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Optizelle v1.3.0

OptimoJoe
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Contents

1 Introduction

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

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

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, second-order 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:

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
//
// f(x,y)=(1-x)^2+100(y-x^2)^2
//
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];
    }
};
//---Objective1---

//---Preconditioner0---
// Define a perfect preconditioner for the Hessian
struct RosenHInv :
    public Optizelle::Operator <double,Optizelle::Rm,Optizelle::Rm>
{
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;
        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---

    //---Extract0---
    // Print out the reason for convergence
    std::cout << "The algorithm converged due to: " <<
        Optizelle::OptimizationStop::to_string(state.opt_stop) <<
        std::endl;

    // Print out the final answer
    std::cout << "The optimal point is: (" << state.x[0] << ','
        << 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

Code

```
% In this example, we setup and minimize the Rosenbrock function.
function rosenbrock(fname)
    % 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);
end
```

Language Optizelle Parameters

Code

```
"Optizelle" :{
  "msg_level" :1,
  "iter_max" :50,
  "eps_trunc" :1e-12
},
```

Language Optizelle Output

Code

```
iter      f(x)      ||grad||   ||dx||
1         2.42e+01  2.33e+02   .
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 converged due to: 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.

2 Installation

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

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 → Settings → System → Apps & features → Optizelle → Uninstall

macOS

1. Drag the folder `/Applications/Optizelle` to the trash
2. Drag the file `/Library/LaunchAgents/com.optimojoe.optizelle.plist` to the trash

Linux/Unix

1. When installed locally using the `tar.gz` package, delete the installation folder
2. When installed using the `rpm` or `deb` packages, use the package manager to remove Optizelle
3. 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	1.3.0	BSD	✓	✓	✓	✓	✓	✓
JsonCpp	1.9.2	Public	✓	✓	✓	✓		✓
BLAS/LAPACK	3.9.0	BSD	✓	✓	✓	✓		✓
CMake	3.17.1	BSD	✓	✓	✓	✓	✓	✓
WiX	3.11.2	MS-RL						✓
GCC	9.3.0	GPL	✓	✓	✓	✓		✓
TeX Live	2019	Various					✓	
Python	3.8.2	Python		✓				
NumPy	1.18.3	BSD		✓				
MATLAB	R2020a	Custom			✓			
JSONLab	1.9.8	BSD			✓	✓		
Octave	5.2.0	GPL				✓		

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. `cd build`
3. `ccmake ..`
4. Configure the build.
5. `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 `OCTAVE_PATH`
3. Add `/some/path/share/optizelle/python` to the `PYTHONPATH`

where `/some/path` denotes the path found in the `CMAKE_INSTALL_PREFIX` 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
3. 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_PREFIX`.

macOS Add a plist file to `/Library/LaunchAgents` or `~/Library/LaunchAgents`. For example

```
<?xml version="1.0" encoding="UTF-8"?>
<!DOCTYPE plist PUBLIC "-//Apple//DTD PLIST 1.0//EN"
"http://www.apple.com/DTDs/PropertyList-1.0.dtd">
<plist version="1.0"><dict>
    <key>Label</key>
    <string>Optizelle.startup</string>
    <key>ProgramArguments</key>
    <array>
        <string>sh</string>
        <string>-c</string>
        <string>
            launchctl setenv MATLABPATH $MATLABPATH:/some/path/share/optizelle/matlab
            launchctl setenv OCTAVE_PATH $OCTAVE_PATH:/some/path/share/optizelle/octave
            launchctl setenv PYTHONPATH $PYTHONPATH:/some/path/share/optizelle/python
        </string>
  </array>
  <key>RunAtLoad</key>
  <true/>
</dict></plist>
```

where `/some/path` denotes the installation path found in the CMake variable CMAKE_INSTALL_PREFIX. Note, we must close the Terminal application and then reboot for the changes to take affect.

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
```

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	PATH
Default	Varies
Dependency	None
Enables	None
Autodetect?	No
Description	Install location of Optizelle.

Flag	ENABLE_DOCUMENTATION
Type	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
Type	BOOL
Default	OFF
Dependency	ENABLE_DOCUMENTATION
Enables	None
Autodetect?	No
Description	When ON, the manual uses A4 paper. Otherwise, the manual uses Letter paper.

Flag	ENABLE_CPP
Type	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
Type	STRING
Default	None
Dependency	ENABLE_CPP
Enables	None
Autodetect?	No
Description	C++ compiler specific flags.

Flag	CMAKE_BUILD_TYPE
Type	STRING
Default	None
Dependency	ENABLE_CPP
Enables	None
Autodetect?	No
Description	Generally set to either RELEASE or DEBUG. Set to RELEASE for production libraries. Set to DEBUG to allow profiling through utilities such as OProfile.

Flag	ENABLE_OPENMP
Type	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
Type	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

Type BOOL

Default OFF

Dependency ENABLE_CPP

Enables JSONCPP_ARCHIVE

Autodetect? No

Description Builds JsonCpp from source.

Flag JSONCPP_ARCHIVE

Type FILEPATH

Default None

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 LAPACK. 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 PATH

Default 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 `$JSONCPP_INCLUDE_DIR/json/`

.

Flag JSONCPP_LIBRARY

Type 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
Type	BOOL
Default	OFF
Dependency	ENABLE_CPP
Enables	None
Autodetect?	No
Description	Enables the build of unit tests that help validate the Optizelle code. Execute these unit tests by running `ctest` in the CMake build directory.

Flag	ENABLE_PYTHON
Type	BOOL
Default	OFF
Dependency	ENABLE_CPP
Enables	PYTHON_INCLUDE_DIR, PYTHON_LIBRARY, PYTHON_EXECUTABLE, ENABLE_PYTHON_EXAMPLES, ENABLE_PYTHON_UNIT
Autodetect?	No
Description	Enables the build of the Python wrappers for Optizelle.

Flag	PYTHON_INCLUDE_DIR
Type	FILEPATH
Default	None
Dependency	ENABLE_PYTHON
Enables	None
Autodetect?	Yes
Description	A path that indicates where the Python headers have been installed. We do not prefix these headers, so we look directly in the directory provided here.

Flag	PYTHON_LIBRARY
Type	FILEPATH
Default	None
Dependency	ENABLE_PYTHON
Enables	None
Autodetect?	Yes

Description	Complete path and library for Python.

Flag	`PYTHON_EXECUTABLE`
Type	`FILEPATH`
Default	None
Dependency	`ENABLE_PYTHON`
Enables	None
Autodetect?	Yes
Description	Complete path and executable for Python.

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

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

Type 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 MATLAB_LIBRARY

Type 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
Type	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
Type	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.

Flag	ENABLE_OCTAVE
Type	BOOL
Default	OFF
Dependency	ENABLE_CPP
Enables	OCTAVE_INCLUDE_DIR, OCTAVE_LIBRARY, OCTAVE_EXECUTABLE, ENABLE_BUILD_JSONLAB, JSONLAB_DIR, 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.

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.

Flag `OCTAVE_EXECUTABLE`

Type `FILEPATH`

Default None

Dependency `ENABLE_OCTAVE`

Enables None

Autodetect? No

Description Complete path and executable for Octave.

Flag `ENABLE_OCTAVE_EXAMPLES`

Type `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
Type	BOOL
Default	OFF
Dependency	ENABLE_MATLAB or ENABLE_OCTAVE
Enables	JSONLAB_ARCHIVE
Autodetect?	No
Description	Builds jsonlab from source.

Flag	JSONLAB_ARCHIVE
Type	FILEPATH
Default	None
Dependency	ENABLE_BUILD_JSONLAB
Enables	None
Autodetect?	No
Description	Location of the json archive downloaded from GitHub.

Flag	JSONLAB_DIR
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
Indication	During compilation, `undefined reference to `__imp_Py_InitModule4'`
Description	Tells Python to use Windows 64-bit specific code

In addition, the following flags may need to be added to the CMAKE_Fortran_FLAGS variable when the compilation also builds BLAS/LAPACK

Flag	`-Wl,--allow-multiple-definition`
Platform	Windows
Interface	C++
Indication	During compilation, `multiple definition of `_gfortran_st_write_done'`
Description	Fixes a bug that occurs when BLAS/LAPACK is compiled with MinGW

3 Basic API

We organize Optizelle's algorithms into four different categories:

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

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
```
#include "optizelle/optizelle.h"
#include "optizelle/vspaces.h"
#include "optizelle/json.h"
```

Language Python

Code
```
import Optizelle
```

Language MATLAB/Octave

Code
```
global Optizelle
setupOptizelle();
```

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

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

we require that

$$\begin{aligned} f &: X \to \mathbb{R} \\ g &: X \to Y \\ h &: X \to Z. \end{aligned}$$

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, $x \succeq y \Longleftrightarrow x_i \geq y_i$ for all $1 \leq i \leq m$. 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		**Equality Constrained**	
$\min\limits_{x \in X}$	$f(x)$	$\min\limits_{x \in X}$	$f(x)$
		st	$g(x) = 0$
Inequality Constrained		**Constrained**	
$\min\limits_{x \in X}$	$f(x)$	$\min\limits_{x \in X}$	$f(x)$
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

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(x) \\ \vdots \\ \frac{\partial f}{\partial x_m}(x) \end{bmatrix},$$

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

In code, we specify this function as:

Language C++

Structure `Optizelle::ScalarValuedFunction`

Interface Inheritance

Code

```
namespace Optizelle{
    // A scalar valued function interface, f : X -> R
    template <
        typename Real,
        template <typename> class XX
    >
    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
        virtual void hessvec(Vector const & x,Vector const & dx,Vector & H_dx)
            const = 0;

        // Allow a derived class to deallocate memory
        virtual ~ScalarValuedFunction() {}
    };
}
```

Language Python

Structure `Optizelle.ScalarValuedFunction`

Interface Inheritance

Code

```
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")

    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")
```

Language MATLAB/Octave

Structure `Optizelle.ScalarValuedFunction`

Interface Members present

Code

```
% A simple scalar valued function interface, f : X -> R
err_svf=@(x)error(sprintf( ...
    'The %s function is not defined in a ScalarValuedFunction.',x));
Optizelle.ScalarValuedFunction = struct( ...
    'eval',@(x)err_svf('eval'), ...
    'grad',@(x)err_svf('grad'), ...
    'hess_vec',@(x,dx)err_svf('hess_vec'));
```

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
//
// f(x,y)=(1-x)^2+100(y-x^2)^2
//
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:

Language C++

Code

```
// Squares its input
template <typename Real>
Real sq(Real const & x){
    return x*x;
}

// Define a simple objective where
//
// f(x,y)=x^2+y^2
//
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]
```

Language MATLAB/Octave

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); ...
        2.*dx(2)];
end
```

3.4 (Optional) Define the constraints

In the optimization problems

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

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

$$\left.\begin{array}{ll} \min\limits_{x \in X} & f(x) \\ \text{st} & h(x) \succeq 0 \end{array}\right\} \rightsquigarrow \left\{\begin{array}{ll} \min\limits_{x \in X, z \in Z} & f(x) \\ \text{st} & h(x) - z = 0 \\ & z \succeq 0 \end{array}\right.$$

and

$$\left.\begin{array}{ll}\min\limits_{x\in X} & f(x)\\ \text{st} & g(x)=0\\ & h(x)\succeq 0\end{array}\right\}\rightsquigarrow\left\{\begin{array}{ll}\min\limits_{x\in X,z\in Z} & f(x)\\ \text{st} & \begin{bmatrix}g(x)\\ h(x)-z\end{bmatrix}=\begin{bmatrix}0\\0\end{bmatrix}\\ & z\succeq 0.\end{array}\right.$$

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 $\langle x,y\rangle=x^Ty$ 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

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

In code, these derivatives become:

Language C++

Structure `Optizelle::VectorValuedFunction`

Interface Inheritance

Code

```
namespace Optizelle{
    // A vector valued function interface, f : X -> Y
    template <
        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")
```

Language MATLAB/Octave

Structure `Optizelle.VectorValuedFunction`

Interface Members present

Code

```
% A vector valued function interface, f : X -> Y
err_vvf=@(x)error(sprintf( ...
    'The %s function is not defined in a VectorValuedFunction.',x));
Optizelle.VectorValuedFunction = struct( ...
    'eval',@(x)err_vvf('eval'), ...
    'p',@(x,dx)err_vvf('p'), ...
    'ps',@(x,dy)err_vvf('ps'), ...
    'pps',@(x,dx,dy)err_vvf('pps'));
```

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

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

Then, we have that

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

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

Language C++

Code

```
// Define a simple equality constraint
//
// g(x,y)= [ (x-2)^2 + (y-2)^2 = 1 ]
//
struct MyEq
    :public Optizelle::VectorValuedFunction<double,Optizelle::Rm,Optizelle::Rm>
{
    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];
    }
};
```

Language Python

Code

```
# 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]
```

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) [ ...
        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

$$\begin{aligned} P_l \delta x \approx & R^{-1} R^{-*} \delta x, \\ P_r \delta x = & \delta x. \end{aligned}$$

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

```
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() {}
    };
}
```

Language Python

Structure `Optizelle.Operator`

Interface Inheritance

Code

```
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")
```

Language MATLAB/Octave

Structure `Optizelle.Operator`

Interface Members present

Code

```
% 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'));
```

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 `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 C++

Code

```
// Define a perfect preconditioner for the Hessian
struct RosenHInv :
    public Optizelle::Operator <double,Optizelle::Rm,Optizelle::Rm>
{
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]);
    }
};
```

Language Python

Code

```
# 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]))
```

Language MATLAB/Octave

Code

```
% 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
```

For our simple equality constraint

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

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

```
// 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.));
    }
};
```

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

```
Optizelle::Unconstrained <Real,XX>::State::t state(x);

Optizelle::EqualityConstrained <Real,XX,YY>::State::t state(x,y);

Optizelle::InequalityConstrained <Real,XX,ZZ>::State::t state(x,z);

Optizelle::Constrained <Real,XX,YY,ZZ>::State::t state(x,y,z);
```

Language Python

Code

```
state = Optizelle.Unconstrained.State.t(XX,x)

state = Optizelle.EqualityConstrained.State.t(XX,YY,x,y)

state = Optizelle.InequalityConstrained.State.t(XX,ZZ,x,z)

state = Optizelle.Constrained.State.t(XX,YY,ZZ,x,y,z)
```

Language MATLAB/Octave

Code

```
state = Optizelle.Unconstrained.State.t(XX,x);

state = Optizelle.EqualityConstrained.State.t(XX,YY,x,y);

state = Optizelle.InequalityConstrained.State.t(XX,ZZ,x,z);

state = Optizelle.Constrained.State.t(XX,YY,ZZ,x,y,z);
```

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

```
// 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);
```

Language Python

Code

```
# 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)
```

Language MATLAB/Octave

Code
```
% 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);
```

In our Simple equality constrained example, we have:

Language C++

Code
```
// 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);
```

Language Python

Code
```
# 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)
```

Language MATLAB/Octave

Code
```
% 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);
```

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

```
Optizelle::json::Unconstrained <Real,XX>::read(fname,state);

Optizelle::json::EqualityConstrained <Real,XX,YY>::read(fname,state);

Optizelle::json::InequalityConstrained <Real,XX,ZZ>::read(fname,state);

Optizelle::json::Constrained <Real,XX,YY,ZZ>::read(fname,state);
```

Language Python

Code

```
Optizelle.json.Unconstrained.read(XX,fname,state)

Optizelle.json.EqualityConstrained.read(XX,YY,fname,state)

Optizelle.json.InequalityConstrained.read(XX,ZZ,fname,state)

Optizelle.json.Constrained.read(XX,YY,ZZ,fname,state)
```

Language MATLAB/Octave

Code

```
state = Optizelle.json.Unconstrained.read(XX,fname,state);

state = Optizelle.json.EqualityConstrained.read(XX,YY,fname,state);

state = Optizelle.json.InequalityConstrained.read(XX,ZZ,fname,state);

state = Optizelle.json.Constrained.read(XX,YY,ZZ,fname,state);
```

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

```
// Read the parameters from file
Optizelle::json::Unconstrained <double,Optizelle::Rm>::read(fname,state);
```

Language Python

Code

```
# Read the parameters from file
Optizelle.json.Unconstrained.read(Optizelle.Rm,fname,state)
```

Language MATLAB/Octave

Code

```
% Read the parameters from file
state=Optizelle.json.Unconstrained.read(Optizelle.Rm,fname,state);
```

This becomes the following in our Simple equality constrained example:

Language C++

Code

```
// Read the parameters from file
Optizelle::json::EqualityConstrained <double,Optizelle::Rm,Optizelle::Rm>
    ::read(fname,state);
```

Language Python

Code

```
# Read the parameters from file
Optizelle.json.EqualityConstrained.read(Optizelle.Rm,Optizelle.Rm,fname,state)
```

Language MATLAB/Octave

Code

```
% Read the parameters from file
state = Optizelle.json.EqualityConstrained.read( ...
    Optizelle.Rm,Optizelle.Rm,fname,state);
```

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

```
Optizelle::Unconstrained <Real,XX>::Functions::t fns;

Optizelle::EqualityConstrained <Real,XX,YY>::Functions::t fns;

Optizelle::InequalityConstrained <Real,XX,ZZ>::Functions::t fns;

Optizelle::Constrained <Real,XX,YY,ZZ>::Functions::t fns;
```

Language Python

Code

```
fns = Optizelle.Unconstrained.Functions.t()

fns = Optizelle.EqualityConstrained.Functions.t()

fns = Optizelle.InequalityConstrained.Functions.t()

fns = Optizelle.Constrained.Functions.t()
```

Language MATLAB/Octave

Code

```
fns = Optizelle.Unconstrained.Functions.t;

fns = Optizelle.EqualityConstrained.Functions.t;

fns = Optizelle.InequalityConstrained.Functions.t;

fns = Optizelle.Constrained.Functions.t;
```

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	`PH`
Type	`Operator`
Problem Class	Unconstrained, Equality Constrained, Inequality Constrained, Constrained
Required	No
Description	Preconditioner for the Hessian of the objective function, $\nabla^2 f(x)$.

Element	`g`
Type	`VectorValuedFunction`
Problem Class	Equality Constrained, Constrained
Required	Yes
Description	Equality constraint.

Element	`PSchur_left`
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`
Type	`Operator`
Problem Class	Equality Constrained, Constrained
Required	No
Description	Right Schur preconditioner for derivative of the equality constraint, $g'(x)g'(x)^*$.

Element	`h`
Type	`VectorValuedFunction`
Problem Class	Inequality Constrained, Constrained
Required	Yes
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
```
// 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));
```

Language Python

Code
```
# Create the bundle of functions
fns=Optizelle.Unconstrained.Functions.t()
fns.f=Rosenbrock()
fns.PH=RosenHInv()
```

Language MATLAB/Octave

Code
```
% Create the bundle of functions
fns=Optizelle.Unconstrained.Functions.t;
fns.f=Rosenbrock();
fns.PH=RosenHInv();
```

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

Language C++

Code
```
// 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));
```

Language Python

Code
```
# Create a bundle of functions
fns=Optizelle.EqualityConstrained.Functions.t()
fns.f=MyObj()
fns.g=MyEq()
fns.PSchur_left=MyPrecon()
```

Language MATLAB/Octave

Code
```
% Create a bundle of functions
fns=Optizelle.EqualityConstrained.Functions.t;
fns.f=MyObj();
fns.g=MyEq();
fns.PSchur_left=MyPrecon();
```

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
```
Optizelle::Unconstrained<Real,XX>::Algorithms::getMin(
    msg,fns,state);

Optizelle::EqualityConstrained<Real,XX,YY>::Algorithms::getMin(
    msg,fns,state);

Optizelle::InequalityConstrained<Real,XX,ZZ>::Algorithms::getMin(
    msg,fns,state);

Optizelle::Constrained<Real,XX,YY,ZZ>::Algorithms::getMin(
    msg,fns,state);
```

Language Python

Code
```
Optizelle.Unconstrained.Algorithms.getMin(XX,msg,fns,state)

Optizelle.EqualityConstrained.Algorithms.getMin(XX,YY,msg,fns,state)

Optizelle.InequalityConstrained.Algorithms.getMin(XX,ZZ,msg,fns,state)

Optizelle.Constrained.Algorithms.getMin(XX,YY,ZZ,msg,fns,state)
```

Language MATLAB/Octave

Code
```
state = Optizelle.Unconstrained.Algorithms.getMin(XX,msg,fns,state);

state = Optizelle.EqualityConstrained.Algorithms.getMin(XX,YY,msg,fns,state);

state = Optizelle.InequalityConstrained.Algorithms.getMin(XX,ZZ,msg,fns,state);

state = Optizelle.Constrained.Algorithms.getMin(XX,YY,ZZ,msg,fns,state);
```

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
```
// Solve the optimization problem
Optizelle::Unconstrained <double,Optizelle::Rm>::Algorithms
    ::getMin(Optizelle::Messaging::stdout,fns,state);
```

Language Python

Code
```
# Solve the optimization problem
Optizelle.Unconstrained.Algorithms.getMin(
    Optizelle.Rm,Optizelle.Messaging.stdout,fns,state)
```

Language MATLAB/Octave

Code
```
% Solve the optimization problem
state = Optizelle.Unconstrained.Algorithms.getMin( ...
    Optizelle.Rm,Optizelle.Messaging.stdout,fns,state);
```

With the Simple equality constrained example, this becomes:

Language C++

Code
```
// Solve the optimization problem
Optizelle::EqualityConstrained <double,Rm,Rm>::Algorithms::getMin(
    Optizelle::Messaging::stdout,fns,state);
```

Language Python

Code
```
# Solve the optimization problem
Optizelle.EqualityConstrained.Algorithms.getMin(
    Optizelle.Rm,Optizelle.Rm,Optizelle.Messaging.stdout,fns,state)
```

Language MATLAB/Octave

Code
```
% Solve the optimization problem
state = Optizelle.EqualityConstrained.Algorithms.getMin( ...
    Optizelle.Rm,Optizelle.Rm,Optizelle.Messaging.stdout,fns,state);
```

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

```
// Print out the reason for convergence
std::cout << "The algorithm converged due to: " <<
    Optizelle::OptimizationStop::to_string(state.opt_stop) <<
    std::endl;

// Print out the final answer
std::cout << "The optimal point is: (" << state.x[0] << ','
    << state.x[1] << ')' << std::endl;
```

Language Python

Code

```
# 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]))
```

Language MATLAB/Octave

Code

```
% 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));
```

In our Simple equality constrained example, this becomes:

Language C++

Code

```
// Print out the reason for convergence
std::cout << "The algorithm converged due to: " <<
    Optizelle::OptimizationStop::to_string(state.opt_stop) <<
    std::endl;

// Print out the final answer
std::cout << std::scientific << std::setprecision(16)
    << "The optimal point is: (" << state.x[0] << ','
<< state.x[1] << ')' << std::endl;
```

Language Python

Code

```
# 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]))
```

Language MATLAB/Octave

Code

```
% 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));
```

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
        ├── optizelle.h
        ├── json.h
        └── vspaces.h
```

where `/some/path` 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.

4 Optimization parameters

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

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.

Type `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 `OptimizationStop`

Values
```
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
```

Type `Operators`

Values
```
Identity,       // Identity approximation
Zero,           // Zero approximation
ScaledIdentity, // Scaled identity approximation
                //
                // || grad || / (2 delta) I
                //
                // Use this for trust-region steepest descent
                // rather than Identity since it forces the
                // iterate into the trust region
BFGS,           // BFGS approximation
InvBFGS,        // Inverse BFGS approximation
SR1,            // SR1 approximation
InvSR1,         // Inverse SR1 approximation
UserDefined     // User defined operator (such as the true
                // Hessian for Newton's method)
```

Type `LineSearchDirection`

Values

```
// 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
```

Type LineSearchKind

Values

```
GoldenSection, // Golden-section search
BackTracking,  // BackTracking search
TwoPointA,     // Barzilai and Borwein's method A
TwoPointB      // Barzilai and Borwein's method B
```

Type OptimizationLocation

Values

```
// Occurs at the start of the optimization function
BeginningOfOptimization,

// Occurs before the initial function and gradient evaluation
BeforeInitialFuncAndGrad,

// Occurs after the initial function and gradient evaluation
AfterInitialFuncAndGrad,

// Occurs just before the main optimization loop
BeforeOptimizationLoop,

// Occurs at the beginning of the optimization loop
BeginningOfOptimizationLoop,

// Occurs just before we take the optimization step x+dx
BeforeSaveOld,

// Occurs just before we take the optimization step x+dx
BeforeStep,

// Occurs before we calculate our new step.
BeforeGetStep,
```

```
// Occurs during a user defined get step calculation.
GetStep,

// 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,

// Occurs just after the gradient computation with the new
// trial step
AfterGradient,

// Occurs before we update our quasi-Newton information.
BeforeQuasi,

// Occurs after we update our quasi-Newton information.
AfterQuasi,

// This occurs after we check our stopping condition. This is
// where the equality and inequality algorithms adjust the
// stopping conditions.
AfterCheckStop,

// This occurs last in the optimization loop. At this point,
// we have already incremented our optimization iteration and
// checked our stopping condition
EndOfOptimizationIteration,

// This occurs prior to the computation of the line search
BeforeLineSearch,

// This occurs after a rejected trust-region step
AfterRejectedTrustRegion,

// This occurs after a rejected line-search step
AfterRejectedLineSearch,

// This occurs prior to checking the predicted versus actual
// reduction in a trust-region method.
BeforeActualVersusPredicted,

// This occurs at the end of all optimization
EndOfOptimization
```

Type `ProblemClass`

Values

```
Unconstrained,      // Unconstrained optimization
EqualityConstrained, // Equality constrained optimization
InequalityConstrained, // Inequality constrained optimization
Constrained         // Fully constrained optimization
```

Type DiagnosticScheme

Values

```
Never,           // Never compute our diagnostic checks
DiagnosticsOnly, // No optimization. Only diagnostics.
EveryIteration   // Every iteration at the start of the iteration
```

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
```

Type ToleranceKind

Values

```
Relative,        // Relative stopping tolerances
Absolute,        // Absolute stopping tolerances
```

Type QuasinormalStop

Values

```
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
                      // point failed, so we regressed to the
                      // Cauchy point
```

Type TruncatedStop

Values

```
NotConverged,           // Algorithm has not converged
NegativeCurvature,      // Negative curvature detected
RelativeErrorSmall,     // 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.
```

Type `Cone`

Values

```
Linear,          // Nonnegative orthant
Quadratic,       // Second order cone
Semidefinite     // Cone of positive semidefinite matrices
```

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 `state.eps_grad > Real(0.)`

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

Unconstrained $\|\nabla f(\mathrm{x}))\| \leq \mathrm{eps\_grad} \cdot \mathrm{norm\_gradtyp}$,

Equality $\|\nabla f(\mathrm{x}) + g'(\mathrm{x})^* \mathrm{y}\| \leq \mathrm{eps\_grad} \cdot \mathrm{norm\_gradtyp}$,

Inequality	$\|\nabla f(\mathtt{x}) - h'(\mathtt{x})^*\mathtt{z}\| \leq \mathtt{eps\_grad} \cdot \mathtt{norm\_gradtyp}$,
Constrained	$\|\nabla f(\mathtt{x}) + g'(\mathtt{x})^*\mathtt{y} - h'(\mathtt{x})^*\mathtt{z}\| \leq \mathtt{eps\_grad} \cdot \mathtt{norm\_gradtyp}$.

At each iteration, we output the norm on the left of the inequality under the label `||grad||`.

Name `eps_dx`

Type `Real`

Valid Value `state.eps_dx > Real(0.)`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `1e-16`

Description Tolerance for the step length stopping criteria reported in `opt_stop`. We satisfy this stopping criteria when

$$\|\mathtt{dx}\| < \mathtt{eps\_dx} \cdot \mathtt{norm\_dxtyp}.$$

At each iteration, we output the norm on the left of the inequality under the label `||dx||`.

Name `stored_history`

Type `Natural`

Valid Value `// Any`

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`

Type `Natural`

Valid Value `state.iter > 0`

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`

Type `Natural`

Valid Value `state.iter_max > 0`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `std::numeric_limits <Integer>::max()`

Description Maximum number of optimization iterations for the stopping criteria reported in `opt_stop`. We satisfy this stopping criteria when

$$\texttt{iter} \geq \texttt{iter\_max}$$

Name `glob_iter`

Type `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`

Type `Natural`

Valid Value `state.glob_iter_max > 0`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `10`

Description Maximum number of globalization iterations that we take before we exit the optimization. In other words, we only allow this many failed trust-region or line-search iterations before we exit the algorithm.

Name `glob_iter_total`

Type `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

1. 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`.
3. 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 equality 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 `state.trunc_iter_max > 0`

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_orthog_storage_max`

Type `Natural`

Valid Value `state.trunc_orthog_storage_max > 0`

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`

Type `Natural`

Valid Value `state.trunc_orthog_iter_max > 0`

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 orgthogonalize 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`

Type `TruncatedStop`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `TruncatedStop::RelativeErrorSmall`

Description Reason why truncated CG exited when solving the optimality system. We output `trunc_stop` at each iteration under the label `trunc_stop`.

Name `trunc_err`

Type `Real`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description Relative error in the solution returned by the truncated CG when solving the optimality system. We output `trunc_err` at each iteration under the label `trunc_err`.

Name `eps_trunc`

Type `Real`

Valid Value `state.eps_trunc > Real(0.)`

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 accommodate the null space projection, we currently ignore this quantity if problems with equality constraints.

Name `H_type`

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
```
state.norm_gradtyp >= Real(0.)
|| (state.iter==1 && state.norm_gradtyp!=state.norm_gradtyp)
```

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description Norm of a typical gradient defined as

Unconstrained	$\|\nabla f(\mathtt{x}_0)\|$,
Equality	$\|\nabla f(\mathtt{x}_0) + g'(\mathtt{x}_0)^*\mathtt{y}_0\|$,
Inequality	$\|\nabla f(\mathtt{x}_0) - h'(\mathtt{x}_0)^*\mathtt{z}_0\|$,
Constrained	$\|\nabla f(\mathtt{x}_0) + g'(\mathtt{x}_0)^*\mathtt{y}_0 - h'(\mathtt{x}_0)^*\mathtt{z}_0\|$,

where $\mathtt{x}_0$, $\mathtt{y}_0$, and $\mathtt{z}_0$ 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
```
state.norm_dxtyp >= Real(0.)
|| (state.iter==1 && state.norm_dxtyp!=state.norm_dxtyp)
```

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description 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.

Name `x`

Type `X_Vector`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `X::copy(x_user,x);`

Description Optimization variable.

Name `grad`

Type `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, $\nabla f(\texttt{x})$.

Name `dx`

Type `X_Vector`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `X::init(x_user)`

Description 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||`.

Name `x_old`

Type `X_Vector`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `X::init(x_user)`

Description Optimization variable from the last iteration.

Name `grad_old`

Type `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 from the last iteration.

Name `dx_old`

Type `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

JSON Param No

Default `// Empty`

Description Difference in prior gradients,

$$[\nabla f(\mathtt{x_{iter}}) - \nabla f(\mathtt{x_{iter-1}}), \ldots, \nabla f(\mathtt{x_{iter-stored\_history}}) - \nabla f(\mathtt{x_{iter-stored\_history-1}})].$$

We use this list in our quasi-Newton methods.

Name `oldS`

Type `List(X_Vector)`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `// Empty`

Description Difference in prior optimization steps,

$$[x_{\texttt{iter}} - x_{\texttt{iter}-1}, \ldots, x_{\texttt{iter}-\texttt{stored\_history}} - x_{\texttt{iter}-\texttt{stored\_history}-1}].$$

We use this list in our quasi-Newton methods.

Name `f_x`

Type `Real`

Valid Value `state.f_x == state.f_x || state.iter==1`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description Current value of the objective function, $f(\texttt{x})$. We output `f_x` at each iteration under the label `f(x)`.

Name `f_xpdx`

Type `Real`

Valid Value `state.f_xpdx == state.f_xpdx || state.iter==1`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description Value of the objective function at the trial step, $f(\texttt{x} + \texttt{dx})$.

Name `msg_level`

Type `Natural`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `1`

Description 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.

Name `safeguard_failed_max`

Type `Natural`

Valid Value `state.safeguard_failed_max >=1`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `5`

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`

Type `Real`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `std::numeric_limits <Real>::quiet_NaN()`

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

Default `std::numeric_limits <Real>::quiet_NaN()`

Description 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`.

Name `eps_kind`

Type `ToleranceKind`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `ToleranceKind::Absolute`

Description Kind of stopping tolerance used by the algorithms.

Name `delta`

Type `Real`

Valid Value `state.delta >= Real(0.)`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `1.`

Description 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`.

Name `eta1`

Type `Real`

Valid Value `state.eta1 > Real(0.) && state.eta1 < Real(1.)`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `.1`

Description When the actual versus predicted reduction for a trust-region method is below this threshold, we reject the step. Otherwise, we accept it.

Name `eta2`

Type `Real`

Valid Value `state.eta2 > state.eta1 && state.eta2 < Real(1.)`

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`

Type `Real`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description Actual reduction in the merit function between the current iterate and the iterate after taking the trial step,

$$\texttt{ared} \equiv \texttt{merit}(\texttt{x}) - \texttt{merit}(\texttt{x} + \texttt{dx}).$$

We use the following merit functions, $\texttt{merit} : \texttt{X\_Vector} \to \texttt{Real}$,

Unconstrained	$f(\texttt{x})$,
Equality	$f(\texttt{x}) + \langle \texttt{y}, g(\texttt{x}) \rangle + \texttt{rho}\|\|g(\texttt{x})\|\|^2$,
Inequality	$f(\texttt{x}) - \texttt{mu} \cdot \texttt{barr}(h(\texttt{x}))$,

Constrained $f(\mathtt{x}) + \langle \mathtt{y}, g(\mathtt{x})\rangle + \mathtt{rho}||g(\mathtt{x})||^2 - \mathtt{mu} \cdot \mathtt{barr}(h(\mathtt{x}))$.

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 `std::numeric_limits<Real>::quiet_NaN()`

Description Predicted reduction in the merit function between the current iterate and the iterate after taking the trial step,

$$\mathtt{pred} \equiv \mathtt{model}(0) - \mathtt{model}(\mathtt{dx}).$$

We use the following model functions, $\mathtt{model} : \mathtt{X\_Vector} \to \mathtt{Real}$,

Unconstrained

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

Equality

$$\begin{aligned} &f(\mathtt{x}) + \langle \mathtt{y}, g(\mathtt{x})\rangle + \mathtt{rho}||g(\mathtt{x})||^2 \\ &+\langle \nabla f(\mathtt{x}) + g'(\mathtt{x})^*\mathtt{y}, \mathtt{dx}\rangle \\ &+\tfrac{1}{2}\langle H(\mathtt{x})\mathtt{dx} + (g''(\mathtt{x})\mathtt{dx})^*\mathtt{y}, \mathtt{dx}\rangle, \end{aligned}$$

Inequality

$$\begin{aligned} &f(\mathtt{x}) - \mathtt{mu} \cdot \mathtt{barr}(h(\mathtt{x})) \\ &+\langle \nabla f(\mathtt{x}) - \mathtt{mu} \cdot h'(\mathtt{x})^* L(h(\mathtt{x}))^{-1} e, \mathtt{dx}\rangle \\ &+\tfrac{1}{2}\langle H(\mathtt{x})\mathtt{dx} + h'(\mathtt{x})^* L(h(\mathtt{x}))^{-1}(h'(\mathtt{x})\mathtt{dx} \circ \mathtt{z}), \mathtt{dx}\rangle, \end{aligned}$$

Constrained

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

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`

Type `Real`

Valid Value `state.alpha0 >= Real(0.)`

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 `std::numeric_limits <Real>::quiet_NaN()`

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`

Type `Real`

Valid Value `state.c1 > Real(0.) && state.c1 < Real(1.)`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `1e-4`

Description Sufficient decrease parameter. When we set `algorithm_class` to LineSearch, we only take a step when `merit`$(\texttt{x} + \texttt{alpha} \cdot \texttt{dx}) <$ `merit`$(\texttt{x}) +$ `c1` $\cdot$ `alpha`$\langle \tilde{x},$ `dx`$\rangle$ where we define $\tilde{x}$ as

Unconstrained	$\nabla f($`x`$)$,
Equality	$\nabla f($`x`$) + g'($`x`$)^*$`y`,
Inequality	$\nabla f($`x`$) -$ `mu` $\cdot\, h'($`x`$)^* L(h($`x`$))^{-1} e$,
Constrained	$\nabla f($`x`$) + g'($`x`$)^*$`y` $-$ `mu` $\cdot\, h'($`x`$)^* L(h($`x`$))^{-1} e$.

Here, $L(h(x))^{-1}$ denotes the inverse of the linear operator induced by the Jordan product, `linv`; and e denotes the identity element in the pseudo-Euclidean-Jordan algebra, `id`. We describe each of these operations further in the section Customized vector spaces.

Name `ls_iter`

Type Natural

Valid Value // Any

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param No

Default 0

Description Current number of iterations used in the line search. We use this to determine the amount of computational effort used by Optizelle during the last iteration. As a note, we output ls_iter at each iteration under the label ls_iter.

Name ls_iter_max

Type Natural

Valid Value state.ls_iter_max > 0

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default 5

Description Maximum number of iterations used in the line search before checking the sufficient decrease condition. We 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 state.eps_ls > Real(0.)

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
```
(state.kind!=LineSearchKind::GoldenSection
   || state.ls_iter_max >= 2) &&
(state.kind!=LineSearchKind::TwoPointA ||
   state.kind!=LineSearchKind::TwoPointB ||
   state.dir==LineSearchDirection::SteepestDescent)
```

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`

Type `FunctionDiagnostics`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `FunctionDiagnostics::NoDiagnostics`

Description Function diagnostics on the Lagrangian.

Name `x_diag`

Type `VectorSpaceDiagnostics`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `VectorSpaceDiagnostics::NoDiagnostics`

Description Vector space diagnostics on X.

Name `dscheme`

Type `DiagnosticScheme`

Valid Value `// Any`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

JSON Param Yes

Default `DiagnosticScheme::Never`

Description Which diagnostic scheme, if any, to employ.

Name `y`

Type `Y_Vector`

Valid Value `// Any`

Problem Class Equality Constrained, Constrained

JSON Param No

Default

```
// Equality constrained
// argmin_y || grad f(x) + g'(x)*y ||
//
// Constrained
// argmin_y || grad f(x) + g'(x)*y - h'(x)*z ||
```

Description Equality multiplier (dual variable or Lagrange multiplier.)

Name `dy`

Type `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 `state.zeta > Real(0.) && state.zeta < Real(1.)`

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`

Type `Real`

Valid Value `state.eta0 > Real(0.) && state.eta0 < Real(1.)-state.eta1`

Problem Class Equality Constrained, Constrained

JSON Param Yes

Default `0.5`

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

Name `rho`

Type Real

Valid Value `state.rho >= Real(1.)`

Problem Class Equality Constrained, Constrained

JSON Param Yes

Default `1.0`

Description Penalty parameter for the augmented-Lagrangian. In problems with equality constraints, this term appears in the merit functions

Equality	$f(\mathtt{x}) + \langle \mathtt{y}, g(\mathtt{x}) \rangle + \mathtt{rho} \|\|g(\mathtt{x})\|\|^2,$
Constrained	$f(\mathtt{x}) + \langle \mathtt{y}, g(\mathtt{x}) \rangle + \mathtt{rho} \|\|g(\mathtt{x})\|\|^2 - \mathtt{mu} \cdot \mathtt{barr}(h(\mathtt{x})).$

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

Name `rho_old`

Type Real

Valid Value `state.rho_old >= Real(1.)`

Problem Class Equality Constrained, Constrained

JSON Param No

Default `rho`

Description Penalty parameter from the last iteration.

Name `rho_bar`

Type Real

Valid Value `state.rho_bar > Real(0.)`

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 `state.eps_constr > Real(0.)`

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

$$\|g(x)\| < \texttt{eps\_constr} \cdot \texttt{norm\_gxtyp}.$$

At each iteration, we output the norm on the left of the inequality under the label `||g(x)||`. Note, since this value tunes a *relative* 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 `state.xi_qn > Real(0.) && state.xi_qn < Real(1.)`

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 `state.xi_pg > Real(0.) && state.xi_pg < Real(1.)`

Problem Class Equality Constrained, Constrained

JSON Param Yes

Default `1e-4`

Description Relative stopping tolerance for the augmented system solve associated with the projection of the gradient prior to solving the tangential subproblem.

Name `xi_proj`

Type `Real`

Valid Value `state.xi_proj > Real(0.) && state.xi_proj < Real(1.)`

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 `state.xi_tang > Real(0.) && state.xi_tang < Real(1.)`

Problem Class Equality Constrained, Constrained

JSON Param Yes

Default `1e-4`

Description Relative stopping tolerance for the augmented system solve associated with the tangential step computation after solving the tangential subproblem.

Name `xi_lmh`

Type `Real`

Valid Value `state.xi_lmh > Real(0.) && state.xi_lmh < Real(1.)`

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 `// state.xi_all > Real(0.) && state.xi_all < Real(1.)`

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 `state.xi_lmg > Real(0.)`

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 `state.xi_4 > Real(1.)`

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`

Type `Real`

Valid Value `// Any`

Problem Class Equality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

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
```
state.PSchur_left_type == Operators::Identity ||
state.PSchur_left_type == Operators::UserDefined
```

Problem Class Equality Constrained, Constrained

JSON Param Yes

Default `Operators::Identity`

Description Left preconditioner for the augmented system. For a full discussion of this preconditioner, see the section (Optional) Define the preconditioners.

Name `PSchur_right_type`

Type `Operators`

Valid Value
```
state.PSchur_right_type == Operators::Identity ||
state.PSchur_right_type == Operators::UserDefined
```

Problem Class Equality Constrained, Constrained

JSON Param Yes

Default `Operators::Identity`

Description Right preconditioner for the augmented system. For a full discussion of this preconditioner, see the section (Optional) Define the preconditioners.

Name `augsys_iter_max`

Type `Natural`

Valid Value `state.augsys_iter_max > 0`

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`

Type 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

Type 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

Type 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

Type 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`

Description Number of iterations taken during the last iterate by the augmented system solve during the equality multiplier solve.

Name `augsys_qn_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 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

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 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

Type 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`

Type `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 tangential 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`

Type `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`

Type `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

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`

Type `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`

Type `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`

Type `Y_Vector`

Valid Value `// Any`

Problem Class Equality Constrained, Constrained

JSON Param No

Default `Y::init(y_user)`

Description Equality constraint evaluated a `x`, $g(\texttt{x})$. We use this in the quasi-normal step as well as in the computation of the linear Taylor series at `x` in the direction `dx_n`. As a note, we output the norm of this vector each iteration under the label `||g(x)||`.

Name `norm_gxtyp`

Type `Real`

Valid Value
```
state.norm_gxtyp >= Real(0.)
|| (state.iter==1 && state.norm_gxtyp!=state.norm_gxtyp)
```

Problem Class Equality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

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
```
state.norm_gpsgxtyp >= Real(0.)
|| (state.iter==1 &&
    state.norm_gpsgxtyp!=state.norm_gpsgxtyp)
```

Problem Class Equality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description Norm of a typical value of $g'(\mathtt{x})^* g(\mathtt{x})$, which we define to be the value of this quantity 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 becomes $\partial x = -g'(x)^* g(x)$. 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. Generally, 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.

Name `gpxdxn_p_gx`

Type `Y_Vector`

Valid Value `// Any`

Problem Class Equality Constrained, Constrained

JSON Param No

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`

Type `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`

Type `Real`

Valid Value `// Any`

Problem Class Equality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description Norm of `gpxdxn_p_gx`. We use this in the penalty parameter computation and predicted 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`

Type `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`

Type `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`

Type `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`

Type `X_Vector`

Valid Value `// Any`

Problem Class Equality Constrained, Constrained

JSON Param No

Default `X::init(x_user)`

Description Hessian applied to the normal step. We require this in `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 $f(\mathtt{x}) + g'(\mathtt{x}) * \mathtt{y} + H\mathtt{dx\_n}$ 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`

Type `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`

Description Inequality multiplier (dual variable or Lagrange multiplier.)

Name `dz`

Type `Z_Vector`

Valid Value `// Any`

Problem Class Inequality Constrained, Constrained

JSON Param No

Default `Z::init(z_user)`

Description Step in the inequality multiplier. Every iteration we set z=z+dz.

Name `h_x`

Type `Z_Vector`

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 `state.mu > Real(0.)`

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`

Type `Real`

Valid Value `state.mu_est == state.mu_est || state.iter == 1`

Problem Class Inequality Constrained, Constrained

JSON Param No

Default `std::numeric_limits<Real>::quiet_NaN()`

Description Current interior-point estimate. We define this as

$$\texttt{mu\_est} \equiv \frac{\langle \texttt{z}, \texttt{h\_x} \rangle}{\langle e, e \rangle}.$$

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.

Name mu_typ

Type Real

Valid Value state.mu_typ > Real(0.) || state.iter==1

Problem Class Inequality Constrained, Constrained

JSON Param No

Default std::numeric_limits<Real>::quiet_NaN()

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 state.eps_mu > Real(0.)

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. $|\texttt{mu} - \texttt{mu\_typ} \cdot \texttt{eps\_mu}| \leq \texttt{mu\_typ} \cdot \texttt{eps\_mu}$
2. $|\texttt{mu} - \texttt{mu\_est}| \leq \texttt{mu}$

Name sigma

Type Real

Valid Value state.sigma > Real(0.) && state.sigma < Real(1.)

Problem Class Inequality Constrained, Constrained

JSON Param Yes

Default `0.1`

Description Rate that we decrease the interior point parameter.

Name `gamma`

Type `Real`

Valid Value `state.gamma > Real(0.) && state.gamma < Real(1.)`

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 `std::numeric_limits <Real>::quiet_NaN()`

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.

Name `z_diag`

Type	`VectorSpaceDiagnostics`
Valid Value	`// Any`
Problem Class	Inequality Constrained, Constrained
JSON Param	Yes
Default	`VectorSpaceDiagnostics::NoDiagnostics`
Description	Vector space diagnostics on Z.

5 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

Min `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

Min `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

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

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

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

Min `msg_level` 1

Description Current interior-point estimate. We use this value within our complementary slackness stopping condition described by the parameter eps_mu. 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 eps_mu.

Name merit(x)

State Param None

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

Min 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

Min 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 eps_trunc and indirectly affect it with the parameters trunc_orthog_storage_max and trunc_orthog_iter_max.

Name trunc_stop

State Param trunc_stop

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

Min msg_level 2

Description Why truncated CG terminated. Although we shorten the strings, we describe each possible outcome in the enumerated type TruncatedStop.

Name ared

State Param ared

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

Min msg_level 2

Description Actual reduction in the merit function between the current iterate and the iterate after taking the trial step.

Name pred

State Param pred

Problem Class 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 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

Min msg_level 2

Description Trust-region radius.

Name ls_iter

State Param ls_iter

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

Min msg_level 2

Description Number of iterations taken by the line search. We tune the maximum number of line-search iterations with the parameter ls_iter_max and indirectly control the number of iterations with the parameter eps_ls.

Name `alpha`

State Param `alpha`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

Min `msg_level` 2

Description Actual line-search step length.

Name `alpha0`

State Param `alpha0`

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

Min `msg_level` 2

Description Base line-search step length.

Name `qn_stop`

State Param `qn_stop`

Problem Class Equality Constrained, Constrained

Min `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

Min `msg_level` 2

Description Interior point parameter.

Name `alpha_x`

State Param `alpha_x`

Problem Class Inequality Constrained, Constrained

Min msg_level 2

Description Amount we truncate dx in order to maintain feasibility with respect to the inequality constraint.

Name alpha_z

State Param alpha_z

Problem Class Inequality Constrained, Constrained

Min 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

Min 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

Min msg_level 3

Description Total number of globalization iterations taken across all iterations.

Name trc_itr_tot

State Param trunc_iter_total

Problem Class Unconstrained, Equality Constrained, Inequality Constrained, Constrained

Min msg_level 3

Description 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.

Name ||dx_n||

State Param Equality Constrained, Constrained

Problem Class None

Min msg_level 3

Description Norm of the quasinormal step, dx_n, taken during the last iteration.

Name ||dx_t||

State Param Equality Constrained, Constrained

Problem Class None

Min msg_level 3

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

Name qn_iter

State Param augsys_qn_iter

Problem Class Equality Constrained, Constrained

Min msg_level 3

Description 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

Min msg_level 3

Description 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.

Name qn_fail

State Param augsys_qn_failed

Problem Class Equality Constrained, Constrained

Min msg_level 3

Description Number of failed quasinormal augmented system solves.

Name pg_iter

State Param augsys_pg_iter

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

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

Min `msg_level` 3

Description Error in the last augmented system solve when projecting the gradient prior to the tangential subproblem.

Name `pg_err_trg`

State Param `augsys_pg_err_target`

Problem Class Equality Constrained, Constrained

Min `msg_level` 3

Description Target error in the last augmented system solve when projecting the gradient prior to the tangential subproblem.

Name `pg_fail`

State Param `augsys_pg_failed`

Problem Class Equality Constrained, Constrained

Min `msg_level` 3

Description Number of failed projected gradient augmented system solves.

Name `pr_iter`

State Param `augsys_proj_iter`

Problem Class Equality Constrained, Constrained

Min `msg_level` 3

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

Min `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

Min msg_level 3

Description 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 error from the last such solve.

Name pr_err_trg

State Param augsys_proj_err_target

Problem Class Equality Constrained, Constrained

Min 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

Min 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

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

Min 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

Min 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

Min msg_level 3

Description Number of failed tangential step augmented system solves.

Name lm_iter

State Param augsys_lmh_iter

Problem Class Equality Constrained, Constrained

Min 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

Min msg_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

Min `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

Min `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

Min `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

Min `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.

6 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

```
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;
    }
}
```

Language Python

Structure `Optizelle.Messaging.t`

Interface Function matches type

Code

```
def t(msg):
    """At its core, we take in a string and then write it somewhere"""
    raise Optizelle.Exception.t("Undefined messaging function")
```

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
```
// Define a custom messaging object
void mymessaging(std::string const & msg) {
    std::cout << "PRINT: " << msg << std::endl;
}
```

Language Python

Code
```
# Define a custom messaging object
def mymessaging(msg):
    """Prints out normal diagnostic information"""
    sys.stdout.write("PRINT: %s\n" %(msg))
```

Language MATLAB/Octave

Code
```
% Define a custom messaging object
function MyMessaging(msg)
    fprintf('PRINT: %s\n',msg);
end
```

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

```
namespace Optizelle {namespace Exception {
    struct t : public std::runtime_error {
        using std::runtime_error::runtime_error;
    };
}}
```

Language Python

Structure `Optizelle.Exception.t`

Interface Exception handling

Code

```
class t(Exception):
    """Type for Optizell's exceptions"""
    pass
```

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

Language C++

Code

```
    // 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
        Optizelle::Exception::to_stderr(e);
    }
```

Language Python

Code

```
# 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 = str(e)

    # Print the error message directly
    print(e)
```

Language MATLAB/Octave

Code

```
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
```

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	`init(x)`
	$init \leftarrow \xi(W)$ 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 `copy`

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 MATLAB/Octave, return the vector x

.

Name `scal`

Definition	**C++**	`scal(alpha,x)`
		$x \leftarrow \alpha x$
	Python	`scal(alpha,x)`
		$x \leftarrow \alpha x$
	MATLAB/Octave	`scal(alpha,x)`
		$scal \leftarrow \alpha x$

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, overwrite y with $\alpha x + y$. In MATLAB/Octave, return $\alpha x + y$.

Name `innr`

Definition	**C++**	`innr(x,y)`
		$innr \leftarrow \langle x, y \rangle$
	Python	`innr(x,y)`
		$innr \leftarrow \langle x, y \rangle$
	MATLAB/Octave	`innr(x,y)`
		$innr \leftarrow \langle x, y \rangle$

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:

Name `prod`

Definition	**C++**	`prod(x,y,z)`
		$z \leftarrow x \circ y$
	Python	`prod(x,y,z)`
		$z \leftarrow x \circ y$
	MATLAB/Octave	`prod(x,y)`
		$prod \leftarrow x \circ y$

Description In 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

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

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.

Name `id`

Definition

C++	`id(x)`
	$x \leftarrow e$
Python	`id(x)`
	$x \leftarrow e$
MATLAB/Octave	`id(x)`
	$id \leftarrow e$

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)`
	$z \leftarrow L(x)^{-1}y$
Python	`linv(x,y,z)`
	$z \leftarrow L(x)^{-1}y$
MATLAB/Octave	`linv(x,y)`
	$linv \leftarrow L(x)^{-1}y$

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, $L(x) = \text{Diag}(x)$, where $\text{Diag}(x)$ denotes the diagonal matrix with x on the diagonal. For second-order cone constraints, $L(x) = \text{Arw}(x)$ where we define $\text{Arw}(x)$ as

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

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

Return the result of the barrier function applied to a vector. Here, the function $\phi : Z \to \mathbb{R}$ denotes the barrier 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++	`srch(x,y)`
	$srch \leftarrow \arg\max\{\alpha \in \mathbb{R} : \alpha x + y \succeq 0, \alpha \geq 0\}$
Python	`srch(x,y)`
	$srch \leftarrow \arg\max\{\alpha \in \mathbb{R} : \alpha x + y \succeq 0, \alpha \geq 0\}$
MATLAB/Octave	`srch(x,y)`
	$srch \leftarrow \arg\max\{\alpha \in \mathbb{R} : \alpha x + y \succeq 0, \alpha \geq 0\}$

Description

Return how far we can move in the direction x from the point y before violating nonnegativity. In other words, the function `srch` denotes the search function used to maintain strict feasibility with respect to the inequality constraint. We define this as

$$\arg\max\{\alpha \in \mathbb{R} : \alpha x + y \succeq 0, \alpha \geq 0\}$$

where we assume $y \succ 0$. Hence, α denotes the maximum distance we can move in the direction x from y so that $\alpha x + y$ remains feasible. Note, sometimes this number is infinite. If this is the case, 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(x)`
	$symm \leftarrow \pi(x)$ where $\pi(x \circ y) = \pi(y \circ x)$

Description In C++ and Python, overwrite x with its symmetrization. In MATLAB/Octave, return the symmetrization of x. Here, the function $\pi : Z \to Z$ denotes the symmetrization operator. We require this operator since we relax the commutativity requirement from the Euclidean-Jordan algebra. For linear bound constraints and second-order cone constraints, this operation does nothing. In addition, for semidefinite constraints where $X \circ Y = \frac{XY+YX}{2}$, this operation does nothing. However, for semidefinite constraints where $X \circ Y = XY$, we may use symmetrization,

$$\pi(X) = \frac{X + X^T}{2},$$

or more generally the *similar symmetrization* operator,

$$\pi_P(X) = \frac{(PXP^{-1} + (PXP^{-1})^T}{2},$$

where we require P to be nonsingular.

Next, we require these vector-space functions be encapsulated in the following structures:

Language C++

Interface Templated struct with static members and a single typedef called `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 methods. 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 `@staticmethod`.

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

```
// 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.)
    static void copy(Vector const & x, Vector & y) {
        for(Natural i=0;i<x.size();i++){
            y[i]=x[i];
        }
    }

    // x <- alpha * x
    static void scal(const Real& alpha, Vector & x) {
        for(Natural i=0;i<x.size();i++){
            x[i]=alpha*x[i];
        }
    }

    // x <- 0
    static void zero(Vector & x) {
        for(Natural i=0;i<x.size();i++){
            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++){
            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++)
            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++)
        x[i]=Real(dis(gen));
}
// Jordan product, z <- x o y.
static void prod(Vector const & x, Vector const & y, Vector & z) {
    for(Natural i=0;i<x.size();i++)
        z[i]=x[i]*y[i];
}

// Identity element, x <- e such that x o e = x.
static void id(Vector & x) {
    for(Natural i=0;i<x.size();i++)
        x[i]=Real(1.);
}

// Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o y.
static void linv(Vector const & x,Vector const & y,Vector & z) {
    for(Natural i=0;i<x.size();i++)
        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++)
        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++) {
        if(x[i] < Real(0.)) {
            Real alpha0 = -y[i]/x[i];
            alpha = alpha0 < alpha ? alpha0 : alpha;
        }
    }

    return alpha;
}

// Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric
// 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 range(0,len(x)):
            x[i]=alpha*x[i]

    @staticmethod
    def zero(x):
        """x <- 0"""
        for i in range(0,len(x)):
            x[i]=0.

    @staticmethod
    def axpy(alpha,x,y):
        """y <- alpha * x + y"""
        for i in range(0,len(x)):
            y[i]=alpha*x[i]+y[i]

    @staticmethod
    def innr(x,y):
        """<- <x,y>"""
        return functools.reduce(lambda z,xy:xy[0]*xy[1]+z,zip(x,y),0.)

    @staticmethod
    def rand(x):
        """x <- random"""
        for i in range(0,len(x)):
            x[i]=random.uniform(0.,1.)

    @staticmethod
    def prod(x,y,z):
        """Jordan product, z <- x o y"""
        for i in range(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 range(0,len(x)):
            x[i]=1.

    @staticmethod
    def linv(x,y,z):
        """Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o y"""
        for i in range(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 > 0"
        alpha = float("inf")
        for i in range(0,len(x)):
            if x[i] < 0:
                alpha0 = -y[i]/x[i]
                if alpha0 < alpha:
                    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;

    % <- 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 o e = x.
    self.id = @(x)tostruct(ones(size(x.data)));

    % Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o 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
```

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:

Language	C++
Vector	`Optizelle::SQL::Vector`
Operations	`Optizelle::SQL`

Language	MATLAB/Octave
Vector	`Optizelle.SQL.create` (produces a structure array)
Operations	`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 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, `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	`x.blkType(k)`
Number of blocks	`x.numblocks()`

In order to access the elements of a MATLAB/Octave SQL vector, `x`, we note that the cones are stored in the cell array `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 ith element of the kth block when this block is quadratic or linear, we use the syntax `x.data{k}(i)`. To access the (i,j)th element of the kth block when the block is semidefinite, we use the syntax `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
//
// f(x,y)=(x-3)^2+(y-2)^2
//
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
//
// h(x,y) = [ y >= |x| ]
// h(x,y) = (y,x) >=_Q 0
//
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
    if(argc!=2) {
        std::cerr << "simple_quadratic_cone <parameters>" << std::endl;
        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: " <<
        Optizelle::OptimizationStop::to_string(state.opt_stop) << std::endl;

    // Print out the final answer
    std::cout << std::setprecision(16) << std::scientific
        << "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:

Language C++

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
//
// f(x,y)=-x+y
//
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
//
// h(x,y) = [ y x ] >= 0
//          [ x 1 ]
//
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);
    }
};

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;
        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);

    // 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: " <<
        Optizelle::OptimizationStop::to_string(state.opt_stop) << std::endl;

    // Print out the final answer
    std::cout << std::setprecision(16) << std::scientific
        << "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 (0.5,.25)

function simple_sdp_cone(fname)
    % Read in the name for the input file
    if nargin ~=1
        error('simple_sdp_cone <parameters>');
    end

    % Execute the optimization
    main(fname);
end

% Define a simple objective where
%
% f(x,y)=-x+y
%
function self = MyObj()

    % Evaluation
    self.eval = @(x) -x(1)+x(2);

    % Gradient
    self.grad = @(x) [
        -1.;
        1.];

    % Hessian-vector product
    self.hessvec = @(x,dx) [
        0;
        0];
end

% Define a simple SDP inequality
%
% h(x,y) = [ y x ] >= 0
%          [ x 1 ]
%
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 = @(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

```
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() {}
    };
}
```

Language Python

Structure `Optizelle.StateManipulator`

Interface Inheritance

Code

```
class StateManipulator(object):
    """A function that has free reign to manipulate or analyze the state"""
    def eval(self,fns,state,loc):
        """Application"""
        pass
```

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

```
Optizelle::Unconstrained<Real,XX>::Algorithms::getMin(
    msg,fns,state,smanip);

Optizelle::EqualityConstrained<Real,XX,YY>::Algorithms::getMin(
    msg,fns,state,smanip);

Optizelle::InequalityConstrained<Real,XX,ZZ>::Algorithms::getMin(
    msg,fns,state,smanip);

Optizelle::Constrained<Real,XX,YY,ZZ>::Algorithms::getMin(
    msg,fns,state,smanip);
```

Language Python

Code

```
Optizelle.Unconstrained.Algorithms.getMin(XX,msg,fns,state,smanip)

Optizelle.EqualityConstrained.Algorithms.getMin(XX,YY,msg,fns,state,smanip)

Optizelle.InequalityConstrained.Algorithms.getMin(XX,ZZ,msg,fns,state,smanip)

Optizelle.Constrained.Algorithms.getMin(XX,YY,ZZ,msg,fns,state,smanip)
```

Language MATLAB/Octave

Code

```
state = Optizelle.Unconstrained.Algorithms.getMin( ...
    XX,msg,fns,state,smanip);

state = Optizelle.EqualityConstrained.Algorithms.getMin( ...
    XX,YY,msg,fns,state,smanip);

state = Optizelle.InequalityConstrained.Algorithms.getMin( ...
    XX,ZZ,msg,fns,state,smanip);

state = Optizelle.Constrained.Algorithms.getMin( ...
    XX,YY,ZZ,msg,fns,state,smanip);
```

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

```
// 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_";
            ss << std::setw(4) << std::setfill('0') << state.iter;
            ss << ".json";

            // Write the restart file
            Optizelle::json::Unconstrained <double,MyVS>::write_restart(
                ss.str(),state);
            break;
        } default:
            break;
        }
    }
};
```

Language Python

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
```
// Solve the optimization problem
Optizelle::Unconstrained <double,MyVS>::Algorithms
    ::getMin(mymessaging,fns,state,MyRestartManipulator());
```

Language Python

Code
```
# Solve the optimization problem
Optizelle.Unconstrained.Algorithms.getMin(
    MyVS,mymessaging,fns,state,MyRestartManipulator())
```

Language MATLAB/Octave

Code
```
% Solve the optimization problem
state=Optizelle.Unconstrained.Algorithms.getMin( ...
    MyVS(),@MyMessaging,fns,state,MyRestartManipulator());
```

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

```
Optizelle::json::Unconstrained <Real,XX>::write_restart(
   fname,state);
Optizelle::json::Unconstrained <Real,XX>::read_restart(
   fname,x,state);

Optizelle::json::EqualityConstrained <Real,XX,YY>::write_restart(
   fname,state);
Optizelle::json::EqualityConstrained <Real,XX,YY>::read_restart(
   fname,x,y,state);

Optizelle::json::InequalityConstrained <Real,XX,ZZ>::write_restart(
   fname,state);
Optizelle::json::InequalityConstrained <Real,XX,ZZ>::read_restart(
   fname,x,z,state);

Optizelle::json::Constrained <Real,XX,YY,ZZ>::write_restart(
   fname,state);
Optizelle::json::Constrained <Real,XX,YY,ZZ>::read_restart(
   fname,x,y,z,state);
```

Language Python

Code

```
Optizelle.json.Unconstrained.write_restart(XX,fname,state);
Optizelle.json.Unconstrained.read_restart(XX,fname,x,state);

Optizelle.json.EqualityConstrained.write_restart(XX,YY,fname,state);
Optizelle.json.EqualityConstrained.read_restart(XX,YY,fname,x,y,state);

Optizelle.json.InequalityConstrained.write_restart(XX,ZZ,fname,state);
Optizelle.json.InequalityConstrained.read_restart(XX,ZZ,fname,x,z,state);

Optizelle.json.Constrained.write_restart(XX,YY,ZZ,fname,state);
Optizelle.json.Constrained.read_restart(XX,YY,ZZ,fname,x,y,z,state);
```

Language MATLAB/Octave

Code

```
Optizelle.json.Unconstrained.write_restart(XX,fname,state);
state = Optizelle.json.Unconstrained.read_restart(XX,fname,x);

Optizelle.json.EqualityConstrained.write_restart(XX,YY,fname,state);
state = Optizelle.json.EqualityConstrained.read_restart(XX,YY,fname,x,y);

Optizelle.json.InequalityConstrained.write_restart(XX,ZZ,fname,state);
state = Optizelle.json.InequalityConstrained.read_restart(XX,ZZ,fname,x,z);

Optizelle.json.Constrained.write_restart(XX,YY,ZZ,fname,state);
state = Optizelle.json.Constrained.read_restart(XX,YY,ZZ,fname,x,y,z);
```

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

```
// 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);
```

Language Python

Code

```
# 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)
```

Language MATLAB/Octave

Code

```
% 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);
```

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

```
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; }
        };
    }
}
```

Language Python

Code

```
Optizelle.json.Serialization.serialize.register(serialize,vector_type)
Optizelle.json.Serialization.deserialize.register(deserialize,vector_type)
```

Language MATLAB/Octave

Code

```
Optizelle.json.Serialization.serialize('register',serialize,check);
Optizelle.json.Serialization.deserialize('register',deserialize,check);
```

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++

Code

```
// 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
                // [ 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++)
                    x_json << x[i] << ", ";
                x_json << x.back() << " ]";

                // 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++)
                    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++)
                    ss >> 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 json representation
    x_json="[ "
    for i in range(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)
```

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

```
// 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/";
                fname << name << ".";
                fname << std::setw(4) << std::setfill('0') << iter;
                fname << ".txt";

                // Actually write the vector there
                std::ofstream fout(fname.str());
                if(fout.fail()) {
                    std::stringstream msg;
                    msg << "While writing the variable " << name
                        << " 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++)
                    fout << x[i] << std::endl;

                // Close out the file
                fout.close();

                // Use this filename as the json string
                std::stringstream x_json;
                x_json << "\"" << fname.str() << "\"";
                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++)
                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++)
                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 range(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 range(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)
```

Language MATLAB/Octave

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++

Type `std::list`

Language Python

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:

Type `Reals`

Description List of `Real` numbers and labels.

Type `Naturals`

Description List of `Natural` numbers and labels.

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.

Type `X_Vectors`

Description List of `X_Vector` vectors and labels.

Type `Y_Vectors`

Description List of `Y_Vector` vectors and labels.

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

```
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.X_Vectors()
ys = Optizelle.EqualityConstrained.Restart.Y_Vectors()
reals = Optizelle.EqualityConstrained.Restart.Reals()
nats = Optizelle.EqualityConstrained.Restart.Naturals()
params = Optizelle.EqualityConstrained.Restart.Params()
Optizelle.EqualityConstrained.Restart.release(
    XX,YY,state,xs,ys,reals,nats,params)
Optizelle.EqualityConstrained.Restart.capture(
    XX,YY,state,xs,ys,reals,nats,params)

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

Language MATLAB/Octave

Code

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

```
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;
[xs zs reals nats params] = Optizelle.InequalityConstrained.Restart.release( ...
    XX,ZZ,state);
state = Optizelle.InequalityConstrained.Restart.capture( ...
    XX,ZZ,state,xs,zs,reals,nats,params);

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 1

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

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

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

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 composite-step 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

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

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

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

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

$$\begin{aligned} \min_{k\in\mathbb{R}^2, u\in\mathbb{R}^m} \quad & \tfrac{1}{2}\|u-d\|^2 \\ \text{st} \quad & (k_1A + k_2B)u = f - k_1\hat{A} - k_2\hat{B}. \end{aligned}$$

For brevity, we specify that

$$\begin{aligned} C(k) =& k_1A + k_2B \\ g(k) =& f - k_1\hat{A} - k_2\hat{B}, \end{aligned}$$

which allows us to reformulate the discretized parameter estimation problem as

$$\begin{aligned} \min_{k\in\mathbb{R}^2, u\in\mathbb{R}^m} \quad & \tfrac{1}{2}\|u-d\|^2 \\ \text{st} \quad & C(k)u = g(k). \end{aligned}$$

We call the above formulation the *full-space formulation*. Alternatively, we can solve for u in the constraints and instead solve

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

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

$$\begin{aligned} C_1'(k) = A, \quad & C_2'(k) = B, \\ g_1'(k) = -\hat{A}, \quad & g_2'(k) = -\hat{B}. \end{aligned}$$

Then,

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

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

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

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

$$\begin{aligned} G'_{k_i}(k,u) =& C_i'u - g_i'(k) \\ G'_u(k,u) =& C(k). \end{aligned}$$

This implies that the total derivative and its adjoint are

$$\begin{aligned} G'(k,u) &= \begin{bmatrix} C_1'u - g_1'(k) & C_2'u - g_2'(k) & C(k) \end{bmatrix} \\ G'(k,u)^* &= \begin{bmatrix} (C_1'u - g_1'(k))^T \\ (C_2'u - g_2'(k))^T \\ C(k)^T \end{bmatrix}. \end{aligned}$$

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

$$(G''(k,u)(\partial k, \partial u))^* \partial y = \begin{bmatrix} 0 & 0 & \partial y^T C_1'(k) \\ 0 & 0 & \partial y^T C_2'(k) \\ C_1'(k)^T \partial y & C_2'(k)^T \partial y & 0 \end{bmatrix} \begin{bmatrix} \partial k_1 \\ \partial k_2 \\ \partial u \end{bmatrix}$$

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

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

7 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

$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & x^2 + y^2 \\ \text{st} \quad & (x-2)^2 + (y-2)^2 = 1 \end{aligned}$$

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
//
// f(x,y)=x^2+y^2
//
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---

//---EqualityConstraint0---
// Define a simple equality constraint
//
// g(x,y)= [ (x-2)^2 + (y-2)^2 = 1 ]
//
struct MyEq
    :public Optizelle::VectorValuedFunction<double,Optizelle::Rm,Optizelle::Rm>
{
    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;
        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---

//---Extract0---
// Print out the reason for convergence
std::cout << "The algorithm converged due to: " <<
    Optizelle::OptimizationStop::to_string(state.opt_stop) <<
    std::endl;

// Print out the final answer
std::cout << std::scientific << std::setprecision(16)
    << "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

#---Objective0---
# 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---

#---EqualityConstraint0---
# 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
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---

#---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.EqualityConstrained.write_restart(
    Optizelle.Rm,Optizelle.Rm,"solution.json",state)
```

Language MATLAB/Octave

Code

```
% 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

    % 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 = @(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); ...
        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
%---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
    Optizelle.json.EqualityConstrained.write_restart( ...
        Optizelle.Rm,Optizelle.Rm,'solution.json',state);
end
```

7.2 Simple inequality constrained

In our Simple inequality constrained example, we optimize the formulation

$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & (x+1)^2 + (y+1)^2 \\ \text{st} \quad & x + 2y \geq 1 \\ & 2x + y \geq 1 \end{aligned}$$

with the code:

Language C++

Code

```
// Optimize a simple optimization problem with an optimal solution
// of (1/3,1/3)
```

```
#include "optizelle/optizelle.h"
#include "optizelle/vspaces.h"
#include "optizelle/json.h"
#include <iostream>
#include <iomanip>
#include <cstdlib>

// Squares its input
template <typename Real>
Real sq(Real const & x){
    return x*x;
}

// Define a simple objective where
//
// f(x,y)=(x+1)^2+(y+1)^2
//
struct MyObj
    : public Optizelle::ScalarValuedFunction <double,Optizelle::Rm>
{
    typedef Optizelle::Rm <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 simple inequalities
//
// h(x,y)= [ x + 2y >= 1 ]
//         [ 2x + y >= 1 ]
//
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 <parameters>" << std::endl;
        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: " <<
        Optizelle::OptimizationStop::to_string(state.opt_stop) <<
        std::endl;

    // Print out the final answer
    std::cout << std::scientific << std::setprecision(16)
        << "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
# 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.*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.)

# 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)
```

Language MATLAB/Octave

Code

```
% 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
%
% 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 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

$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & (x+1)^2 + (y+1)^2 \\ \text{st} \quad & x + 2y = 1 \\ & 2x + y \geq 1 \end{aligned}$$

with the code:

Language C++

Code

```
// Optimize a simple optimization problem with an optimal
// solution of (1/3,1/3)

#include "optizelle/optizelle.h"
```

```
#include "optizelle/vspaces.h"
#include "optizelle/json.h"
#include <iostream>
#include <iomanip>
#include <cstdlib>

// Squares its input
template <typename Real>
Real sq(Real const & x){
    return x*x;
}

// Define a simple objective where
//
// f(x,y)=(x+1)^2+(y+1)^2
//
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
//
// g(x,y)= [ x + 2y = 1 ]
//
struct MyEq
    :public Optizelle::VectorValuedFunction<double,Optizelle::Rm,Optizelle::Rm>
{
```

```
    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.*x[1]-1.;
    }

    // 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
//
// h(x,y)= [ 2x + y >= 1 ]
//
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);
    }
};

int main(int argc,char* argv[]){
    // Read in the name for the input file
    if(argc!=2) {
        std::cerr << "simple_constrained <parameters>" << std::endl;
        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: " <<
        Optizelle::OptimizationStop::to_string(state.opt_stop) <<
        std::endl;

    // Print out the final answer
    std::cout << std::scientific << std::setprecision(16)
        << "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
# 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.*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 = @(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 = @(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 = @(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.)
    static void copy(Vector const & x, Vector & y) {
        for(Natural i=0;i<x.size();i++){
            y[i]=x[i];
        }
    }

    // x <- alpha * x
    static void scal(const Real& alpha, Vector & x) {
        for(Natural i=0;i<x.size();i++){
            x[i]=alpha*x[i];
        }
    }

    // x <- 0
    static void zero(Vector & x) {
        for(Natural i=0;i<x.size();i++){
            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++){
            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++)
            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++)
            x[i]=Real(dis(gen));
    }
    // Jordan product, z <- x o y.
```

```
    static void prod(Vector const & x, Vector const & y, Vector & z) {
        for(Natural i=0;i<x.size();i++)
            z[i]=x[i]*y[i];
    }

    // Identity element, x <- e such that x o e = x.
    static void id(Vector & x) {
        for(Natural i=0;i<x.size();i++)
            x[i]=Real(1.);
    }

    // Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o y.
    static void linv(Vector const & x,Vector const & y,Vector & z) {
        for(Natural i=0;i<x.size();i++)
            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++)
            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++) {
            if(x[i] < Real(0.)) {
                Real alpha0 = -y[i]/x[i];
                alpha = alpha0 < alpha ? alpha0 : alpha;
            }
        }

        return alpha;
    }

    // Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric
    // 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
//
// f(x,y)=(1-x)^2+100(y-x^2)^2
//
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;
}
//---Messaging1---

//---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 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++)
                    x_json << x[i] << ", ";
                x_json << x.back() << " ]";

                // 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++)
                    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++)
                    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_";
            ss << std::setw(4) << std::setfill('0') << state.iter;
            ss << ".json";

            // 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;
        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: " <<
        Optizelle::OptimizationStop::to_string(state.opt_stop) << std::endl;

    // Print out the final answer
    std::cout << "The optimal point is: (" << state.x[0] << ','
    << 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
```

```
import functools

#---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 range(0,len(x)):
            x[i]=alpha*x[i]

    @staticmethod
    def zero(x):
        """x <- 0"""
        for i in range(0,len(x)):
            x[i]=0.

    @staticmethod
    def axpy(alpha,x,y):
        """y <- alpha * x + y"""
        for i in range(0,len(x)):
            y[i]=alpha*x[i]+y[i]

    @staticmethod
    def innr(x,y):
        """<- <x,y>"""
        return functools.reduce(lambda z,xy:xy[0]*xy[1]+z,zip(x,y),0.)

    @staticmethod
    def rand(x):
        """x <- random"""
        for i in range(0,len(x)):
            x[i]=random.uniform(0.,1.)

    @staticmethod
    def prod(x,y,z):
        """Jordan product, z <- x o y"""
        for i in range(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 range(0,len(x)):
            x[i]=1.

    @staticmethod
    def linv(x,y,z):
        """Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o y"""
        for i in range(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 > 0"
        alpha = float("inf")
        for i in range(0,len(x)):
            if x[i] < 0:
                alpha0 = -y[i]/x[i]
                if alpha0 < alpha:
                    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 range(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

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.

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
        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 o e = x.
    self.id = @(x)tostruct(ones(size(x.data)));

    % Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o 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

$$\begin{aligned} \min_{x \in \mathbb{R}^2} \quad & (x+1)^2 + (y+1)^2 \\ \text{st} \quad & x + 2y = 1 \\ & 2x + y \geq 1 \end{aligned}$$

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)

#include "optizelle/optizelle.h"
#include "optizelle/vspaces.h"
#include "optizelle/json.h"
#include <iostream>
#include <iomanip>
#include <cstdlib>
#include <cstring>

// Grab Optizelle's Natural type
using Optizelle::Natural;

// 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.)
    static void copy(Vector const & x, Vector & y) {
        for(Natural i=0;i<x.size();i++){
            y[i]=x[i];
```

```
    }
}

// x <- alpha * x
static void scal(Real const & alpha, Vector & x) {
    for(Natural i=0;i<x.size();i++){
        x[i]=alpha*x[i];
    }
}

// x <- 0
static void zero(Vector & x) {
    for(Natural i=0;i<x.size();i++){
        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++){
        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++)
        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++)
        x[i]=Real(dis(gen));
}
// Jordan product, z <- x o y.
static void prod(Vector const & x, Vector const & y, Vector & z) {
    for(Natural i=0;i<x.size();i++)
        z[i]=x[i]*y[i];
}

// Identity element, x <- e such that x o e = x.
static void id(Vector & x) {
    for(Natural i=0;i<x.size();i++)
        x[i]=Real(1.);
}

// Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o y.
static void linv(Vector const & x,Vector const & y,Vector & z) {
```

```
        for(Natural i=0;i<x.size();i++)
            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++)
            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++) {
            if(x[i] < Real(0.)) {
                Real alpha0 = -y[i]/x[i];
                alpha = alpha0 < alpha ? alpha0 : alpha;
            }
        }

        return alpha;
    }

    // Symmetrization, x <- symm(x) such that L(symm(x)) is a symmetric
    // 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
//
// f(x,y)=(x+1)^2+(y+1)^2
//
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
//
// g(x,y)= [ x + 2y = 1 ]
//
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.*x[1]-1.;
    }

    // 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
//
// h(x,y)= [ 2x + y >= 1 ]
//
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/";
                fname << name << ".";
                fname << std::setw(4) << std::setfill('0') << iter;
                fname << ".txt";

                // Actually write the vector there
                std::ofstream fout(fname.str());
                if(fout.fail()) {
                    std::stringstream msg;
                    msg << "While writing the variable " << name
                        << " 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++)
                    fout << x[i] << std::endl;

                // Close out the file
                fout.close();

                // Use this filename as the json string
                std::stringstream x_json;
                x_json << "\"" << fname.str() << "\"";
                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++)
                    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++)
                    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 <
    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) {
        // 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_";
            ss << std::setw(4) << std::setfill('0') << state.iter;
            ss << ".json";

            // 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 <parameters>"<< std::endl;
        std::cerr << "simple_constrained_advanced_api <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: " <<
        Optizelle::OptimizationStop::to_string(state.opt_stop) <<
        std::endl;
```

```
    // Print out the final answer
    std::cout << std::scientific << std::setprecision(16)
        << "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

Code

```
# Optimize a simple optimization problem with an optimal solution
# of (1/3,1/3)

import Optizelle
import sys
import copy
import array
import math
import functools

# 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 range(0,len(x)):
            x[i]=alpha*x[i]

    @staticmethod
    def zero(x):
        """x <- 0"""
        for i in range(0,len(x)):
            x[i]=0.

    @staticmethod
    def axpy(alpha,x,y):
```

```
    """y <- alpha * x + y"""
    for i in range(0,len(x)):
        y[i]=alpha*x[i]+y[i]

@staticmethod
def innr(x,y):
    """<- <x,y>"""
    return functools.reduce(lambda z,xy:xy[0]*xy[1]+z,zip(x,y),0.)

@staticmethod
def rand(x):
    """x <- random"""
    for i in range(0,len(x)):
        x[i]=random.uniform(0.,1.)

@staticmethod
def prod(x,y,z):
    """Jordan product, z <- x o y"""
    for i in range(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 range(0,len(x)):
        x[i]=1.

@staticmethod
def linv(x,y,z):
    """Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o y"""
    for i in range(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 functools.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 > 0"
    alpha = float("inf")
    for i in range(0,len(x)):
        if x[i] < 0:
            alpha0 = -y[i]/x[i]
            if alpha0 < alpha:
                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.*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 >= 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 range(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 range(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,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

% 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 o e = x.
    self.id = @(x)tostruct(ones(size(x.data)));

    % Jordan product inverse, z <- inv(L(x)) y where L(x) y = x o 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

% 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) 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
```

8 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.

Algorithm Trust-region Newton

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. *Trust-Region Methods*. SIAM, 2000.
- Jorge Nocedal and Stephen J. Wright. *Numerical Optimization*. 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. *Numerical Optimization*. 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 *pseudo* because we do not require commutativity in the Jordan product. Specifically, our derivation begins from the optimality conditions

$$\begin{aligned} \nabla f(x) - h'(x)^* z &= 0, \\ h(x) &\succeq 0, \\ z &\succeq 0, \\ h(x) \circ z &= 0 \end{aligned}$$

in the case of inequality constrained problems and

$$\begin{aligned} \nabla f(x) + g'(x)^* y - h'(x)^* z &= 0, \\ g(x) &= 0, \\ h(x) &\succeq 0, \\ z &\succeq 0, \\ h(x) \circ z &= 0 \end{aligned}$$

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

$$\begin{aligned} \mathrm{grad}(x, y) - h'(x)^* z &= 0, \\ h(x) &\succeq 0, \\ z &\succeq 0, \\ h(x) \circ z &= 0 \end{aligned}$$

where

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

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

$$\begin{aligned} \mathrm{grad}(x, y) - h'(x)^* z &= 0 \\ h(x) &\succ 0 \\ z &\succ 0 \\ h(x) \circ z &= \mu e. \end{aligned}$$

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

$$\begin{aligned} \mathrm{grad}(x, y) - h'(x)^* z &= 0, \\ h(x) \circ z &= \mu e, \end{aligned}$$

which yields the system

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

where

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

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

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

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

$$\texttt{z} = \texttt{mu} \cdot L(h(\texttt{x}))^{-1}e.$$

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

$$\begin{aligned} h(\texttt{x} + \texttt{alpha\_x} \cdot \texttt{dx}) &\geq (1 - \texttt{gamma})h(x) \\ \texttt{z} + \texttt{alpha\_z} \cdot \texttt{dz} &\geq (1 - \texttt{gamma})z) \\ h(\texttt{x} + \texttt{alpha\_x\_qn} \cdot \texttt{dx\_n}) &\geq (1 - \texttt{gamma} \cdot \texttt{zeta})h(x) \end{aligned}$$

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 $\texttt{mu} = \texttt{sigma} \cdot \texttt{mu}$ when one of the following global or local convergence criteria is satisfied

1. $\log(\texttt{norm\_gradtyp}) - \log(\|\text{gradstep}(x,y,z)\|) < \log(\texttt{mu\_typ}) - \log(\texttt{mu\_est})$

2. $\|\text{gradstep}(x, y, z)\| < \texttt{eps\_grad} \cdot \texttt{norm\_gradtyp}$
3. $\log(\texttt{norm\_gradtyp}) - \log(\|\text{gradstop}(x, y, z)\|) < \log(\texttt{mu\_typ}) - \log(\texttt{mu\_est})$
4. $\|\text{gradstop}(x, y, z)\| < \texttt{eps\_grad} \cdot \texttt{norm\_gradtyp}$

where

$$\text{gradstop}(x, y, z) = \begin{cases} \nabla f(x) - h'(x)^* z & \text{Inequality constrained,} \\ \nabla f(x) + g'(x)^* y - h'(x)^* z & \text{Constrained.} \end{cases}$$

$$\text{gradstep}(x, y, z) = \begin{cases} \nabla f(x) - \mu h'(x)^* L(h(x))^{-1} e & \text{Inequality constrained} \\ \nabla f(x) + W(\nabla^2 f(x)\texttt{dx\_n}) + g'(x)^* y - \mu h'(x)^* L(h(x))^{-1} e & \text{Constrained.} \end{cases}$$

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

1. $\log(\texttt{norm\_gxtyp}) - \log(\|g(\texttt{x})\|) < \log(\texttt{mu\_typ}) - \log(\texttt{mu\_est})$
2. $\|g(\texttt{x})\| < \texttt{eps\_constr} \cdot \texttt{norm\_gxtyp}$

In addition, we must converge `mu_est` locally

$$|\texttt{mu} - \texttt{mu\_est}| < \texttt{mu}$$

and not have converged `mu` globally

$$|\texttt{mu} - \texttt{eps\_mu} \cdot \texttt{mu\_typ}| \geq \texttt{eps\_mu} \cdot \texttt{mu\_typ}.$$

Finally, we also require that $\texttt{iter} > 1$, 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 $x \circ \nabla \texttt{barr}(x) = e$. In our `Rm` and `SQL` vector spaces, we use the log-barrier functions:

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

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

$$\texttt{z} = \texttt{mu} \cdot L(h(\texttt{x}))^{-1} e.$$

This guarantees that

1. $h(\texttt{x}) \circ \texttt{z} = \texttt{mu} \cdot e$
2. $\texttt{mu\_est} = \texttt{mu}$

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.

9 Licenses

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

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9.6 GCC

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GCC RUNTIME LIBRARY EXCEPTION

Version 3.1, 31 March 2009

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The "Compilation Process" transforms code entirely represented in
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$Id: LICENSE.TL 52869 2019-11-20 02:36:55Z karl $

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9.8 Python

A. HISTORY OF THE SOFTWARE
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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, which became
Zope Corporation. In 2001, the Python Software Foundation (PSF, see
https://www.python.org/psf/) was formed, a non-profit organization
created specifically to own Python-related Intellectual Property.
Zope Corporation was 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 from	Year	Owner	GPL-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
2.1.2	2.1.1	2002	PSF	yes
2.1.3	2.1.2	2002	PSF	yes
2.2 and above	2.1.1	2001-now	PSF	yes

Footnotes:

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(2) According to Richard Stallman, 1.6.1 is not GPL-compatible,
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Thanks to the many outside volunteers who have worked under Guido's
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more than your reasonable cost of physically performing this
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