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.,

$$\min f(x), x \in \mathcal{M}.$$

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`

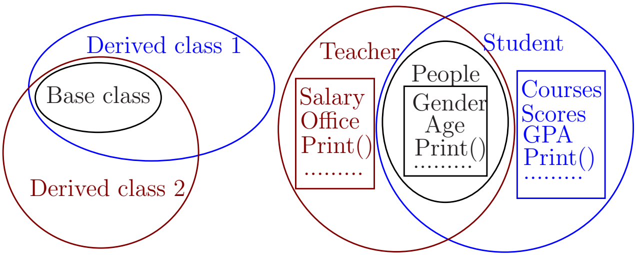
- C++ is a popular and object-oriented programming language
    - Not difficult to maintain
    - Built in other packages
    - Reliable computational time
- Use standard linear algebra packages, BLAS and LAPACK

Framework

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

Riemannian trust-region Newton (RTRNewton)	[ABG07]
Riemannian trust-region symmetric rank-one update (RTRSR1)	[HAG15]
Limited-memory RTRSR1 (LRTRSR1)	[HAG15]
Riemannian trust-region steepest descent (RTRSD)	[AMS08]
Riemannian line-search Newton (RNewton)	[AMS08]
Riemannian Broyden family (RBroydenFamily)	[HGA14]
Riemannian BFGS (RWRBFGS and RBFGS)	[RW12, HGA14]
Limited-memory RBFGS (LRBFGS)	[HGA14]
Riemannian conjugate gradients (RCG)	[NW06, AMS08, SI13]
Riemannian steepest descent (RSD)	[AMS08]

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 η_k
- Trust region based methods
  - Approximately solve the local model $\eta_k = \mathrm{argmin}_{\|\eta\| \in \mathbb{D}} f(x_k) + g(\mathrm{grad}\, f(x_k), \eta) + \frac{1}{2} g(\mathcal{B}_k \eta, \eta)$ and accept or reject $\tilde{x}_{k+1} = R_{x_k}(\eta_k)$ based on the quality of the approximation
  - $\mathcal{B}_k$ is the Hessian approximation
  - Different algorithms use different Hessian approximation

Solvers

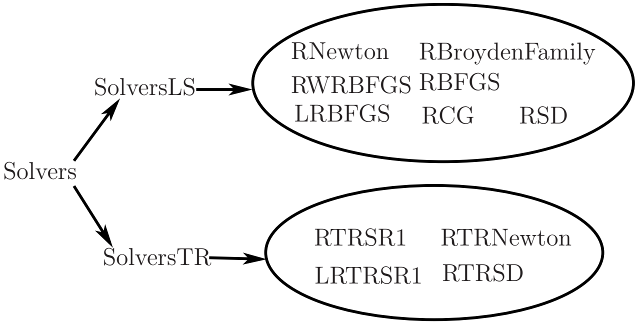
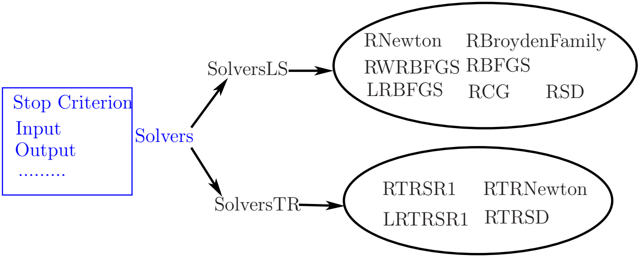


Figure: Relationships among classes of solvers in the package. Arrows are from base class to derived class.

Solvers



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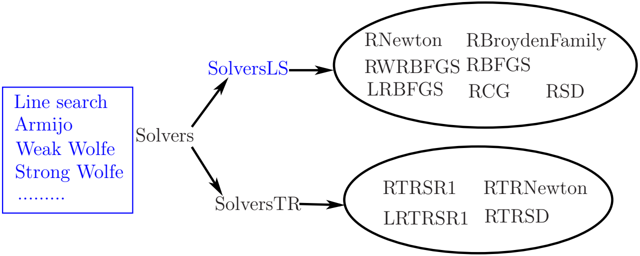

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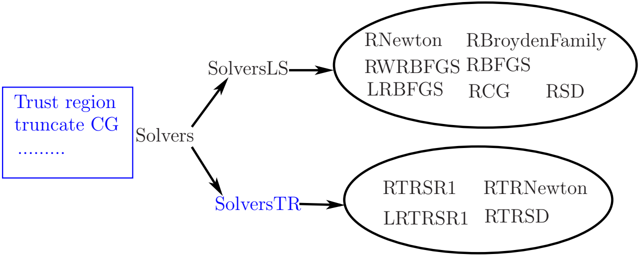
Solvers



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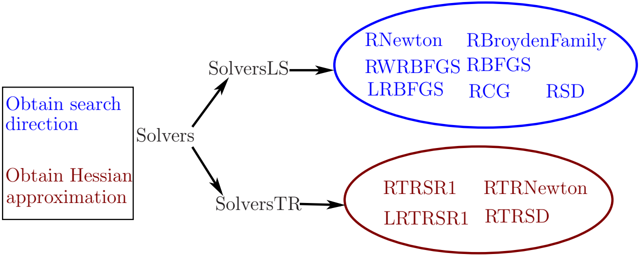

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Space

- Copy-on-Write strategy is used

```
>> 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

Space

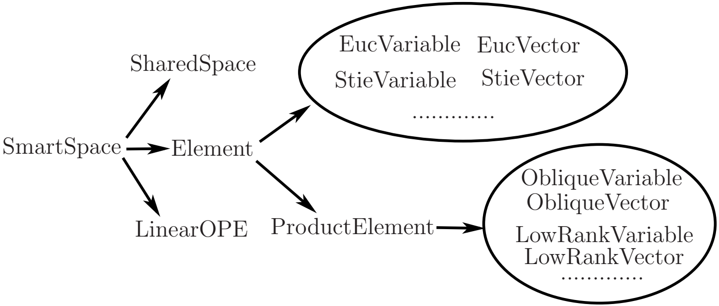

Figure: Relationships among classes of variables and tangent vectors in the package. Arrows are from base class to derived class.

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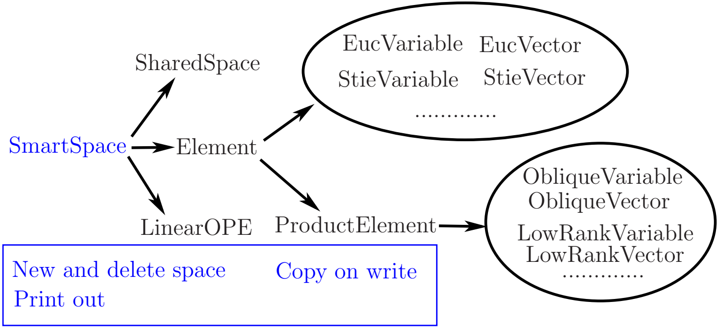

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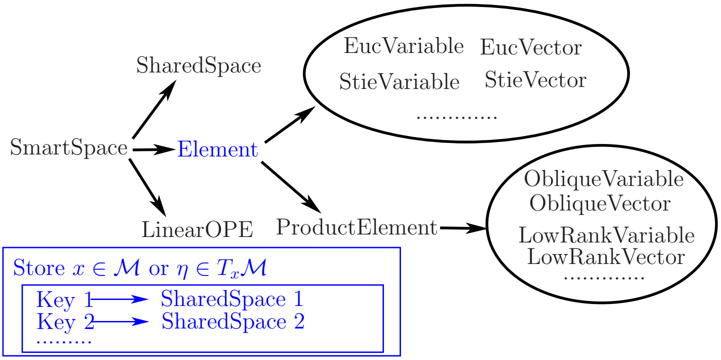

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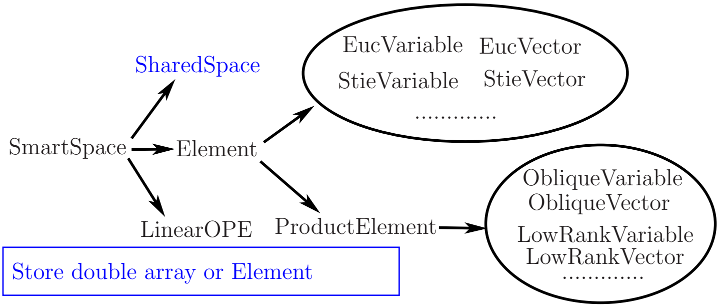

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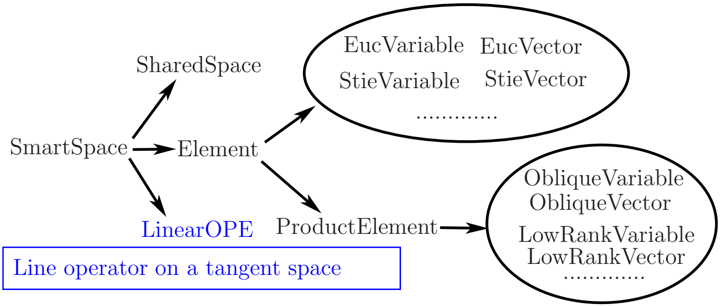

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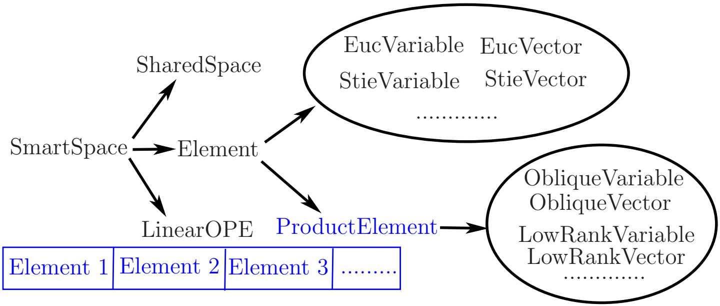

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Manifold

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.

Manifold

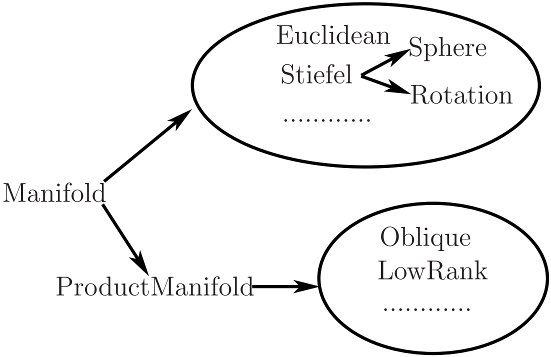
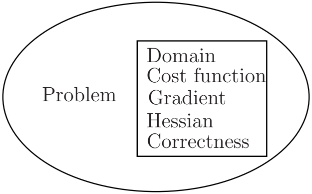


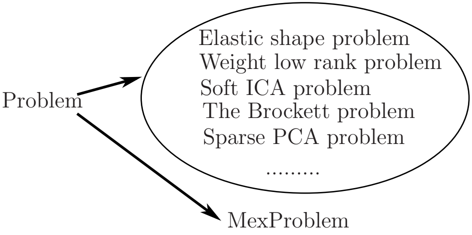
Figure: Relationships among classes of Manifolds in the package. Arrows are from base class to derived class.

Problem



- 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

Installation

Only Matlab environment is shown.

- Set up the mex environment properly. Follow the webpage: `www.mathworks.com/support/compilers/R2014b/index.html`
- Run "GenerateMyMex.m"
- Use "MyMex.m" to compile code

```
>> 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

```
[Xf, fv, gfv, gf0, iter, nf, ng, nR, nV, nVp, nH, time, FS, GFS, TS] =
DriverOPT(fh, gfh, Hh, SolverParams, ManiParams, HasHHR, initialX)
```

An Example

- The Brockett cost function: Minimize

$$\mathrm{trace}(X^T BXD) \tag{1}$$

  such that $x \in \mathrm{St}(p, n)$, where $B \in \mathbb{R}^{n\times n}$, $B = B^T$, $D = \mathrm{diag}(\mu_1, \mu_2, \ldots, \mu_p)$ and $\mu_1 > \mu_2 > \ldots > \mu_p$.
- The columns of a global minimizer, $X^* e_i$, are eigenvectors for the p smallest eigenvalues, λ_i, ordered so that $\lambda_1 \leq \cdots \leq \lambda_p$ [AMS08, §4.8].

Interface of 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

$$\mathrm{trace}(X_1^T B_1 X_1 D_1) + \mathrm{trace}(X_2^T B_2 X_2 D_2) + \mathrm{trace}(X_3^T B_3 X_3 D_3) \tag{2}$$

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

Future Work

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

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