Orthogonalization-free Approaches for Optimization Problems on Stiefel Manifold

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Optimization Problem with Orthogonality Constraints

General form

$$\min_{X \in \mathbb{R}^{n \times p}} \quad f(X)$$
$$\text{s. t.} \quad X^\top X = I. \qquad \text{(OCP)}$$

- $n > p$
- $p(p+1)/2$ constraints –– nonconvex
- Stiefel manifold:

$$\mathcal{S}_{n,p} := \{X \in \mathbb{R}^{n \times p} \mid X^\top X = I\}.$$

Why interesting?

- Special manifold optimization
- Emerging application

Emerging Applications

Homogeneous quadratic objective
– Rayleigh-Ritz trace maximization

$$\max_{X \in \mathbb{R}^{n \times p}} \quad f(X) := \mathbf{tr}(X^\top A X),$$
$$\text{s. t.} \quad X^\top X = I.$$

- Subspace approaches:
  - LOBPCG: Knyazev 2001,
  - LMSVD: Liu-Wen-Zhang 2013,
  - ARRABIT: Wen-Zhang 2017
- Penalty function approaches:
  - EIGPEN: Wen-Yang-Liu-Zhang 2016,
  - SLRP: Liu-Wen-Zhang 2015

Emerging Applications (Cont'd)

Smooth objective

– Discretized Kohn-Sham total energy minimization

$$\min\ E(X) \quad \text{s. t.} \quad X^\top X = I, \quad X \in \mathbb{R}^{n\times p},$$

where, for $\rho(X) := \text{diag}(XX^\top)$,

$$E(X) := \frac{1}{4}\text{tr}(X^\top LX) + \frac{1}{2}\text{tr}(X^\top V_{ion}X) + \frac{1}{2}\sum_i \sum_l |x_i^\top w_l|^2 + \frac{1}{4}\rho^\top L^\dagger \rho + \frac{1}{2}e^\top \epsilon_{xc}(\rho).$$

1. Kinetic energy (L: discretizede Laplacian operator)
2. Local ionic potential energy (V_{ion}: discretized ionic pseudopotentials)
3. Nonlocal ionic potential energy (w_l: projection function)
4. Hartree potential energy ($L^\dagger$: pseudo-inverse of L)
5. Exchange correlation energy (ϵ_{xc}: interaction between electrons)

- Self-Consistent Field Iteration: Gao-Yang-Meza 2009, Liu-Wang-Wen-Y. 2014, Liu-Wen-Wang-Ulbrich-Y. 2015
- Optimization: Yang-Meza-Wang 2007, Wen-Milzarek-Ulbrich-Zhang 2013, Dai-Liu-Zhang-Zhou, 2017

Emerging Applications (Cont'd)

Smooth objective (Cont'd) – Spectral Clustering

- Ratio cut: Chen-Liu-Y. 2020

$$\begin{aligned} \min_{X\in\mathbb{R}^{n\times p}} \quad & \mathrm{tr}(X^\top LX), \\ \text{s. t.} \quad & X^\top X = I, \\ & X \geq 0, \\ & e^\top XX^\top e = n. \end{aligned}$$

- Connected subgraph: Liu-Ng-Zhang-Zhang 2018

$$\begin{aligned} \min_{X\in\mathbb{R}^{n\times n}, H\in\mathbb{R}^{n\times p}} \quad & f(X,H) = \mathrm{tr}[H^\top \mathcal{L}(A\circ X)H] - \beta\cdot\mathrm{tr}(AX), \\ \text{s. t.} \quad & X \in [0,1]^{n\times n} \cap \mathcal{S}^n_A, \\ & H^\top H = I_d. \end{aligned}$$

Emerging Applications (Cont'd)

Nonsmooth objective – statistic data analysis

- Sparse principal component analysis: Joliliffe-Reendafilov-Uddin 2003, Zou-Xue 2018

$$\min_{X \in \mathbb{R}^{n\times p}} \quad -\frac{1}{2}\mathrm{tr}\left(X^\top L X\right) + \gamma \|X\|_1$$
$$\text{s. t.} \quad X^\top X = I_p,$$

- Sparse variable PCA: Ulfarsson-Solo 2008, Chen-Zou-Cook 2010; regularized discriminative feature selection: Tang-Liu 2012

$$\min_{X \in \mathbb{R}^{n\times p}} \quad \frac{1}{2}\mathrm{tr}\left(X^\top M X\right) + \sum_{j=1}^{n} \gamma_j \left\|X_{j\cdot}\right\|_2$$
$$\text{s. t.} \quad X^\top X = I_p,$$

- Dual principal component pursuit: Xu-Caramanis-Sanghavi 2010

$$\min_{W \in \mathbb{R}^{n\times p}} \quad \left\|W^\top Y\right\|_1$$
$$\text{s. t.} \quad W^\top W = I_p,$$

Part I. Smooth Objective

Many Existing Methods, including

Optimization on matrix manifolds

- Steepest descent: Helmke-Moore 1994; Udriste 1994
- Conjugate gradient: Edelman-Arias-Smith 1998; Brace-Manton 2006; Smith 1994; Gallivan-Absil 2010
- Newton: Smith 1994; Edelman-Arias-Smith 1998
- Quasi-Newton: Edelman-Arias-Smith 1998; Brace-Manton 2006; Gallivan-Absil 2010; Huang-Gallivan-Absil 2015
- Trust region: Absil-Baker-Gallivan 2007
- Geodesic search in canonical metric: Abrudan-Eriksson-Koivunen 2008
- Cayley transformation: Nishimori-Akaho 2005

Searching in tangent space

- Projection-based method: Manton 2002; Absil-Mahony-Sepulchre 2008; Dai-Zhang-Zhou 2019
- Constraint preserving update scheme: Wen-Yin 2012; Jiang-Dai 2014
- Structured Quasi-Newton: Hu-Jiang-Lin-Wen-Yuan 2018
- Regularized Newton: Hu-Wen-Milzarek-Yuan 2017

Other type of works

- Splitting and alternating: Lai-Osher 2014; Rosman-Tai-Kimmel-Bruckstein 2014
- Multiplier correction framework including GR/GP, CBCD: Gao-Liu-Chen-Y. 2018, SIAM Journal on Optimization

Bottleneck (when p is large)

Feasibility/Orthogonalization

- **Orthonormalization — lacks of concurrency**
- **Column-wise parallelization — lacks of scalability**

Our Approach: infeasible method

- **Key point: efficient in serial**
- **To keep the structure: penalty function method**
- **Nonsmooth penalty function is intractable**

$$\min_{X \in \mathbb{R}^{n \times p}} \quad f(X) + \gamma \|X^\top X - I_p\|_1$$

Augmented Lagrangian Method (ALM)

Augmented Lagrangian penalty function

(Powell 1969; Hestenes 1969)

$$\mathcal{L}(X, \Lambda) := f(X) - \frac{1}{2}\mathrm{tr}\left(\Lambda(X^\top X - I_p)\right) + \frac{\beta}{4}\left\|X^\top X - I_p\right\|_\mathrm{F}^2.$$

- Exact penalty function

ALM with dual ascend

1. Choose an initial point X_0, Λ_0, $k = 0$
2. Update X_k by $X_{k+1} = \arg\min_X \; \mathcal{L}(X, \Lambda_k)$
3. Update Λ_k by $\Lambda_{k+1} = \Lambda_k - \tau_k \beta(X_{k+1}^\top X_{k+1} - I_p)$

- Solving subproblem with fixed multiplier
- Updating multiplier by dual ascent
- Numerically inefficient

Motivation: First-order Optimality

First-order Optimality (OCP)

$$\begin{cases} \nabla f(X) - X\Lambda & = & 0; \\ X^\top X & = & I. \end{cases}$$

Lagrangian multipliers: $\Lambda = X^T \nabla f(X)$
at any first-order stationary point.

Updating multipliers in closed-form

$$\Lambda_{k+1} := \Phi(X_k^T \nabla f(X_k)),$$

$\Phi : \mathbb{R}^{n\times n} \mapsto \mathbb{S}^n$ is defined by $\Phi(A) := \frac{1}{2}(A + A^\top)$.

Explicit Multiplier Updating Scheme

Gao-Liu-Y. 2019, SIAM Journal on Scientific Computing

Proximal Linearized Augmented Lagrangian Method (PLAM)

- $\Lambda_k = \Phi(X_k^\top \nabla f(X_k))$, $\quad \Phi(M) = \frac{1}{2}(M + M^\top)$
- Gradient step in $\min \mathcal{L}(X, \Lambda_k)$:

$$X_{k+1} = X_k - \eta_k \nabla_X \mathcal{L}(X_k, \Lambda_k).$$

- Exact penalty, global convergence, local linear convergence
- Comparable with existent algorithms with subtly selected β

Column-wise block minimization of PLAM (PCAL)

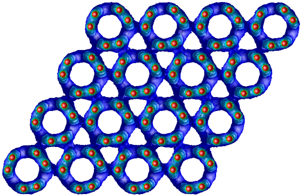
- Column-wise normalization:

$$(X_{k+1})_i = (X_k - \eta_k \nabla_X \mathcal{L}(X_k, \Lambda_k)_i / \|(X_k - \eta_k \nabla_X \mathcal{L}(X_k, \Lambda_k)_i\|_2$$

- Not sensitive with β
- Comparable with feasible algorithms
- Much better scalability in parallel computing

PCAL Applied in Electronic Structure Calculation

Gao-Hu-Kuang-Liu, An Orthogonalization-free Parallelizable Framework for All-electron Calculations in Density Funcitonal Theory, arXiv:2007.14228



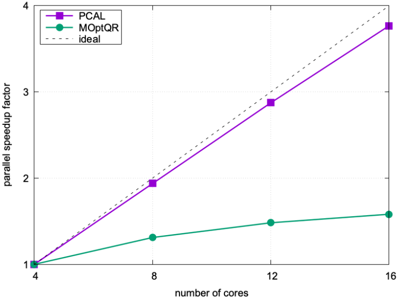


Figure 1: Calculation on AFEABIC: C_{384} with $n = 380233$, $p = 1152$. Left: the isosurface of the electron density at value 0.2. Right: the speedup factor for this example.

Still Not Perfect

PLAM & PCAL

- Understanding of the merit function

$$h(X) := f(X) - \frac{1}{2}\text{tr}\left(\Phi\left(X^\top \nabla f(X)\right)(X^\top X - I_p)\right) + \frac{\beta}{4}\left\|X^\top X - I_p\right\|_\text{F}^2$$

- Why PCAL is better?
- Possible extension: second-order method?

Exact Penalty Function

Is $h(x)$ an exact penalty function?

- If X^* is a first-order stationary point of (OCP), then

$$\nabla h(X^*) = 0.$$

- How about the other way round?

$$\nabla h(X) = 0 \Rightarrow X^\top X = I_p?$$

A crucial Issue:

$h(X)$ **may be unbounded from below – an example**

- $f(X) = \frac{1}{4}\left\|X^\top X\right\|_{\mathrm{F}}^2$
- $h(X) = \frac{1}{4}\left\|X^\top X\right\|_{\mathrm{F}}^2 - 2\mathrm{tr}\left((X^\top X)^2(X^\top X - I_p)\right) + \frac{\beta}{4}\left\|X^\top X - I_p\right\|_{\mathrm{F}}^2$
- $\|X\|_{\mathrm{F}} \to +\infty \Rightarrow h(X) \to -\infty.$

A New Penalty Model

Xiao-Liu-Y., A Class of Smooth Exact Penalty Function Methods for Optimization Problems with Orthogonality Constraints, optimization online: 2020/02/7607

Restrict $h(X)$ in a bounded set

$$\min_{X \in \mathcal{M}} \quad h(X). \qquad \text{(PenC)}$$

- $\mathcal{M}$ is convex and compact, $\mathcal{S}_{n,p} \subset \mathcal{M}$
- Projection to $\mathcal{M}$ can be easily calculated

Possible choices of $\mathcal{M}$:

- Ball ($\mathcal{B}$) with radius $K \geq \sqrt{p}$
- Convex hull of Stiefel manifold: $\{X \in \mathbb{R}^{n \times p} | \, \|X\|_2 \leq 1\}$
- Convex hull of Oblique manifold: $\{X \in \mathbb{R}^{n \times p} | \, \|(X)_i\|_2 \leq 1\}$
- ...

Assumptions

Assumption 1

$f(X)$ is differentiable, $\nabla f(X)$ is Lipschitz continuous.

- Does not imply the existence of $\nabla h(X)$

Assumption 2

$f(X)$ is twice continuous differentiable, and $\nabla^2 f(X)$ is Lipschitz continuous for each $X \in \mathbb{R}^{n\times p}$.

- Does not imply the existence of $\nabla^2 h(X)$

Constants

- $M_0 := \sup_{X\in\mathcal{M}} \max\{1, \|\nabla f(X)\|_{\mathrm{F}}\}$, $\quad M_1 := \sup_{X\in\mathcal{M}} \max\{1, \|\Lambda(X)\|_{\mathrm{F}}\}$;
- $C_1 := \sup_{X\in\mathcal{M}} \tilde{h}(X) - \inf_{X\in\mathcal{M}} \tilde{h}(X)$, $\quad L_1 := \sup_{X\in\mathcal{M}} \frac{1}{\|X-Y\|_2} \|\Lambda(X) - \Lambda(Y)\|_2$;
- $L_2 := \sup_{X\in\mathcal{M}, Y\in\mathbb{R}^{n\times p}} \limsup_{t\to 0} \frac{\|\nabla\tilde{h}(X+tY) - \nabla\tilde{h}(X)\|_{\mathrm{F}}}{t\|Y\|_{\mathrm{F}}}$, $M_3 := \sup_{X\in\mathcal{M}} \max\{1, \|\nabla^2 f(X)\|_{\mathrm{F}}\}$.

Properties of Penalty Model

First-order Stationarity

Theorem 1

Suppose Assumption 1 holds. Let $\tilde{X}$ *be a first-order stationary point of* (PenC) *with* $\beta \geq \max\{2(M_0 + M_1), 2pL_1\}$, *then either* $\tilde{X}$ *is a first-order stationary point of problem* (OCP) *, or* $\sigma_{\min}(\tilde{X}^\top \tilde{X}) \leq \frac{2M_1 + \sqrt{2}L_1}{2\beta}$.

Lemma 1

Suppose Assumption 1 holds. Let $0 < \delta \leq \frac{1}{3}$ *and* $\beta \geq \max\left\{2(M_0 + M_1), 2pL_1, \left(3M_1 + \frac{3\sqrt{2}}{2}L_1\right), \ \frac{2C_1}{\delta^2}\right\}$. *For any* $X \in \mathcal{M}$, *it holds that*

$$\sup_{\|X^\top X - I_p\|_{\mathrm{F}} \leq \delta} h(X) < \inf_{\|X^\top X - I_p\|_{\mathrm{F}} \geq 2\delta} h(X).$$

Moreover, any global minimizer X^* *of PenC satisfies* $X^{*\top} X^* = I_p$ *which further implies that it is a global minimizer of problem* (OCP) *.*

Properties of Penalty Model (Cont'd)

Second-order Stationarity

Theorem 2

Suppose Assumption 2 holds, and $\mathcal{M}$ is chosen as
$\mathcal{B} := \{X \in \mathbb{R}^{n\times p} | \, \|X\|_{\mathrm{F}} \leq K, K > \sqrt{p}\}$ *and*
$\beta \geq \max\left\{2(M_0 + M_1), 2pL_1, 6M_1 + 3\sqrt{2}L_1, 2L_2 + 1, \frac{6L_2+12KM_2+1}{5}\right\}$.
Then, any second-order stationary point $\tilde{X}$ of (PenC) *satisfies* $\tilde{X}^\top \tilde{X} = I_p$. *Moreover, $\tilde{X}$ is a second-order stationary point of problem* (OCP) *.*

Algorithm

Problem reformulation

$$\begin{aligned} \min \quad & f(X) \\ \text{s.t.} \quad & X^\top X = I_p, \end{aligned} \quad \Rightarrow \quad \min_{X \in \mathcal{B}} \quad h(X).$$

- $K > \sqrt{p}$

Gradient of $h(X)$

$$\begin{aligned} \nabla h(X) = & \nabla f(X) - X\Lambda(X) + \beta X(X^\top X - I_p) \\ & -\frac{1}{2}\left(\nabla f(X)(X^\top X - I_p) + \nabla^2 f(X)[X(X^\top X - I_p)]\right) \end{aligned}$$

Denote $G(X) := \nabla f(X) - X\Lambda(X) + \beta X(X^\top X - I_p)$

- Exact gradient involves $\nabla^2 f(X)$, unaffordable
- Omit the red part

First-order Method for Penalty Model with Compact Convex Constraints (PenCF)

1. Choose an initial guess X_0, set $k = 0$;
2. Compute $\Lambda(X_k)$;
3. Update X_k by

$$X_{k+1} = X_k - \eta_k(\nabla f(X_k) - X_k\Lambda(X_k) + \beta X_k(X_k^\top X_k - I_p));$$

4. If $\|X_{k+1}\|_F \geq K$, project X_{k+1} back to $\mathcal{B}$;
5. If certain stopping criterion is satisfied, return X_{k+1}; Otherwise, set $k := k + 1$ and go to Step 2.

Global Convergence

Theorem 3

Suppose Assumption 1 holds, $\delta \in \left(0, \frac{1}{3}\right]$, $K \geq \sqrt{p + \delta \sqrt{p}}$, *and* $\beta \geq \max\left\{2(M_0 + M_1), 2pL_1, \;\; 3M_1 + \frac{3\sqrt{2}}{2}L_1\right\}$. *Let* $\{X_k\}$ *be the iterate sequence generated by PenCF initiated from* $X_0 \in \mathcal{M}$ *satisfying* $\|X_0^\top X_0 - I_p\|_{\mathrm{F}} \leq \delta$, *and the stepsize* $\eta_k \in \left[\frac{1}{2}\bar{\eta}, \bar{\eta}\right]$, *where* $\bar{\eta} = \min\left\{\frac{\delta}{8KM_4}, \frac{\beta\delta^2}{9K^2L_1M_4^2}, \frac{1}{45(L_0+M_1)+137\beta}\right\}$, $M_4 = M_0 + M_1K + \beta\delta K$.
Then, the iterate sequence $\{X_k\}$ *has at least one cluster point, and each cluster point of* $\{X_k\}$ *is a stationary point of problem* (OCP) *.*
More precisely, for any $N \geq 1$, *it holds that*

$$\min_{0\leq i\leq N-1} \max\left\{\|X_i^\top X_i - I_p\|_{\mathrm{F}}, \|G_i\|_{\mathrm{F}}\right\} \leq \max\left\{\frac{2\sqrt{3}}{3M_1}, 1\right\} \cdot \sqrt{\frac{5C_1 + \frac{5}{4}\beta\delta^2}{N\bar{\eta}}},$$

where $G_i = G(X_i)$.

Local Convergence Rate

Theorem 4

Suppose Assumption 2 holds, X^* is an isolated local minimizer of (OCP), and we denote

$$\tau := \inf_{Y^\top X^* + X^{*\top} Y = 0} \frac{\nabla^2 f(X^*)[Y,Y] - \mathrm{tr}\left(Y^\top Y \Lambda(X^*)\right)}{\|Y\|_F^2}.$$

The algorithm parameters satisfy $\beta \geq \frac{1}{2}M_3 + \frac{\sqrt{3}M_0}{3} + \frac{1}{2}\tau$ and $\eta_k \in [\frac{\bar{\eta}}{2}, \bar{\eta}]$, where $\bar{\eta} \geq M_3 + \frac{2\sqrt{3}M_0}{3} + 2\beta$. Then, there exists $\varepsilon > 0$ such that starting from any X_0 satisfying $\|X_0 - X^*\|_F < \varepsilon$, the iterate sequence $\{X_k\}$ generated by PenCF converges to X^* Q-linearly.

PLAM and PCAL – Further Explanation

PLAM

- $\mathcal{M} = \mathbb{R}^{n \times p}$
- $h(x)$ is not bounded below: small $\beta \Rightarrow$ divergence

PCAL

- $\mathcal{M} = \mathcal{OB}_{n,p}$
- (PenC) is bounded below: accept smaller β

PenCF

- $\mathcal{M} = \{X \in \mathbb{R}^{n \times p} \mid \|X\|_{\mathrm{F}} \leq K\} \Rightarrow$ cheap projection
- Constraint becomes inactive when close to $\mathcal{S}_{n,p}$

Both PLAM and PCAL can be regarded as applying approximate gradient method to solve corresponding (PenC) .

- better than ALM
- Comparable with existing retraction-based first-order methods

Preliminary Numerical Experiments

Running Platform

- ThundeRobot personal computer with an Intel Core i7-9700 CPU @ 3.6GHz×8 and 16 GB of RAM
- Ubuntu 18.04
- MATLAB R2018b

Stopping criteria

- Substationarity: $\|\nabla f(X_k) - X_k \Lambda(X_k)\|_F \leq 10^{-8}$
- Max iteration: 2000 for PenCF, 10 for PenCS.

Testing Problems

Problem 1

Simplified Kohn-Sham total energy minimization including the non-classical and quantum interaction between electrons.

$$\begin{aligned} \min_{X \in \mathbb{R}^{n \times p}} \quad & \frac{1}{2} tr\left(X^\top L X\right) + \frac{1}{4} \rho^\top L^\dagger \rho - \frac{3\gamma}{4} \rho^\top \rho^{\frac{1}{3}} \\ \text{s.t.} \quad & X^\top X = I_p, \end{aligned}$$

where $\rho = \mathrm{Diag}\left(XX^\top\right)$ *and* γ *is a constant.*

Testing Problems (Cont'd)

Problem 2

Minimizing quadratic function over Stiefel manifold

$$\begin{aligned} \min_{X \in \mathbb{R}^{n \times p}} \quad & tr\left(X^\top A X\right) + tr\left(G^\top X\right) \\ \text{s.t.} \quad & X^\top X = I_p. \end{aligned}$$

Both A and G are randomly generated with Gaussian distribution.

Default Setting

Barzilai-Borwein stepsize: Barzilai-Borwein 1988

$$\eta_k^{\mathrm{BB1}} := \frac{|\langle S_{k-1}, Y_{k-1}\rangle|}{\langle S_{k-1}, S_{k-1}\rangle}, \quad \text{or} \quad \eta_k^{\mathrm{BB2}} := \frac{\langle Y_{k-1}, Y_{k-1}\rangle}{|\langle S_{k-1}, Y_{k-1}\rangle|},$$

where

$$\begin{aligned} S_k &= X_k - X_{k-1}, \\ Y_k &= \nabla_X \mathcal{L}(X_k, \Lambda_k) - \nabla_X \mathcal{L}(X_{k-1}, \Lambda_{k-1}) \end{aligned}$$

Alternating BB strategy: Dai-Fletcher 2005

$$\eta_k^{\mathrm{ABB}} := \begin{cases} \eta_k^{\mathrm{BB1}}, & \text{for odd } k, \\ \eta_k^{\mathrm{BB2}}, & \text{for even } k. \end{cases}$$

Post-process by Orthonormalization

Why Post-process?

- To attain high accuracy on feasibility
- To maintain mild accuracy on the substationarity

How to Post-process?

- $X_k^{\mathrm{orth}} := UV^\top$, economy-size SVD: $X_k = U\Sigma V$

Proposition 1

Suppose Assumption 1 holds, $\beta \geq 1 + 2L_0 + 2L_1 + 2M_1$ and $X \in \mathcal{M}$. Let $X = U\Sigma V^\top$ be the economy-size SVD for X and $\mathrm{orth}(X) = UV^\top$. Then, it holds that

$$h(X^{\mathrm{orth}}) \leq h(X) - \frac{1}{4}\left\|X^\top X - I_p\right\|_{\mathrm{F}}^2 .$$

Experiments on Kohn-Sham DFT

Problem generation

- Yang-Meza-Lee-Wang 2009 KSSOLV a Matlab toolbox for solving the Kohn-Sham equations, *ACM Trans. Math. Softw. 36, 135*
- Downloadable from http://crd-legacy.lbl.gov/~chao/KSSOLV/

Testing Methods

- SCF: self-consistent field method
- TRDCM: trust-region direct constrained minimization Meza-Wang-Yang 2007
- MOptQR: optimization algorithms on manifold with retraction based on QR factorization + BB step size Boumal-Mishra-Absil-Sepulchre, 2014(version 4.0 2018)
  (downloadable from http://www.manopt.org)
- OptM: algorithm by Wen-Yin 2013 (BB stepsize)
  (downloadable from http://optman.blogs.rice.edu)
- PCAL: algorithm by Gao-Liu-Yuan 2019 $\eta = \eta_{ABB}, \beta = 1$
  (downloadable from http://lsec.cc.ac.cn/~liuxin/index.html)
- PenCF: $\eta = \eta_{\mathrm{ABB}}, \beta = 1, K = 1.1\sqrt{p}$.

Solver	E_{tot}	Substationarity	Iteration	Feasibility	CPU time(s)
alanine, $n = 12671, p = 18$					
SCF	-6.1161921213050e+01	3.14e-09	20	7.31e-15	21.63
TRDCM	-6.1161921213046e+01	2.28e-06	200	4.91e-15	150.53
ManOptQR	-6.1161921213050e+01	5.68e-09	185	3.89e-15	30.10
OptM	-6.1161921213050e+01	2.30e-09	105	3.79e-14	18.23
PCAL	-6.1161921213050e+01	5.94e-09	106	3.63e-15	19.47
PenCF	-6.1161921213050e+01	5.96e-09	113	3.55e-15	18.92
al, $n = 16879, p = 12$					
SCF	-1.5769678051112e+01	1.08e-01	200	5.59e-15	175.33
TRDCM	-1.5803817596149e+01	3.33e-08	200	3.68e-15	133.41
ManOptQR	-1.5630343515632e+01	9.67e-01	2000	6.39e-15	311.84
OptM	-1.5803791154679e+01	2.47e-09	1942	1.10e-14	303.16
PCAL	-1.5803817596151e+01	1.90e-08	2000	1.54e-12	310.82
PenCF	-1.5803817596151e+01	9.93e-09	1722	1.67e-14	266.62
benzene, $n = 8407, p = 15$					
SCF	-3.7225751362902e+01	3.45e-09	17	7.21e-15	9.20
TRDCM	-3.7225751362902e+01	8.83e-09	44	6.77e-15	16.68
ManOptQR	-3.7225751362902e+01	1.27e-09	135	2.62e-15	11.97
OptM	-3.7225751362902e+01	2.42e-09	99	2.17e-14	9.20
PCAL	-3.7225751362902e+01	9.13e-09	89	2.44e-15	8.72
PenCF	-3.7225751362902e+01	5.70e-09	95	3.04e-15	8.72
c12h26, $n = 5709, p = 37$					
SCF	-8.1536091936606e+01	3.19e-09	23	1.15e-14	29.92
TRDCM	-8.1536091936555e+01	6.80e-06	200	9.83e-15	149.25
ManOptQR	-8.1536091936606e+01	9.26e-09	822	5.56e-15	141.71
OptM	-8.1536091936606e+01	1.41e-09	120	9.51e-14	23.07
PCAL	-8.1536091936606e+01	9.05e-09	117	1.19e-14	24.45
PenCF	-8.1536091936606e+01	8.54e-09	108	5.95e-15	20.85

Solver	E_{tot}	Substationarity	Iteration	Feasibility	CPU time(s)
glutamine, $n = 16517, p = 29$					
SCF	-9.1839425243648e+01	3.75e-09	23	8.69e-15	71.50
TRDCM	-9.1839425243571e+01	9.55e-06	200	8.11e-15	496.17
ManOptQR	-9.1839425243648e+01	6.01e-09	119	6.61e-15	59.35
OptM	-9.1839425243648e+01	1.18e-09	143	5.67e-15	71.75
PCAL	-9.1839425243648e+01	9.28e-09	127	9.53e-15	66.50
PenCF	-9.1839425243648e+01	5.02e-09	128	5.99e-15	62.64
graphene16, $n = 3071, p = 37$					
SCF	-9.4032618962855e+01	6.28e-02	200	1.24e-14	129.52
TRDCM	-9.4046217544979e+01	8.13e-06	200	9.09e-15	104.55
ManOptQR	-9.4046217545036e+01	7.08e-09	746	5.61e-15	77.18
OptM	-9.4046217545036e+01	1.66e-09	298	5.01e-15	31.89
PCAL	-9.4046217545036e+01	8.83e-09	276	5.44e-15	32.45
PenCF	-9.4046217545036e+01	6.07e-09	270	5.44e-15	28.41
ptnio, $n = 4069, p = 43$					
SCF	-2.2678884272587e+02	5.39e-09	99	1.50e-14	88.09
TRDCM	-2.2678883639168e+02	2.89e-04	200	1.05e-14	136.59
ManOptQR	-2.2678884272587e+02	9.52e-09	697	5.01e-15	100.67
OptM	-2.2678884272587e+02	2.40e-09	864	4.52e-15	125.62
PCAL	-2.2678884272587e+02	9.70e-09	699	5.36e-15	110.28
PenCF	-2.2678884272587e+02	7.83e-09	693	4.38e-15	95.34
ctube661, $n = 12599, p = 48$					
SCF	-1.3463843176502e+02	6.79e-09	19	1.39e-14	62.98
TRDCM	-1.3463843176491e+02	1.05e-05	200	1.04e-14	487.15
ManOptQR	-1.2304610718869e+02	7.04e+00	2000	6.70e-15	967.80
OptM	-1.3463843176501e+02	1.97e-09	120	5.91e-15	64.29
PCAL	-1.3463843176502e+02	8.39e-09	112	5.75e-15	61.94
PenCF	-1.3463843176502e+02	3.17e-09	120	7.61e-15	59.55

Second-order Methods

Suppose computing $\nabla^2 f(X)$ is affordable

- To compute $\nabla h(X)$ becomes affordable:

$$\begin{aligned}\nabla h(X) = \nabla f(X) - X\Lambda(X) + \beta X(X^\top X - I_p) \\ - \left(\nabla f(X)(X^\top X - I_p) + \nabla^2 f(X)[X(X^\top X - I_p)]\right)\end{aligned}$$

- To compute $\nabla^2 h(X)$ is still intractable
- Solution: approximate $\nabla^2 h(X)$ by ∇f and $\nabla^2 f$

Motivation: delete high-order terms in Hessian

$$
\begin{aligned}
\nabla^2 h(X)[D,D] =& \nabla^2 f(X)[D,D] \\
&- \mathrm{tr}\left(\Lambda(X)D^\top D - D^\top \nabla f(X)\Phi(D^\top X) - X^\top \nabla^2 f(X)[D]\Phi(D^\top X)\right) \\
&- \frac{1}{2}\mathrm{tr}\left(\left(D^\top \nabla^2 f(X)[D] + \frac{1}{2}X^\top \nabla^3 f(X)[D,D]\right)(X^\top X - I_p)\right) \\
&+ \mathrm{tr}\left(\beta X^\top X D^\top D + \beta D^\top X X^\top D + \beta X^\top D X^\top D - \beta D^\top D\right).
\end{aligned}
$$

$$
\begin{aligned}
W(X)[D,D] :=& \nabla^2 f(X)[D,D] \\
&- \mathrm{tr}\left(\Lambda(X)D^\top D - D^\top \nabla f(X)\Phi(D^\top X) - X^\top \nabla^2 f(X)[D]\Phi(D^\top X)\right) \\
&+ \mathrm{tr}\left(\beta X^\top X D^\top D + \beta D^\top X X^\top D + \beta X^\top D X^\top D - \beta D^\top D\right).
\end{aligned}
$$

- $\left\|W(X) - \nabla^2 h(X)\right\|_\mathrm{F} \to 0$ as $\left\|X^\top X - I_p\right\|_\mathrm{F} \to 0$

Second-order Method

Subproblem

$$\begin{aligned} \min \quad & \frac{1}{2} W(X_k)[D, D] + \mathrm{tr}\left(D^\top \nabla h(X_k)\right) \\ \text{s.t.} \quad & \|X_k + D\|_{\mathrm{F}} \le K. \end{aligned} \qquad \text{(TRS)}$$

- Trust region subproblem: computing global minimizer is tractable
- $\nabla h(X)$ is sufficiently small $\Rightarrow$ inactive constraint

Second-order Method for Penalty Model with Compact Convex Constraints (PenCS)

1. Choose an initial guess X_0, set $k = 0$;
2. Compute stepsize η_k;
3. Compute D_k by solving (TRS) , set $X_{k+1} = X_k + \eta_k D_k$;
4. If certain stopping criterion is satisfied, return X_{k+1}; Otherwise, set $k := k + 1$ and go to Step 2.

Theoretical Results

Theorem 5

Suppose Assumption 2 holds. X^* *is an isolated local minimizer of (OCP) with*

$$\tau := \inf_{Y^\top X^* + X^{*\top} Y = 0} \frac{\nabla^2 f(X^*)[Y,Y] - tr\left(Y^\top Y \Lambda(X^*)\right)}{\|Y\|_F^2} > 0\,.$$

When $\delta \in (0, \frac{1}{3})$, $K \geq \sqrt{p + \delta\sqrt{p}}$,
$\beta \geq \max\left\{2pL_1, \frac{2p(M_0+M_1)}{3}, 6M_1 + 12L_1, \frac{2(L_2+pM_1)}{3}, 2L_2 + 1, \frac{4L_2^2+\tau^2}{\tau}\right\}$ *and stepsize* $\eta_k = 1$, *there exists a sufficiently small* ε *such that when* $\|X_0 - X^*\|_F \leq \varepsilon$, X_k *generated by PenCS converges to* X^* *quadratically.*

Numerical Tests for PenCS

Problem 3

Kohn-Sham total energy minimization including the non-classical and quantum interaction between electrons.

$$\min_{X \in \mathbb{R}^{n\times p}} \quad \frac{1}{2} tr\left(X^\top L X\right) + \frac{\alpha}{4} tr\left(\rho^\top L^\dagger \rho\right)$$
$$\text{s.t.} \quad X^\top X = I_p,$$

where $\rho = \mathrm{Diag}\,(XX^\top)$ *and* α *is a constant.*

Preliminary Numerical Experiments

Testing methods

- ARNT: Adaptive regularized Newton method
  Hu-Wen-Milzarek-Yuan 2017
- RTR: Riemann trust-region method
  Absil-Baker-Gallivan 2007,
  Boumal-Mishra-Absil-Sepulchre 2013
  (downloadable from https://github.com/NicolasBoumal/manopt)
- PenCS: $\beta = \|\nabla h(X_0)\|_F$, $K = 1.1\sqrt{p}$, $b_1 = 1$.

Implementation

- L is tri-diagonal (gallery('tridiag', n, $-1, 2, -1$))
- X_0 is computed by GR-BB with KKT violation $\leq 10^{-4}$
- Orthonormalization process in the last step for PenCS

Numerical Tests for Different n

Solver	fval	iter.	inner iter.	substationarity	feasibility	CPU time(s)
$(n,p,\alpha) = (5000, 80, 1)$						
ARNT	1.114821e+04	100	511	1.55e-09	5.34e-15	11.16
RTR	1.114821e+04	15	1757	8.51e-12	5.01e-15	17.30
PenCS	1.114821e+04	4	1124	7.33e-12	5.25e-15	10.81
$(n,p,\alpha) = (8000, 80, 1)$						
ARNT	1.114821e+04	100	579	1.23e-09	5.10e-15	16.51
RTR	1.114821e+04	14	1337	9.75e-12	6.68e-15	23.61
PenCS	1.114821e+04	3	988	8.34e-12	5.30e-15	16.72
$(n,p,\alpha) = (10000, 80, 1)$						
ARNT	1.114821e+04	100	1444	2.32e-09	4.91e-15	34.72
RTR	1.114821e+04	10	1275	7.92e-12	5.19e-15	28.71
PenCS	1.114821e+04	3	1108	9.88e-12	6.29e-15	22.76
$(n,p,\alpha) = (15000, 80, 1)$						
ARNT	1.114821e+04	100	1221	1.25e-09	5.08e-15	50.25
RTR	1.114821e+04	9	1268	9.96e-12	4.96e-15	45.98
PenCS	1.114821e+04	3	1145	8.21e-12	5.24e-15	37.47
$(n,p,\alpha) = (20000, 80, 1)$						
ARNT	1.114821e+04	100	553	3.14e-09	4.56e-15	49.28
RTR	1.114821e+04	9	1266	9.29e-12	5.78e-15	62.61
PenCS	1.114821e+04	3	1025	8.06e-12	5.46e-15	48.48

Table 1: Comparison with fixed p and α.

Numerical Tests for Different p

Solver	fval	iter.	inner iter.	substationarity	feasibility	CPU time(s)
$(n, p, \alpha) = (10000, 50, 1)$						
ARNT	2.810709e+03	100	269	2.50e-09	3.90e-15	8.18
RTR	2.810709e+03	5	821	7.31e-12	3.84e-15	10.28
PenCS	2.810709e+03	3	663	8.09e-12	5.01e-15	8.26
$(n, p, \alpha) = (10000, 80, 1)$						
ARNT	1.114821e+04	100	1444	2.32e-09	4.91e-15	34.98
RTR	1.114821e+04	10	1275	7.92e-12	5.19e-15	28.64
PenCS	1.114821e+04	3	1108	9.88e-12	6.29e-15	22.83
$(n, p, \alpha) = (10000, 100, 1)$						
ARNT	2.156071e+04	100	4656	3.28e-09	6.10e-15	114.23
RTR	2.156071e+04	14	3257	9.43e-12	5.75e-15	91.45
PenCS	2.156071e+04	3	1270	9.24e-12	6.54e-15	37.24
$(n, p, \alpha) = (10000, 120, 1)$						
ARNT	3.702321e+04	100	4821	2.92e-09	6.48e-15	153.30
RTR	3.702321e+04	41	3056	1.02e-11	7.76e-15	112.14
PenCS	3.702321e+04	4	1613	8.97e-12	8.19e-15	55.69
$(n, p, \alpha) = (10000, 140, 1)$						
ARNT	5.853571e+04	100	3879	2.70e-09	6.21e-15	159.86
RTR	5.853571e+04	41	2821	1.47e-11	6.74e-15	123.79
PenCS	5.853571e+04	6	1397	9.15e-12	1.62e-15	63.66

Table 2: Comparison with fixed n and α.

Part II. Nonsmooth Objective

How About Nonsmooth Cases?

Extension to nonsmooth cases – seems impossible

- Main idea: closed-form expression of the multipliers at any stationary point
- $\Lambda = \nabla f(X)^\top X$ – gradient is involved
- Nonsmooth cases: gradient is not available

Extension to nonsmooth cases – special cases

- Sparse variable PCA
- Regularized discriminative feature selection

$\ell_{2,1}$ Norm Regularization Minimization with Orthogonality Constraints

Xiao-Liu-Y., Exact Penalty Function for $\ell_{2,1}$ Norm Minimization over the Stiefel Manifold, optimization online: 2020/07/7908

General form

$$\begin{array}{ll} \min\limits_{X \in \mathbb{R}^{n\times p}} & f(X) + r(X) \\ \text{s.t.} & X^\top X = I. \qquad \text{(OCPR)} \end{array}$$

- $f : \mathbb{R}^{n\times p} \longmapsto \mathbb{R}$
- $r(X) = \sum_{j=1}^{n} \gamma_j \|X(j,:)\|_2$, $X_{j\cdot} := X(j,:)^\top, X_{\cdot i} = X(:,i)$
- $n > p$
- $p(p+1)/2$ constraints –– nonconvex
- Stiefel manifold:

$$\mathcal{S}_{n,p} := \{X \in \mathbb{R}^{n\times p} |\, X^\top X = I\}.$$

Existing Approaches

Subgradient methods

- Subgradient method on Riemann manifold: Ferreira-Oliveria 1998
- ε subgradient method: Grohs-Hosseini 2016
- Gradient sampling method: Hosseini-Uschmajew 2017
- ......

How to fully exploit the composite structure ?

Existing Approaches (Cont'd)

ADMM-based proximal gradient methods

- Splitting for orthogonality constrained problems (SOC): Lai-Osher 2014
- Manifold ADMM (MADMM): Kovnatsky-Glashoff-Bornstein 2016
- PAMAL: Chen-Ji-You 2016

Properties of these approaches

- Simple subproblems
- Multiple-block alternating updating ⇒ usually not very efficient;
- Updating multiplier via dual-ascend ⇒ many parameters need to be tuned.

Existing Approaches (Cont'd)

Proximal gradient approaches

- Proximal gradient method on manifold (ManPG): Chen-Ma-So-Zhang 2020

$$\min_{D \in \mathcal{T}_{X_k}} \ \langle D, \nabla f(X_k) \rangle + r(X_k + D) + \frac{\|D\|_{\mathrm{F}}^2}{2\eta_k} \quad \text{(proximal mapping)}$$

- Riemannian proximal gradient method: Huang-Wei 2019

Computational cost per outer iteration

- No closed-form solution for proximal mapping ⇒ semismooth Newton method: Qi-Sun 1993 Sun-Sun 2002
- Orthonormalization process is required in each iteration ⇒ lacks scalability

First-order Optimal Condition

Definition 1

(Yang-Zhang-Song 2014)
A point $X \in \mathcal{S}_{n,p}$ is called as first-order stationary point of (OCPR) if and only if it satisfies

$$0 \in \mathcal{P}_{\mathcal{T}_X}\left(\nabla f(X) + \partial r(X)\right),$$

where $\mathcal{T}_X$ denotes the tangent space at X,
$\mathcal{P}_{\mathcal{T}_X}(\mathcal{Y}) := \{Y - X\Phi(Y^\top X) \mid Y \in \mathcal{Y} \subseteq \mathbb{R}^{n\times p}\}$ consists of all the projection points of $Y \in \mathcal{Y}$ onto the tangent space $\mathcal{T}_X$, and ∂R stands for the Clarke subdifferential of R.

Equivalent version

- There exists $D \in \partial r(X)$ and $\Lambda \in \mathbb{R}^{p\times p}$:

$$\begin{cases} X\Lambda = \nabla f(X) + D \\ \Lambda = \Lambda^\top \\ X^\top X = I_p \end{cases}$$

Motivation: Exact Penalty Model with Compact Convex Constraints

Smooth case

- $\Lambda(X) = \Phi(X^\top \nabla f(X))$;

$$\begin{aligned} &\min \ f(X) \\ &\ \text{s.t. } X^\top X = I_p \\ \Longrightarrow &\min_{X \in \mathcal{M}} f(X) - \frac{1}{2}\left\langle \Lambda(X), X^\top X - I_p \right\rangle + \frac{\beta}{4}\left\| X^\top X - I_p \right\|_{\mathrm{F}}^2 . \end{aligned}$$

$\ell_{2,1}$-norm regularized case

$$\Lambda(X) \in \Phi\left(X^\top \nabla f(X) + X^\top \partial r(X)\right)$$

- Can we choose $\Lambda(X)$ for (OCPR) by its first-order optimality conditions?

Motivation: Explicit Expression

Expression for $\partial r(X)$

- $\partial r(X) = [\gamma_1 \partial(\|X_{1\cdot}\|_2), \gamma_2 \partial(\|X_{2\cdot}\|_2), ..., \gamma_n \partial(\|X_{n\cdot}\|_2)]^\top$
- $\partial(\left\|X_{j\cdot}\right\|_2) = \begin{cases} \frac{X_{j\cdot}^\top}{\|X_{j\cdot}\|_2}, & \text{if } \left\|X_{j\cdot}\right\|_2 \neq 0, \\ u_j \text{ satisfying } \left\|u_j\right\|_2 = 1\ , & \text{otherwise.} \end{cases}$
- For any $D \in \partial r(X)$,

$$X^\top D = \sum_{i=1}^{n} \gamma_i S(X_{i\cdot}), \qquad \text{where} \quad S(x) := \begin{cases} \frac{xx^\top}{\|x\|_2}, & \text{if } x \neq 0; \\ 0, & \text{otherwise.} \end{cases}$$

- $S(x)$ Lipschitz continuous.

Hence,

$$\Lambda(X) = \Phi(X^\top \nabla f(X)) + \sum_{i=1}^{n} \gamma_i S(X_{i\cdot})$$

- Closed-form expression;
- Lipschitz continuous.

Penalty Function

Exact penalty function

$$h(X) := f(X) - \frac{1}{2}\left\langle \Lambda(X), X^\top X - I_p \right\rangle + \frac{\beta}{4}\left\|X^\top X - I_p\right\|_{\mathrm{F}}^2 + r(X),$$

where

$$\Lambda(X) = \Phi(X^\top \nabla f(X)) + \sum_{j=1}^{n} \gamma_i S(X_{i\cdot}).$$

- X^* is a first-order stationary point of (OCPR) $\Rightarrow 0 \in \partial h(X^*)$;

* $0 \in \partial h(X) \Rightarrow X^\top X = I_p$?

h may be unbounded from below - the example in smooth case is also true for nonsmooth case

- $f(X) = \frac{1}{4}\left\|X^\top X - I_p\right\|_{\mathrm{F}}^2$, $\gamma_i = 0$;
- $h(X) = \frac{1}{4}\left\|X^\top X\right\|_{\mathrm{F}}^2 - 2\mathrm{tr}\left((X^\top X)^2(X^\top X - I_p)\right) + \frac{\beta}{4}\left\|X^\top X - I_p\right\|_{\mathrm{F}}^2$

$\Rightarrow \|X\|_{\mathrm{F}} \to +\infty \Rightarrow h(X) \to -\infty$.

A New Penalty Model

Restrict h in a bounded set

$$\min_{X \in \mathcal{M}} \quad h(X). \qquad \text{(PenC)}$$

- $\mathcal{M}$ is a convex compact set, $\mathcal{S}_{n,p} \subset \mathcal{M}$

$\Rightarrow$ Projection to $\mathcal{M}$ can be easily calculated

Several Examples

- Ball with radius K in F-norm : $\mathcal{B} := \{X \in \mathbb{R}^{n \times p} \mid \|X\|_{\mathrm{F}} \leq K\}$
- Closure of Oblique manifold : $\{X \in \mathbb{R}^{n \times p} \mid \|X_{\cdot i}\|_2 \leq 1\}$
- ...

Assumptions

Assumption 3

- $f(X)$ *is differentiable and* $\nabla f(X)$ *is Lipschitz continuous.*

Constants

- $M_0 := \sup_{X \in \mathcal{M}} \|\nabla f(X)\|_{\mathrm{F}}$;
- $M_1 := \sup_{X \in \mathcal{M}} \|\Lambda(X)\|_2$;
- $M_2 := \sup_{X \in \mathcal{M}} r(X)$;
- $C_1 := \sup_{X \in \mathcal{M}} \tilde{h}(X) - \inf_{X \in \mathcal{M}} \tilde{h}(X)$;
- $L_0 := \sup_{X,Y \in \mathcal{M}} \frac{\|\nabla f(X) - \nabla f(Y)\|_{\mathrm{F}}}{\|X-Y\|_{\mathrm{F}}}$;
- $L_1 := \sup_{X \in \mathcal{M}, Y \in \mathcal{M}} \frac{\|\Lambda(X) - \Lambda(Y)\|_{\mathrm{F}}}{\|X-Y\|_{\mathrm{F}}}$;
- $L_r := \sup_{X \in \mathcal{M}, D \in \partial r(X)} \|D\|_{\mathrm{F}}$;
- $\bar{\gamma} = \sum_{i=1}^{n} \gamma_i$.

Properties of Penalty Model

Theorem 6

Suppose Assumption 3 holds. Let $\tilde{X}$ *be a first-order stationary point of (PenC) with* $\beta \geq \max\{2(M_0 + M_1), 2pL_1\}$, *then either* $\tilde{X}$ *is a first-order stationary point of (OCPR), or* $\sigma_{\min}(\tilde{X}^\top \tilde{X}) \leq \frac{2M_1 + \sqrt{2}L_1}{2\beta}$.

Lemma 7

For any $0 < \delta \leq \frac{1}{3}$, *when*
$\beta \geq \max\left\{2(M_0 + M_1), 2pL_1, \left(3M_1 + \frac{3\sqrt{2}}{2}L_1\right), \frac{2C_1}{\delta^2}\right\}$, *we have*

$$\sup_{\|X^\top X - I_p\|_F \leq \delta} h(X) < \inf_{\|X^\top X - I_p\|_F \geq 2\delta} h(X).$$

Moreover, any global minimizer X^* *of (PenC) satisfies* $X^* \in \mathcal{S}_{n,p}$, *which further implies that it is a global minimizer of problem* (OCPR) *.*

Algorithm

Problem reformulation

$$\begin{aligned} \min_{X \in \mathbb{R}^{n\times p}} \quad & f(X) + r(X) \\ \text{s.t.} \quad & X^\top X = I_p, \end{aligned} \quad \Rightarrow \quad \min_{X \in \mathcal{B}} \quad h(X).$$

- $\mathcal{B} := \{X \in \mathbb{R}^{n\times p} \mid \|X\|_{\mathrm{F}} \leq K\}$ where $K > \sqrt{p}$.

Difficulties in computing proximal mapping

$$h(X) := f(X) + \frac{\beta}{4}\left\|X^\top X - I_p\right\|_{\mathrm{F}}^2 - \frac{1}{2}\left\langle \Lambda(X), X^\top X - I_p \right\rangle + r(X).$$

- $f(X) + \frac{\beta}{4}\left\|X^\top X - I_p\right\|_{\mathrm{F}}^2$: smooth
- $r(X)$: nonsmooth, row-wise separable
- $\frac{1}{2}\left\langle \Lambda(X), X^\top X - I_p \right\rangle$: nonconvex, nonsmooth $\Rightarrow$ approximate

Proximal Gradient Method for Solving PenC with Exact Lambda (PenCPG)

1. Choose X_0, set $k = 0$;
2. Choose stepsize η_k;
3. Compute $D_k = \nabla f(X_k) + \beta X_k \left[({X_k}^\top X_k - I_p) - \Lambda(X_k) \right]$;
4. Update X_k by

$$X_{k+1} = \arg \min_{X \in \mathbb{R}^{n \times p}} \quad \langle X - X_k, D_k \rangle + r(X) + \frac{\|X - X_k\|_\mathrm{F}^2}{2\eta_k}$$

5. If $\|X_{k+1}\|_\mathrm{F} > K$, project X_{k+1} back to $\mathcal{B}$;
6. If certain stopping criterion is satisfied, return X_{k+1}; Otherwise, set $k := k + 1$ and go to Step 2.

Global Convergence

Theorem 8

Suppose Assumption 3 holds. Let $0 < \delta \le \frac{1}{3}$, $K \ge \frac{\sqrt{6p}}{2}$ *and* $\beta \ge \max\{6M_1, \max\{2p, 12\sqrt{6}\}L_1, 2(M_0 + M_1), \frac{2C_1}{\delta^2}\}$. *Suppose that* $\{X_k\}$ *is the iterate sequence generated by PenCPG, starting from the initial point* $X_0 \in \mathcal{B}$ *satisfying* $\left\|X_0^\top X_0 - I_p\right\|_{\mathrm{F}} \le \frac{\delta}{2}$, *and adopting the stepsize* $\eta_k \in [\frac{1}{2}\eta^+, \eta^+]$ *where*

$$\eta^+ = \min\left\{\frac{1}{L_0 + 4\beta + \frac{\sqrt{6}}{2}L_1 + M_1}, \frac{1}{15\left(M_0 + \frac{2\sqrt{3p}}{3}M_1 + \frac{2\sqrt{3}}{9}\beta + L_r\right)}, \frac{1}{4\left(L_0 + 4\beta + M_1\right)}\right\}.$$

Then $\{X_k\}$ *exists clustering point and any clustering point is a first-order stationary point of (OCPR). More precisely, for any* $N \ge 1$, *it holds that*

$$\min_{0 \le k \le N-1} \|X_{k+1} - X_k\|_{\mathrm{F}} \le \sqrt{\frac{(16C_1 + \beta\delta^2)\eta^+}{2N}}.$$

Global Convergence (Cont'd)

Remark 1

The sublinear convergence rate of $\|X_{k+1} - X_k\|_{\mathrm{F}}$ *illustrated in Theorem 8 actually tells us that PenCPG terminates after* $O(1/\epsilon^2)$ *iterations, if the stopping criterion is set as* $\|X_{k+1} - X_k\|_{\mathrm{F}} < \epsilon$*. Meanwhile, we have* $\left\|X_{k+1}{}^\top X_{k+1} - I_p\right\|_{\mathrm{F}} < \frac{6\sqrt{6}}{\eta^+\beta}\epsilon$*.*

PenCPG and ManPG - A Comparison

ManPG

- Proximal gradient method ⇒ outperforms ADMM and subgradient methods, fewer parameters
- Difficult proximal mapping ⇒ expensive

$$\min_{D \in \mathcal{T}_{X_k}(\mathbb{S}_{n,p})} \quad \langle D, \nabla f(X_k) \rangle + r(D) + \frac{1}{2\eta_k} \|D - X_k\|_{\mathrm{F}}^2 .$$

- Feasible, retraction based ⇒ orthonormalization process lacks scalability

PenCPG

- Proximal gradient method
- Explicit solution for proximal mapping ⇒ easy to compute
- Infeasible, only requires matrix-matrix multiplication ⇒ high scalability

Comparison on Computational Complexity

ManPG		
Computing gradient	$\nabla f(X_k)$	1 first-order oracle
Computing Riemann gradient	$\nabla f(X_k) - X_k \Phi({X_k}^\top \nabla f(X_k))$	$4np^2$
Retraction[1]	$qr(X_{k+1})$	$2np^2$
SSN for proximal subproblem[2,3]	$E(\Lambda_k)\text{vec}(\Lambda_{k+1}) = -D(\Lambda_k)$	$2np^2 \cdot l_{CG}$
total	1 first-order oracle + $6np^2$ + $2np^2 \cdot l_{CG}$	

PenCPG		
Computing gradient	$\nabla f(X_k)$	1 first-order oracle
Computing D_k	D_k	$6np^2$
Solving subproblem	thresholding	$2np$
Retraction	no retraction in PenCPG	0
total	1 first-order oracle + $6np^2$	

[1] Grad-Schmidt orthonormalization

[2] l_{CG} denotes the total iterations in CG method for solving the linear system, and ManPG can take multiple SSN steps in each iteration.

[3] $l_{CG} \gg 1$.

Preliminary Numerical Experiments

Running Platform

- Intel(R) Xeon(R) Silver 4110 CPU @ 2.10GHz and 394GB RAM
- Ubuntu 18.10
- MATLAB R2018a

Stopping Criteria

- Substationarity: $\frac{\|X_{k+1}-X_k\|_\mathrm{F}}{\eta_k} \leq 10^{-4}$;
- Max iteration: 20000 for PenCPG.

Testing Problems

- Problem 1: Sparse variable PCA
- Problem 2: Canonical correlation analysis

Default Setting

A possible choice of fixed β

$\beta := \|\nabla f(X_0)\|_{\mathrm{F}} + \bar{\gamma}$.

BB Stepsize for Nonsmooth Optimization

Wen-Yin-Goldfarb-Zhang 2010, Chen-Hager-Yashtini-Zhang 2013

$$\eta_k^{\mathrm{BB1}} := \frac{\langle S_{k-1}, S_{k-1} \rangle}{|\langle S_{k-1}, Y_{k-1} \rangle|}, \quad \text{or} \quad \eta_k^{\mathrm{BB2}} := \frac{|\langle S_{k-1}, Y_{k-1} \rangle|}{\langle Y_{k-1}, Y_{k-1} \rangle},$$

where

$$\begin{aligned} S_k &= X_k - X_{k-1}, \\ Y_k &= \left[\nabla f(X_k) - X_k \Lambda(X_k) + \beta X_k ({X_k}^\top X_k - I_p) \right] \\ &\quad - \left[\nabla f(X_{k-1}) - X_{k-1} \Lambda(X_{k-1}) + \beta X_{k-1} ({X_{k-1}}^\top X_{k-1} - I_p) \right] \end{aligned}$$

Post-process by Orthonormalization

Projection after convergence

- Obtain X_k, and economy-size SVD: $X_k = U\Sigma V^\top$;
- Return $X^{\mathrm{orth}} := UV^\top$.

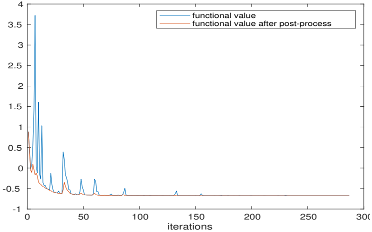
Proposition 2

Given $\delta \in \left(0, \frac{1}{3}\right]$, $K \geq \sqrt{p + \delta\sqrt{p}}$. *Then for*
$\beta \geq \max\{6M_1, 36L_1, 2(M_0 + M_1), \frac{2C_1}{\delta^2}, 2\,(L_0 + L_1 + 3M_1 + 2M_2)\}$.
Suppose PenCPG starts with initial value $\left\|{X_0}^\top X_0 - I_p\right\|_{\mathrm{F}} \leq \frac{\delta}{2}$ *with stepsize* $\eta_k \in [\frac{1}{2}\eta^+, \eta^+]$, *and generates a sequence* $\{X_k\}$. *Then for any* $k > 0$, *let* X_k *has compact SVD* $U_k\Sigma_k {V_k}^\top$ *and define* $X^{orth} = U_k {V_k}^\top$, *then*

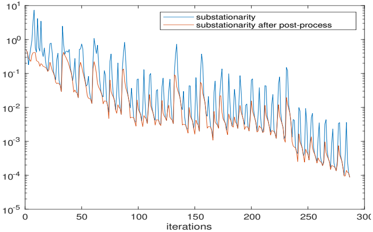
$$h(X_k) \geq h(X^{\mathrm{orth}}). \quad (1)$$

- Eliminate feasibility violation
- Reduce penalty function value

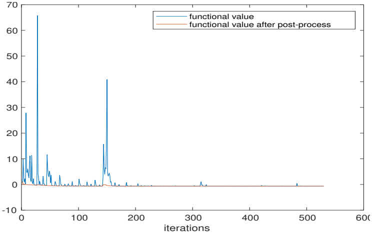
Numerical Experiments for Post-process



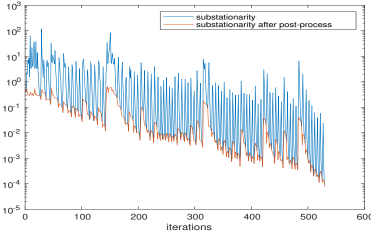
(a) Functional value, $\beta = s$.



(b) Substationarity, $\beta = s$.



(c) Functional value, $\beta = 10s$.



(d) Substationarity, $\beta = 10s$.

Figure 2: Problem 1 with $n = 500$, $p = 4$, $\gamma = 0.09$.

Experiments for Sparse Variable PCA

Problem generation

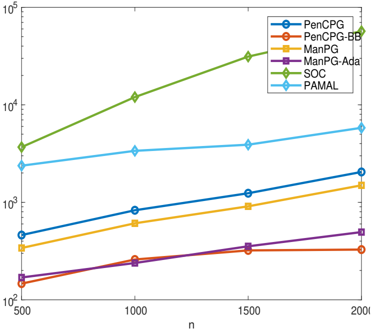
- Randomly generate uniformly distributed samples, $N = 200$, and set A as their covariance matrix; $\gamma_i = \frac{b}{2}\sqrt{\log(2n)/50}$
- 10 experiments with random initial points

Testing Algorithms

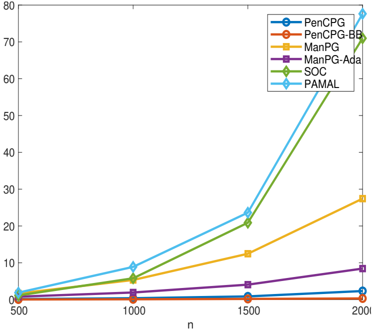
Testing methods

- SOC: Splitting method for orthogonality constrained problems, Lai-Osher 2014 ;
- PAMAL: Proximal alternating minimized augmented Lagrangian, Chen-Ji-You 2016 ;
- ManPG : Manifold proximal gradient method, Chen-Ma-So-Zhang 2020 ;
- ManPG-Ada: Accelerated version of ManPG, Chen-Ma-So-Zhang 2020 ;
- PenCPG: $\beta = s, K = 10\sqrt{p}$, fixed stepsize $\eta_k = \frac{1}{2s}$;
- PenCPG-BB: PenCPG with BB1 stepsize, $\beta = s, K = 10\sqrt{p}$.

Numerical Results on n



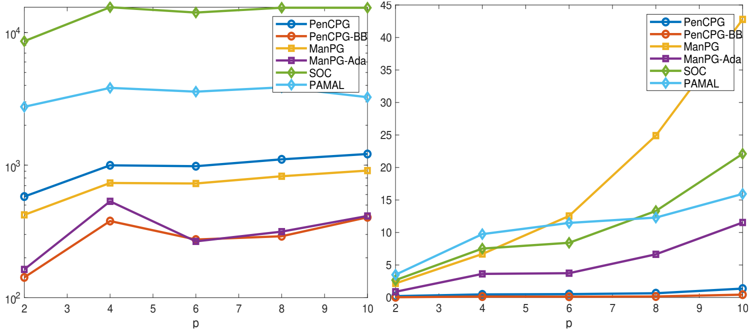
(a) Iterations



(b) CPU time

- Comparable in the aspect of iterations
- Less CPU time

Numerical Results on p



(a) Iterations (b) CPU time

- Cheap proximal mapping $\Rightarrow$ high scalability

Conclusion

Contributions

- PLAM and PCAL – updating multipliers by closed-form expression
- PenC model – an **exact penalty model** with simple convex constraint
  - Fist-order approaches: PCAL, PenCF
  - Second-order approach: PenCS
  - Algorithm for $\ell_{2,1}$ regularized objective: PenCPG

Further development

- Extension to general nonsmooth cases: SLPG

Thanks for your attention!

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