A C++ Riemannian Optimization Library

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Goal

Develop a library to find an optimum of a real-valued function $f$ on a Riemannian manifold, i.e.,

$$\min f(x), x \in M.$$ 

Many libraries exist, e.g. ManOpt [BMAS14].

- Reliable computational time
- Interfaces for various languages users
- Can be built in other packages
C++ Package

Available on http://www.math.fsu.edu/~whuang2/ROPTLIB

- C++ is a popular and object-oriented programming language
  - Not difficult to maintain
  - Built in other packages
  - Reliable computational time

- Use standard linear algebra packages, BLAS and LAPACK
The framework partly inspires by ManOpt [BMAS14] and GenRTR [ABG07], and include four parts:

- **Solvers**: State-of-the-art algorithms
- **Space**: Storing elements on manifolds, tangent vectors and linear operators
- **Manifold**: Operations of manifolds
- **Problem**: Cost function, gradient, etc.
Inheritance

- Multiple base classes $\rightarrow$ a derived class
- Make it easy to maintain the code
- Overwrite a function, e.g. Print()
### Solvers

**Table: Riemannian algorithms in the package**

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<th>Reference(s)</th>
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<td>Riemannian steepest descent (RSD)</td>
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</table>
Solvers

- Line search based methods
  - \( x_{k+1} = R_{x_k}(t_k \eta_k) \)
  - Line search algorithm is used to find a step size \( t_k \)
  - Different algorithms use different search direction \( \eta_k \)

- Trust region based methods
  - Approximately solve the local model
    \[ \eta_k = \arg\min_{\|\eta\| \in \mathcal{D}} f(x_k) + g(\nabla f(x_k), \eta) + \frac{1}{2} g(B_k \eta, \eta) \]
    and accept or reject \( \tilde{x}_{k+1} = R_{x_k}(\eta_k) \) based on the quality of the approximation
  - \( B_k \) is the Hessian approximation
  - Different algorithms use different Hessian approximation
Figure: Relationships among classes of solvers in the package. Arrows are from base class to derived class.
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Solvers

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Copy-on-Write strategy is used

```matlab
>> A = randn(1000, 1000);
>> tic; B = A; toc  \%\% 0.000006 seconds
>> tic; B(1,1) = 1; toc  \%\% 0.006373 seconds.
```

- Elements on Product of manifolds
  - Consecutive memory
  - Spatial locality
- Shared memory

Memory of $x \in \mathcal{M}$

```
x x related temp data
```
Figure: Relationships among classes of variables and tangent vectors in the package. Arrows are from base class to derived class.
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Define basic operations on Manifold

- Metric
- Retraction
- Vector transport
- Projection onto tangent space
- Euclidean gradient to Riemannian gradient
- Euclidean Hessian to Riemannian Hessian
- etc

Provide functions to check correctness of operations.
Figure: Relationships among classes of Manifolds in the package. Arrows are from base class to derived class.
Define cost function, gradient and action of Hessian
Convert Euclidean gradient and action of Euclidean Hessian to Riemannian gradient and action of Riemannian Hessian
Check correctness of gradient and action of Hessian
Problem

"MexProblem" is the bridge between C++ and Matlab
It converts function handles of Matlab to C++ functions
Only Matlab environment is shown.

- Set up the mex environment properly. Follow the webpage:
- Run "GenerateMyMex.m"
- Use "MyMex.m" to compile code

```matlab
>> GenerateMyMex
Generate MyMex.m file...
>> MyMex TestStieBrockett
Building with 'g++ -4.7'.
MEX completed successfully.
```
Interface of Matlab

- Run “MyMex DriverMexProb” to obtain the driver “DriverMexProb” for Matlab
- “DriverMexProb” is wrapped by the matlab script “DriverOPT.m”
- “DriverOPT.m” can be called by

\[
[X_f, f_v, g_fv, g_f0, \text{iter}, n_f, n_g, n_R, n_V, n_Vp, n_H, \text{time}, F_S, G_F, T_S] = \\
\text{DriverOPT}(f_h, g_fh, H_h, \text{SolverParams}, \text{ManiParams}, \text{HasHHR}, \text{initialX})
\]
An Example

- The Brockett cost function: Minimize

\[ \text{trace}(X^T BXD) \]  

such that \( x \in \mathcal{St}(p, n) \), where \( B \in \mathbb{R}^{n \times n} \), \( B = B^T \), \( D = \text{diag}(\mu_1, \mu_2, \ldots, \mu_p) \) and \( \mu_1 > \mu_2 > \cdots > \mu_p \).

- The columns of a global minimizer, \( X^* e_i \), are eigenvectors for the \( p \) smallest eigenvalues, \( \lambda_i \), ordered so that \( \lambda_1 \leq \cdots \leq \lambda_p \) [AMS08, §4.8].
Interface of Matlab

```matlab
function output = testBrockett()
    n = 5; p = 2; % size of the Stiefel manifold
    B = randn(n, n); B = B + B'; % data matrix
    D = sparse(diag(p : -1 : 1)); % data matrix
    fhandle = @(x)f(x, B, D); % cost function handle
    gfhandle = @(x)gf(x, B, D); % gradient
    Hesshandle = @(x, eta)Hess(x, eta, B, D); % Hessian

    SolverParams.method = 'RSD'; % Use RSD solver
    ManiParams.name = 'Stiefel'; % Domain is the Stiefel manifold
    ManiParams.n = n; % assign size to manifold parameter
    ManiParams.p = p; % assign size to manifold parameter
    initialX.main = orth(randn(n, p)); % initial iterate

    % call the driver
    output = DriverOPT(fhandle, gfhandle, Hesshandle, SolverParams, ManiParams, initialX);
end

function [output, x] = f(x, B, D)
    x.BUD = B * x.main * D;
    output = x.main(:)’ * x.BUD(:);
end

function [output, x] = gf(x, B, D)
    output.main = 2 * x.BUD;
end

function [output, x] = Hess(x, eta, B, D)
    output.main = 2 * B * eta.main * D;
end
```
An Example

- Summation of three Brockett cost functions: Minimize

\[
\text{trace}(X_1^T B_1 X_1 D_1) + \text{trace}(X_2^T B_2 X_2 D_2) + \text{trace}(X_3^T B_3 X_3 D_3)
\]

such that \((X_1, X_2, X_3) \in \text{St}(p, n) \times \text{St}(p, n) \times \text{St}(q, m)\), where \(B_1, B_2 \in \mathbb{R}^{n \times n}, B_3 \in \mathbb{R}^{m \times m}, B_1 = B_1^T, B_2 = B_2^T, B_3 = B_3^T,\)
\[D_1 = \text{diag}(\mu_1, \mu_2, \ldots, \mu_p), \mu_1 \geq \mu_2 \geq \ldots \geq \mu_p,\]
\[D_2 = \text{diag}(\nu_1, \nu_2, \ldots, \nu_p), \nu_1 \geq \nu_2 \geq \ldots \geq \nu_p,\]
\[D_3 = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_q), \text{ and } \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_q.\]
Future Work

- Interface with ManOpt
- More manifolds
- Interfaces for other languages, e.g., python
- Automatic differentiation
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