector & z) {
       for(Natural i=0;i<x.size();i++)</pre>
           z[i]=y[i]/x[i];
    }
    // Barrier function, barr <- barr(x) where x o grad barr(x) = e.
    static Real barr(Vector const & x) {
       Real z=Real(0.);
       for(Natural i=0;i<x.size();i++)</pre>
           z+=log(x[i]);
       return z;
    }
    // Line search, srch <- argmax {alpha i > 0 : alpha x + y >= 0}
    // where y > 0.
    static Real srch(Vector const & x,Vector const & y) {
       // Line search parameter
       Real alpha=std::numeric_limits <Real>::infinity();
       // Search for the optimal linesearch parameter.
       for(Natural i=0;i<x.size();i++) {</pre>
           if(x[i] < Real(0.)) {</pre>
               Real alpha0 = -y[i]/x[i];
               alpha = alpha0 < alpha ? alpha0 : alpha;</pre>
           }
       }
       return alpha;
    }
    // Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric</pre>
    // operator.
    static void symm(Vector & x) { }
};
//---VectorSpace1---
// Squares its input
template <typename Real>
Real sq(Real x){
```

```
return x*x;
}
// Define the Rosenbrock function where
11
// f(x,y)=(1-x)^2+100(y-x^2)^2
11
struct Rosenbrock : public Optizelle::ScalarValuedFunction <double,MyVS> {
   typedef MyVS <double> X;
    // Evaluation of the Rosenbrock function
   double eval(X::Vector const & x) const {
       return sq(1.-x[0])+100.*sq(x[1]-sq(x[0]));
   }
   // Gradient
   void grad(
       X::Vector const & x,
       X::Vector & g
   ) const {
       g[0] = -400 * x[0] * (x[1] - sq(x[0])) - 2 * (1 - x[0]);
       g[1]=200*(x[1]-sq(x[0]));
   }
    // Hessian-vector product
   void hessvec(
       X::Vector const & x,
       X::Vector const & dx,
       X::Vector & H_dx
   ) const {
       H_dx[0] = (1200 * sq(x[0]) - 400 * x[1] + 2) * dx[0] - 400 * x[0] * dx[1];
       H_dx[1] = -400 * x[0] * dx[0] + 200 * dx[1];
   }
};
// Define a perfect preconditioner for the Hessian
struct RosenHInv : public Optizelle::Operator <double,MyVS,MyVS> {
public:
   typedef MyVS <double> X;
   typedef X::Vector X_Vector;
private:
   X_Vector& x;
public:
   RosenHInv(X::Vector& x_) : x(x_) {}
   void eval(const X_Vector& dx,X_Vector &result) const {
       auto one_over_det=1./(80000.*sq(x[0])-80000.*x[1]+400.);
       result[0]=one_over_det*(200.*dx[0]+400.*x[0]*dx[1]);
       result[1]=one_over_det*
           (400.*x[0]*dx[0]+(1200.*x[0]*x[0]-400.*x[1]+2.)*dx[1]);
   }
};
//---Messaging0---
// Define a custom messaging object
void mymessaging(std::string const & msg) {
   std::cout << "PRINT: " << msg << std::endl;</pre>
}
```

```
//---Messaging1---
//---Serialization0---
// Define serialization routines for {\rm MyVS}
namespace Optizelle {
   namespace json {
       template <>
       struct Serialization <double,MyVS> {
           static std::string serialize(
               typename MyVS <double>::Vector const & x,
               std::string const & name,
               Natural const & iter
           ) {
               // Create a string with the format
               // [ x1, x2, ..., xm ].
               std::stringstream x_json;
               x_json.setf(std::ios::scientific);
               x_json.precision(16);
               x_json << "[ ";</pre>
               for(Natural i=0;i<x.size()-1;i++)</pre>
                   x_json << x[i] << ", ";
               x_json << x.back() << " ]";</pre>
               // Return the string
               return x_json.str();
           }
           static MyVS <double>::Vector deserialize(
               typename MyVS <double>::Vector const & x_,
               std::string const & x_json_
           ) {
               // Make a copy of x_json_
               auto x_json = x_json_;
               // Filter out the commas and brackets from the string
               char formatting[] = "[],";
               for(Natural i=0;i<3;i++)</pre>
                   x_json.erase(
                      std::remove(x_json.begin(),x_json.end(),formatting[i]),
                      x_json.end());
               // Create a new vector that we eventually return
               auto x = std::vector <double>(x_.size());
               // Create a stream out of x_json
               std::stringstream ss(x_json);
               // Read in each of the elements
               for(auto i=0;i<x.size();i++)</pre>
                   ss >> x[i];
               // Return the result
               return std::move(x);
           }
       };
   }
}
//---Serialization1---
```

```
//---RestartManipulator0---
// Define a state manipulator that writes out the optimization state at
// each iteration.
struct MyRestartManipulator
    : Optizelle::StateManipulator <Optizelle::Unconstrained <double,MyVS> >
{
   void eval(
       typename Optizelle::Unconstrained <double,MyVS>
           ::Functions::t const & fns,
       typename Optizelle::Unconstrained <double,MyVS>
           ::State::t & state,
       Optizelle::OptimizationLocation::t const & loc
    ) const {
       switch(loc) {
       // At the end of the optimization iteration, write the restart file
       case Optizelle::OptimizationLocation::EndOfOptimizationIteration: {
           // Create a reasonable file name
           std::stringstream ss;
           ss << "rosenbrock_advanced_api_";</pre>
           ss << std::setw(4) << std::setfill('0') << state.iter;</pre>
           ss << ".json";</pre>
           // Write the restart file
           Optizelle::json::Unconstrained <double,MyVS>::write_restart(
               ss.str(),state);
           break;
       } default:
           break;
       }
   }
};
//---RestartManipulator1---
int main(int argc, char* argv[]) {
    // Read in the name for the parameters and optional restart file
    if(!(argc==2 || argc==3)) {
       std::cerr << "rosenbrock_advanced_api <parameters>" << std::endl;</pre>
       std::cerr << "rosenbrock_advanced_api <parameters> <restart>"
           << std::endl;
       exit(EXIT_FAILURE);
   }
    auto pname = argv[1];
    auto rname = argc==3 ? argv[2] : "";
    // Generate an initial guess for Rosenbrock
    auto x = std::vector <double> {-1.2, 1.};
    // Create an unconstrained state based on this vector
   Optizelle::Unconstrained <double,MyVS>::State::t state(x);
    //---ReadRestart0---
    // If we have a restart file, read in the parameters
    if(argc==3)
       Optizelle::json::Unconstrained <double,MyVS>::read_restart(
           rname,x,state);
```

```
// Read additional parameters from file
    Optizelle::json::Unconstrained <double,MyVS>::read(pname,state);
    //---ReadRestart1---
    // Create the bundle of functions
   Optizelle::Unconstrained <double,MyVS>::Functions::t fns;
    fns.f.reset(new Rosenbrock);
    fns.PH.reset(new RosenHInv(state.x));
    //---Solver0---
    // Solve the optimization problem
   Optizelle::Unconstrained <double,MyVS>::Algorithms
       ::getMin(mymessaging,fns,state,MyRestartManipulator());
    //---Solver1---
   // Print out the reason for convergence
   std::cout << "The algorithm converged due to: " <<</pre>
       Optizelle::OptimizationStop::to_string(state.opt_stop) << std::endl;</pre>
    // Print out the final answer
    std::cout << "The optimal point is: (" << state.x[0] << ','</pre>
    << state.x[1] << ')' << std::endl;
    //---WriteRestart0---
    // Write out the final answer to file
   Optizelle::json::Unconstrained <double,MyVS>::write_restart(
       "solution.json",state);
   //---WriteRestart1---
}
```

```
Language
               Python
Code
               # In this example, we duplicate the Rosenbrock example while demonstrating
                # some of the more advanced API features such as custom vector spaces,
               # messaging objects, and restarts.
                import Optizelle
                import sys
                import copy
                import array
                import math
               #---VectorSpace0---
                # Defines the vector space used for optimization.
                class MyVS(object):
                   @staticmethod
                   def init(x):
                       """Memory allocation and size setting"""
                       return copy.deepcopy(x)
                   @staticmethod
                   def copy(x,y):
                       """y <- x (Shallow. No memory allocation.)"""
                       y[:]=x[:]
                   @staticmethod
```

```
def scal(alpha,x):
   """x <- alpha * x"""
   for i in xrange(0,len(x)):
       x[i]=alpha*x[i]
@staticmethod
def zero(x):
   """x <- 0"""
   for i in xrange(0,len(x)):
       x[i]=0.
@staticmethod
def axpy(alpha,x,y):
   """y <- alpha * x + y"""
   for i in xrange(0,len(x)):
       y[i]=alpha*x[i]+y[i]
@staticmethod
def innr(x,y):
   """<- <x,y>"""
   return reduce(lambda z,xy:xy[0]*xy[1]+z,zip(x,y),0.)
@staticmethod
def rand(x):
   """x <- random"""
   for i in xrange(0,len(x)):
       x[i]=random.uniform(0.,1.)
@staticmethod
def prod(x,y,z):
   """Jordan product, z <- x o y"""
   for i in xrange(0,len(x)):
       z[i]=x[i]*y[i]
@staticmethod
def id(x):
   """Identity element, x <- e such that x o e = x"""
   for i in xrange(0,len(x)):
       x[i]=1.
@staticmethod
def linv(x,y,z):
   ""Jordan product inverse, z \le inv(L(x)) y where L(x) y = x \circ y""
   for i in xrange(0,len(x)):
       z[i]=y[i]/x[i]
@staticmethod
def barr(x):
   """Barrier function, <- barr(x) where x o grad barr(x) = e"""
   return reduce(lambda x,y:x+math.log(y),x,0.)
@staticmethod
def srch(x,y):
   """Line search, <- argmax {alpha \in Real >= 0 : alpha x + y >= 0} where y >
   alpha = float("inf")
   for i in xrange(0,len(x)):
       if x[i] < 0:
```

```
alpha0 = -y[i]/x[i]
               if alpha0 < alpha:</pre>
                   alpha=alpha0
       return alpha
    @staticmethod
   def symm(x):
       """Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric operator
       pass
#---VectorSpace1---
# Squares its input
sq = lambda x:x*x
# Define the Rosenbrock function where
#
# f(x,y)=(1-x)^{2}+100(y-x^{2})^{2}
#
class Rosenbrock(Optizelle.ScalarValuedFunction):
   # Evaluation of the Rosenbrock function
   def eval(self,x):
       return sq(1.-x[0])+100.*sq(x[1]-sq(x[0]))
   # Gradient
   def grad(self,x,grad):
       grad[0] = -400 * x[0] * (x[1] - sq(x[0])) - 2*(1 - x[0])
       grad[1]=200*(x[1]-sq(x[0]))
   # Hessian-vector product
   def hessvec(self,x,dx,H_dx):
       H_dx[0] = (1200*sq(x[0])-400*x[1]+2)*dx[0]-400*x[0]*dx[1]
       H_dx[1] = -400 * x[0] * dx[0] + 200 * dx[1]
# Define a perfect preconditioner for the Hessian
class RosenHInv(Optizelle.Operator):
   def eval(self,state,dx,result):
       x = state.x
       one_over_det=1./(80000.*sq(x[0])-80000.*x[1]+400.)
       result[0]=one_over_det*(200.*dx[0]+400.*x[0]*dx[1])
       result[1]=(one_over_det*
           (400.*x[0]*dx[0]+(1200.*x[0]*x[0]-400.*x[1]+2.)*dx[1]))
#---Messaging0---
# Define a custom messaging object
def mymessaging(msg):
    """Prints out normal diagnostic information"""
   sys.stdout.write("PRINT: %s\n" %(msg))
#---Messaging1---
#---Serialization0---
def serialize_MyVS(x,name,iter):
    """Serializes an array for the vector space MyVS"""
   # Create the json representation
   x_json="[ "
   for i in xrange(0,len(x)):
       x_json += str(x[i]) + ", "
```

```
x_json=x_json[0:-2]
   x_json +=" ]"
   return x_json
def deserialize_MyVS(x,x_json):
   """Deserializes an array for the vector space MyVS"""
   # Eliminate all whitespace
   x_json="".join(x_json.split())
   # Check if we're a vector
   if x_json[0:1]!="[" or x_json[-1:]!="]":
       raise TypeError("Attempted to deserialize a non-array vector.")
   # Eliminate the initial and final delimiters
   x_json=x_json[1:-1]
   # Create a list of the numbers involved
   x_json=x_json.split(",")
   # Convert the strings to numbers
   x_json=map(lambda x:float(x),x_json)
   # Create a MyVS vector
   return array.array('d',x_json)
# Register the serialization routines for arrays
def MySerialization():
   Optizelle.json.Serialization.serialize.register(
       serialize_MyVS,array.array)
   Optizelle.json.Serialization.deserialize.register(
       deserialize_MyVS,array.array)
#---Serialization1---
#---RestartManipulator0---
# Define a state manipulator that writes out the optimization state at
# each iteration.
class MyRestartManipulator(Optizelle.StateManipulator):
   def eval(self,fns,state,loc):
       # At the end of the optimization iteration, write the restart file
       if loc == Optizelle.OptimizationLocation.EndOfOptimizationIteration:
           # Create a reasonable file name
           ss = "rosenbrock_advanced_api_%04d.json" % (state.iter)
           # Write the restart file
           Optizelle.json.Unconstrained.write_restart(MyVS,ss,state)
#---RestartManipulator1---
# Register the serialization routines
MySerialization()
# Read in the name for the input file
if not(len(sys.argv)==2 or len(sys.argv)==3):
   sys.exit("python rosenbrock_advanced_api.py <parameters>\n" +
            "python rosenbrock_advanced_api.py <parameters> <restart>")
pname = sys.argv[1]
```

```
rname = sys.argv[2] if len(sys.argv)==3 else ""
               # Generate an initial guess for Rosenbrock
               x = array.array('d', [-1.2,1.0])
               # Create an unconstrained state based on this vector
               state=Optizelle.Unconstrained.State.t(MyVS,x)
               #---ReadRestart0---
               # If we have a restart file, read in the parameters
               if len(sys.argv)==3:
                   Optizelle.json.Unconstrained.read_restart(MyVS,rname,x,state)
               # Read additional parameters from file
               Optizelle.json.Unconstrained.read(MyVS,pname,state)
               #---ReadRestart1---
               # Create the bundle of functions
               fns=Optizelle.Unconstrained.Functions.t()
               fns.f=Rosenbrock()
               fns.PH=RosenHInv()
               #---Solver0---
               # Solve the optimization problem
               Optizelle.Unconstrained.Algorithms.getMin(
                   MyVS,mymessaging,fns,state,MyRestartManipulator())
               #---Solver1---
               # Print out the reason for convergence
               print("The algorithm converged due to: %s" % (
                   Optizelle.OptimizationStop.to_string(state.opt_stop)))
               # Print out the final answer
               print("The optimal point is: (%e,%e)" % (state.x[0],state.x[1]))
               #---WriteRestart0---
               # Write out the final answer to file
               Optizelle.json.Unconstrained.write_restart(MyVS,"solution.json",state)
               #---WriteRestart1---
Language
               MATLAB/Octave
               % In this example, we duplicate the Rosenbrock example while demonstrating
               % some of the more advanced API features such as custom vector spaces,
               % messaging objects, and restarts.
               function rosenbrock_advanced_api(pname,rname)
                   % Read in the name for the input file
                   if ~(nargin==1 || nargin==2)
                      error(sprintf('%s\n%s', ...
                          'rosenbrock_advanced_api(parameters)\n', ...
                          'rosenbrock_advanced_api(parameters,restart)'));
                   end
                   % Execute the optimization
                   if nargin==1
```

Code

```
main(pname);
   else
       main(pname,rname);
    end
end
%----VectorSpace0----
% Convert a vector to structure
function y = tostruct(x)
   y = struct('data',x);
end
% Defines the vector space used for optimization.
function self = MyVS()
   % Memory allocation and size setting
   self.init = @(x) x;
   % <- x (Shallow. No memory allocation.)
   self.copy = @(x) x;
   % <- alpha * x
   self.scal = @(alpha,x) tostruct(alpha*x.data);
   % <- 0
   self.zero = @(x) tostruct(zeros(size(x.data)));
   % <- alpha * x + y
   self.axpy = @(alpha,x,y) tostruct(alpha * x.data + y.data);
   %<- <x,y>
   self.innr = @(x,y)x.data'*y.data;
   % <- random
   self.rand = @(x)tostruct(randn(size(x.data)));
   % Jordan product, z <- x o y.
   self.prod = @(x,y)tostruct(x.data .* y.data);
   % Identity element, x < -e such that x \circ e = x.
   self.id = @(x)tostruct(ones(size(x.data)));
   % Jordan product inverse, z \leftarrow inv(L(x)) y where L(x) y = x \circ y.
    self.linv = @(x,y)tostruct(y.data ./ x.data);
   % Barrier function, barr <- barr(x) where x o grad barr(x) = e.
   self.barr = @(x)sum(log(x.data));
   % Line search, srch <- argmax {alpha \in Real >= 0 : alpha x + y >= 0}
   % where y > 0.
   self.srch = @(x,y) feval(@(z)min([min(z(find(z>0)));inf]),-y.data ./x.data);
   % Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric
   % operator.
    self.symm = @(x)x;
end
```

```
%---VectorSpace1---
% Squares its input
function z = sq(x)
   z=x*x;
end
\% Define the Rosenbrock function where
%
% f(x,y)=(1-x)^2+100(y-x^2)^2
%
function self = Rosenbrock()
   % Evaluation of the Rosenbrock function
   self.eval = @(x) feval(@(x)sq(1.-x(1))+100.*sq(x(2)-sq(x(1))),x.data);
   % Gradient
   self.grad = @(x) tostruct(feval(@(x)[
       -400.*x(1)*(x(2)-sq(x(1)))-2.*(1.-x(1));
       200.*(x(2)-sq(x(1)))],x.data));
   % Hessian-vector product
   self.hessvec = @(x,dx) tostruct(feval(@(x,dx)[
       (1200.*sq(x(1))-400.*x(2)+2)*dx(1)-400.*x(1)*dx(2);
       -400.*x(1)*dx(1)+200.*dx(2)],x.data,dx.data));
end
\% Define a perfect preconditioner for the Hessian
function self = RosenHInv()
   self.eval = @(state,dx) eval(state,dx);
end
function result = eval(state,dx)
   x = state.x.data;
   dx = dx.data;
   one_over_det=1./(80000.*sq(x(1))-80000.*x(2)+400.);
   result = tostruct([
       one_over_det*(200.*dx(1)+400.*x(1)*dx(2));
       one_over_det*...
           (400.*x(1)*dx(1)+(1200.*x(1)*x(1)-400.*x(2)+2.)*dx(2))]);
end
%---Messaging0---
% Define a custom messaging object
function MyMessaging(msg)
   fprintf('PRINT: %s\n',msg);
end
%---Messaging1---
%---Serialization0---
\% Define serialization routines for MyVS
function MySerialization()
   global Optizelle;
   Optizelle.json.Serialization.serialize( ...
       'register', ...
       @(x,name,iter)strrep(mat2str(x.data'),' ',', '), ...
       @(x)isstruct(x) && isfield(x,'data') && isvector(x.data));
   Optizelle.json.Serialization.deserialize( ...
```

```
'register', ...
       @(x,x_json)tostruct(str2num(x_json)'), ...
       @(x)isstruct(x) && isfield(x,'data') && isvector(x.data));
end
%---Serialization1---
%---RestartManipulator0---
\% Define a state manipulator that writes out the optimization state at
% each iteration.
function smanip=MyRestartManipulator()
   smanip=struct('eval',@(fns,state,loc)MyRestartManipulator_(fns,state,loc));
end
function state=MyRestartManipulator_(fns,state,loc)
   global Optizelle;
   % At the end of the optimization iteration, write the restart file
   if(loc == Optizelle.OptimizationLocation.EndOfOptimizationIteration)
       % Create a reasonable file name
       ss = sprintf('rosenbrock_advanced_api_%04d.json',state.iter);
       % Write the restart file
       Optizelle.json.Unconstrained.write_restart(MyVS(),ss,state);
   end
end
%---RestartManipulator1---
% Actually runs the program
function main(pname,rname)
   % Grab the Optizelle library
   global Optizelle;
   setupOptizelle();
   % Register the serialization routines
   MySerialization();
   % Generate an initial guess for Rosenbrock
   x = tostruct([-1.2;1.]);
   \% Create an unconstrained state based on this vector
   state=Optizelle.Unconstrained.State.t(MyVS(),x);
   %---ReadRestart0---
   % If we have a restart file, read in the parameters
   if(nargin==2)
       state = Optizelle.json.Unconstrained.read_restart(MyVS(),rname,x);
   end
   % Read additional parameters from file
   state=Optizelle.json.Unconstrained.read(MyVS(),pname,state);
   %---ReadRestart1---
   % Create the bundle of functions
   fns=Optizelle.Unconstrained.Functions.t;
   fns.f=Rosenbrock();
   fns.PH=RosenHInv();
```

```
%---Solver0---
% Solve the optimization problem
state=Optizelle.Unconstrained.Algorithms.getMin( ...
MyVS(),@MyMessaging,fns,state,MyRestartManipulator());
%---Solver1---
% Print out the reason for convergence
fprintf('The algorithm converged due to: %s\n', ...
Optizelle.OptimizationStop.to_string(state.opt_stop));
% Print out the final answer
fprintf('The optimal point is: (%e,%e)\n',state.x.data(1),state.x.data(2));
%---WriteRestart0---
% Write out the final answer to file
Optizelle.json.Unconstrained.write_restart(MyVS(),'solution.json',state);
%---WriteRestart1---
end
```

7.5 Simple constrained advanced API

In our Simple constrained advanced API example, we optimize the formulation

$$\min_{\substack{x \in \mathbb{R}^2 \\ \text{st}}} \qquad (x+1)^2 + (y+1)^2$$
$$x+2y = 1$$
$$2x+y \ge 1$$

which uses the same formulation as our example Simple constrained. It differs in that we implement a restart mechanism that writes our variables to an external file. By using the features described in our chapter Advanced API, we accomplish this with the code:

Language	C++
Code	// Optimize a simple optimization problem with an optimal // solution of $(1/3, 1/3)$
	<pre>#include "optizelle/optizelle.h" #include "optizelle/vspaces.h" #include "optizelle/json.h" #include <iostream> #include <iostream> #include <cstdlib> #include <cstdlib> #include <cstring> // Grab Optizelle's Natural type</cstring></cstdlib></cstdlib></iostream></iostream></pre>
	<pre>using Optizelle::Natural; // Defines the vector space used for optimization. template <typename real=""> struct MyVS {</typename></pre>
	<pre>typedef std::vector <real> Vector; // Memory allocation and size setting static Vector init(Vector const & x) { return std::move(Vector(x.size())); }</real></pre>

```
// y <- x (Shallow. No memory allocation.)</pre>
static void copy(Vector const & x, Vector & y) {
    for(Natural i=0;i<x.size();i++){</pre>
       y[i]=x[i];
    }
}
// x <- alpha * x
static void scal(Real const & alpha, Vector & x) {
    for(Natural i=0;i<x.size();i++){</pre>
       x[i]=alpha*x[i];
    }
}
// x <- 0
static void zero(Vector & x) {
    for(Natural i=0;i<x.size();i++){</pre>
       x[i]=0.;
    }
}
// y <- alpha * x + y
static void axpy(Real const & alpha, Vector const & x, Vector & y) {
    for(Natural i=0;i<x.size();i++){</pre>
       y[i]=alpha*x[i]+y[i];
    }
}
// innr <- <x,y>
static Real innr(Vector const & x,Vector const & y) {
    Real z=0;
    for(Natural i=0;i<x.size();i++)</pre>
       z+=x[i]*y[i];
   return z;
}
// x <- random
static void rand(Vector & x){
    std::mt19937 gen(1);
    std::uniform_real_distribution<Real> dis(Real(0.),Real(1.));
    for(Natural i=0;i<x.size();i++)</pre>
       x[i]=Real(dis(gen));
}
// Jordan product, z <- x \circ y.
static void prod(Vector const & x, Vector const & y, Vector & z) {
    for(Natural i=0;i<x.size();i++)</pre>
       z[i]=x[i]*y[i];
}
// Identity element, x \leftarrow e such that x \circ e = x.
static void id(Vector & x) {
    for(Natural i=0;i<x.size();i++)</pre>
       x[i]=Real(1.);
}
// Jordan product inverse, z \le inv(L(x)) y where L(x) y = x \circ y.
```

static void linv(Vector const & x,Vector const & y,Vector & z) {

```
for(Natural i=0;i<x.size();i++)</pre>
           z[i]=y[i]/x[i];
   }
    // Barrier function, barr <- barr(x) where x o grad barr(x) = e.
   static Real barr(Vector const & x) {
       Real z=Real(0.);
       for(Natural i=0;i<x.size();i++)</pre>
           z + = log(x[i]);
       return z;
   }
    // Line search, srch <- argmax {alpha \in Real >= 0 : alpha x + y >= 0}
    // where y > 0.
   static Real srch(Vector const & x,Vector const & y) {
       // Line search parameter
       Real alpha=std::numeric_limits <Real>::infinity();
       // Search for the optimal linesearch parameter.
       for(Natural i=0;i<x.size();i++) {</pre>
           if(x[i] < Real(0.)) {</pre>
               Real alpha0 = -y[i]/x[i];
               alpha = alpha0 < alpha ? alpha0 : alpha;</pre>
           }
       }
       return alpha;
   }
   // Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric</pre>
   // operator.
   static void symm(Vector & x) { }
};
// Squares its input
template <typename Real>
Real sq(Real const & x){
   return x*x;
}
// Define a simple objective where
11
// f(x,y)=(x+1)^2+(y+1)^2
11
struct MyObj : public Optizelle::ScalarValuedFunction <double,MyVS> {
   typedef MyVS <double> X;
    // Evaluation
   double eval(const X::Vector& x) const {
       return sq(x[0]+1.)+sq(x[1]+1.);
   }
   // Gradient
   void grad(
       X::Vector const & x,
       X::Vector & grad
    ) const {
```

```
grad[0]=2*x[0]+2;
       grad[1]=2*x[1]+2;
   }
   // Hessian-vector product
   void hessvec(
       X::Vector const & x,
       X::Vector const & dx,
       X::Vector & H_dx
   ) const {
       H_dx[0]=2.*dx[0];
       H_dx[1]=2.*dx[1];
   }
};
// Define a simple equality
11
// g(x,y)= [ x + 2y = 1 ]
11
struct MyEq :public Optizelle::VectorValuedFunction<double,MyVS,MyVS> {
   typedef MyVS <double> X;
   typedef MyVS <double> Y;
   // y=g(x)
   void eval(
       X::Vector const & x,
       Y::Vector & y
   ) const {
       y[0] = x[0] + 2 \cdot x[1] - 1 \cdot;
   }
   // y=g'(x)dx
   void p(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector & y
   ) const {
       y[0] = dx[0]+2.*dx[1];
   }
   // xhat=g'(x)*dy
   void ps(
       X::Vector const & x,
       Y::Vector const & dy,
       X::Vector & xhat
   ) const {
       xhat[0] = dy[0];
       xhat[1] = 2.*dy[0];
   }
   // xhat=(g''(x)dx)*dy
   void pps(
       X::Vector const & x,
       X::Vector const & dx,
       Y::Vector const & dy,
       X::Vector & xhat
   ) const {
```

```
X::zero(xhat);
   }
};
// Define a simple inequality
11
// h(x,y) = [2x + y > = 1]
11
struct MyIneq :public Optizelle::VectorValuedFunction<double,MyVS,MyVS> {
   typedef MyVS <double> X;
   typedef MyVS <double> Z;
   // z=h(x)
   void eval(
       X::Vector const & x,
       Z::Vector & z
   ) const {
       z[0]=2.*x[0]+x[1]-1.;
   }
   // z=h'(x)dx
   void p(
       X::Vector const & x,
       X::Vector const & dx,
       Z::Vector & z
   ) const {
       z[0] = 2.*dx[0]+dx[1];
   }
   // xhat=h'(x)*dz
   void ps(
       X::Vector const & x,
       Z::Vector const & dz,
       X::Vector & xhat
   ) const {
       xhat[0] = 2.*dz[0];
       xhat[1] = dz[0];
   }
   // xhat=(h''(x)dx)*dz
   void pps(
       X::Vector const & x,
       X::Vector const & dx,
       Z::Vector const & dz,
       X::Vector & xhat
   ) const {
       X::zero(xhat);
   }
};
//---Serialization0---
// Define serialization routines for MyVS
namespace Optizelle {
   namespace json {
       template <>
       struct Serialization <double,MyVS> {
           static std::string serialize(
```

```
typename MyVS <double>::Vector const & x,
   std::string const & name,
   Natural const & iter
) {
   // Create the filename where we put our vector
   std::stringstream fname;
   fname << "./restart/";</pre>
   fname << name << ".";</pre>
   fname << std::setw(4) << std::setfill('0') << iter;</pre>
   fname << ".txt";</pre>
   // Actually write the vector there
   std::ofstream fout(fname.str());
   if(fout.fail()) {
       std::stringstream msg;
       msg << "While writing the variable " << name</pre>
           << " to file on iteration " << iter
           << ", unable to open the file: "
           << fname.str() << ".";
       throw Optizelle::Exception::t(msg.str());
   }
   fout.setf(std::ios::scientific);
   fout.precision(16);
   for(Natural i=0;i<x.size();i++)</pre>
       fout << x[i] << std::endl;</pre>
   // Close out the file
   fout.close();
   // Use this filename as the json string
   std::stringstream x_json;
   x_json << "\"" << fname.str() << "\"";</pre>
   return x_json.str();
}
static MyVS <double>::Vector deserialize(
   typename MyVS <double>::Vector const & x_,
   std::string const & x_json_
) {
   // Make a copy of x_json_
   auto x_json = x_json_;
   // Filter out the quotes and newlines from the string
   auto formatting = "\"\n";
   for(auto i=0;i<2;i++)</pre>
       x_json.erase(
           std::remove(x_json.begin(),x_json.end(),formatting[i]),
           x_json.end());
   // Open the file for reading
   std::ifstream fin(x_json.c_str());
   if(!fin.is_open())
       throw Optizelle::Exception::t(
           "Error while opening the file " + x_json + ": " +
           strerror(errno));
   // Create a new vector that we eventually return
   auto x = std::vector <double> (x_.size());
```

```
// Read in each of the elements
              for(auto i=0;i<x.size();i++)</pre>
                  fin >> x[i];
              // Return the result
              return std::move(x);
           }
       };
   }
}
//---Serialization1---
// Define a state manipulator that writes out the optimization state at
// each iteration.
struct MyRestartManipulator : Optizelle::StateManipulator <</pre>
   Optizelle::Constrained <double,MyVS,MyVS,MyVS> >
{
   void eval(
       typename Optizelle::Constrained <double,MyVS,MyVS,MyVS>
           ::Functions::t const & fns,
       typename Optizelle::Constrained <double,MyVS,MyVS,MyVS>
           ::State::t & state,
       Optizelle::OptimizationLocation::t const & loc
   ) const {
       switch(loc) {
       \ensuremath{\prime\prime}\xspace At the end of the optimization iteration, write the restart file
       case Optizelle::OptimizationLocation::EndOfOptimizationIteration: {
           // Create a reasonable file name
           std::stringstream ss;
           ss << "simple_constrained_advanced_api_";</pre>
           ss << std::setw(4) << std::setfill('0') << state.iter;</pre>
           ss << ".json";</pre>
           // Write the restart file
           Optizelle::json::Constrained <double,MyVS,MyVS,MyVS>::write_restart(
              ss.str(),state);
           break;
       } default:
           break;
       }
   }
};
int main(int argc, char* argv[]){
   // Read in the name for the parameters and optional restart file
   if(!(argc==2 || argc==3)) {
       std::cerr << "simple_constrained_advanced_api <pre>parameters> <restart>"
           << std::endl;
       exit(EXIT_FAILURE);
   }
   auto pname = argv[1];
   auto rname = argc==3 ? argv[2] : "";
   // Generate an initial guess for the primal
   auto x = std::vector <double> {2.1, 1.1};
```

```
// Allocate memory for equality multiplier
                   auto y = std::vector <double> (1);
                   // Allocate memory for the inequality multiplier
                   auto z = std::vector <double> (1);
                   // Create an optimization state
                   Optizelle::Constrained <double,MyVS,MyVS,MyVS>::State::t state(x,y,z);
                   // If we have a restart file, read in the parameters
                   if(argc==3)
                       Optizelle::json::Constrained <double,MyVS,MyVS,MyVS>::read_restart(
                           rname,x,y,z,state);
                   // Read the parameters from file
                   Optizelle::json::Constrained <double,MyVS,MyVS,MyVS>::read(pname,state);
                   // Create a bundle of functions
                   Optizelle::Constrained <double,MyVS,MyVS,MyVS>::Functions::t fns;
                   fns.f.reset(new MyObj);
                   fns.g.reset(new MyEq);
                   fns.h.reset(new MyIneq);
                   // Solve the optimization problem
                   Optizelle::Constrained <double,MyVS,MyVS,MyVS>::Algorithms
                       ::getMin(Optizelle::Messaging::stdout,fns,state,MyRestartManipulator());
                   // Print out the reason for convergence
                   std::cout << "The algorithm converged due to: " <<</pre>
                       Optizelle::OptimizationStop::to_string(state.opt_stop) <<</pre>
                       std::endl;
                   // Print out the final answer
                   std::cout << std::scientific << std::setprecision(16)</pre>
                       << "The optimal point is: (" << state.x[0] << ','
                       << state.x[1] << ')' << std::endl;
                   // Write out the final answer to file
                   Optizelle::json::Constrained <double,MyVS,MyVS,MyVS>::write_restart(
                       "solution.json",state);
                   // Successful termination
                   return EXIT_SUCCESS;
               }
Language
               Python
               # Optimize a simple optimization problem with an optimal solution
               # of (1/3,1/3)
                import Optizelle
                import sys
                import copy
                import array
                import math
```

Code

```
# Defines the vector space used for optimization.
class MyVS(object):
   @staticmethod
   def init(x):
       """Memory allocation and size setting"""
       return copy.deepcopy(x)
   @staticmethod
   def copy(x,y):
       """y <- x (Shallow. No memory allocation.)"""</pre>
       y[:]=x[:]
   @staticmethod
   def scal(alpha,x):
       """x <- alpha * x"""
       for i in xrange(0,len(x)):
           x[i]=alpha*x[i]
   @staticmethod
   def zero(x):
       """x <- 0"""
       for i in xrange(0,len(x)):
           x[i]=0.
   @staticmethod
   def axpy(alpha,x,y):
       """y <- alpha * x + y"""
       for i in xrange(0,len(x)):
           y[i]=alpha*x[i]+y[i]
   @staticmethod
   def innr(x,y):
       """<- <x,y>"""
       return reduce(lambda z,xy:xy[0]*xy[1]+z,zip(x,y),0.)
   @staticmethod
   def rand(x):
       """x <- random"""
       for i in xrange(0,len(x)):
           x[i]=random.uniform(0.,1.)
   @staticmethod
   def prod(x,y,z):
       """Jordan product, z <- x o y"""
       for i in xrange(0,len(x)):
           z[i]=x[i]*y[i]
    @staticmethod
   def id(x):
       """Identity element, x < -e such that x \circ e = x"""
       for i in xrange(0,len(x)):
           x[i]=1.
   @staticmethod
   def linv(x,y,z):
       ""Jordan product inverse, z \le inv(L(x)) y where L(x) y = x \circ y""
```

```
for i in xrange(0,len(x)):
           z[i]=y[i]/x[i]
   @staticmethod
   def barr(x):
       """Barrier function, <- barr(x) where x o grad barr(x) = e"""
       return reduce(lambda x,y:x+math.log(y),x,0.)
   @staticmethod
   def srch(x,y):
       """Line search, <- argmax {alpha \in Real >= 0 : alpha x + y >= 0} where y >
       alpha = float("inf")
       for i in xrange(0,len(x)):
           if x[i] < 0:
               alpha0 = -y[i]/x[i]
               if alpha0 < alpha:</pre>
                  alpha=alpha0
       return alpha
   @staticmethod
   def symm(x):
       """Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric operator
       pass
# Squares its input
sq = lambda x:x*x
# Define a simple objective where
#
# f(x,y)=(x+1)^2+(y+1)^2
#
class MyObj(Optizelle.ScalarValuedFunction):
   # Evaluation
   def eval(self,x):
       return sq(x[0]+1.)+sq(x[1]+1.)
   # Gradient
   def grad(self,x,grad):
       grad[0]=2.*x[0]+2.
       grad[1]=2.*x[1]+2.
   # Hessian-vector product
   def hessvec(self,x,dx,H_dx):
       H_dx[0]=2.*dx[0]
       H_dx[1]=2.*dx[1]
# Define a simple equality
#
# g(x,y)= [ x + 2y = 1 ]
#
class MyEq(Optizelle.VectorValuedFunction):
   # y=g(x)
   def eval(self,x,y):
       y[0] = x[0] + 2 \cdot x[1] - 1.
```

```
\# y=g'(x)dx
   def p(self,x,dx,y):
       y[0] = dx[0]+2.*dx[1]
   # xhat=g'(x)*dy
   def ps(self,x,dy,xhat):
       xhat[0] = dy[0]
       xhat[1]= 2.*dy[0]
   # xhat=(g''(x)dx)*dy
   def pps(self,x,dx,dy,xhat):
       MyVS.zero(xhat)
# Define simple inequalities
#
# h(x,y) = [2x + y \ge 1]
#
class MyIneq(Optizelle.VectorValuedFunction):
   \# z=h(x)
   def eval(self,x,z):
       z[0]=2.*x[0]+x[1]-1.
   \# z=h'(x)dx
   def p(self,x,dx,z):
       z[0] = 2.*dx[0]+dx[1]
   # xhat=h'(x)*dz
   def ps(self,x,dz,xhat):
       xhat[0] = 2.*dz[0]
       xhat[1] = dz[0]
   # xhat=(h''(x)dx)*dz
   def pps(self,x,dx,dz,xhat):
       MyVS.zero(xhat)
#---Serialization0---
def serialize_MyVS(x,name,iter):
   """Serializes an array for the vector space MyVS"""
   # Create the filename where we put our vector
   fname = "./restart/%s.%04d.txt" % (name,iter)
   # Actually write the vector there
   fout = open(fname,"w");
   for i in xrange(0,len(x)):
       fout.write("%1.16e\n" % x[i])
   # Close out the file
   fout.close()
   # Use this filename as the json string
   x_json = "\"%s\"" % fname
   return x_json
def deserialize_MyVS(x_,x_json):
    """Deserializes an array for the vector space MyVS"""
```

```
# Eliminate all whitespace
   x_json="".join(x_json.split())
   # Eliminate the initial and final delimiters
   x_json=x_json[1:-1]
   # Open the file for reading
   fin = open(x_json,"r")
   # Allocate a new vector to return
   x = copy.deepcopy(x_)
   # Read in each of the elements
   for i in xrange(0,len(x)):
       x[i] = float(fin.readline())
   # Close out the file
   fin.close()
   # Return the result
   return x
# Register the serialization routines for arrays
def MySerialization():
   Optizelle.json.Serialization.serialize.register(
       serialize_MyVS,array.array)
   Optizelle.json.Serialization.deserialize.register(
       deserialize_MyVS,array.array)
#---Serialization1---
# Define a state manipulator that writes out the optimization state at
# each iteration.
class MyRestartManipulator(Optizelle.StateManipulator):
   def eval(self,fns,state,loc):
       # At the end of the optimization iteration, write the restart file
       if loc == Optizelle.OptimizationLocation.EndOfOptimizationIteration:
           # Create a reasonable file name
           ss = "simple_constrained_advanced_api_%04d.json" % (state.iter)
           # Write the restart file
           Optizelle.json.Constrained.write_restart(
             MyVS, MyVS, MyVS, ss, state)
# Register the serialization routines
MySerialization()
# Read in the name for the input file
if not(len(sys.argv)==2 or len(sys.argv)==3):
   sys.exit("python simple_constrained_advanced_api.py <parameters>\n" +
           "python simple_constrained_advanced_api.py parameters> <restart>")
pname = sys.argv[1]
rname = sys.argv[2] if len(sys.argv)==3 else ""
# Generate an initial guess
x = array.array('d', [2.1,1.1])
```

```
# Allocate memory for the equality multiplier
               y = array.array('d', [0.])
               # Allocate memory for the inequality multiplier
               z = array.array('d',[0.])
               # Create an optimization state
               state=Optizelle.Constrained.State.t(MyVS,MyVS,MyVS,x,y,z)
               # If we have a restart file, read in the parameters
               if len(sys.argv)==3:
                   Optizelle.json.Constrained.read_restart(MyVS,MyVS,MyVS,rname,x,y,z,state)
               # Read the parameters from file
               Optizelle.json.Constrained.read(MyVS,MyVS,MyVS,pname,state)
               # Create a bundle of functions
               fns=Optizelle.Constrained.Functions.t()
               fns.f=MyObj()
               fns.g=MyEq()
               fns.h=MyIneq()
               # Solve the optimization problem
               Optizelle.Constrained.Algorithms.getMin(
                   MyVS,MyVS,Optizelle.Messaging.stdout,fns,state,MyRestartManipulator())
               # Print out the reason for convergence
               print("The algorithm converged due to: %s" % (
                   Optizelle.OptimizationStop.to_string(state.opt_stop)))
               # Print out the final answer
               print("The optimal point is: (%e,%e)" % (state.x[0],state.x[1]))
               # Write out the final answer to file
               Optizelle.json.Constrained.write_restart(MyVS,MyVS,MyVS,"solution.json",state)
Language
               MATLAB/Octave
Code
               \% Optimize a simple optimization problem with an optimal solution
               % of (1/3,1/3)
               function simple_constrained_advanced_api(pname,rname)
                   % Read in the name for the input file
                   if ~(nargin==1 || nargin==2)
                      error(sprintf('%s\n%s', ...
                          'simple_constrained_advanced_api(parameters)\n', ...
                          'simple_constrained_advanced_api(parameters,restart)'));
                   end
                   % Execute the optimization
                   if nargin==1
                      main(pname);
                   else
                      main(pname,rname);
                   end
               end
```

```
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```

```
% Convert a vector to structure
function y = tostruct(x)
   y = struct('data',x);
end
\% Defines the vector space used for optimization.
function self = MyVS()
   % Memory allocation and size setting
   self.init = Q(x) x;
   % <- x (Shallow. No memory allocation.)
   self.copy = @(x) x;
   % <- alpha * x
   self.scal = @(alpha,x) tostruct(alpha*x.data);
   % <- 0
   self.zero = @(x) tostruct(zeros(size(x.data)));
   % <- alpha * x + y
   self.axpy = @(alpha,x,y) tostruct(alpha * x.data + y.data);
   %<- <x,y>
   self.innr = @(x,y)x.data'*y.data;
   % <- random
   self.rand = @(x)tostruct(randn(size(x.data)));
   % Jordan product, z <- x o y.
   self.prod = @(x,y)tostruct(x.data .* y.data);
   % Identity element, x < -e such that x \circ e = x.
   self.id = @(x)tostruct(ones(size(x.data)));
   % Jordan product inverse, z \le inv(L(x)) y where L(x) y = x \circ y.
   self.linv = @(x,y)tostruct(y.data ./ x.data);
   % Barrier function, barr <- barr(x) where x o grad barr(x) = e.
   self.barr = @(x)sum(log(x.data));
   % Line search, srch <- argmax {alpha i >= 0 : alpha x + y >= 0}
   % where y > 0.
   self.srch = @(x,y) feval(@(z)min([min(z(find(z>0)));inf]),-y.data ./x.data);
   % Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric
   % operator.
   self.symm = @(x)x;
end
% Squares its input
function z = sq(x)
   z=x*x;
end
% Define a simple objective where
```

```
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```

```
%
% f(x,y)=(x+1)^2+(y+1)^2
%
function self = MyObj()
   % Evaluation
   self.eval = @(x) feval(@(x)sq(x(1)+1.)+sq(x(2)+1.),x.data);
   % Gradient
   self.grad = @(x) tostruct(feval(@(x)[
       2.*x(1)+2.;
       2.*x(2)+2.],x.data));
   % Hessian-vector product
   self.hessvec = @(x,dx) tostruct(feval(@(x,dx)[
       2.*dx(1);
       2.*dx(2)],x.data,dx.data));
end
% Define a simple equality
%
% g(x,y) = [x + 2y = 1]
%
function self = MyEq()
   % y=g(x)
   self.eval = @(x) tostruct(feval(@(x)[x(1)+2.*x(2)-1.],x.data));
   % y=g'(x)dx
   self.p = @(x,dx) tostruct(feval(@(x,dx)[dx(1)+2.*dx(2)],x.data,dx.data));
   \% xhat=g'(x)*dy
   self.ps = @(x,dy) tostruct(feval(@(x,dy)[
       dy(1);
       2.*dy(1)],x.data,dy.data));
   % xhat=(g''(x)dx)*dy
   self.pps = @(x,dx,dy) tostruct(zeros(2,1));
end
% Define simple inequalities
%
% h(x,y) = [2x + y > = 1]
%
function self = MyIneq()
   % z=h(x)
   self.eval = @(x) tostruct(feval(@(x)[
       2.*x(1)+x(2)-1],x.data));
   % z=h'(x)dx
   self.p = @(x,dx) tostruct(feval(@(x,dx)[
       2.*dx(1)+dx(2)],x.data,dx.data));
   % xhat=h'(x)*dz
   self.ps = @(x,dz) tostruct(feval(@(x,dz)[
       2.*dz(1)
```

```
dz(1)],x.data,dz.data));
   \% hat=(h''(x)dx)*dz
   self.pps = @(x,dx,dz) tostruct([ 0. ]);
end
%---Serialization0---
\% Define the serialize routine for MyVS
function x_json=serialize_MyVS(x,name,iter)
   % Create the filename where we put our vector
   fname=sprintf('./restart/%s.%04d.txt',name,iter);
   % Actually write the vector there
   dlmwrite(fname, x.data);
   % Use this filename as the json string
   x_json = sprintf('\"%s\"',fname);
end
\% Define the deserialize routine for MyVS
function x=deserialize_MyVS(x_,x_json)
   % Filter out the quotes and newlines from the string
   x_json = strrep(x_json,'"',');
   x_json = strrep(x_json, sprintf('\n'),');
   % Read the data into x
   x=tostruct(dlmread(x_json));
end
% Define serialization routines for MyVS
function MySerialization()
   global Optizelle;
   Optizelle.json.Serialization.serialize( ...
       'register', ...
       @(x,name,iter)serialize_MyVS(x,name,iter), ...
       @(x)isstruct(x) && isfield(x,'data') && isvector(x.data));
   Optizelle.json.Serialization.deserialize( ...
       'register', ...
       @(x,x_json)deserialize_MyVS(x,x_json), ...
       @(x)isstruct(x) && isfield(x,'data') && isvector(x.data));
end
%---Serialization1---
\% Define a state manipulator that writes out the optimization state at
% each iteration.
function smanip=MyRestartManipulator()
   smanip=struct('eval',@(fns,state,loc)MyRestartManipulator_(fns,state,loc));
end
function state=MyRestartManipulator_(fns,state,loc)
   global Optizelle;
   \% At the end of the optimization iteration, write the restart file
   if(loc == Optizelle.OptimizationLocation.EndOfOptimizationIteration)
       % Create a reasonable file name
       ss = sprintf('simple_constrained_advanced_api_%04d.json',state.iter);
       % Write the restart file
```

```
Optizelle.json.Constrained.write_restart( ...
          MyVS(),MyVS(),MyVS(),ss,state);
   end
end
% Actually runs the program
function main(pname,rname)
   % Grab the Optizelle library
   global Optizelle;
   setupOptizelle();
   % Register the serialization routines
   MySerialization();
   % Generate an initial guess
   x = tostruct([2.1;1.1]);
   % Allocate memory for the equality multiplier
   y = tostruct([0.]);
   % Allocate memory for the inequality multiplier
   z = tostruct([0.]);
   % Create an optimization state
   state = Optizelle.Constrained.State.t(MyVS(),MyVS(),MyVS(),x,y,z);
   \% If we have a restart file, read in the parameters
   if(nargin==2)
       state = Optizelle.json.Constrained.read_restart( ...
           MyVS(),MyVS(),MyVS(),rname,x,y,z);
   end
   % Read the parameters from file
   state = Optizelle.json.Constrained.read(MyVS(),MyVS(),MyVS(),pname,state);
   % Create a bundle of functions
   fns = Optizelle.Constrained.Functions.t;
   fns.f = MyObj();
   fns.g = MyEq();
   fns.h = MyIneq();
   % Solve the optimization problem
   state = Optizelle.Constrained.Algorithms.getMin( ...
       MyVS(),MyVS(),MyVS(),Optizelle.Messaging.stdout,fns,state, ...
       MyRestartManipulator());
   % Print out the reason for convergence
   fprintf('The algorithm converged due to: %s\n', ...
       Optizelle.OptimizationStop.to_string(state.opt_stop));
   % Print out the final answer
   fprintf('The optimal point is: (%e,%e)\n',state.x.data(1),state.x.data(2));
   % Write out the final answer to file
   Optizelle.json.Constrained.write_restart( ...
       MyVS(),MyVS(),MyVS(),'solution.json',state);
```

 end

Algorithmic discussion

In the following chapter, we give a brief discussion of the algorithms we include within Optizelle and references to more detailed descriptions.

- Algorithm Barzilai-Borwein
- **Description** We implement the Barzilai-Borwein algorithm by setting dir to SteepestDescent and kind to either TwoPointA or TwoPointB. Specifically, TwoPointA and TwoPointB refer to the algorithms generated by equation (5) and (6) in Barzilai and Borwein's paper, respectively. Since this algorithm requires two points before it may commence, we use a GoldenSection search on the first iteration.
 - Jonathan Barzilai and Jonathan M. Borwein. Two-point step size gradient methods. *IMA Journal of Numerical Analysis*, 8(1):141–148, 1988.
- Algorithm Golden-section search
- **Description** We implement a straightforward golden-section search. For historical significance, we refer to Kiefer's paper, but a much more complete description can be found in Bazaraa, Sherali, and Shetty's book.
 - J. Kiefer. Sequential minimax search for a maximum. Proceedings of the American Mathematical Society, 4(3):502–506, 1953.
 - Mokhtar S. Bazaraa, Hanif D. Sherali, and C. M. Shetty. *Nonlinear Programming: Theory And Algorithms*. Wiley-Interscience, 3rd edition, 2006.

Algorithm BFGS

- **Description** Our BFGS implementation uses a limited-memory, iterative reformulation of the algorithm based on a generic inner product. Our limited-memory implementation differs from that of Byrd, Nocedal, and Schnabel's because we do not form a compact representation, but instead use a scratch space whose size is equal to stored_history. In addition, since we do not check the Wolfe conditions, we do a hard check to insure that BFGS operator remains positive definite. We refer to the collection of 1970s papers for historical significance, but note that a much better presentation of the algorithm can be found in Nocedal and Wright's book.
 - C. G. Broyden. The convergence of a class of double-rank minimization algorithms: 2. the new algorithm. *IMA Journal of Applied Mathematics*, 6(3):222–231, 1970.
 - R. Fletcher. A new approach to variable metric algorithms. *The Computer Journal*, 13(3):317–322, 1970.

- D. Goldfarb. A family of variable metric updates derived by variational means. Mathematics of Computation, 24:23–26, 1970.
- D. F. Shanno. Conditioning of quasi-Newton methods for function minimization. Mathematics of Computation, 24(111):647–656, 1970.
- Richard H. Byrd, Jorge Nocedal, and Robert B. Schnabel. Representations of quasi-Newton matrices and their use in limited memory methods. *Mathematical Programming*, 63(2):129–156, 1994.
- Jorge Nocedal and Stephen J. Wright. *Numerical Optimization*. Springer, 2nd edition, 2006.

Algorithm SR1

- **Description** Similar to BFGS, our SR1 implementation uses a limited-memory, iterative reformulation of the algorithm based on a generic inner product. As before, our limited-memory implementation differs from that of Byrd, Nocedal, and Schnabel's because we do not form a compact representation, but instead use a scratch space whose size is equal to **stored_history**. We refer to Broyden's paper for historical significance, but note that a much better presentation of the algorithm can be found in Nocedal and Wright's book.
 - C. G. Broyden. Quasi-Newton methods and their application to function minimization. *Mathematics of Computation*, 21:368–381, 1967.
 - Richard H. Byrd, Jorge Nocedal, and Robert B. Schnabel. Representations of quasi-Newton matrices and their use in limited memory methods. *Mathematical Programming*, 63(2):129–156, 1994.
 - Jorge Nocedal and Stephen J. Wright. *Numerical Optimization*. Springer, 2nd edition, 2006.

Algorithm Nonlinear-CG

- **Description** We use a standard implementation of nonlinear-CG. On the first iteration, we move in the steepest descent direction, but use the specified nonlinear-CG direction on subsequent iterations. Since we do not check the strong-Wolfe condition, we do a hard check to insure a descent direction. If we do not, we negate the search direction. Although we reference the original papers from Hestenes and Stiefel, Fletcher and Reeves, and Polak and Ribiere, Nocedal and Wright give a nicer presentation. In addition, Hager and Zhang present a nice overview of the different nonlinear-CG variations in their survey paper.
 - Magnus R. Hestenes and Eduard Stiefel. Methods of conjugate gradients for solving linear systems. Journal of Research of the National Bureau of Standards, 49(6):409–436, 1952.
 - R. Fletcher and C. M. Reeves. Function minimization by conjugate gradients. *The Computer Journal*, 7(2):149–154, 1964.
 - E. Polak and G. Ribiere. Note sur la convergence de méthodes de directions conjuguées. *Revue Française d'Informatique et de Recherche Opérationnelle*, 16:35– 43, 1969.
 - Jorge Nocedal and Stephen J. Wright. *Numerical Optimization*. Springer, 2nd edition, 2006.
 - William W. Hager and Hongchao Zhang. A survey of nonlinear conjugate gradient methods. *Pacific Journal of Optimization*, 2(1):35–58, January 2006.

0	0
Description	Our trust-region Newton implementation uses truncated-CG to solve the trust-region subproblem. Both Conn, Gould, and Toint's as well as Nocedal and Wright's book give good descriptions of the algorithm.
	• Andrew R. Conn, Nicholas I. M. Gould, and Philippe L. Toint. <i>Trust-Region Methods</i> . SIAM, 2000.
	• Jorge Nocedal and Stephen J. Wright. <i>Numerical Optimization</i> . Springer, 2nd edition, 2006.
Algorithm	Newton-CG
Description	We base our Newton-CG algorithm on truncated CG and not a Hessian modification. Nocedal and Wright's book describes this algorithm.
	• Jorge Nocedal and Stephen J. Wright. <i>Numerical Optimization</i> . Springer, 2nd edition, 2006.
Algorithm	Truncated CG
Description	 Our version of truncated CG actually possesses the ability to over orthogonalize against previous Krylov vectors, which is controlled by the parameters trunc_orthog_storage_max and trunc_orthog_iter_max. In addition, we have added a safeguard procedure for the interior point method that insures truncated CG always produces a solution feasible with respect to the inequality constraint. This safeguard process is similar to the one used by Byrd, Hribar, and Nocedal in their NITRO algorithm. Finally, for the inexact composite-step SQP method, we use the heuristic described in appendix B by Heinkenschloss and Ridzal to detect instability in the algorithm. Historically, Toint and Steihaug give a description of truncated-CG in their respective papers. For a modern treatment of truncated-CG see Conn, Gould, and Toint's book. Ph. L. Toint. Towards an efficient sparsity exploiting Newton method for minimization. pages 57–88. 1981. Trond Steihaug. The conjugate gradient method and trust regions in large scale optimization. SIAM Journal on Numerical Analysis, 20(3):626–637, 1983. Andrew R. Conn, Nicholas I. M. Gould, and Philippe L. Toint. Trust-Region Methods. SIAM, 2000. Richard H. Byrd, Mary E. Hribar, and Jorge Nocedal. An interior point algorithm for large-scale nonlinear programming. SIAM Journal on Optimization, 9(4):877–900, 1999. Matthias Heinkenschloss and Denis Ridzal. A matrix-free trust-region sqp method for equality constrained optimization. SIAM Journal on Optimization, 24(3):1507–1541, 2014.
Algorithm	Interior-point method
-	-
Description	Our interior point method is based on a new derivation of the primal-dual interior point equations based on pseudo-Euclidean-Jordan algebras. We say <i>pseudo</i> because we do not require commutativity in the Jordan product. Specifically, our derivation begins from the optimality conditions
	$\nabla f(x) - h'(x)^* z = 0,$
	$h(x) \succeq 0,$

Algorithm

Trust-region Newton

 $z \succeq 0,$ $h(x) \circ z = 0$

in the case of inequality constrained problems and

$$abla f(x) + g'(x)^* y - h'(x)^* z = 0,$$

 $g(x) = 0,$
 $h(x) \succeq 0,$
 $z \succeq 0,$
 $h(x) \circ z = 0$

in the case of constrained problems. Here, \circ denotes the Jordan product that we refer to as **prod**. Since we use a composite-step SQP method for constrained problems, we ignore the feasibility condition, g(x) = 0, in the constrained problem. Simply, we handle feasibility with respect to this constraint with the quasi-normal step. This allows us to reduce both sets of optimality conditions to

$$grad(x, y) - h'(x)^* z = 0,$$
$$h(x) \succeq 0,$$
$$z \succeq 0,$$
$$h(x) \circ z = 0$$

where

$$\operatorname{grad}(x,y) = \begin{cases} \nabla f(x) & \text{Inequality constrained problems,} \\ \nabla f(x) + g'(x)^*y & \text{Constrained problems.} \end{cases}$$

Then, using a standard interior-point formulation, we perturb the optimality conditions into

$$grad(x, y) - h'(x)^* z = 0$$
$$h(x) \succ 0$$
$$z \succ 0$$
$$h(x) \circ z = \mu e.$$

where e denotes the identity element in the pseudo-Euclidean-Jordan algebra, which we refer to as **id**. Next, we apply Newton's method to the nonlinear system of equations

$$grad(x, y) - h'(x)^* z = 0,$$

$$h(x) \circ z = \mu e,$$

which yields the system

$$\begin{bmatrix} \operatorname{hess}(x,y) & -h'(x)^* \\ h'(x) \cdot \circ z & h(x) \circ \cdot \end{bmatrix} \begin{bmatrix} \delta x \\ \delta z \end{bmatrix} = \begin{bmatrix} -\operatorname{grad}(x,y) + h'(x)^* z \\ -h(x) \circ z + \mu e \end{bmatrix}$$

where

$$\operatorname{hess}(x,y) = \begin{cases} \nabla^2 f(x) & \text{Inequality constrained problems,} \\ \nabla^2 f(x) + (g''(x) \cdot)^* y & \text{Constrained problems.} \end{cases}$$

Using the second equation in the Newton system, we solve for δz and find that

$$\delta z = -z + L(h(x))^{-1}(-h'(x)\delta x \circ z + \mu e)$$

where $L(h(x))^{-1}$ denotes the inverse of the linear operator induced by the Jordan product, \circ , which we refer to as **linv**. In other words, $h(x) \circ z = L(h(x))z$. Then, we plug this equation into the first equation and reduce our Newton system to

$$[hess(x,y) + h'(x)^* (L(h(x))^{-1}(h'(x) \cdot \circ z))] \delta x = -\operatorname{grad}(x,y) + \mu h'(x)^* (L(h(x))^{-1}e).$$

At this point, we solve the Newton system using truncated CG. As a note, when using a line-search method that is not Newton-CG, we using a different scheme and instead set

$$\mathbf{z} = \mathbf{m}\mathbf{u} \cdot L(h(\mathbf{x}))^{-1}e.$$

This gives us a log-barrier algorithm for these methods. In short, without solving a Newton system, the equations for dz don't make sense, so we instead fallback on a log-barrier method, which does not require them. In order to maintain strict feasibility of h(x) and z we safeguard our steps dx and dz using the fraction to the boundary rule

$$\begin{split} h(\mathbf{x} + \mathtt{alpha}_{\mathbf{x}} \cdot \mathtt{dx}) \geq & (1 - \mathtt{gamma})h(x) \\ \mathbf{z} + \mathtt{alpha}_{\mathbf{z}} \cdot \mathtt{dz} \geq & (1 - \mathtt{gamma})z) \\ h(\mathbf{x} + \mathtt{alpha}_{\mathbf{x}}\mathtt{qn} \cdot \mathtt{dx}\mathtt{n}) \geq & (1 - \mathtt{gamma} \cdot \mathtt{zeta})h(x) \end{split}$$

Note, the last inequality only occurs in constrained problems. When we enforce these rules depends on the algorithm. Specifically, trust-region methods enforce these bounds during the truncated-CG solve of the optimality conditions. Since truncated CG may violate the inequality bounds periodically throughout the optimality solve, we save the last feasible iterate during the computation. When we exit, we take the last feasible iterate and step and compute the safeguard search, which satisfies the fraction to the boundary rule above. In order to prevent too many discarded steps due to the safeguard, we limit the maximum number of infeasible steps that we allow to be **safeguard_failed_max**. Although our process is slightly different than their paper, how we embed the safeguard into truncated CG is similar to what Byrd, Hribar, and Nocedal do in their implementation of NITRO. In a line-search method, we safeguard the step prior to the line search. Specifically, we shorten alpha0 so that the maximum step length taken by the line search does not exceed our fraction to the boundary rule. Finally, in the inexact composite step SQP method, we also safeguard our quasi-normal step by enforcing the fraction to the boundary rule during the dogleg computation. In each case, we calculate the distance to the boundary with the user-defined function srch. In our Rm and SQL vector spaces, we use a closed form formula for linear and second-order cones and the Arnoldi algorithm for semidefinite cones. We reduce mu prior to the truncated-CG solve for the optimality system and set $\mathbf{mu} = \mathbf{sigma} \cdot \mathbf{mu}$ when one of the following global or local convergence criteria is satisfied

- 1. $\log(\texttt{norm_gradtyp}) \log(\|\texttt{gradstep}(x, y, z)\|) < \log(\texttt{mu_typ}) \log(\texttt{mu_est})$
- 2. $\|\operatorname{gradstep}(x, y, z)\| < \operatorname{eps_grad} \cdot \operatorname{norm_gradtyp}$
- 3. $\log(\operatorname{norm_gradtyp}) \log(||\operatorname{gradstop}(x, y, z)||) < \log(\operatorname{mu_typ}) \log(\operatorname{mu_est})$
- 4. $\|\operatorname{gradstop}(x, y, z)\| < \operatorname{eps_grad} \cdot \operatorname{norm_gradtyp}$

where

$$\begin{aligned} \operatorname{gradstop}(x,y,z) &= \begin{cases} \nabla f(x) - h'(x)^* z & \operatorname{Inequality \ constrained,} \\ \nabla f(x) + g'(x)^* y - h'(x)^* z & \operatorname{Constrained.} \end{cases} \\ \\ \operatorname{gradstep}(x,y,z) &= \begin{cases} \nabla f(x) - \mu h'(x)^* L(h(x))^{-1} e & \operatorname{Inequality \ constrained,} \\ \nabla f(x) + W(\nabla^2 f(x) \mathrm{d} \mathbf{x}_{-} \mathbf{n}) + g'(x)^* y - \mu h'(x)^* L(h(x))^{-1} e & \operatorname{Constrained.} \end{cases} \end{aligned}$$

and W denotes the projection onto nullspace of g'(x). Next, we must satisfy one of the following global or local convergence criteria

1. $\log(\operatorname{norm_gxtyp}) - \log(||g(\mathbf{x})||) < \log(\operatorname{mu_typ}) - \log(\operatorname{mu_est})$

2. $\|g(\mathbf{x})\| < eps_constr \cdot norm_gxtyp$

In addition, we must converge **mu_est** locally

$$|mu - mu_est| < mu$$

and not have converged **mu** globally

$$|mu - eps_mu \cdot mu_typ| \ge eps_mu \cdot mu_typ.$$

Finally, we also require that iter > 1, so that we don't reduce **mu** on the first iteration. For globalization, in both trust-region and line-search methods, we modify our merit function with the addition of a barrier function, which we refer to as **barr**. Specifically, we allow any barrier function such that $x \circ \nabla barr(x) = e$. In our Rm and SQL vector spaces, we use the log-barrier functions:

Linear	$\langle \log(x), e \rangle,$
Quadratic	$\frac{1}{2}\log(x_0^2-\langle \bar{x},\bar{x}\rangle),$
Semidefinite	$\log(\det(x)).$

where $\langle \cdot, \cdot \rangle$ refers to the ℓ^2 inner product. In order to compute the semidefinite barrier function, we Choleski factor x into $u^T u$ since

$$\log(\det(x)) = \log(\det(u^{T}u)) = \log(\det(u^{T})\det(u)) = \log(\det(u)^{2}) = 2\log(\det(u))$$

and the determinant of an upper triangular matrix can be calculated quickly. As our final step, since we don't require our Jordan product to be commutative, we forcibly symmetrize both δx and δz using the symm operator in our vector space. As far as the initial inequality multiplier, we set

$$\mathbf{z} = \mathbf{m}\mathbf{u} \cdot L(h(\mathbf{x}))^{-1}e.$$

This guarantees that

1. $h(\mathbf{x}) \circ \mathbf{z} = \mathbf{m} \mathbf{u} \cdot e$

2. $mu_est = mu$

In other words, our initial inequality multiplier puts us on the central path specified by the parameter **mu**. Historically, we are not the first to use Euclidean-Jordan algebras in an interior point algorithm. Alizadeh and Schmieta describe their use for semidefinite programming and Alizadeh and Goldfarb describe their use in second-order cone programming. Nevertheless, we drop the commutativity requirement in our algorithm. Part of the reason we drop the commutativity requirement is that in the SDP case we essentially generate the same optimality conditions as equation (4.10) in Helmberg, Rendl, Vanderbei, and Wolkowicz's SDP paper. In fact, our symmetrization in the SQL vector space is identical to equation (4.30) in the same paper, which later became known as the HKM search direction. Beyond the HKM symmetrization, we allow any similar symmetrization operator, which Zhang describes in his paper.

- Farid Alizadeh and Stefan Schmieta. Symmetric cones, potential reduction methods and word-by-word extensions. In Henry Wolkowicz, Romesh Saigal, and Lieven Vandenberghe, editors, *Handbook of Semidefinite Programming*, volume 27 of *International Series in Operations Research & Management Science*, pages 195–233. Springer US, 2000.
- F. Alizadeh and D. Goldfarb. Second-order cone programming. *Mathematical Programming*, 95(1):3–51, 2003.
- Christoph Helmberg, Franz Rendl, Robert J. Vanderbei, and Henry Wolkowicz. An interior-point method for semidefinite programming. SIAM Journal on Optimization, 6(2):342–361, 1996.
- Yin Zhang. On extending some primal-dual interior-point algorithms from linear programming to semidefinite programming. *SIAM Journal on Optimization*, 8(2):365–386, 1998.
- Richard H. Byrd, Mary E. Hribar, and Jorge Nocedal. An interior point algorithm for large-scale nonlinear programming. *SIAM Journal on Optimization*, 9(4):877–900, 1999.

Algorithm Inexact composite-step SQP

- **Description** We implement a modified version of inexact composite-step SQP method that Ridzal devised in his Ph.D. thesis and later refined in a technical report by Ridzal, Aguiló, and Heinkenschloss. Our implementation adds several safe-guards in order to more directly account for round-off error within the algorithm, which generally affects the augmented system solves. As one example, when solving the augmented system for the quasi-normal step, if the Cauchy point brings us to optimality, GMRES may not be able to practically satisfy the tolerances the algorithm specifies. Therefore, we detect this case directly and terminate the augmented system solve.
 - Denis Ridzal. Trust-Region SQP Methods with Inexact Linear System Solves for Large-Scale Optimization. PhD thesis, Rice University, 2006.
 - Denis Ridzal, Miguel Aguiló, and Matthias Heinkenschloss. Numerical study of matrix-free trust-region SQP method for equality constrained optimization. Technical Report SAND2011-9346, Sandia National Laboratories, 2011.
 - Matthias Heinkenschloss and Denis Ridzal. A matrix-free trust-region sqp method for equality constrained optimization. *SIAM Journal on Optimization*, 24(3):1507–1541, 2014.

In the following chapter, we detail Optizelle's license as well as the license of all of its dependencies.

9.1 Optizelle

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- * US National Labs (Los Alamos, Livermore, Sandia) ASC Parallel Visualization Initiative.
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9.5 WiX

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9.8 Python

A. HISTORY OF THE SOFTWARE

Python was created in the early 1990s by Guido van Rossum at Stichting Mathematisch Centrum (CWI, see http://www.cwi.nl) in the Netherlands as a successor of a language called ABC. Guido remains Python's principal author, although it includes many contributions from others.

In 1995, Guido continued his work on Python at the Corporation for National Research Initiatives (CNRI, see http://www.cnri.reston.va.us) in Reston, Virginia where he released several versions of the software.

In May 2000, Guido and the Python core development team moved to BeOpen.com to form the BeOpen PythonLabs team. In October of the same year, the PythonLabs team moved to Digital Creations (now Zope Corporation, see http://www.zope.com). In 2001, the Python Software Foundation (PSF, see http://www.python.org/psf/) was formed, a non-profit organization created specifically to own Python-related Intellectual Property. Zope Corporation is a sponsoring member of the PSF.

All Python releases are Open Source (see http://www.opensource.org for the Open Source Definition). Historically, most, but not all, Python releases have also been GPL-compatible; the table below summarizes the various releases.

Release	Derived	Year	Owner	GPL-
	from			compatible? (1)
0.9.0 thru 1.2		1991-1995	CWI	yes
1.3 thru 1.5.2	1.2	1995-1999	CNRI	yes
1.6	1.5.2	2000	CNRI	no
2.0	1.6	2000	BeOpen.com	no
1.6.1	1.6	2001	CNRI	yes (2)
2.1	2.0+1.6.1	2001	PSF	no
2.0.1	2.0+1.6.1	2001	PSF	yes
2.1.1	2.1+2.0.1	2001	PSF	yes
2.2	2.1.1	2001	PSF	yes
2.1.2	2.1.1	2002	PSF	yes
2.1.3	2.1.2	2002	PSF	yes
2.2.1	2.2	2002	PSF	yes
2.2.2	2.2.1	2002	PSF	yes
2.2.3	2.2.2	2003	PSF	yes
2.3	2.2.2	2002-2003	PSF	yes
2.3.1	2.3	2002-2003	PSF	yes
2.3.2	2.3.1	2002-2003	PSF	yes
2.3.3	2.3.2	2002-2003	PSF	yes
2.3.4	2.3.3	2004	PSF	yes
2.3.5	2.3.4	2005	PSF	yes
2.4	2.3	2004	PSF	yes
2.4.1	2.4	2005	PSF	yes
2.4.2	2.4.1	2005	PSF	yes
2.4.3	2.4.2	2006	PSF	yes
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2.5	2.4	2006	PSF	yes
2.5.1	2.5	2007	PSF	yes
2.5.2	2.5.1	2008	PSF	yes
2.5.3	2.5.2	2008	PSF	yes
2.6	2.5	2008	PSF	yes

2.6.1	2.6	2008	PSF	yes
2.6.2	2.6.1	2009	PSF	yes
2.6.3	2.6.2	2009	PSF	yes
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