Optimization on Stiefel Sets by Linear Search

A brief introduction to a typical gradient-based algorithm

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[1] I mainly take reference to: "A feasible method for optimization with orthogonality constraints" by Z. Wen, and W. Yin. 2010; and "Notes on Optimization on Stiefel Manifold" by H. D. Tagare, 2011. The latter is the most accessible document I've found about this topic.

Overview

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Stiefel manifold

Optimization on Stiefel sets

People aimed to develop a procedure to tackle this (non-convex for sure) optimization problem.

$$\min_{X_k \in \mathbb{R}^{n \times p}} F(X_1, X_2, ..., X_K) \qquad \text{subject to } X_k^T X_k = I_p$$

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Definition of Stiefel manifold

Stiefel manifold, or sometimes called Stiefel set, is a set of semi-orthogonal matrices of size $n \times p$, denoted by

$$\mathcal{V}_p(\mathbb{R}^n) \triangleq \{X \in \mathbb{R}^{n \times p} | X^T X = I_p\},$$

where I_p is the identity matrix of size $p \times p$.

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We have nothing to do with the formal definition(s) of manifold, and it suffices to just consider the above thing as a special set. However, it is good to regard a "manifold" as a space that locally resembles Euclidean space near each point.[2]

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Why do we care about it? – For useful applications.

Low-rank nearest correlation estimation

Let $C \in \mathbb{S}^n$ be a given be a given symmetric matrix and $H \geqslant 0$ be a nonnegative (weight) matrix. The low-rank nearest correlation estimation problem is given by

$$\min_{Q \in \mathbb{S}_+^n} \|H \odot (Q - C)\|_F^2, \qquad \text{subject to } Q_{ii} = 1,\ \forall i \in [n];\ \ \operatorname{rank}(Q) \leqslant r,$$

where $\mathbb{S}_+^n$ denotes the set of $n \times n$ positive semi-definite matrices.

The problem tries to find a correlation matrix[3] (which is Q) from an estimate C.
C may not be PSD, since it's usually a noisy estimate.
The rank constraint makes the problem not convex.

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Reformulation of the above

One can express the rank constraints explicitly as $Q = U^T U$ with $U = [U_1, ..., U_n] \in \mathbb{R}^{r \times n}$ with $\|U_i\|_2 = 1, \quad \forall i \in [n]$. And we have

$$\min_{Q \in \mathbb{S}^n_+} \|H \odot (U^T U - C)\|_F^2, \quad \text{subject to } \|U_i\|_2 = 1,\ \forall i \in [n] \iff U_i \in \mathcal{V}_1(\mathbb{R}^r)\ \forall i \in [n]$$

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Gradient descent?

Let's ease ourselve with the (easier, though still hard) problem of

$$\min_{X \in \mathbb{R}^{n \times p}} F(X) \qquad \text{subject to } X^T X = I_p \iff X \in \mathcal{V}_p(\mathbb{R}^n).$$

General gradient-based methods in Euclidean spaces

We usually use this iteration to reach a minimizer:

$$X_{t+1} \leftarrow X_t - \gamma_t \nabla F(X_t)$$

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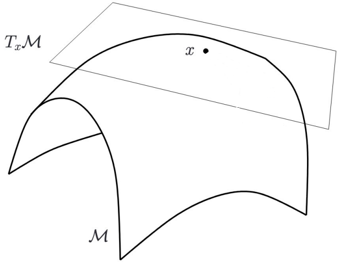
Difficulties come with the feasible set $\mathcal{V}_p(\mathbb{R}^n)$:

- Non-convexity: $\mathcal{V}_p(\mathbb{R}^n)$ is not convex, since $\pm I_{n,p} \in \mathcal{V}_p(\mathbb{R}^n)$, but $0 \notin \mathcal{V}_p(\mathbb{R}^n)$.
- (In)feasibility: hard to stay inside the constraint set: $\mathcal{V}_p(\mathbb{R}^n)$.

Hopefully, we want to adapt such successful way in Euclidean spaces into our new $\mathcal{V}_p(\mathbb{R}^n)$, after some modification if needed.

And, we are not aiming to find a global-minimizer-approaching algorithm, because doing so on a manifold $\mathcal{M}$ is really hard. Instead, what we are trying to obtain is an algorithm to generate a decreasing sequence of feasible X_t's.

Tangent space of an $X \in \mathcal{M}(= \mathcal{V}_p(\mathbb{R}^n))$



Tangent space of $X \in \mathcal{M}$

The tangent space (of X) is a "bridge" connecting the ambient $\mathbb{R}^{n\times p}$ and $\mathcal{M}$. Before taking a step from current $X = X_t$ towards some X_{t+1}, we first want to find the deepest decreasing direction at the tangent plane of X_t.[a]

[a] By the informal definition of manifold.

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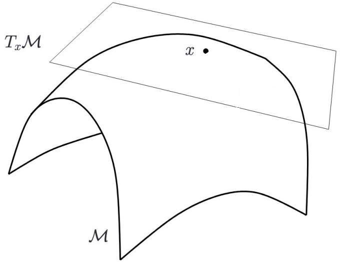

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Pick any $X \in \mathcal{V}_p(\mathbb{R}^n)$, the tangent space of X is denoted as $T_X(\mathcal{V}_p(\mathbb{R}^n))$. Our next goal is to investigate the (directional) derivative starting from X towards the direction $Z \in T_X(\mathcal{V}_p(\mathbb{R}^n))$. Before that, we recall the usual case for $Z \in \mathbb{R}^{n\times p}$:

Directional derivative of F at $X \in \mathcal{M}$ towards direction $Z \in \mathbb{R}^{n\times p}$

$$\mathcal{D}F_X[Z] \triangleq \lim_{t\to 0^+} \frac{F(X+tZ)-F(X)}{t} = \langle \mathcal{D}F_X \cdot Z \rangle_E$$

Overview

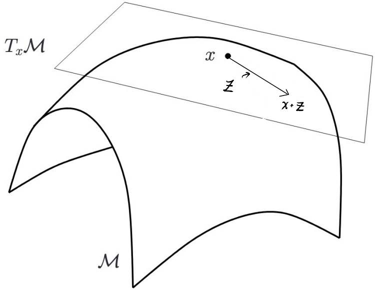
Characterising $T_X(\mathcal{V}_p(\mathbb{R}^n))$

For any $X \in \mathcal{V}_p(\mathbb{R}^n)$, we know $X = [x_1, ..., x_p]$ is made up of p orthonormal columns. Pick another $n - p$ new orthonormal vectors: $v_1, ..., v_{n-p}$ such that $\{x_1, ..., x_p, v_1, ..., v_{n-p}\}$ is a basis of $\mathbb{R}^n$. Define $X_\perp \triangleq [v_1, ..., v_{n-p}] \in \mathbb{R}^{n\times(n-p)}$.

Lemma

$Z = XA + X_\perp B \in T_X(\mathcal{V}_p(\mathbb{R}^n))$, if and only if $A = -A^T$, aka, A is a skew-symmetric matrix.

Side note: $0 \in T_X(\mathcal{V}_p(\mathbb{R}^n))$. The tangent space $T_X(\mathcal{V}_p(\mathbb{R}^n))$ takes X as origin.



Inner product representation of directional derivative

In previous slides, we stated that fix any $X \in \mathcal{V}_p(\mathbb{R}^n)$, for any $Z \in \mathbb{R}^{n\times p}$ (whatever direction),

$$\mathcal{D}F_X[Z] = \sum_{i,j} \frac{\partial F}{\partial X_{i,j}} Z_{i,j} = \mathbf{tr}(G^T Z) = \langle G \cdot Z \rangle_E \in \mathbb{R},$$

where $G = [\frac{\partial F}{\partial X_{i,j}}] \in \mathbb{R}^{n\times p}$. We always use G to denote the usual (Euclidean) gradient of F at X.

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Inner product representation

Fix any $X \in \mathcal{V}_p(\mathbb{R}^n)$, we say G represents[a] the (linear) operator $\mathcal{D}F_X : \underbrace{\mathbb{R}^{n\times p}}_{Z\in} \to \mathbb{R}$ – which is the directional derivative – under Euclidean standard inner product $\langle \cdot \rangle_E$.

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We then restrict $Z \in T_X \subset \mathbb{R}^{n\times p}$. Because we only move inside the T_X. We want to find (1) a matrix W, and (2) an inner product $\langle\cdot\rangle_C$, such that W represents $\mathcal{D}F_X|_{T_X} : T_X \to \mathbb{R}$ under that inner product. Aka, $\forall Z \in T_X$,

$$\mathcal{D}F_X[Z] = \langle W \cdot Z \rangle_C$$

Theorem (Representation of gradient only wrt directions in tangent space.)

Pick any $X \in \mathcal{M} = \mathcal{V}_p(\mathbb{R}^n)$. Analog to G represents the action of $\mathcal{D}F_X$ on $\mathbb{R}^{n\times p}$ under the standard matrix inner product $\langle\cdot\rangle_E$;
W, with $W \triangleq (GX^T - XG^T)X$, represents the action of $\mathcal{D}F_X$ on T_X under another inner product $\langle\cdot\rangle_C$ defined as $\langle Q \cdot H\rangle_C \triangleq \mathbf{tr}(Q^T(I - \frac{1}{2}XX^T)H)$.

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Proof.

Write $G = XG_1 + X_\perp G_2$. Suppose $Z \in T_X$, then $Z = XZ_1 + X_\perp Z_2$, $Z_1 = -Z_1^T$. $\mathcal{D}F_X[Z] = \mathbf{tr}(G^TZ) = \mathbf{tr}(G_1^TZ_1) + \mathbf{tr}(G_2^TZ_2)$. Write $G_1 = G_{1,sym} + G_{1,skew}$. We proceed by $\mathbf{tr}(G_1^TZ_1) + \mathbf{tr}(G_2^TZ_2) = \mathbf{tr}(G_{1,skew}^TZ_1) + \mathbf{tr}(G_2^TZ_2)$.

We want to find some $U = XU_1 + X_\perp U_2 \in T_X$ (by previous lemma $U_1 = -U_1^T$) such that $\langle U \cdot Z\rangle_C = \mathcal{D}F_X[Z]$.

$\langle U \cdot Z\rangle_C = \mathbf{tr}((XU_1 + X_\perp U_2)^T(I - \frac{1}{2}XX^T)(XZ_1 + X_\perp Z_2)) = \frac{\mathbf{tr}(U_1^TZ_1)}{2} + \mathbf{tr}(U_2^TZ_2)$.
Set $U_1 \leftarrow 2G_{1,skew}$ and $U_2 \leftarrow G_2$. We surprisingly achieve that.

Last, rewrite U with X and $G = [\frac{\partial F}{\partial X_{ij}}]$. Using $G_{1,skew} = \frac{G_1 - G_1^T}{2} = \frac{X^TG - G^TX}{2}$.

$$U = 2XG_{1,skew} + X_\perp G_2 = G - XG^TX = (GX^T - XG^T)X.$$

□

Overview

Descent curve

Suppose now we are at some initial guess $X_0 \in \mathcal{M}$. And by previous analysis, we know the direction we should move (on the tangent plane) is $-W$.
Should we move to $\hat{X}_1 \leftarrow X_0 - \gamma_0 W = X_0 - \gamma_0(GX_0^T - X_0 G^T)X_0$, where γ_0 is some stepsize?

Not really, because ${\hat{X}_1}^T \hat{X}_1 \notin \mathcal{M}$. We are moving out of the manifold!

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Not really, because $\hat{X}_1{}^T \hat{X}_1 \notin \mathcal{M}$. We are moving out of the manifold!
We don't need to worry. Some genius came up with good ideas.
When we are at X, we can consider a curve parameterized by $\tau \geqslant 0$:

$$Y(\tau) = (I + \frac{\tau}{2}A)^{-1}(I - \frac{\tau}{2}A)X,$$

where $A = GX^T - XG^T$. Such curve has some good properties:

(1) $\forall \tau \geqslant 0$, $Y(\tau)^T Y(\tau) = I_p$. (one-line proof using $A = -A^T$)

(2) $Y'(0) = -AX$. It starts towards the deepest step on the tangent plane.

(3) $\frac{dF(Y(\tau))}{d\tau}|_{\tau=0} = -\frac{1}{2}\|A\|_F^2 < 0$ if $A \neq 0$.
Hence[4] $\exists$ some $\tau > 0$ such that $F(Y(\tau)) < F(X)$. (Such τ can be found via linear search.)

[4] Thanks to the smoothness of $\mathcal{M}$.

Retraction in general

In general, **retraction** is some map that sends out-of-manifold elements back to the manifold $\mathcal{M}$.

Cayley-transform based retraction

The retraction map we just discussed is termed as a "Cayley-transform" based one. Because "Cayley-transform" means something like:

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with U being skew-symmetric.

Of course, there are other kinds of retractions, e.g.,

Projection based retraction

Let $\xi \leftarrow -\gamma G$ (G always denote the usual gradient $G = [\frac{\partial F}{\partial X_{ij}}]$). One can also consider $X \to (X + \xi)(I + \xi^T \xi)^{-\frac{1}{2}}$. One can actually prove[a] $(X + \xi)(I + \xi^T \xi)^{-\frac{1}{2}} = \Pi_{\mathcal{V}_p(\mathbb{R}^n)}(X + \xi)$.

[a] Lemma 1 of "Weakly convex optimization over Stiefel Manifold using Riemannian subgradient-type methods", 2021

Overview

Simulation results on the "nearest correlation" problem

TABLE 5.6
Computational results for the Low-Rank nearest correlation problem.

	Major			PenCorr			Algorithm 2		
p	resi	CPU	feasi	resi	CPU	feasi	resi	CPU	feasi
Ex1, $H = I$									
2	1.564201e+02	8.34	1.2e-13	1.564172e+02	53.20	4.3e-09	1.686832e+02	0.25	3.5e-15
5	7.883390e+01	4.54	1.4e-13	7.883423e+01	10.34	3.1e-08	7.882875e+01	1.12	3.7e-15
10	3.868525e+01	5.25	5.2e-15	3.868518e+01	6.30	2.9e-07	3.868258e+01	1.01	4.0e-15
20	1.570825e+01	12.64	5.6e-15	1.570796e+01	5.31	7.8e-08	1.570688e+01	1.26	5.1e-15
50	4.140789e+00	142.30	7.1e-15	4.139455e+00	2.29	5.2e-07	4.139235e+00	5.71	5.9e-15
100	1.471204e+00	928.58	9.5e-15	1.466498e+00	2.56	2.4e-07	1.467395e+00	19.46	8.0e-15
125	1.055070e+00	1731.39	9.4e-15	1.048114e+00	2.85	3.0e-08	1.049154e+00	24.65	8.1e-15
Ex1, random H									
2	9.106583e+02	14.64	1.4e-13	9.109902e+02	163.18	4.6e-07	9.778999e+02	0.76	3.6e-15
5	4.536099e+02	31.42	1.2e-13	4.537458e+02	91.15	7.7e-07	4.535966e+02	2.04	3.9e-15
10	2.204165e+02	67.21	5.1e-15	2.204421e+02	69.79	5.4e-07	2.204043e+02	2.08	4.2e-15
20	8.812054e+01	218.99	5.4e-15	8.812887e+01	69.65	3.6e-07	8.851307e+01	3.36	4.9e-15
50	2.203931e+01	2022.31	7.1e-15	2.191649e+01	94.46	8.6e-07	2.188864e+01	27.36	6.0e-15
100	7.110542e+00	9649.30	9.2e-15	6.389784e+00	121.00	2.6e-07	6.457456e+00	39.97	8.0e-15
125	5.030963e+00	13801.88	1.0e-14	4.179018e+00	151.09	9.6e-07	4.348972e+00	48.05	8.8e-15
Ex2, $H = I$									
5	4.127677e+02	10.63	1.6e-13	4.128428e+02	172.70	6.5e-08	4.127542e+02	2.72	5.3e-15
10	3.265122e+02	46.72	6.2e-15	3.263352e+02	185.19	1.2e-07	3.262344e+02	2.73	5.6e-15
20	2.887315e+02	27.11	7.6e-15	2.887228e+02	88.19	3.2e-08	2.886782e+02	9.87	6.6e-15
50	2.763023e+02	78.99	1.0e-14	2.762742e+02	51.40	7.5e-08	2.762733e+02	11.74	8.8e-15
100	2.758067e+02	260.08	1.4e-14	2.757853e+02	9.44	1.7e-08	2.757854e+02	6.35	1.1e-14
150	2.758095e+02	925.63	1.7e-14	2.757853e+02	9.44	1.7e-08	2.757854e+02	7.40	1.3e-14
250	2.758087e+02	1676.32	2.1e-14	2.757853e+02	9.44	1.7e-08	2.757854e+02	11.11	1.6e-14
Ex2, H given by T. Fushiki									
5	1.141113e+04	407.47	2.6e-13	1.147849e+04	2480.31	5.7e-07	1.140483e+04	35.89	5.1e-15
10	7.586522e+03	1299.88	6.1e-15	7.638036e+03	2305.20	2.8e-07	7.586921e+03	33.17	5.8e-15
20	5.200671e+03	1733.57	7.3e-15	5.219117e+03	2062.14	2.7e-07	5.194958e+03	30.54	6.1e-15
50	3.712916e+03	4154.29	9.0e-15	3.718507e+03	1356.16	2.0e-09	3.711896e+03	21.99	7.8e-15
100	3.503209e+03	6426.36	1.2e-14	3.507128e+03	906.02	3.3e-07	3.502541e+03	22.05	9.7e-15
150	3.501124e+03	8734.17	1.6e-14	3.505351e+03	824.69	3.1e-07	3.500676e+03	27.78	1.1e-14
250	3.501170e+03	15595.92	2.0e-14	3.505351e+03	864.67	3.1e-07	3.500654e+03	40.59	1.4e-14

Remarks

"Algorithm 2" is the proposed method.

resi: objective value.
CPU: running time (sec).
feasi: infeasibility.

All 3 metrics are "the lower the better".

Improvement is achieved in running time, especially for the nontrivial H cases.[a]

[a] Thanks to an efficient implementation of the original Cayley transform.

Codebase repository

The authors put their MatLab codes – with quite high-quality implementation – of this problem to GitHub.[5] There are some more extensions, but the usage are similar.

$$\min_{X \in \mathbb{R}^{n \times p}} F(X) \qquad \text{subject to } X^T X = I_p$$

Anyone can use their API in the following way:

```
X0 = 1/np.sqrt(n) * np.ones((n, p));
opts.record = 0;
opts.mxitr  = 2000;
opts.xtol = 1e-20;
opts.gtol = 1e-20;
opts.ftol = 1e-20;

[X, out]= OptStiefelGBB(X0, @fun, opts, arg1, arg2, arg3);


    function [F, G] = fun(X, arg1, arg2, arg3)
            F = ... ## Define your function here
            G = ... ## Calculate the usual gradient here
    end
```

[5] https://github.com/optsuite/OptM