

New matrix norms for structured matrix estimation

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Sparse Representations, Numerical Linear Algebra,
and Optimization workshop
BIRS, Banff, Oct 5-10, 2014

Outline

- 1 Atomic norms
- 2 Sparse matrices with disjoint column supports
- 3 Low-rank matrices with sparse factors

The screenshot shows the homepage of 'Homemade Gifts Made Easy'. At the top left is a logo with two stylized tulips. The title 'Homemade Gifts Made Easy' is centered at the top. To the right of the title is a row of four small images: a bowl of food, a pink rose, a bouquet of flowers, and a gift box. Below the title is a main content area with the heading 'How to Make Paper Lanterns'. Under this heading are three images of red paper lanterns in different stages of construction. Below the images is a paragraph of text: 'Looking for instructions on how to make paper lanterns? My husband designed an easy template for making paper lanterns in a cute round shape. They look a bit oriental, don't you think?'. To the left of the main content is a sidebar with 'Welcome' and 'Occasions' sections. To the right is a search bar and a 'FREE Homemade Gifts Newsletter!' sign-up box.

Homemade Gifts Made Easy

How to Make Paper Lanterns

Looking for instructions on how to make paper lanterns? My husband designed an easy template for making paper lanterns in a cute round shape. They look a bit oriental, don't you think?

FREE Homemade Gifts Newsletter!

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Atomic Norm (Chandrasekaran et al., 2012)

Definition

Given a set of atoms \mathcal{A} , the associated atomic norm is

$$\|x\|_{\mathcal{A}} = \inf\{t > 0 \mid x \in t \operatorname{conv}(\mathcal{A})\}.$$

NB: This is really a norm if \mathcal{A} is centrally symmetric and spans \mathbb{R}^p

Primal and dual form of the norm

$$\|x\|_{\mathcal{A}} = \inf \left\{ \sum_{a \in \mathcal{A}} c_a \mid x = \sum_{a \in \mathcal{A}} c_a a, \quad c_a > 0, \forall a \in \mathcal{A} \right\}$$

$$\|x\|_{\mathcal{A}}^* = \sup_{a \in \mathcal{A}} \langle a, x \rangle$$

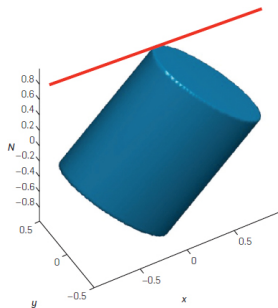
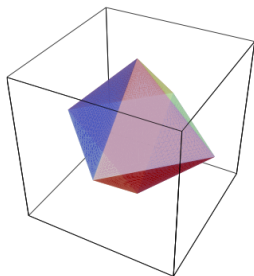
Examples

- Vector ℓ_1 -norm: $x \in \mathbb{R}^p \mapsto \|x\|_1$

$$\mathcal{A} = \{ \pm \mathbf{e}_k \mid 1 \leq k \leq p \}$$

- Matrix trace norm: $Z \in \mathbb{R}^{m_1 \times m_2} \mapsto \|Z\|_*$ (sum of singular value)

$$\mathcal{A} = \{ ab^T : a \in \mathbb{R}^{m_1}, b \in \mathbb{R}^{m_2}, \|a\|_2 = \|b\|_2 = 1 \}$$



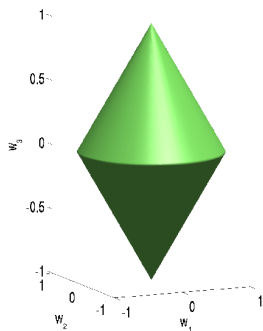
Group lasso (Yuan and Lin, 2006)

For $x \in \mathbb{R}^p$ and $\mathcal{G} = \{g_1, \dots, g_G\}$ a partition of $[1, p]$:

$$\|x\|_{1,2} = \sum_{g \in \mathcal{G}} \|x_g\|_2$$

is the atomic norm associated to the set of atoms

$$\mathcal{A}_g = \bigcup_{u \in \mathbb{R}^p : \text{supp}(u) = g, \|u\|_2 = 1}$$



$$\mathcal{G} = \{\{1, 2\}, \{3\}\}$$

$$\begin{aligned} \|x\|_{1,2} &= \|(x_1, x_2)^T\|_2 + \|x_3\|_2 \\ &= \sqrt{x_1^2 + x_2^2} + \sqrt{x_3^2} \end{aligned}$$

Group lasso with overlaps

How to generalize the group lasso when the groups overlap?

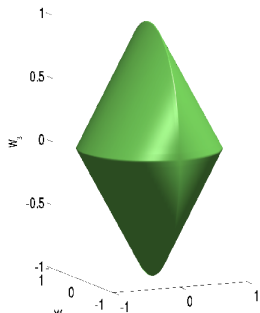
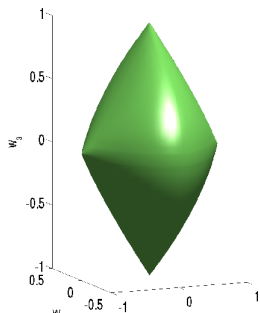
- Set features to zero by groups (Jenatton et al., 2011)

$$\|x\|_{1,2} = \sum_{g \in \mathcal{G}} \|x_g\|_2$$

- Select support as a union of groups (Jacob et al., 2009)

$$\|x\|_{\mathcal{A}_G},$$

see also MKL (Bach et al., 2004)



$$\mathcal{G} = \{\{1,2\}, \{2,3\}\}$$

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Joint work with...

Kevin Vervier, Pierre Mahé, Jean-Baptiste Veyrieras (Biomerieux)



Alexandre d'Aspremont (CNRS/ENS)



Columns with disjoint supports

$$X = \begin{array}{|c|c|c|} \hline \square & \blacksquare & \square \\ \hline \blacksquare & \square & \square \\ \hline \square & \square & \blacksquare \\ \hline \blacksquare & \square & \square \\ \hline \square & \square & \blacksquare \\ \hline \square & \blacksquare & \square \\ \hline \square & \square & \square \\ \hline \square & \square & \blacksquare \\ \hline \blacksquare & \square & \square \\ \hline \blacksquare & \square & \square \\ \hline \end{array}$$

- Motivation: multiclass or multitask classification problems where we want to select features specific to each class or task
- Example: recognize identify and emotion of a person from an image (Romera-Paredes et al., 2012), or hierarchical coarse-to-fine classifier (Xiao et al., 2011; Hwang et al., 2011)

Penalty for orthogonal columns

- For $X = [x_1, \dots, x_p] \in \mathbb{R}^{n \times p}$ we want

$$x_i^\top x_j = 0 \quad \text{for } i \neq j$$

- A natural "relaxation":

$$\Omega(X) = \sum_{i \neq j} \left| x_i^\top x_j \right|$$

- But not convex

Convex penalty for orthogonal columns

$$\Omega_K(X) = \sum_{i=1}^p K_{ii} \|x_i\|^2 + \sum_{i \neq j} K_{ij} |x_i^\top x_j|$$

Theorem (Xiao et al., 2011)

If \bar{K} is positive semidefinite, then Ω_K is convex, where

$$\bar{K}_{ij} = \begin{cases} |K_{ii}| & \text{if } i = j, \\ -|K_{ij}| & \text{otherwise.} \end{cases}$$

Can we be tighter?

$$\Omega_K(X) = \sum_{i=1}^p \|x_i\|^2 + \sum_{i \neq j} K_{ij} |x_i^\top x_j|$$

- Let \mathcal{O} be the set of matrices of unit Frobenius norm, with orthogonal columns

$$\mathcal{O} = \left\{ X \in \mathbb{R}^{n \times p} : X^\top X \text{ is diagonal and } \text{Trace}(X^\top X) = 1 \right\}$$

- Note that

$$\forall X \in \mathcal{O}, \quad \Omega_K(X) = 1$$

- The atomic norm $\|X\|_{\mathcal{O}}$ associated to \mathcal{O} is the tightest convex penalty to recover the atoms in \mathcal{O} !

Optimality of Ω_K for $p = 2$

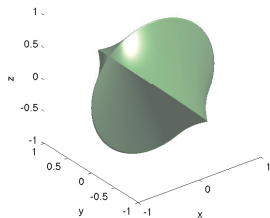
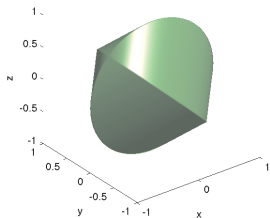
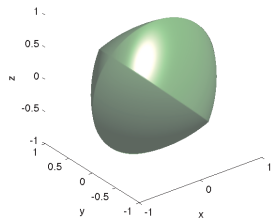
Theorem (Vervier, Mahé, d'Aspremont, Veyrieras and V., 2014)

For any $X \in \mathbb{R}^{n \times 2}$,

$$\Omega_K(X) = \|X\|_0^2$$

with

$$K = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$



Case $p > 2$

- $\Omega_K(X) \neq \|X\|_{\mathcal{O}}^2$
- But sparse combinations of matrices in \mathcal{O} may not be interesting anyway...

Theorem (Vervier et al., 2014)

For any $p \geq 2$, let K be a symmetric p -by- p matrix with non-negative entries and such that,

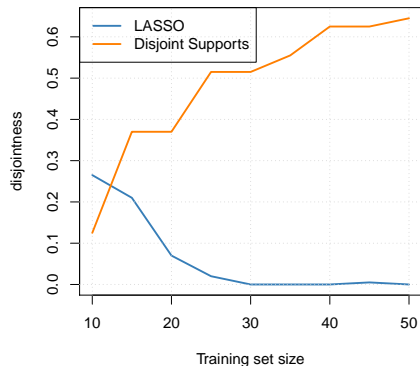
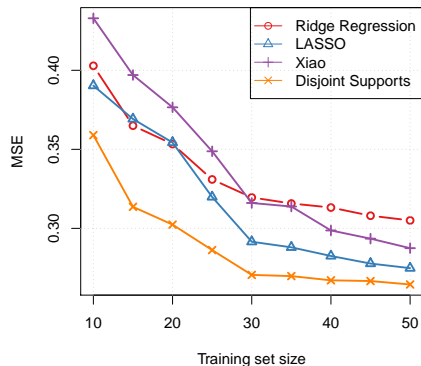
$$\forall i = 1, \dots, p \quad K_{ii} = \sum_{j \neq i} K_{ij}.$$

Then

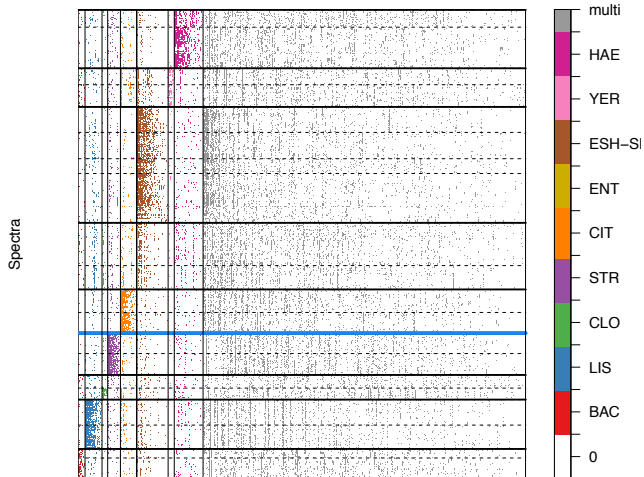
$$\Omega_K(X) = \sum_{i < j} K_{ij} \|x_i, x_j\|_{\mathcal{O}}^2.$$

Simulations

Regression $Y = XW + \epsilon$, W has disjoint column support, $n = p = 10$



Example: multiclass classification of MS spectra



Features

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- 3 Low-rank matrices with sparse factors

Joint work with...

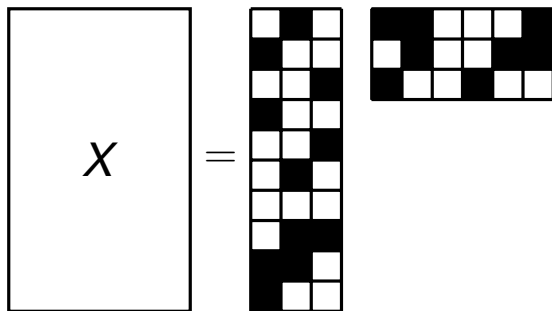
Emile Richard (Stanford)



Guillaume Obozinski (Ecole des Ponts - ParisTech)



Low-rank matrices with sparse factors



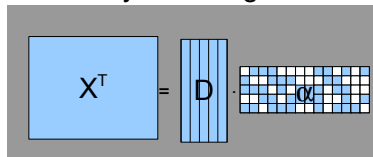
$$X = \sum_{i=1}^r u_i v_i^T$$

- factors not orthogonal a priori
- \neq from assuming the SVD of X is sparse

Dictionary Learning

$$\min_{\substack{A \in \mathbb{R}^{k \times n} \\ D \in \mathbb{R}^{p \times k}}} \sum_{i=1}^n \|x_i - D\alpha_i\|_2^2 + \lambda \sum_{i=1}^n \|\alpha_i\|_1 \quad \text{s.t.} \quad \forall j, \|d_j\|_2 \leq 1.$$

Dictionary Learning

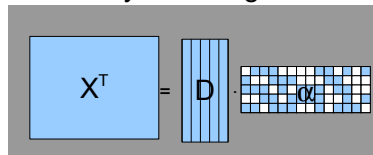


- e.g. overcomplete dictionaries for natural images
- sparse decomposition
- (Elad and Aharon, 2006)

Dictionary Learning / Sparse PCA

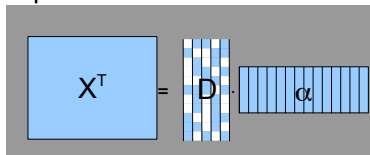
$$\min_{\substack{A \in \mathbb{R}^{k \times n} \\ D \in \mathbb{R}^{p \times k}}} \sum_{i=1}^n \|x_i - D\alpha_i\|_2^2 + \lambda \sum_{i=1}^n \|\alpha_i\|_1 \quad \text{s.t.} \quad \forall j, \|d_j\|_2 \leq 1.$$

Dictionary Learning



- e.g. overcomplete dictionaries for natural images
- sparse decomposition
- (Elad and Aharon, 2006)

Sparse PCA



- e.g. microarray data
- sparse dictionary
- (Witten et al., 2009; Bach et al., 2008)

Sparsity of the loadings vs sparsity of the dictionary elements

- **Low rank factorization with “community structure”**

Modeling clusters or community structure in social networks or recommendation systems (Richard et al., 2012).

- **Subspace clustering (Wang et al., 2013)**

Up to an unknown permutation, $X^T = [X_1^T \ \dots \ X_K^T]$ with X_k low rank, so that there exists a low rank matrix Z_k such that $X_k = Z_k X_k$. Finally,

$$X = ZX \quad \text{with} \quad Z = \text{BkDiag}(Z_1, \dots, Z_K).$$

- **Sparse PCA from $\hat{\Sigma}_n$**

- **Sparse bilinear regression**

$$y = x^T Mx' + \varepsilon$$

Existing approaches

- Bi-convex formulations

$$\min_{U, V} \mathcal{L}(UV^T) + \lambda(\|U\|_1 + \|V\|_1),$$

with $U \in \mathbb{R}^{n \times r}$, $V \in \mathbb{R}^{p \times r}$.

- Convex formulation for **sparse and low rank**

$$\min_Z \mathcal{L}(Z) + \lambda\|Z\|_1 + \mu\|Z\|_*$$

- Doan and Vavasis (2013); Richard et al. (2012)
- factors not necessarily sparse as r increases.

A new formulation for sparse matrix factorization

Assumptions:

$$X = \sum_{i=1}^r a_i b_i^\top$$

- All left factors a_i have support of size k .
- All right factors b_i have support of size q .

Goals:

Propose a convex formulation for sparse matrix factorization that

- is able to handle multiple sparse factors
- permits to identify the sparse factors themselves
- leads to better statistical performance than ℓ_1 /trace norm.

Propose algorithms based on this formulation.

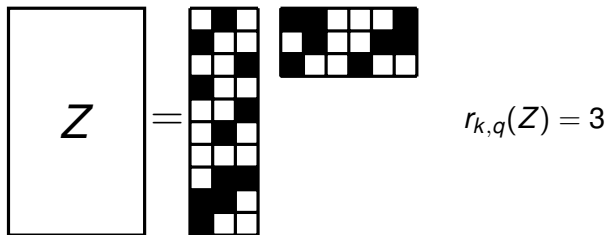
The (k, q) -rank of a matrix

- Sparse unit vectors:

$$\mathcal{A}_j^n = \{ \mathbf{a} \in \mathbb{R}^n : \|\mathbf{a}\|_0 \leq j, \|\mathbf{a}\|_2 = 1 \}$$

- (k, q) -rank of a $m_1 \times m_2$ matrix Z :

$$r_{k,q}(Z) = \min \left\{ r : Z = \sum_{i=1}^r c_i \mathbf{a}_i \mathbf{b}_i^\top, (\mathbf{a}_i, \mathbf{b}_i, c_i) \in \mathcal{A}_k^{m_1} \times \mathcal{A}_q^{m_2} \times \mathbb{R}_+ \right\}$$
$$= \min \left\{ \|\mathbf{c}\|_0 : Z = \sum_{i=1}^{\infty} c_i \mathbf{a}_i \mathbf{b}_i^\top, (\mathbf{a}_i, \mathbf{b}_i, c_i) \in \mathcal{A}_k^{m_1} \times \mathcal{A}_q^{m_2} \times \mathbb{R}_+ \right\}$$



The (k, q) trace norm (Richard et al., 2014)

For a matrix $Z \in \mathbb{R}^{m_1 \times m_2}$, we have

combinatorial penalty	$\ Z\ _0$		$\text{rank}(Z)$
convex relaxation	$\ Z\ _1$		$\ Z\ _*$

The (k, q) trace norm (Richard et al., 2014)

For a matrix $Z \in \mathbb{R}^{m_1 \times m_2}$, we have

	(1, 1)-rank	(k, q)-rank	(m_1, m_2)-rank
combinatorial penalty	$\ Z\ _0$	$r_{k,q}(Z)$	$\text{rank}(Z)$
convex relaxation	$\ Z\ _1$		$\ Z\ _*$

The (k, q) trace norm (Richard et al., 2014)

For a matrix $Z \in \mathbb{R}^{m_1 \times m_2}$, we have

	(1, 1)-rank	(k, q) -rank	(m_1, m_2) -rank
combinatorial penalty	$\ Z\ _0$	$r_{k,q}(Z)$	$\text{rank}(Z)$
convex relaxation	$\ Z\ _1$	$\Omega_{k,q}(Z)$	$\ Z\ _*$

The (k, q) trace norm $\Omega_{k,q}(Z)$ is the atomic norm associated with

$$\mathcal{A}_{k,q} := \{ab^\top \mid a \in \mathcal{A}_k^{m_1}, b \in \mathcal{A}_q^{m_2}\},$$

namely:

$$\Omega_{k,q}(Z) = \inf \left\{ \|c\|_1 : Z = \sum_{i=1}^{\infty} c_i a_i b_i^\top, (a_i, b_i, c_i) \in \mathcal{A}_k^{m_1} \times \mathcal{A}_q^{m_2} \times \mathbb{R}_+ \right\}$$

Some properties of the (k, q) -trace norm

Nesting property:

$$\Omega_{m_1, m_2}(Z) = \|Z\|_* \leq \Omega_{k, q}(Z) \leq \|Z\|_1 = \Omega_{1, 1}(Z)$$

Dual norm and reformulation

- Let $\|\cdot\|_{\text{op}}$ denote the operator norm.
- Let $\mathcal{G}_{k, q} = \{(I, J) \subset [1, m_1] \times [1, m_2], |I| = k, |J| = q\}$

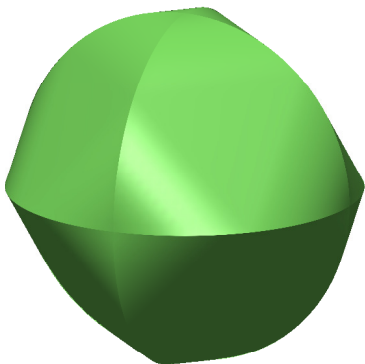
Given that $\|x\|_{\mathcal{A}}^* = \sup_{a \in \mathcal{A}} \langle a, x \rangle$, we have

$$\Omega_{k, q}^*(Z) = \max_{(I, J) \in \mathcal{G}_{k, q}} \|Z_{I, J}\|_{\text{op}} \quad \text{and}$$

$$\Omega_{k, q}(Z) = \inf \left\{ \sum_{(I, J) \in \mathcal{G}_{k, q}} \|A^{(I, J)}\|_* : Z = \sum_{(I, J) \in \mathcal{G}_{k, q}} A^{(I, J)}, \text{supp}(A^{(I, J)}) \subset I \times J \right\}$$

Vector case

When $q = m_2 = 1$, $\Omega_{k,1}(x)$ is the k -support norm of Argyriou et al. (2012), i.e., the overlapping group lasso with all groups of size k .



Statistical dimension (Amelunxen et al., 2013)

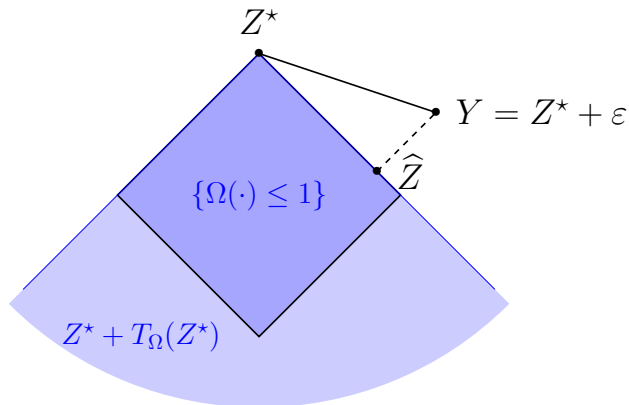


figure inspired by Amelunxen et al. (2013)

$$\mathfrak{S}(Z, \Omega) := \mathbb{E} \left[\left\| \Pi_{T_\Omega(Z)}(\mathcal{G}) \right\|_{\text{Fro}}^2 \right],$$

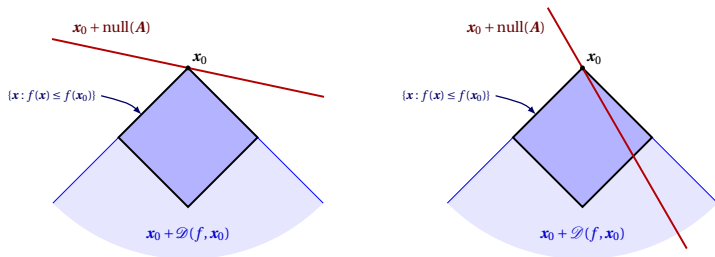


Figure from Amelunxen et al. (2013)

Exact recovery from random measurements

With $\mathcal{X} : \mathbb{R}^p \rightarrow \mathbb{R}^n$ rand. lin. map from the std Gaussian ensemble

$$\hat{Z} = \underset{Z}{\operatorname{argmin}} \Omega(Z) \quad \text{s.th.} \quad \mathcal{X}(Z) = y$$

is equal to Z^* w.h.p. as soon as $n \geq \mathfrak{G}(Z^*, \Omega)$.

Statistical dimension of the (k, q) -trace norm

Theorem (Richard et al., 2014)

Let $A = ab^\top \in \mathcal{A}_{k,q}$ with $I_0 = \text{supp}(a)$ and $J_0 = \text{supp}(b)$.

$$\text{Let } \gamma(a, b) := (k \min_{i \in I_0} a_i^2) \wedge (q \min_{j \in J_0} b_j^2),$$

we have

$$\mathfrak{S}(A, \Omega_{k,q}) \leq \frac{322}{\gamma^2} (k + q + 1) + \frac{160}{\gamma} (k \vee q) \log(m_1 \vee m_2).$$

Summary of results for statistical dimension

Matrix norm	\mathfrak{S}	Vector norm	\mathfrak{S}
ℓ_1	$\Theta(kq \log \frac{m_1 m_2}{kq})$	ℓ_1	$\Theta(k \log \frac{p}{k})$
trace-norm	$\Theta(m_1 + m_2)$	ℓ_2	p
$\ell_1 + \text{trace}$	$\Omega(kq \wedge (m_1 + m_2))$	elastic net	$\Theta(k \log \frac{p}{k})$
(k, q) -trace	$\mathcal{O}((k \vee q) \log (m_1 \vee m_2))$	k -support	$\Theta(k \log \frac{p}{k})$

Lower bound for $\ell_1 + \text{trace}$ norm based on a result of Oymak et al. (2012)

$f = \Theta(g)$ means ($f = \mathcal{O}(g)$ & $g = \mathcal{O}(f)$)

$f = \Omega(g)$ means $g = \mathcal{O}(f)$

Working set algorithm

$$\min_Z \mathcal{L}(Z) + \lambda \Omega_{k,q}(Z)$$

Given a **working set** \mathcal{S} of blocks (I, J) , solve the restricted problem

$$\min_{Z, (A^{(I,J)})_{(I,J) \in \mathcal{S}}} \mathcal{L}(Z) + \lambda \sum_{(I,J) \in \mathcal{S}} \|A^{(I,J)}\|_*$$

$$Z = \sum_{(I,J) \in \mathcal{S}} A^{(I,J)}, \quad \text{supp}(A^{(I,J)}) \subset I \times J.$$

Proposition

The global problem is solved by a solution Z_S of the restricted problem if and only if

$$\forall (I, J) \in \mathcal{G}_{k,q}, \quad \left\| [\nabla \mathcal{L}(Z_S)]_{I,J} \right\|_{\text{op}} \leq \lambda. \quad (*)$$

Working set algorithm

Active set algorithm

Iterate:

- 1 Solve the restricted problem by block coordinate descent (Tseng and Yun, 2009)
- 2 Look for (I, J) that violates (\star)
 - If none exists, terminate the algorithm !
 - Else add the found (I, J) to \mathcal{S}

Problem: step 2 require to solve a rank-1 SPCA problem \rightarrow NP-hard

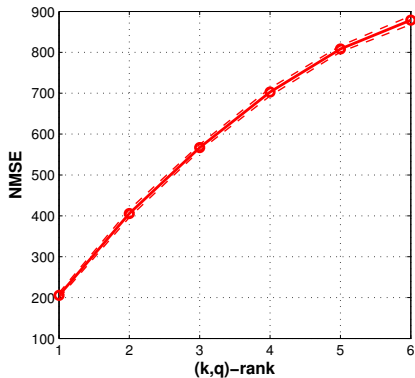
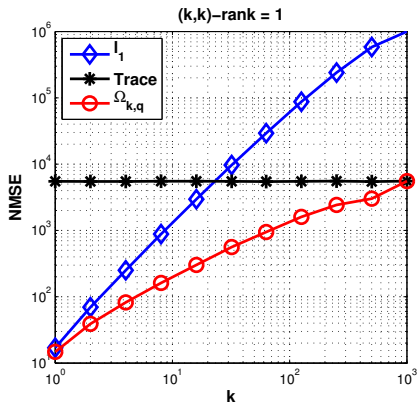
Idea: Leverage the work on algorithms that attempt to solve rank-1 SPCA like

- convex relaxations,
- truncated power iteration method

to heuristically find blocks potentially violating the constraint.

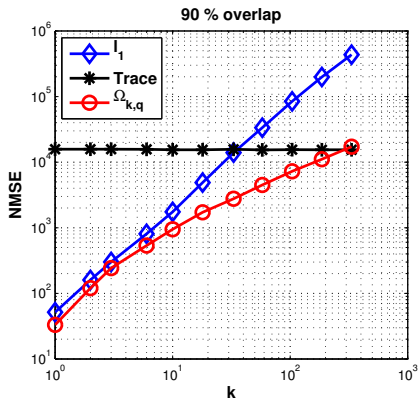
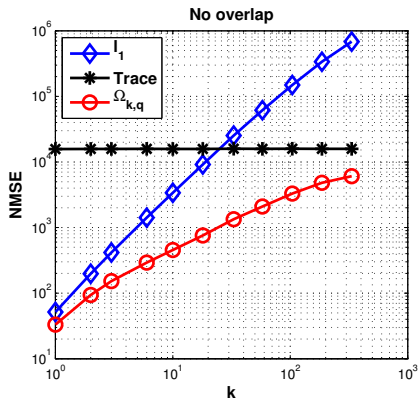
Denoising results

- $Z \in \mathbb{R}^{1000 \times 1000}$ with $Z = \sum_{i=1}^r a_i b_i^\top + \sigma G$ and $a_i b_i^\top \in \mathcal{A}_{k,q}$
- $k = q$
- σ^2 small \Rightarrow $\text{MSE} \propto \mathfrak{G}(ab^\top, \Omega_{k,q}) \sigma^2$

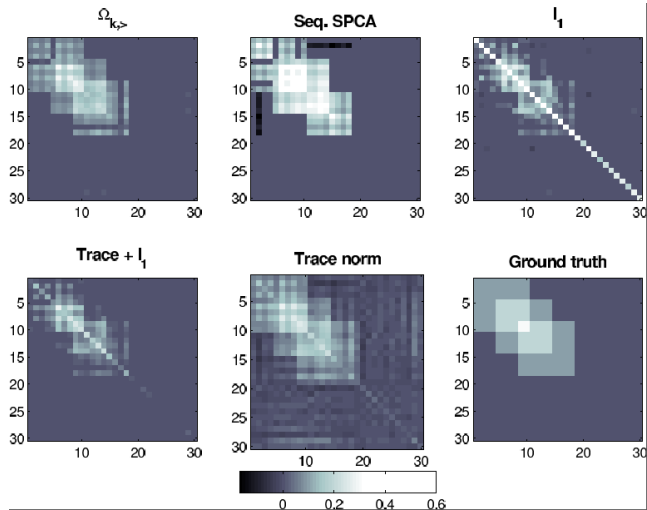


Denoising results

- $[Z \in \mathbb{R}^{300 \times 300}$ and σ^2 small \Rightarrow $\text{MSE} \propto \mathfrak{G}(ab^T, \Omega_{k,q}) \sigma^2]$
- $r = 3$ atoms, with or without overlap



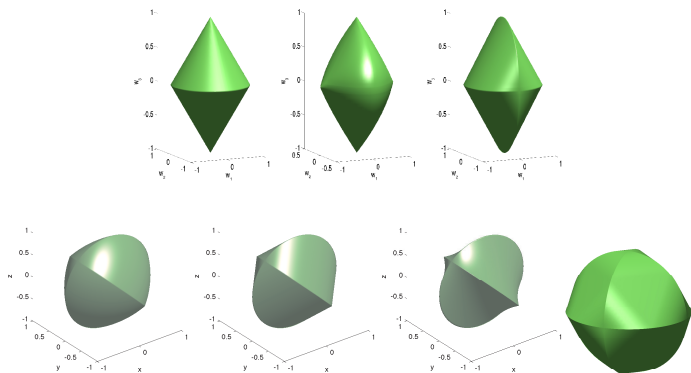
Empirical results for sparse PCA



Sample covariance	Trace	ℓ_1	Trace + ℓ_1	Sequential	$\Omega_{k,\succeq}$
4.20 ± 0.02	0.98 ± 0.01	2.07 ± 0.01	0.96 ± 0.01	0.93 ± 0.08	0.59 ± 0.03

Table 3: Relative error of covariance estimation with different methods.

Conclusion



- Atomic norms for structured sparsity
- Gain in statistical performance at the expense of algorithmic complexity (convex but NP-hard)
- The structure of the convex problem may be exploited to devise new efficient heuristics or relaxations

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