A Block Coordinate Descent Method for Nonsmooth Composite Optimization under Orthogonality Constraints

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Outline of This Talk

Introduction

Introduction

Nonsmooth Composite Optimization under Orth. Constraints

$$\bar{\mathbf{X}} \in \arg\min_{\mathbf{X}\in\mathbb{R}^{n\times r}} \; F(\mathbf{X}) \triangleq f(\mathbf{X}) + h(\mathbf{X}), \;\; s.t. \; \mathbf{X}^{\mathsf{T}}\mathbf{X} = \mathbf{I} \tag{1}$$

Assumptions

1. $f(\cdot)$ is $\mathbf{H}$-smooth with $\mathbf{H} \in \mathbb{R}^{nr\times nr}$ such that:

   $$f(\mathbf{X}^+) \leq f(\mathbf{X}) + \langle \mathbf{X}^+ - \mathbf{X}, \nabla f(\mathbf{X})\rangle + \tfrac{1}{2}\|\mathbf{X}^+ - \mathbf{X}\|_{\mathbf{H}}^2$$

2. $h(\mathbf{X})$: closed, proper, lsc, and potentially non-smooth (limiting subdifferential always exists). Examples: $h(\mathbf{X}) = \|\mathbf{X}\|_p$ with $p \in \{0, 1\}$, and $h(\mathbf{X}) = \mathcal{I}_{\geq 0}(\mathbf{X})$.
3. The subproblem can be solved: $\min_{\mathbf{V}\in\mathrm{St}(k,k)} \; \mathcal{P}(\mathbf{V}) \triangleq \frac{1}{2}\|\mathbf{V}\|_{\mathbf{Q}'}^2 + \langle \mathbf{V}, \mathbf{P}\rangle + h(\mathbf{VZ})$ for any given $\mathbf{Z} \in \mathbb{R}^{k\times r}$, $\mathbf{P} \in \mathbb{R}^{k\times k}$, and $\mathbf{Q}' \in \mathbb{R}^{k^2\times k^2}$.

Introduction

Applications in Data Science

1. Sparse/Nonnegative PCA
2. Deep Neural Networks
3. Fourier Transforms Approximation
4. Electronic Structure Calculation
5. Sharpness Aware Minimization

Introduction: Related Work

Minimizing Smooth Functions under Orth. Constraints

1. Geodesic-like Methods
2. Projection-like Methods
3. Multiplier Correction Methods

Minimizing Nonmooth Functions under Orth. Constraints

1. Subgradient methods
2. Proximal gradient methods
3. Operator splitting methods

Introduction: Related Work

Block Coordinate Descent Methods

1. Gained great attention in non-convex problems: strong optimality guarantees and/or excellent empirical performance
2. Column-wise BCD methods (Shalit & Chechik, ICML 2014) are limited to solve smooth problems with $k = 2$ and $r = n$. Our methods can solve general nonsmooth problems with $k \geq 2$ and $r \leq n$ with stronger optimality guarantees.
3. Another column-wise BCD methods (Gao et al., SISC 2019) are unconstrained multiplier correction methods, parallelizable scheme for solving the proximal subproblems. It can not solve general problem when $h(\mathbf{X}) \neq 0$.

Introduction: Contributions

1. Algorithmically: OBCD algorithm for Problem (1)
2. Theoretically: optimality and convergence analyses
3. Side Contributions: breakpoint searching methods for solving subproblems, and working set selection greedy strategies
4. Empirically: Our methods surpass existing solutions in terms of accuracy and/or efficiency

Proposed Block Coordinate Descent Method

A New Constraint-Preserving Update Scheme

1. Split the set $[1, 2, ..., n]$ into $[\mathrm{B}, \mathrm{B}^c]$, $\mathrm{B} \in \mathbb{N}^k$ is the working set
2. We define $\mathrm{U}_\mathrm{B} \in \mathbb{R}^{n\times k}$ and $\mathrm{U}_{\mathrm{B}^c} \in \mathbb{R}^{n\times(n-k)}$ as:

$$(\mathrm{U}_\mathrm{B})_{ji} = \begin{cases} 1, & \mathrm{B}_i = j; \\ 0, & \text{else.} \end{cases}, (\mathrm{U}_{\mathrm{B}^c})_{ji} = \begin{cases} 1, & \mathrm{B}_i^c = j; \\ 0, & \text{else.} \end{cases}$$

3. Here, $\mathbf{I}_n\mathbf{X} = (\mathrm{U}_\mathrm{B}\mathrm{U}_\mathrm{B}^\mathsf{T} + \mathrm{U}_{\mathrm{B}^c}\mathrm{U}_{\mathrm{B}^c}^\mathsf{T})\mathbf{X} = \mathrm{U}_\mathrm{B}\mathbf{X}(\mathrm{B},:) + \mathrm{U}_{\mathrm{B}^c}\mathbf{X}(\mathrm{B}^c,:)$
$\mathbf{X}(\mathrm{B},:) = \mathrm{U}_\mathrm{B}^\mathsf{T}\mathbf{X} \in \mathbb{R}^{k\times r}$ and $\mathbf{X}(\mathrm{B}^c,:) = \mathrm{U}_{\mathrm{B}^c}^\mathsf{T}\mathbf{X} \in \mathbb{R}^{(n-k)\times r}$.
4. Update k rows of $\mathbf{X}$ via $\mathbf{X}^{t+1}(\mathrm{B},:) \Leftarrow \mathbf{V}\mathbf{X}^t(\mathrm{B},:)$, $\mathbf{V} \in \mathrm{St}(k,k)$
5. The following equivalent expressions hold:

$$\begin{aligned} \mathbf{X}^{t+1}(\mathrm{B},:) = \mathbf{V}\mathbf{X}^t(\mathrm{B},:) \quad &\Leftrightarrow \quad \mathbf{X}^{t+1} = (\mathrm{U}_\mathrm{B}\mathbf{V}\mathrm{U}_\mathrm{B}^\mathsf{T} + \mathrm{U}_{\mathrm{B}^c}\mathrm{U}_{\mathrm{B}^c}^\mathsf{T})\mathbf{X}^t \\ &\Leftrightarrow \quad \mathbf{X}^{t+1} = \mathbf{X}^t + \mathrm{U}_\mathrm{B}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_\mathrm{B}^\mathsf{T}\mathbf{X}^t \end{aligned}$$

A New Constraint-Preserving Update Scheme

1. Suppose the following update scheme is considered:

$$\bar{\mathbf{V}} \in \arg\min_{\mathbf{V}} (f+h)(\mathcal{X}_{\mathrm{B}}^t(\mathbf{V})), \ s.t. \ \underbrace{\mathbf{X}^t + \mathrm{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_{\mathrm{B}}^\top \mathbf{X}^t}_{\triangleq \mathcal{X}_{\mathrm{B}}^t(\mathbf{V})} \in \mathrm{St}(n, r).$$

   And then $\mathbf{X}^{t+1} \Leftarrow \mathcal{X}_{\mathrm{B}}^t(\bar{\mathbf{V}})$.

2. We prove that $\mathcal{X}_{\mathrm{B}}^t(\mathbf{V}) \in \mathrm{St}(n, r)$ can be implied by $\mathbf{V} \in \mathrm{St}(k, k)$, where $k \geq 2$

3. It suffices to consider the following small-sized optimization problem under orth. constraints:

$$\bar{\mathbf{V}} \in \arg\min_{\mathbf{V}} (f+h)(\mathcal{X}_{\mathrm{B}}^t(\mathbf{V})), \ s.t. \ \mathbf{V} \in \mathrm{St}(k, k).$$

   Still difficult to solve when $f + h$ is complex. MM Strategy!

Majorization Minimization Strategy

1. We construct the majorization function:

$$\begin{aligned} f(\mathcal{X}_{\mathrm{B}}^t(\mathbf{V})) - f(\mathbf{X}^t) &\leq \langle \mathcal{X}_{\mathrm{B}}^t(\mathbf{V}) - \mathbf{X}^t, \nabla f(\mathbf{X}^t) \rangle + \tfrac{1}{2} \| \mathcal{X}_{\mathrm{B}}^t(\mathbf{V}) - \mathbf{X}^t \|_{\mathbf{H}}^2 \\ &= \langle \mathrm{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_k) \mathrm{U}_{\mathrm{B}}^{\mathsf{T}} \mathbf{X}^t, \nabla f(\mathbf{X}^t) \rangle + \tfrac{1}{2} \| \mathbf{V} - \mathbf{I}_k \|_{\underline{\mathbf{Q}}}^2 \\ &\leq \langle \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathrm{BB}} \rangle + \tfrac{1}{2} \| \mathbf{V} - \mathbf{I}_k \|_{\mathbf{Q} + \alpha \mathbf{I}}^2 \end{aligned}$$

2. Here, $\mathbf{Q}$ is chosen using one of the following methods:

$$\mathbf{Q} = \underline{\mathbf{Q}} \triangleq (\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathrm{B}})^{\mathsf{T}} \mathbf{H} (\mathbf{Z}^{\mathsf{T}} \otimes \mathrm{U}_{\mathrm{B}}), \text{ with } \mathbf{Z} \triangleq \mathbf{U}_{\mathrm{B}}^{\mathsf{T}} \mathbf{X}^t, \quad (2)$$

$$\mathbf{Q} = \varsigma \mathbf{I}, \text{ with } \|\underline{\mathbf{Q}}\| \leq \varsigma \leq L_f. \quad (3)$$

3. Taking into account into $h(\cdot)$, it suffices to solve to find $\bar{\mathbf{V}}$:

$$\min_{\mathbf{V}} \langle \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^{\mathsf{T}}]_{\mathrm{BB}} \rangle + \tfrac{1}{2} \| \mathbf{V} - \mathbf{I}_k \|_{\mathbf{Q}+\alpha\mathbf{I}}^2 + h(\mathbf{V} \mathrm{U}_{\mathrm{B}}^{\mathsf{T}} \mathbf{X}^t).$$

The Proposed **OBCD** for Problem (1)

Input: an initial feasible solution $\mathbf{X}^0$. Set $k \geq 2$, $t = 0$.

for *t from 0 to T* **do**

(**S1**) Use some strategy to find a working set $\mathtt{B}^t$ for the t-it iteration with $\mathtt{B}^t \in \{1, 2, ..., n\}^k$. Let $\mathtt{B} = \mathtt{B}^t$ and $\mathtt{B}^c = \{1, 2, ..., n\} \setminus \mathtt{B}$.

(**S2**) Choose a suitable matrix $\mathbf{Q} \in \mathbb{R}^{k^2 \times k^2}$ using Equation (2) or Equation (3):

(**S3**) Find a **global optimal solution** or **critical stationary solution** of the following problem:

$$\bar{\mathbf{V}}^t \in \arg\min_{\mathbf{V}} \underbrace{\langle \mathbf{V} - \mathbf{I}_k, [\nabla f(\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T}]_{\mathtt{BB}} \rangle + \tfrac{1}{2}\|\mathbf{V} - \mathbf{I}_k\|^2_{\mathbf{Q}+\alpha\mathbf{I}} + h(\mathbf{V}\mathrm{U}_{\mathtt{B}}^\mathsf{T}\mathbf{X}^t)}_{\triangleq \mathcal{K}(\mathbf{V};\mathbf{X}^t,\mathtt{B})}.$$

(**S4**) $\mathbf{X}^{t+1}(\mathtt{B},:) = \bar{\mathbf{V}}^t\mathbf{X}^t(\mathtt{B},:)$

On Solving the Small-Sized Subproblems

1. When $h(\cdot) = 0$, $\mathbf{Q} = \varsigma \mathbf{I}$, it can be solved globally using small-sized SVD.
2. When $h(\mathbf{X}) = \|\mathbf{X}\|_p$, $p \in \{0, 1\}$, $h(\mathbf{X}) = \mathcal{I}_{\geq 0}(\mathbf{X})$, and $k = 2$, it can be solved globally using a novel BSM (discussed later).
3. One can use other heuristic methods to find a local solution.
4. We are particularly interested in the case when $k = 2$. Any orthogonal matrix $\mathbf{V} \in \mathrm{St}(2, 2)$ can be expressed as a Givens rotation matrix $\mathbf{V}_\theta^{\mathrm{rot}} \triangleq \left(\begin{smallmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{smallmatrix}\right)$ or Jacobi reflection matrix $\mathbf{V}_\theta^{\mathrm{ref}} \triangleq \left(\begin{smallmatrix} -\cos(\theta) & \sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{smallmatrix}\right)$.

Optimality Analysis and Convergence Analysis

Basis Representation of Orthogonal Matrices

1. The update scheme $\mathbf{X}^{+} \Leftarrow \mathbf{X} + \mathrm{U}_{\mathrm{B}}(\mathbf{V} - \mathbf{I}_k)\mathrm{U}_{\mathrm{B}}^{\mathsf{T}}\mathbf{X}$ can reach any orthogonal matrix $\mathbf{X} \in \mathrm{St}(n, r)$ for any starting solution $\mathbf{X}^0 \in \mathrm{St}(n, r)$.
2. Both Givens rotation and Jacobi reflection matrices are considered! This is necessary since a reflection matrix cannot be represented through a sequence of rotations.
3. Key strategy: develop a new **Jacobi-Givens-QR** algorithm, that decomposes $\mathbf{X} \in \mathrm{St}(n, n)$ into $\mathbf{X} = \mathbf{QR}$, where $\mathbf{Q} = \mathbf{X}$ and $\mathbf{R} = \mathbf{I}_n$, using C_n^k Givens rotation or Jacobi reflection steps

Optimality Conditions

1. Critical Point. A solution $\check{\mathbf{X}} \in \mathrm{St}(n, r)$ is a critical point of Problem (1) if: $\mathbf{0} \in \partial_{\mathcal{M}} F(\check{\mathbf{X}}) \triangleq \partial F(\check{\mathbf{X}}) \ominus (\check{\mathbf{X}}[\partial F(\check{\mathbf{X}})]^{\mathsf{T}} \check{\mathbf{X}})$.
2. Block-k Stationary Point ($\mathrm{BS_k}$ Point). A solution $\ddot{\mathbf{X}} \in \mathrm{St}(n, r)$ is called a $\mathrm{BS_k}$ point if:

$$\forall \mathtt{B} \in \{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k},\ \mathbf{I}_k \in \arg \min_{\mathbf{V} \in \mathrm{St}(k,k)} \mathcal{K}(\mathbf{V}; \ddot{\mathbf{X}}, \mathtt{B})$$

3. Assume the subproblem can be solved globally. We have:

$$\{\text{critical points}\, \check{\mathbf{X}}\} \supseteq \{\mathrm{BS_2}\text{-points}\, \ddot{\mathbf{X}}\} \supseteq \{\text{global optimal points}\, \bar{\mathbf{X}}\}$$

$$\{\mathrm{BS_k}\text{-}\mathit{points}\, \ddot{\mathbf{X}}\} \supseteq \{\mathrm{BS_{k+1}}\text{-}\mathit{points}\, \ddot{\mathbf{X}}\}$$

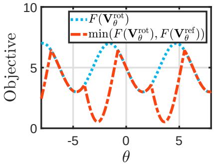
Two Simple Examples for the Optimality Hierarchy

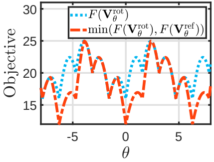
1. Optimality: BS_2-points is stronger than critical points
2. We examine two simple examples:

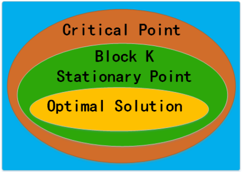
$$\min_{\mathbf{V}\in\mathrm{St}(2,2)} \; F(\mathbf{V}) \triangleq \|\mathbf{V}-\mathbf{A}\|_\mathsf{F}^2, \text{ with } \mathbf{A} = \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix}.$$

$$\min_{\mathbf{V}\in\mathrm{St}(2,2)} \; F(\mathbf{V}) \triangleq \|\mathbf{V}-\mathbf{B}\|_\mathsf{F}^2 + 5\|\mathbf{V}\|_1, \text{ with } \mathbf{B} = \begin{pmatrix} 1 & 0 \\ 1 & 2 \end{pmatrix}.$$

3. Within $[0, 2\pi)$, one unique BS_2-point, 4 and 8 critical points.







Convergence Analysis

Theorem (Subsequence Convergence)

We define $\tilde{c} \triangleq \frac{2}{\alpha} \cdot (F(\mathbf{X}^0) - F(\ddot{\mathbf{X}}))$*. We have:*

*(**a**) The following sufficient decrease condition holds for all* $t \geq 0$*:*

$$\frac{\alpha}{2}\|\mathbf{X}^{t+1} - \mathbf{X}^t\|_\mathsf{F}^2 \leq \frac{\alpha}{2}\|\bar{\mathbf{V}}^t - \mathbf{I}_k\|_\mathsf{F}^2 \leq F(\mathbf{X}^t) - F(\mathbf{X}^{t+1}). \quad (4)$$

*(**b**) If the* $\mathtt{B}^t$ *is selected from* $\{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$ *randomly and uniformly,* **OBCD** finds an ϵ-BS$_k$-*point* of Problem (1) in at most T iterations in the sense of expectation, where $T \geq \lceil \frac{\tilde{c}}{\epsilon} \rceil$.

(***c***) If the $\mathtt{B}^t$ is selected from $\{\mathcal{B}_i\}_{i=1}^{\mathrm{C}_n^k}$ cyclically, **OBCD** finds an ϵ-BS$_k$-*point* of Problem (1) in at most T iterations deterministically, where $T \geq \lceil \frac{\tilde{c}}{\epsilon} + \mathrm{C}_n^k \rceil$.

Convergence Analysis

Assumption (KL Inequality)

The function $F^\circ(\mathbf{X}) = F(\mathbf{X}) + \mathcal{I}_{\mathcal{M}}(\mathbf{X})$ *is a KL function.*

Assumption (Lipschitz Continuity)

There exists positive constants l_f *and* l_h *that:*

$\forall \mathbf{X}, \|\nabla f(\mathbf{X})\|_2 \leq l_f, \|\partial h(\mathbf{X})\|_2 \leq l_h.$

Convergence Analysis

The Key Lemma:

Lemma (Riemannian Subgradient Lower Bound for the Iterates Gap)

The Riemannian subdifferential of $\mathcal{K}(\mathbf{V};\mathbf{X}^t,\mathrm{B}^t)$ *at the point* $\mathbf{V}=\mathbf{I}_k$ *can be computed as:* $\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k;\mathbf{X}^t,\mathrm{B}^t)=\mathrm{U}_{\mathrm{B}^t}^{\mathsf{T}}(\mathbb{D}\ominus\mathbb{D}^{\mathsf{T}})\mathrm{U}_{\mathrm{B}^t}$, *where* $\mathbb{D}=[\nabla f(\mathbf{X}^t)+\partial h(\mathbf{X}^t)][\mathbf{X}^t]^{\mathsf{T}}$. *It holds that:*

$$\mathbb{E}_{\xi^{t+1}}[\mathrm{dist}(\mathbf{0},\partial_{\mathcal{M}}\mathcal{K}(\mathbf{I}_k;\mathbf{X}^{t+1},\mathrm{B}^{t+1}))]\leq\phi\cdot\mathbb{E}_{\xi^t}[\|\bar{\mathbf{V}}^t-\mathbf{I}_k\|_{\mathsf{F}}],$$

where $\phi\triangleq 4(l_f+l_h+L_f)+2\alpha$.

Convergence Analysis

Theorem (Strong Limit-Point Convergence)

(**A Finite Length Property**). The sequence $\{\mathbf{X}^t\}_{t=0}^{\infty}$ has a finite length property that: $\sum_{t=1}^{\infty} \mathbb{E}_{\xi^t}[\|\mathbf{X}^{t+1} - \mathbf{X}^t\|_\mathsf{F}] \leq C < +\infty$ with $C \triangleq 2\sqrt{k} + \frac{4\gamma\phi}{\alpha}\varphi(F(\mathbf{X}^1) - F(\ddot{\mathbf{X}}))$. Here, $\gamma \triangleq (\mathrm{C}_n^k/\mathrm{C}_{n-2}^{k-2})^{1/2}$, ϕ is a universal constant (depends on $\{l_f, l_h, L_f, \alpha\}$), and $\varphi(\cdot)$ is the desingularization function.

Remark: By exploring the KL exponent, one can establish the convergence rate of **OBCD**.

A Breakpoint Searching Method for Subproblems

A Breakpoint Searching Method

1. The general subproblem:
$\min_{\mathbf{V}\in\mathrm{St}(k,k)} \mathcal{P}(\mathbf{V}) \triangleq \frac{1}{2}\|\mathbf{V}\|_{\mathbf{Q}}^2 + \langle \mathbf{V}, \mathbf{P}\rangle + h(\mathbf{VZ})$.
2. When $k = 2$, it boils down to a one-dimensional subproblem:
$\min_{\theta} \ \frac{1}{2}\|\mathbf{V}\|_{\mathbf{Q}}^2 + \langle \mathbf{V}, \mathbf{P}\rangle + h(\mathbf{VZ}),\ s.t.\, \mathbf{V} \in \{\mathbf{V}_\theta^{\mathrm{rot}}, \mathbf{V}_\theta^{\mathrm{ref}}\}$
3. It takes the following quadratic form:

$$\begin{aligned}\bar{\theta} \in \arg\min_{\theta}\ & h\left(\cos(\theta)\mathbf{x} + \sin(\theta)\mathbf{y}\right) + a\cos(\theta) + b\sin(\theta) \\ & + c\cos^2(\theta) + d\cos(\theta)\sin(\theta) + e\sin^2(\theta)\end{aligned}$$

4. Using $\cos(\theta) = \pm 1/\sqrt{1+\tan^2(\theta)}$ and $\sin(\theta) = \pm\tan(\theta)/\sqrt{1+\tan^2(\theta)}$, the problem above only depends on $\tan(\theta) = t$.

A Breakpoint Searching Method

Lemma

We define $\breve{F}(\tilde{c},\tilde{s}) \triangleq a\tilde{c} + b\tilde{s} + c\tilde{c}^2 + d\tilde{c}\tilde{s} + e\tilde{s}^2 + h\left(\tilde{c}\mathbf{x} + \tilde{s}\mathbf{y}\right)$, *and* $w \triangleq c - e$. *The optimal solution* $\bar{\theta}$ *can be computed as:* $[\cos(\bar{\theta}), \sin(\bar{\theta})] \in \arg\min_{[c,s]} \breve{F}(c,s),\ s.t.\ [c,s] \in \{[c_1,s_1],[c_2,s_2],[0,1],[0,-1]\}$, *where* $c_1 \triangleq \frac{1}{\sqrt{1+(\bar{t}_+)^2}}$, $s_1 = \frac{\bar{t}_+}{\sqrt{1+(\bar{t}_+)^2}}$, $c_2 \triangleq \frac{-1}{\sqrt{1+(\bar{t}_-)^2}}$, *and* $s_2 \triangleq \frac{-\bar{t}_-}{\sqrt{1+(\bar{t}_-)^2}}$. *Furthermore,* $\bar{t}_+$ *and* $\bar{t}_-$ *are respectively defined as:*

$$\bar{t}_+ \in \arg\min_t\ p(t) \triangleq \frac{a+bt}{\sqrt{1+t^2}} + \frac{w+dt}{1+t^2} + h\left(\frac{\mathbf{x}+t\mathbf{y}}{\sqrt{1+t^2}}\right), \tag{5}$$

$$\bar{t}_- \in \arg\min_t\ \tilde{p}(t) \triangleq \frac{-a-bt}{\sqrt{1+t^2}} + \frac{w+dt}{1+t^2} + h\left(\frac{-\mathbf{x}-t\mathbf{y}}{\sqrt{1+t^2}}\right). \tag{6}$$

BSM for the ℓ_0 norm Function

1. We consider Problem (5) with $h(\mathbf{x}) = \lambda\|\mathbf{x}\|_0$

$$\bar{t}_+ \in \arg\min_t \; p(t) \triangleq \frac{a+bt}{\sqrt{1+t^2}} + \frac{w+dt}{1+t^2} + \lambda\|\frac{\mathbf{x}+t\mathbf{y}}{\sqrt{1+t^2}}\|_0. \qquad (7)$$

2. Case **(i)**. We assume $(\mathbf{x}+t\mathbf{y})_i = 0$ for some i. Then the solution $\bar{t}$ can be determined using $\bar{t} = \frac{\mathbf{x}_i}{\mathbf{y}_i}$. There are $2r$ breakpoints $\{\frac{\mathbf{x}_1}{\mathbf{y}_1}, \frac{\mathbf{x}_2}{\mathbf{y}_2}, ..., \frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}\}$ for this case.
3. Case **(ii)**. We now assume $(\mathbf{x}+t\mathbf{y})_i \neq 0$ for all i. Then $\lambda\|\mathbf{x}+t\mathbf{y}\|_0 = 2r\lambda$ becomes a constant. Setting the subgradient of $p(t)$ to zero yields: $0 = \nabla p(t) =$ $[b(1+t^2)-(a+bt)t]\cdot\sqrt{1+t^2}\cdot t^\circ + [d(1+t^2)-(w+dt)(2t)]\cdot t^\circ$, where $t^\circ = (1+t^2)^{-2}$.

BSM for the ℓ_0 norm Function

1. Case **(ii)** continue. Dropping $t^\circ > 0$, we obtain: $d(1+t^2) - (w+dt)2t = -(b-at) \cdot \sqrt{1+t^2}$. We obtain real roots for the resulting quartic equation $\{\bar{t}_1, \bar{t}_2, ..., \bar{t}_j\}$ with $1 \leq j \leq 4$, and pick the best one. There are at most 4 breakpoints for this case.
2. In total, it contains at most $2r+4$ breakpoints $\Theta = \{\frac{\mathbf{x}_1}{\mathbf{y}_1}, \frac{\mathbf{x}_2}{\mathbf{y}_2}, ..., \frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}, \bar{t}_1, \bar{t}_2, ..., \bar{t}_j\}$.
3. $(2r+4)$ breakpoints are both necessary and sufficient to find the global solution.

BSM for the ℓ_1 norm Function

1. We consider Problem (5) with $h(\mathbf{x}) = \lambda\|\mathbf{x}\|_1$

$$\bar{t}_+ \in \arg\min_t \; p(t) \triangleq \frac{a+bt}{\sqrt{1+t^2}} + \frac{w+dt}{1+t^2} + \frac{\lambda\|\mathbf{x}+t\mathbf{y}\|_1}{\sqrt{1+t^2}}. \quad (8)$$

2. Case **(i)**. We assume $(\mathbf{x}+t\mathbf{y})_i = 0$ for some i. Then the solution $\bar{t}$ can be determined using $\bar{t} = \frac{\mathbf{x}_i}{\mathbf{y}_i}$. There are $2r$ breakpoints $\{\frac{\mathbf{x}_1}{\mathbf{y}_1}, \frac{\mathbf{x}_2}{\mathbf{y}_2}, ..., \frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}\}$ for this case.
3. Case **(ii)** We assume $(\mathbf{x}+t\mathbf{y})_i \neq 0$ for all i. We have $0 \in \partial p(t) = t^\circ[d(1+t^2) - (w+dt)2t + (b-at)\cdot\sqrt{1+t^2}] + t^\circ\lambda\cdot\sqrt{1+t^2}\cdot[\langle \mathrm{sign}(\mathbf{x}+t\mathbf{y}), \mathbf{y}\rangle(1+t^2) - \|\mathbf{x}+t\mathbf{y}\|_1 t]$, where $t^\circ = (1+t^2)^{-2}$. We define $\mathbf{z} \triangleq \{+\frac{\mathbf{x}_1}{\mathbf{y}_1}, -\frac{\mathbf{x}_1}{\mathbf{y}_1}, +\frac{\mathbf{x}_2}{\mathbf{y}_2}, -\frac{\mathbf{x}_2}{\mathbf{y}_2}, ..., +\frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}, -\frac{\mathbf{x}_{2r}}{\mathbf{y}_{2r}}\} \in \mathbb{R}^{4r\times 1}$ and sort $\mathbf{z}$ in non-descending order.

BSM for the ℓ_1 norm Function

1. Case **(ii)** continue. Given $\bar{t} \neq \mathbf{z}_i$ for all i in this case, the domain $p(t)$ can be divided into $(4r+1)$ non-overlapping intervals: $(-\infty, \mathbf{z}_1), (\mathbf{z}_1, \mathbf{z}_2), ..., (\mathbf{z}_{4r}, +\infty)$. In each interval, $\operatorname{sign}(\mathbf{x} + t\mathbf{y}) \triangleq \mathbf{o}$ can be determined.
2. Given $t^\circ > 0$ and $\|\mathbf{x} + t\mathbf{y}\|_1 = \langle \mathbf{o}, \mathbf{x} + t\mathbf{y} \rangle$, the first-order optimality condition is: $(at - b) \cdot \sqrt{1+t^2} - \lambda \cdot \sqrt{1+t^2} \cdot [\langle \mathbf{o}, \mathbf{y} - t\mathbf{x} \rangle] = [d(1+t^2) - (w + dt)2t]$. We obtain real roots for the resulting quartic equation, and pick the best one. There are at most 4 breakpoints for this case.
3. In total, it contains at most $2r + (4r+1) \times 4$ breakpoints.

BSM for the Function $h(\mathbf{x}) \triangleq I_{\geq 0}(\mathbf{x})$

1. We consider Problem (5) with $h(\mathbf{x}) \triangleq I_{\geq 0}(\mathbf{x})$:

$$\bar{t}_+ \in \arg\min_t \; p(t) \triangleq \tfrac{a+bt}{\sqrt{1+t^2}} + \tfrac{w+dt}{1+t^2}, \;\; s.t. \; \tfrac{\mathbf{x}+t\mathbf{y}}{\sqrt{1+t^2}} \geq \mathbf{0}. \qquad (9)$$

2. We define $I \triangleq \{i|\mathbf{y}_i > 0\}$ and $J \triangleq \{i|\mathbf{y}_i < 0\}$. It is not difficult to verity that $\{x + t\mathbf{y} \geq 0\} \Leftrightarrow \{-\frac{\mathbf{x}_I}{\mathbf{y}_I} \leq t, t \leq -\frac{\mathbf{x}_J}{\mathbf{y}_J}\} \Leftrightarrow \{lb \triangleq \max(-\frac{\mathbf{x}_I}{\mathbf{y}_I}) \leq t \leq \min(-\frac{\mathbf{x}_J}{\mathbf{y}_J}) \triangleq ub\}$. When $lb > ub$, we can directly conclude that the problem has no solution for this case. Now we assume $ub \geq lb$ and define $P(t) \triangleq \min(ub, \max(t, lb))$.

BSM for the Function $h(\mathbf{x}) \triangleq I_{\geq 0}(\mathbf{x})$

1. Case **(ii)** continue. We omit the bound constraint and set the gradient of $p(t)$ to zero, which yields: $0 = \nabla p(t) = [b(1+t^2)-(a+bt)t]\cdot\sqrt{1+t^2}\cdot t^{\circ}+[d(1+t^2)-(w+dt)(2t)]\cdot t^{\circ}$, where $t^{\circ} = (1+t^2)^{-2}$. We obtain all its real roots for the quartic equation.
2. Combining with the bound constraints, we conclude that this problem contains at most $(4+2)$ breakpoints $\{P(\bar{t}_1), P(\bar{t}_2), ..., P(\bar{t}_j), lb, ub\}$ with $1 \leq j \leq 4$.

Greedy Strategies for Working Set Selection

Two New Greedy Strategies

1. Motivation: past studies show that greedy strategies significantly accelerates CD methods: LIBLINEAR, LIBSVM, CD-NMF
2. We propose two Working Set Selection (**WSS**) strategies.
3. **WWS-SV**: selects the index $\text{B} = [\bar{i}, \bar{j}]$ that most violates the first-order optimality condition
4. **WWS-OR**: chooses the index $\text{B} = [\bar{i}, \bar{j}]$ that leads to the maximum objective reduction

WSS: Working Set Selection via Greedy Strategies

Input: $\mathbf{X}^t$ and $\mathbf{G}^t \in \partial F(\mathbf{X}^t)$.

(**S1**) Compute the scoring matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$ using one of the following two strategies:

- Option **WSS-SV** (using Maximum Stationarity Violation Pair):

$$\mathbf{S} = \mathbf{X}^t[\mathbf{G}^t]^\mathsf{T} - \mathbf{G}^t[\mathbf{X}^t]^\mathsf{T}. \tag{10}$$

- Option **WSS-OR** (using Maximum Objective Reduction Pair):

$$\mathbf{S}_{ij} = \min_{\mathbf{V}^\mathsf{T}\mathbf{V}=\mathbf{I}_2} \langle \mathbf{V} - \mathbf{I}_2, \mathbf{T}_{\mathrm{BB}} \rangle, \mathrm{B} = [i,j], \tag{11}$$

where $\mathbf{T} = (\mathbf{G}^t - L_f\mathbf{X}^t)(\mathbf{X}^t)^\mathsf{T} - \alpha\mathbf{I}_n \in \mathbb{R}^{n \times n}$.

(**S2**) Output: $\mathrm{B} = [\bar{i}, \bar{j}] = \arg\max_{i \in [n], j \in [n], i \neq j} |\mathbf{S}_{ij}|$

Remarks on Working Set Selection Strategies

1. For **WSS-SV**, we have:
   $\mathbf{X}^t \in \mathrm{St}(n, r)$ is a critical point $\Leftrightarrow \mathbf{S} = \mathbf{0} \Leftrightarrow \mathbf{S}(\bar{i}, \bar{j}) = 0$.
2. For **WSS-OR**, if $\mathbf{X}^t$ is not a critical point, it holds that:
   $\mathbf{S}(\bar{i}, \bar{j}) < 0$ and $F(\mathbf{X}^{t+1}) < F(\mathbf{X}^t)$.
3. Standard greedy strategies has high computational complexity.
4. Practical strategies: Greedy + Random
5. This reduces to significantly reduced complexity:
   $\mathcal{O}(n^2 r) \Rightarrow \mathcal{O}(pr)$. Here $p \ll \mathrm{C}_n^2$.

Experiments

Experiments for L_0 norm-based SPCA Problem

1. L_0 norm-based Sparse PCA:

$$\min_{\mathbf{X}\in \mathrm{St}(n,r)} \; -\frac{1}{2}\langle \mathbf{X}, \mathbf{C}\mathbf{X}\rangle + \lambda\|\mathbf{X}\|_0.$$

2. **Data Sets**. 10 real-world or random data sets

3. **Compared Methods**. Two operator splitting methods: Linearized ADMM (LADMM) and Smoothing Penalty Method (SPM). Initialized differently with random and identity matrices, resulting in four variants: LADMM(id), SPM(id), LADMM(rnd), and SPM(rnd). We use a random strategy to find the working set for **OBCD**, initializing it with the identity matrix, resulting in **OBCD-R**(id).

Experiments for L_0 norm-based SPCA Problem

1. **Implementations**. All methods are implemented in MATLAB. However, our BSM is developed in C++ and integrated into the MATLAB environment.
2. **Experiment Settings**. We compare the objective values of different methods relative to CPU time over a 30-second runtime.

L_0 Norm-based SPCA with $\lambda = 10000$

data-m-n	$F_{\min}$	LADMM (id)	SPM (id)	LADMM (rnd)	SPM (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 10000$, time limit=30						
w1a-2477-300	2.0e+05	4.12e+04	3.90e+03	2.02e+04	1.70e+05	**0.00e+00**
TDT2-500-1000	2.0e+05	8.27e-01	6.71e-01	1.00e+04	4.00e+04	**0.00e+00**
20News-8000-1000	2.0e+05	3.72e-01	2.00e+04	2.00e+04	4.00e+04	**0.00e+00**
sector-6412-1000	2.0e+05	3.00e+04	2.00e+04	4.99e+00	1.10e+05	**0.00e+00**
E2006-2000-1000	2.0e+05	4.61e-02	9.12e-02	2.00e+04	1.60e+05	**0.00e+00**
MNIST-60000-784	1.5e+05	6.58e+04	4.67e+04	1.01e+05	7.80e+05	**0.00e+00**
Gisette-3000-1000	1.7e+05	6.70e+05	3.26e+05	2.31e+05	5.24e+05	**0.00e+00**
CnnCaltech-3000-1000	2.0e+05	1.18e+06	2.50e+05	1.10e+05	4.80e+05	**0.00e+00**
Cifar-1000-1000	2.0e+05	3.09e+04	9.99e+02	1.79e+05	1.41e+06	**0.00e+00**
randn-500-1000	1.9e+05	1.11e+05	8.10e+05	3.21e+05	1.52e+06	**0.00e+00**

Table: Comparisons of relative objective values $(F(\mathbf{X}) - F_{\min})$ for L_0 norm-based SPCA across all the compared methods. The 1^{st}, 2^{nd}, and 3^{rd} best results are colored with **red**, green and blue, respectively.

L_0 Norm-based SPCA with $\lambda = 1000$

data-m-n	$F_{\min}$	LADMM (id)	SPM (id)	LADMM (rnd)	SPM (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 1000$, time limit=30						
w1a-2477-300	1.5e+04	2.60e+03	3.90e+03	1.48e+03	8.02e+03	**0.00e+00**
TDT2-500-1000	2.0e+04	4.00e+03	6.71e-01	2.00e+03	7.00e+03	**0.00e+00**
20News-8000-1000	2.0e+04	3.00e+03	3.00e+03	5.00e+03	6.00e+03	**0.00e+00**
sector-6412-1000	2.0e+04	1.01e+03	3.00e+03	1.02e+03	1.30e+04	**0.00e+00**
E2006-2000-1000	2.0e+04	2.00e+03	1.16e-01	4.00e+03	1.20e+04	**0.00e+00**
MNIST-60000-784	-6.7e+04	6.38e+04	8.68e+04	2.28e+03	4.30e+04	**0.00e+00**
Gisette-3000-1000	-2.1e+05	4.11e+05	2.02e+05	1.19e+05	8.65e+04	**0.00e+00**
CnnCaltech-3000-1000	1.9e+04	9.09e+03	3.09e+04	2.40e+04	3.09e+04	**0.00e+00**
Cifar-1000-1000	1.6e+04	1.80e+04	9.99e+02	2.40e+04	1.10e+05	**0.00e+00**
randn-500-1000	1.4e+04	2.53e+04	5.81e+04	2.22e+04	4.92e+04	**0.00e+00**

Table: Comparisons of relative objective values $(F(\mathbf{X}) - F_{\min})$ for L_0 norm-based SPCA across all the compared methods. The 1^{st}, 2^{nd}, and 3^{rd} best results are colored with **red**, green and blue, respectively.

L_0 Norm-based SPCA with $\lambda = 100$

data-m-n	$F_{\min}$	LADMM (id)	SPM (id)	LADMM (rnd)	SPM (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 100$, time limit=30						
w1a-2477-300	-2.7e+03	2.28e+03	3.90e+03	1.84e+02	4.14e+02	**0.00e+00**
TDT2-500-1000	2.0e+03	6.00e+02	9.15e-01	3.00e+02	1.10e+03	**0.00e+00**
20News-8000-1000	2.0e+03	7.76e-02	3.87e-01	1.00e+02	1.00e+03	**0.00e+00**
sector-6412-1000	2.0e+03	1.03e+04	8.26e+00	6.12e+02	1.99e+02	**0.00e+00**
E2006-2000-1000	2.0e+03	1.01e+02	1.45e-01	5.50e+03	3.40e+03	**0.00e+00**
MNIST-60000-784	-2.2e+05	5.54e+03	2.23e+05	**0.00e+00**	1.05e+04	1.08e+04
Gisette-3000-1000	-8.8e+05	**0.00e+00**	3.00e+05	6.72e+04	1.62e+04	9.35e+04
CnnCaltech-3000-1000	1.4e+03	1.13e+03	2.96e+03	7.70e+02	7.72e+03	**0.00e+00**
Cifar-1000-1000	-4.3e+04	1.08e+05	2.48e+04	1.83e+04	3.79e+04	**0.00e+00**
randn-500-1000	-3.9e+03	4.10e+03	4.91e+03	3.55e+03	7.03e+03	**0.00e+00**

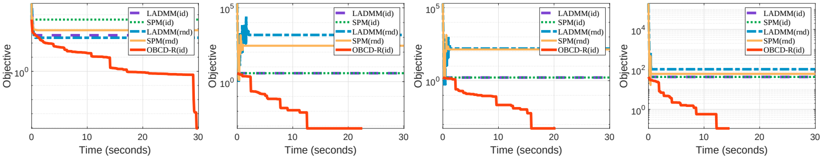
Table: Comparisons of relative objective values ($F(\mathbf{X}) - F_{\min}$) for L_0 norm-based SPCA across all the compared methods. The 1^{st}, 2^{nd}, and 3^{rd} best results are colored with **red**, green and blue, respectively.

L_0 Norm-based SPCA with $\lambda = 10$

data-m-n	F_{min}	LADMM (id)	SPM (id)	LADMM (rnd)	SPM (rnd)	OBCD-R (id)
$r = 20$, $\lambda = 10$, time limit=30						
w1a-2477-300	-5.2e+03	1.92e+03	4.55e+03	3.30e+02	8.05e+02	**0.00e+00**
TDT2-500-1000	2.0e+02	3.74e+00	3.74e+00	1.10e+02	2.70e+02	**0.00e+00**
20News-8000-1000	2.0e+02	1.66e+00	1.66e+00	1.73e+03	1.40e+02	**0.00e+00**
sector-6412-1000	1.6e+02	4.17e+01	4.17e+01	1.09e+02	5.95e+01	**0.00e+00**
E2006-2000-1000	2.0e+02	6.38e-01	6.38e-01	1.15e+03	5.00e+02	**0.00e+00**
MNIST-60000-784	-3.1e+05	2.01e+04	3.13e+05	**0.00e+00**	2.08e+03	6.25e+04
Gisette-3000-1000	-1.0e+06	1.64e+04	1.98e+04	1.15e+04	**0.00e+00**	7.31e+04
CnnCaltech-3000-1000	-4.7e+02	1.05e+03	3.20e+02	1.45e+03	2.66e+02	**0.00e+00**
Cifar-1000-1000	-1.2e+05	**0.00e+00**	8.67e+03	1.20e+04	6.17e+03	1.33e+04
randn-500-1000	-6.3e+03	1.09e+03	9.71e+02	8.90e+02	1.29e+03	**0.00e+00**

Table: Comparisons of relative objective values $(F(\mathbf{X}) - F_{\min})$ for L_0 norm-based SPCA across all the compared methods. The 1^{st}, 2^{nd}, and 3^{rd} best results are colored with **red**, green and blue, respectively.

L_0 Norm-based SPCA



(a) w1a-2477-300 (b) TDT2-500-1000 (c) 20News-8000-1000 (d) sector-6412-100

Figure: The convergence curve of the compared methods for solving L_0 norm-based SPCA with $\lambda = 100$. No matter how long the algorithms run, the other methods remain trapped in poor local minima.

Thank You!