Optimization Algorithms on Riemannian Manifolds with Applications

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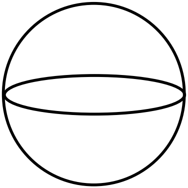
Problem Statements

- Finding an optimum of a real-valued function f on a Riemannian manifold, i.e.,

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

- Finite dimensional manifold
- Roughly speaking, a manifold is a set endowed with coordinate patches that overlap smoothly, e.g.,

sphere: $\{x \in \mathbb{R}^n | \|x\|_2 = 1\}$.



Motivations

Optimization on manifolds is used in many areas [AMS08].

- Numerical linear algebra
- Signal processing
- Data mining
- Statistical image analysis

Frameworks of Optimization

- Line search optimization methods
  - Find a search direction,
  - Apply a line search algorithm and obtain a next iterate.
- Trust region optimization methods
  - Build a local model that approximates the objective function f,
  - Optimize the local model and obtain a candidate of next iterate,
  - If the local model is close to f, then accept the candidate to be next iterate, otherwise, reject the candidate,
  - Update the local model.

Existing Euclidean Optimization Algorithms

There are many algorithms developed for problems in Euclidean space. (see e.g. [NW06]) e.g.,

- Newton-based (requires gradient and Hessian)
- gradient-based (requires gradient only)
  - Steepest descent
  - Quasi-Newton
    - Restricted Broyden Family (BFGS, DFP)
    - Symmetric rank-1 update
- These ideas can be combined with line search or trust region strategies.

Existing Riemannian Optimization Algorithms

The algorithmic and theoretical work on Riemannian manifolds is quite limited.

- Trust region with Newton-Steihaug CG (C. G. Baker [Bak08])
- Riemannian BFGS (C. Qi [Qi11])
- Riemannian BFGS (W. Ring and B. Wirth [RW12])

Quadratic:

$$\lim_{k\to\infty} \frac{dist(x_{k+1}, x^*)}{dist(x_k, x^*)^2} < \infty$$

Superlinear:

$$\lim_{k\to\infty} \frac{dist(x_{k+1}, x^*)}{dist(x_k, x^*)} = 0$$

Linear:

$$\lim_{k\to\infty} \frac{dist(x_{k+1}, x^*)}{dist(x_k, x^*)} < 1$$

Framework of Line Search Optimization Methods

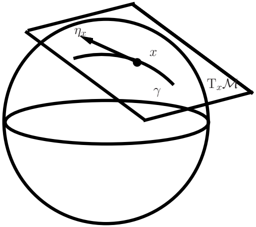
- Line search optimization methods on Euclidean space

$$x_+ = x + \alpha d,$$

  where d is a descent direction and α is a step size.
- Cannot apply to problems on Riemannian manifold directly
  - direction?
  - addition?
- Riemannian concepts can be found in [O'N83, AMS08].

Tangent Space

- γ is a curve on $\mathcal{M}$. The tangent vector shows the direction along γ at x, for which is $\gamma'(0)$, where $\gamma(0) = x$.
- Tangent space at x is the set of all tangent vectors(directions) at x, denoted by $\mathrm{T}_x \mathcal{M}$.
- Tangent space is a linear space.



Riemannian Metric

A Riemannian metric g is defined on each $\mathrm{T}_x\,\mathcal{M}$ as an inner product $g_x : \mathrm{T}_x\,\mathcal{M} \times \mathrm{T}_x\,\mathcal{M} \to \mathbb{R}$. A Riemannian manifold is the combination $(\mathcal{M}, g)$. This results in:

- angle between directions and length of directions
- distance:

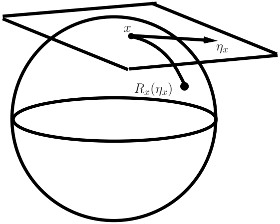
$$d(x, y) = \inf_{\gamma}\{\int_0^1 \|\dot{\gamma}(t)\|_{g_{\gamma(t)}} dt\},$$

  where γ is a curve on $\mathcal{M}$ with $\gamma(0) = x$ and $\gamma(1) = y$.
- neighborhood:

$$\mathcal{B}_\delta(x) = \{y \in \mathcal{M} : d(x, y) < \delta\}.$$

Retraction

Retraction is a mapping from a tangent vector to a point on $\mathcal{M}$, denoted by $R_x(\eta_x)$ where $x \in \mathcal{M}$ and $\eta_x \in \mathrm{T}_x\,\mathcal{M}$.



Framework of Line Search Optimization Methods

- Line search optimization methods on Riemannian manifolds

$$x_+ = R_x(\alpha d),$$

where $d \in \mathrm{T}_x \mathcal{M}$ and α is a step size.

Riemannian Gradient

- The Riemannian gradient $\mathrm{grad}\, f$ of f at x is the unique tangent vector such that

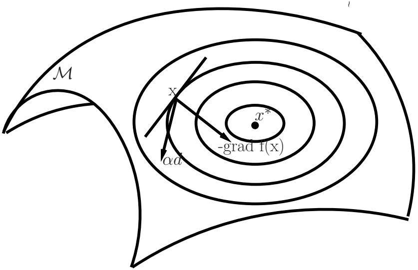
$$\langle \mathrm{grad}\, f(x), \eta \rangle_x = \mathrm{D}\, f(x)[\eta], \forall \eta \in \mathrm{T}_x\, \mathcal{M},$$

  where $\mathrm{D}\, f(x)[\eta]$ denotes the derivative of f along η.
- $\mathrm{grad}\, f(x)$ is the steepest ascent direction.

Search Direction and Step Size

- Search direction
  The angle between $-\operatorname{grad} f$ and d does not approach $\pi/2$.
- Step size
  - f decreases sufficiently,
  - Step size is not too small,
  - e.g., the Wolfe conditions, the Armijo-Goldstein conditions.
- Above conditions are sufficient to guarantee convergence.

- Example: The figure shows the contour curves of f around a minimizer x^*.



Steepest Descent

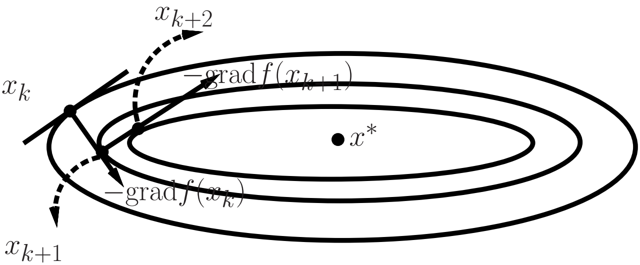
- Riemannian steepest descent (RSD): $d = -\operatorname{grad} f(x)$,
- Converges slowly, i.e., linearly

$$\lim_{k\to\infty} \frac{\operatorname{dist}(x_{k+1}, x^*)}{\operatorname{dist}(x_k, x^*)} < 1$$

- The Riemannian Hessian of f at x is a linear operator on $\mathrm{T}_x \mathcal{M}$.
- Let $\operatorname{Hess} f(x^*)$ denote the Hessian at the minimizer x^* and $\lambda_{\min}$ and $\lambda_{\max}$ respectively denote the smallest and largest eigenvalue of $\operatorname{Hess} f(x^*)$. The smaller $\lambda_{\min}/\lambda_{\max}$ is, the more slowly steepest descent converges. [AMS08, Theorem 4.5.6]

An Example for Steepest Descent

- f is a function defined on a Euclidean space.
- x^* is a minimizer and $\lambda_{\min}/\lambda_{\max}$ is small.
- The following figure shows contour curves of $f(x)$ around x^* and iterates generated by an exact line search algorithm.

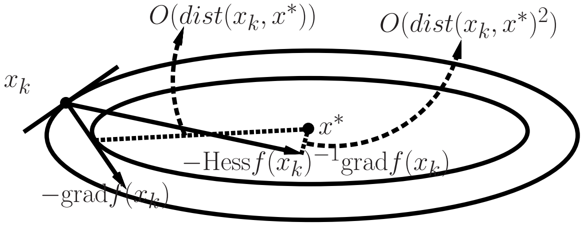


Newton Method

- Riemannian Newton update formula:

$$x_+ = R_x(\alpha[-\operatorname{Hess} f(x)^{-1} \operatorname{grad} f(x)]),$$

  where α is chosen to be 1 when x is close enough to x^*.
- The search direction is not necessarily descent.
- When x_k is close enough to x^*, the search direction is descent.
- Riemannian Newton method converges quadratically [AMS08, Theorem 6.3.2], i.e.,$\lim_{k\to\infty} \frac{\operatorname{dist}(x_{k+1},x^*)}{\operatorname{dist}(x_k,x^*)^2} < \infty$.

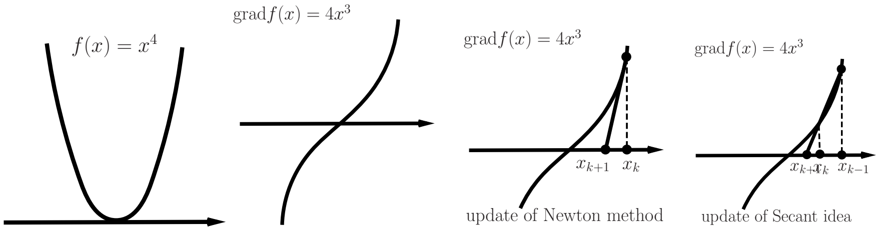


Quasi-Newton Methods

- Steepest descent method
    - Converge slowly
- Newton method
    - Requires the action of the Hessian which may be expensive or unavailable
    - Search direction may be not descent. Therefore, extra considerations are required.
- Quasi-Newton method
    - Approximate the action of the Hessian or its inverse and therefore accelerate the convergent rate
    - Provide an approach to produce a descent direction

Secant Condition

An 1 dimension example to show the idea of the secant condition.



- Newton: $x_{k+1} = x_k - (\mathrm{Hess}\, f(x_k))^{-1}\, \mathrm{grad}\, f(x_k)$
- Secant: $x_{k+1} = x_k - B_k^{-1}\, \mathrm{grad}\, f(x_k)$,
  $B_k(x_k - x_{k-1}) = \mathrm{grad}\, f(x_k) - \mathrm{grad}\, f(x_{k-1})$

Riemannian Secant Conditions

- Euclidean:

$$\mathrm{grad}\, f(x_{k+1}) - \mathrm{grad}\, f(x_k) = B_{k+1}(x_{k+1} - x_k).$$

- Riemannian:
  - $x_{k+1} - x_k$ can be replaced by $R_{x_k}^{-1}(x_{k+1})$
  - $\mathrm{grad}\, f(x_{k+1})$ and $\mathrm{grad}\, f(x_k)$ are in different tangent spaces. A method of comparing tangent vectors in different tangent spaces is required.

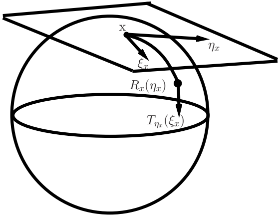
Vector Transport

Vector transport

- Transport a tangent vector from one tangent space to another.
- notation: $\mathcal{T}_{\eta_x}\xi_x$, denotes transport of ξ_x to tangent space of $R_x(\eta_x)$. R is a retraction associated with $\mathcal{T}$.
- An isometric vector transport, denoted by $\mathcal{T}_S$, additionally satisfies

$$g_x(\eta_x, \xi_x) = g_y(\mathcal{T}_{S_{\zeta_x}}\eta_x, \mathcal{T}_{S_{\zeta_x}}\xi_x),$$

where $x, y \in \mathcal{M}$, $y = R_x(\zeta_x)$ and $\eta_x, \xi_x, \zeta_x \in \mathrm{T}_x\,\mathcal{M}$.



Riemannian Secant Conditions

The secant condition of Qi [Qi11]:

$$\operatorname{grad} f(x_{k+1}) - P_{\gamma_k}^{1\leftarrow 0} \operatorname{grad} f(x_k) = \mathcal{B}_{k+1}(P_{\gamma_k}^{1\leftarrow 0} \operatorname{Exp}_{x_k}^{-1} x_{k+1}),$$

where Exp is a particular retraction, called the exponential mapping and P is a particular vector transport, called the parallel translation.

Riemannian Secant Conditions

The secant condition of Ring and Wirth [RW12]:

$$(\mathrm{grad}\, f(x_{k+1})^\flat \mathcal{T}_{R_{\xi_k}} - \mathrm{grad}\, f(x_k)^\flat)\mathcal{T}_{S_{\xi_k}}^{-1} = (\mathcal{B}_{k+1}\mathcal{T}_{S_{\xi_k}}\xi_k)^\flat$$

where $\mathcal{T}_R$ is differentiated retraction of R, i.e.,

$$\mathcal{T}_{R_{\eta_x}}\zeta_x = \frac{d}{dt}R_x(\eta_x + t\zeta_x)|_{t=0}$$

and $\eta_x^\flat$ denotes a function from $\mathrm{T}_x\,\mathcal{M}$ to $\mathbb{R}$, i.e., $\eta_x^\flat \xi_x = g_x(\eta_x, \xi_x)$. Their work is on infinite dimensional manifolds. It is rewritten in a finite dimensional form so that it can be compared to our secant condition.

Riemannian Secant Conditions

- We use

$$\operatorname{grad} f(x_{k+1})/\beta_k - \mathcal{T}_{S_{\xi_k}} \operatorname{grad} f(x_k) = \mathcal{B}_{k+1} \mathcal{T}_{S_{\xi_k}} \xi_k,$$

where $\xi_k = R_{x_k}^{-1}(x_{k+1})$, $\beta_k = \|\xi_k\| / \|\mathcal{T}_{R_{\xi_k}} \xi_k\|$, $\mathcal{T}_R$ is differentiated retraction, and $\mathcal{T}_S$ is an isometric vector transport that satisfies

$$\mathcal{T}_{S_\xi} \xi = \beta \mathcal{T}_{R_\xi} \xi.$$

Euclidean DFP

The Euclidean secant condition and some additional constraints are imposed.

$$\min_B \|B - B_k\|_{W_B}$$
$$\text{s.t. } B = B^T,$$

where W_B is any positive definite matrix satisfying $W_B y_k = s_k$ and $\|A\|_{W_B} = \|W_B^{1/2} A W_B^{1/2}\|_F$.

$$B_{k+1} = (I - \frac{y_k s_k^T}{y_k^T s_k}) B_k (I - \frac{s_k y_k^T}{y_k^T s_k}) + \frac{y_k y_k^T}{y_k^T s_k},$$

where $s_k = x_{k+1} - x_k$ and $y_k = \mathrm{grad}\, f(x_{k+1}) - \mathrm{grad}\, f(x_k)$. This is called Davidon-Fletcher-Powell(DFP) update.

Euclidean BFGS

Let $H_k = B_k^{-1}$.

$$\min_{H} \|H - H_k\|_{W_H}$$
$$\text{s.t. } H = H^T,$$

where W_B is any positive definite matrix satisfying $W_B y_k = s_k$ and $\|A\|_{W_B} = \|W_B^{1/2} A W_B^{1/2}\|_F$.

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}.$$

This is called Broyden-Fletcher-Goldfarb-Shanno(BFGS) update.

Euclidean Broyden Family

The linear combination of BFGS update and DFP update is called Broyden Family update, $(1-\phi_k)BFGS + \phi_k DFP$:

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k} + (\phi_k s_k^T B_k s_k) v_k v_k^T,$$

where

$$v_k = \frac{y_k}{y_k^T s_k} - \frac{B_k s_k}{s_k^T B_k s_k}.$$

If $\phi_k \in [0,1]$, then it is restricted Broyden Family update.

- Properties
  - If $y_k^T s_k > 0$, then B_{k+1} is positive definite if and only if B_k is positive definite.
  - $y_k^T s_k > 0$ is guaranteed by the Wolfe second condition.

Riemannian Broyden Family

Riemannian Restricted Broyden Family update is

$$\mathcal{B}_{k+1} = \tilde{\mathcal{B}}_k - \frac{\tilde{\mathcal{B}}_k s_k (\tilde{\mathcal{B}}_k^* s_k)^\flat}{(\tilde{\mathcal{B}}_k^* s_k)^\flat s_k} + \frac{y_k y_k^\flat}{y_k^\flat s_k} + \phi_k g(s_k, \tilde{\mathcal{B}}_k s_k) v_k v_k^\flat,$$

where $\phi_k \in [0,1]$, $\eta_x^\flat$ denotes a function from $\mathrm{T}_x\,\mathcal{M}$ to $\mathbb{R}$, i.e., $\eta_x^\flat \xi_x = g_x(\eta_x, \xi_x)$, $s_k = \mathcal{T}_{S_{\alpha_k \eta_k}} \alpha_k \eta_k$ and $y_k = \mathrm{grad}\, f(x_{k+1})/\beta_k - \mathcal{T}_{S_{\alpha_k \eta_k}} \mathrm{grad}\, f(x_k)$, $\tilde{\mathcal{B}}_k = \mathcal{T}_{S_{\alpha_k \eta_k}} \circ \mathcal{B}_k \circ \mathcal{T}_{S_{\alpha_k \eta_k}}^{-1}$ and

$$v_k = \frac{y_k}{g(y_k, s_k)} - \frac{\tilde{\mathcal{B}}_k s_k}{g(s_k, \tilde{\mathcal{B}}_k s_k)}.$$

Riemannian Broyden Family

Properties

- If $g(y_k, s_k) > 0$, then $\mathcal{B}_{k+1}$ is positive definite if and only if $\mathcal{B}_k$ is positive definite.
- $g(y_k, s_k) > 0$ is not guaranteed by the most natural way of generalizing the Wolfe second condition for arbitrary retraction and isometric vector transport.
- We impose another condition called the 'locking condition'

$$\mathcal{T}_{S_\xi} \xi = \beta \mathcal{T}_{R_\xi} \xi, \quad \beta = \frac{\|\xi\|}{\|\mathcal{T}_{R_\xi} \xi\|},$$

where $\mathcal{T}_R$ is differentiated retraction.

Line Search Riemannian Broyden Family Method

(1) Given initial x_0 and symmetric positive definite B_0. Let $k = 0$.

(2) Obtain search direction by $\eta_k = -\mathcal{B}_k^{-1} \operatorname{grad} f(x_k)$

(3) Set next iterate $x_{k+1} = R_{x_k}(\alpha_k \eta_k)$, where α_k is set to satisfy the Wolfe conditions

$$f(x_{k+1}) \leq f(x_k) + c_1 \alpha_k g(\operatorname{grad} f(x_k), \eta_k), \quad (1)$$

$$\frac{d}{dt} f(R_{x_k}(t\eta_k))|_{t=\alpha_k} \geq c_2 \frac{d}{dt} f(R_{x_k}(t\eta_k)|_{t=0}. \quad (2)$$

where $0 < c_1 < 0.5 < c_2 < 1$.

(4) Use update formula to obtain $\mathcal{B}_{k+1}$.

(5) If not converged, then $k \leftarrow k + 1$ and go to Step 2.

Euclidean Theoretical Results

- If $f \in C^2$ and strongly convex, then the sequence $\{x_k\}$ generated by a Broyden family algorithm with $\phi_k \in [0, 1-\delta)$ converges to the minimizer x^*, where $\delta > 0$. Furthermore, the convergence rate is linear.
- If additionally, $\mathrm{Hess}\, f$ is Hölder continuous at the minimizer x^*, i.e., there exist $p > 0$ and $L > 0$ such that

$$\|\mathrm{Hess}\, f(x) - \mathrm{Hess}\, f(x^*)\| \leq L\|x - x^*\|^p,$$

for all x in a neighborhood of x^*, then step size $\alpha_k = 1$ satisfies the Wolfe conditions eventually. Moreover, if 1 is chosen to be the step size whenever it satisfies the Wolfe conditions, $\{x_k\}$ converges to x^* superlinearly, i.e.,

$$\lim_{k \to \infty} \frac{\|x_{k+1} - x^*\|_2}{\|x_k - x^*\|_2} = 0.$$

Riemannian Theoretical Results

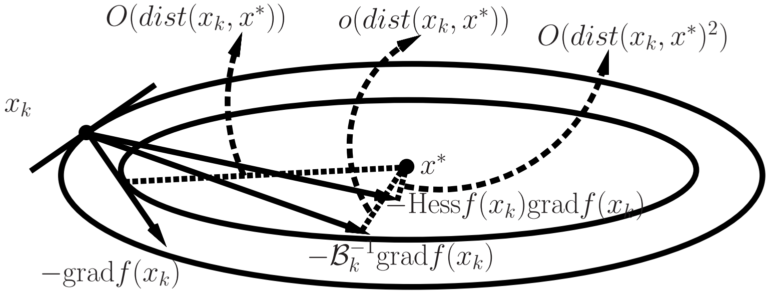
1. The (strong) convexity of a function is generalized to the Riemannian setting and is called (strong) retraction-convexity.
2. Suppose some reasonable assumptions hold. If $f \in C^2$ and strongly retraction-convex, then the sequence $\{x_k\}$ generated by a Riemannian Broyden family algorithm with $\phi_k \in [0, 1-\delta)$ converges to the minimizer x^*, where $\delta > 0$. Furthermore, the convergence rate is linear.
3. If additionally, $\mathrm{Hess}\, f$ satisfies a generalization of Hölder continuity at the minimizer x^*, then step size $\alpha_k = 1$ satisfies the Wolfe conditions eventually. Moreover, if 1 is chosen to be the step size whenever it satisfies the Wolfe conditions, $\{x_k\}$ converges to x^* superlinearly, i.e.,

$$\lim_{k \to \infty} \frac{dist(x_{k+1}, x^*)}{dist(x_k, x^*)} = 0.$$

Convergence Rate

Step size $\alpha_k = 1$:

- Eventually works for Riemannian Broyden family algorithm and Riemannian quasi-Newton algorithm
- Does not work for RSD in general.



Limited-memory RBFGS

Riemannian Restricted Broyden Family requires computing $\tilde{\mathcal{B}}_k = \mathcal{T}_{S_{\alpha_k \eta_k}} \circ \mathcal{B}_k \circ \mathcal{T}_{S_{\alpha_k \eta_k}}^{-1}$.

- Explicit form of $\mathcal{T}_S$ may not exist.
- Even though it exists, matrix multiplication is needed.

Limited-memory

- Similar to Euclidean case, it requires less memory.
- It avoids the requirement of explicit form of $\mathcal{T}_S$.

We only consider limited-memory RBFGS algorithm.

Limited-memory RBFGS

Consider the update of inverse Hessian approximation of RBFGS, $\mathcal{H}_k = \mathcal{B}_k^{-1}$. We have

$$\mathcal{H}_{k+1} = \mathcal{V}_k^{\flat} \tilde{\mathcal{H}}_k \mathcal{V}_k + \rho_k s_k s_k^{\flat}, \text{ where } \rho_k = \frac{1}{g(y_k, s_k)} \text{ and } \mathcal{V}_k = \mathrm{id} - \rho_k y_k s_k^{\flat}.$$

If the number of latest s_k and y_k we use is $m+1$, then

$$\begin{aligned} \mathcal{H}_{k+1} = & \tilde{\mathcal{V}}_k^{\flat} \tilde{\mathcal{V}}_{k-1}^{\flat} \cdots \tilde{\mathcal{V}}_{k-m}^{\flat} \tilde{\mathcal{H}}_{k+1}^0 \tilde{\mathcal{V}}_{k-m} \cdots \tilde{\mathcal{V}}_{k-1} \tilde{\mathcal{V}}_k \\ & + \rho_{k-m} \tilde{\mathcal{V}}_k^{\flat} \tilde{\mathcal{V}}_{k-1}^{\flat} \cdots \tilde{\mathcal{V}}_{k-m+1}^{\flat} s_{k-m}^{(k+1)} s_{k-m}^{(k+1)^{\flat}} \tilde{\mathcal{V}}_{k-m+1} \cdots \tilde{\mathcal{V}}_{k-1} \tilde{\mathcal{V}}_k \\ & + \cdots \\ & + \rho_k s_k^{(k+1)} s_k^{(k+1)^{\flat}}, \end{aligned}$$

where $\tilde{\mathcal{V}}_i = \mathrm{id} - \rho_i y_i^{(k+1)} s_i^{(k+1)^{\flat}}$ and $\mathcal{H}_{k+1}^0 = \frac{g(s_k, y_k)}{g(y_k, y_k)} \mathrm{id}$.

Construct $\mathcal{T}_S$

Methods to construct $\mathcal{T}_S$ satisfying the locking condition

$$\mathcal{T}_{S_\xi} \xi = \beta \mathcal{T}_{R_\xi} \xi, \quad \beta = \frac{\|\xi\|}{\|\mathcal{T}_{R_\xi} \xi\|},$$

for all $\xi \in \mathrm{T}_x \mathcal{M}$.

- Method 1: Modifying an existing isometric vector transport
- Method 2: Construct $\mathcal{T}_S$ when a smooth function of building orthonormal basis of tangent space is known.
- Both ideas use Householder reflection twice.
- Method 3: Given an isometric vector transport $\mathcal{T}_S$, a retraction is obtained by solving $\frac{d}{dt} R_x(t\eta_x) = \mathcal{T}_{S_{t\eta_x}} \eta_x$. In some cases, the closed form of the solution exists.

Framework of Trust Region Optimization Methods

Euclidean trust region method is to build a local model

$$m_k(\eta) = f(x_k) + \mathrm{grad}\, f(x_k)^T \eta + \frac{1}{2}\eta^T B_k \eta$$

and finds

$$\eta_k = \arg \min_{\|\eta\|_2 \leq \delta_k} m_k(\eta),$$

where δ_k is the radius of trust region. The candidate of next iterate is

$$\tilde{x}_{k+1} = x_k + \eta_k.$$

If $(f(x_k) - f(\tilde{x}_k))/(m_k(0) - m_k(\eta_k)$ is big enough, then accept the candidate $x_{k+1} = \tilde{x}_{k+1}$, otherwise, reject the candidate. Finally, update the local model.

Framework of Trust Region Optimization Methods

Riemannian trust region builds a model on the tangent space of current iterate x_k,

$$m_k(\eta) = f(x_k) + g(\mathrm{grad}\, f(x_k), \eta) + \frac{1}{2} g(\eta, \mathcal{B}_k \eta)$$

and finds

$$\eta_k = \arg \min_{\|\eta\| \leq \delta_k} m_k(\eta),$$

where δ_k is the radius of trust region. The candidate of next iterate is

$$\tilde{x}_{k+1} = R_{x_k}(\eta_k).$$

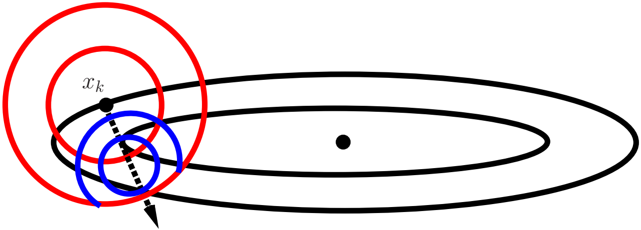
If $(f(x_k) - f(\tilde{x}_k))/(m_k(0) - m_k(\eta_k)$ is big enough, then accept the candidate $x_{k+1} = \tilde{x}_{k+1}$, otherwise, reject the candidate. Finally, update the local model.

Steepest Descent

- Riemannian trust region steepest descent(SD)
  - $\mathcal{B}_k = \mathrm{id}$,
  - If the local model is solved exactly, then

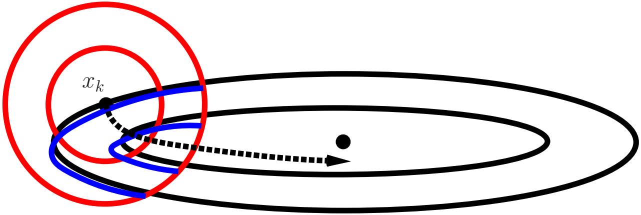
$$\eta_k = -\min(1, \delta_k / \| \mathrm{grad}\, f(x_k) \|)\, \mathrm{grad}\, f(x_k),$$

  - Converges linearly.



Newton Method

- Riemannian trust region Newton method
  - $\mathcal{B}_k = \mathrm{Hess}\, f(x_k)$,
  - Converges quadratically [Bak08],
  - In [Bak08], the local model is not required to be solved exactly and a Riemannian truncated conjugate gradient is proposed.



Quasi-Newton Method

Symmetric rank-1 update

- Euclidean: $B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{(y_k - B_k s_k)^T s_k}$,
- Riemannian: $\mathcal{B}_{k+1} = \tilde{\mathcal{B}}_k + \frac{(y_k - \tilde{\mathcal{B}}_k s_k)(y_k - \tilde{\mathcal{B}}_k s_k)^\flat}{g(s_k, y_k - \tilde{\mathcal{B}}_k s_k)}$,
  where $\tilde{\mathcal{B}}_k = \mathcal{T}_{S_{\eta_k}} \circ \mathcal{B}_k \circ \mathcal{T}_{S_{\eta_k}}^{-1}$.
- Properties:
  - It does not preserve positive definiteness of $\mathcal{B}_k$,
  - It produces better Hessian approximation as an operator.

  These properties suggest we use trust region.

Riemannian Trust region with symmetric rank-1 method (RTR-SR1)

(1) Given $\tau_1, c \in (0,1)$, $\tau_2 > 1$, initial x_0, and symmetric B_0. Let $k = 0$.

(2) Obtain η_k by (approximately) solving the local model $m_k(\eta)$

(3) Set the candidate of next iterate $\tilde{x}_{k+1} = R_{x_k}(\eta_k)$.

(4) Let $\rho_k = (f(x_k) - f(\tilde{x}_k))/(m_k(0) - m_k(\eta_k)$. If $\rho_k > c$, then $x_{k+1} = \tilde{x}_{k+1}$, otherwise $x_{k+1} = x_k$.

(5) Update the local model by first using update formula to obtain $\mathcal{B}_{k+1}$ and setting

$$\delta_{k+1} = \begin{cases} \tau_2 \delta_k, & \text{if } \rho_k > 0.75 \text{ and } \|\eta\| \geq 0.8\delta_k; \\ \tau_1 \delta_k, & \text{if } \rho_k < 0.1; \\ \delta_k, & \text{otherwise.} \end{cases}$$

(6) If not converge, then $k \leftarrow k + 1$ and go to Step 2.

Euclidean Theoretical Results

- If f is Lipschitz continuously differentiable and bounded below and the $\|B_k\| \leq C$ for some constant C, then the sequence $\{x_k\}$ generated by trust region with symmetric rank-1 update method converges to a stationary point x^*. [NW06]
- Suppose some reasonable assumptions hold. If $f \in C^2$ and the $\mathrm{Hess}\, f$ is Lipschitz continuous around the minimizer x^*, then the sequence $\{x_k\}$ converges to x^* $n+1$-step superlinearly, i.e.,

$$\lim_{k \to \infty} \frac{\|x_{k+n+1} - x^*\|_2}{\|x_k - x^*\|_2} = 0,$$

where n is the dimension of the domain. [BKS96]

Riemannian Theoretical Results

- Global convergence property has been proved in [Bak08] and is applicable for RTR-SR1.
- Suppose some reasonable assumptions hold. If $f \in C^2$ and the $\mathrm{Hess}\, f$ satisfies a Riemannian generalization version of Lipschitz continuity around the minimizer x^*, then the sequence $\{x_k\}$ converges to x^* $d+1$-step superlinearly, i.e.,

$$\lim_{k \to \infty} \frac{\mathrm{dist}(x_{k+d+1}, x^*)}{\mathrm{dist}(x_k, x^*)} = 0,$$

where d is the dimension of the manifold.

Limited-memory RTR-SR1

- Same motivation as limited-memory RBFGS
  - Less storage complexity,
  - Avoid some expensive operations.
- Similar techniques
  - Use a few previous s_k and y_k to approximate the action of the Hessian.

Important Theorems

Dennis and Moré conditions give necessary and sufficient conditions for a sequence $\{x_k\}$ converging superlinearly to x^* [DM77]. We have generalized to

- Riemannian Dennis Moré conditions for root solving
- Riemannian Dennis Moré conditions for optimization

Optimization for Partly Smooth Functions

- f is called partly smooth on $\mathcal{S}$ if it is continuously differentiable on an open dense subset.
- Gradient sampling algorithm (GS) [BLO05],
  - Global convergence analysis.
  - Works for non-Lipschitz continuous functions empirically.
- BFGS [LO13],
  - Modify the line search algorithm,
  - Modify the stopping criterion,
  - No convergence analysis.
  - Does not work for non-Lipschitz continuous functions empirically.

Optimization for Partly Smooth Functions

Complexity

- GS,
  - Many gradient evaluations in each iteration
  - Each iteration needs to solve a convex quadratic program.
- BFGS,
  - Less gradient evaluations than GS
  - Solving a convex quadratic program is needed when the sequence is close to convergence.
- Solving a convex quadratical program is expensive.

Optimization for Riemannian Partly Smooth Functions

- Generalized the framework of GS to the Riemannian setting.
- Generalized the modifications of BFGS to the Riemannian setting.
- Empirical performance testing.

General Implementations

- All the discussions about Riemannian optimization algorithms are general,
- General implementations for Riemannian manifolds that can be represented by $\mathbb{R}^n$ are given,
    - $\mathcal{M}$ is a subset of $\mathbb{R}^n$,
    - $\mathcal{M}$ is a quotient manifold with total space be a subset of $\mathbb{R}^n$,
    - $\mathcal{M}$ is a product of two or more manifolds each of which is any of the first two types.

General Implementations

The discussions include

- Representation of metric, linear operator and vector transports,
    - n-dimensional representation,
    - d-dimensional representation (intrinsic approach),
- Constructions and implementations of the vector transports.

Implementations for Four Specific Manifolds

Providing detailed efficient implementations for four particular manifolds:

- the sphere,
- the compact Stiefel manifold,
- the orthogonal group,
- the Grassmann manifold.

Experiments

Four cost functions are tested:

- the Brockett cost function on the Stiefel manifold,
- the Rayleigh quotient function on the Grassmann manifold,
- the Lipschitz minmax function on the sphere,
- the non-Lipschitz minmax function on the sphere.

Experiments

Ten algorithms are compared

- RBFGS,
- Riemannian Broyden family using Davidon's update ϕ [Dav75],
- Riemannian Broyden family using a problem specific ϕ,
- Limited-memory RBFGS,
- Riemannian SD,
- Riemannian GS,
- RTR-SR1,
- Limited-memory RTR-SR1,
- RTR-SD,
- RTR-Newton [Bak08].

Experiments

Systematic comparisons are made. The following are shown in the dissertation.

- Performance of different retractions and vector transports,
- Performance of different choices of ϕ_k,
- Performance of different algorithms,
- The locking condition yield robustness and reliability of Riemannian Broyden family in our framework. Empirical evidence shows it is not necessary but behavior then is often difficult to predict.
- The value of limited-memory versions for large scaled problems,
- The value of Riemannian GS for non-Lipschitz continuous function on a manifold.

Applications

- Applications with smooth enough cost functions,
  - The joint diagonalization problem for independent component analysis,
  - The synchronization of rotation problem,
  - Rotation and reparameterization problem of closed curves in elastic shape analysis,
  - Secant-based nonlinear dimension reduction.
- Application with a partly smooth cost function.
  - Secant-based nonlinear dimension reduction.

The Joint Diagonalization Problem for Independent Component Analysis

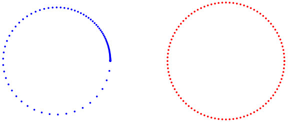
- Independent component analysis (ICA)
  - Determine an independent component form of a random vector,
  - Determine a few components of an independent component form of a random vector.
- Different cost functions are used [AG06], [TCA09]. We used the joint diagonalization cost function[TCA09].
  - The previous algorithm used is RTR-Newton. It is relatively slow when the number of samples are large.
  - RTR-SR1 and LRBFGS are the two fastest algorithms when the number of samples are large.

The Synchronization of Rotation Problem

- The Synchronization of Rotation Problem is to find N unknown rotations $R_1, \ldots R_N$ from M noisy measurements, H_{ij} of $\tilde{H}_{ij} = R_i R_j^T$.
- A review and a Riemannian approach for this problem can be found in [BSAB12].
- Using Riemannian optimization algorithms for the Riemannian approach, we showed that RBFGS and limited-memory RBFGS are the two fastest and reliable algorithms.

Rotation and Reparameterization Problem of Closed Curves in Elastic Shape Analysis

- In elastic shape analysis, a shape is invariant to
  - Scaling
  - Translation
  - Rotation
  - Reparametrization
    - shape1: $x = \cos(2\pi t^3), y = \sin(2\pi t^3), t \in [0, 1]$
    - shape2: $x = \cos(2\pi t), y = \sin(2\pi t), t \in [0, 1]$
- Our work is based on the framework of [SKJJ11].



Rotation and Reparameterization Problem of Closed Curves in Elastic Shape Analysis

- Elastic shape space is a quotient space. When two closed curves are compared, an important problem in elastic space analysis is to find the best rotation and reparametrization function.
- Previous algorithm is a coordinate relaxation of rotation and reparameterization.
  - Rotation: Singular value decomposition
  - Reparameterization: dynamic programming
  - One iteration
- Difficulties
  - High complexity.
  - Not robust when more iterations are used.

Rotation and Reparameterization Problem of Closed Curves in Elastic Shape Analysis

Gradient methods:

- Hessian is unknown,
- Infinite dimensional problem,
- Riemannian quasi-Newton algorithms can be applied,
  - Work for closed curves problem,
  - Reliable and much faster than the coordinate relaxation algorithm.

Secant-based Nonlinear Dimension Reduction

- Suppose $\mathcal{M}$ is a d-dimensional manifold embedded in $\mathbb{R}^n$. The idea is to find a projection $\pi_{[U]} = U(U^T U)^{-1} U^T$ such that $\pi_{[U]}|_{\mathcal{M}}$ is easy to invert, i.e., maximize $k_{\pi_{[U]}}$ where

$$k_{\pi_{[U]}} = \inf_{x,y \in \mathcal{M}, x \neq y} \frac{\|\pi_{[U]}(x-y)\|_2}{\|x-y\|_2}.$$

- The cost function $\phi([U]) = \|\pi_{[U]}(x-y)\|_2 / \|x-y\|_2$ is partly smooth.
- An alternative smooth cost function $F([U])$ is proposed in [BK05].
- Discretization is needed to approximate F and ϕ, called $\tilde{F}$ and $\tilde{\phi}$ respectively.

Secant-based Nonlinear Dimension Reduction

- Previous method used in [BK05] is Riemannian conjugate gradient algorithm for $\tilde{F}([U])$.
- An example (used in [BK00] and [BK05]) is tested
  - For the smooth function $\tilde{F}$, RBFGS and LRBFGS is the two fastest algorithms.
  - For the partly smooth function $\tilde{\phi}$, RBFGS is the fastest algorithm.
  - Even though Riemannian GS is relatively slow, it can escape from local optima and usually find the global optimum.
  - $\tilde{F}$ is a worse cost function than $\tilde{\phi}$ in the sense the global optimum of $\tilde{F}$ may be non-invertible.

Conclusions

- Generalized Broyden family update and symmetric rank-1 update to the Riemannian setting; combined them with line search and trust region strategy respectively and provided complete convergence analysis.
- Generalized limited-memory version of SR1 and BFGS to the Riemannian setting.
- The main work of generalizing quasi-Newton algorithms to Riemannian setting is finished.
- Generalized GS and modified version of BFGS to the Riemannian setting.
- Developed general, detailed and efficient implementations for Riemannian optimization.
- Empirical performances are accessed by experiments and four applications.

Thank you!

Thank you!

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