# Relaxations convexes pour l'estimation de matrices à facteurs parcimonieux

Guillaume Obozinski

Ecole des Ponts - ParisTech

Collaboration avec Emile Richard et Jean-Philippe Vert

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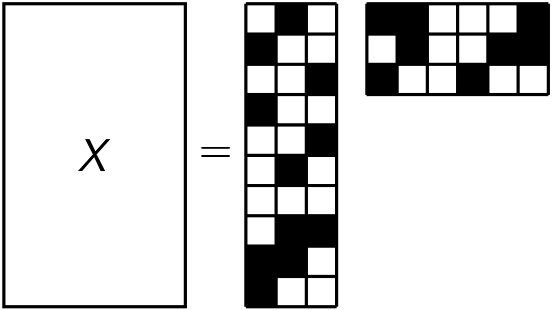
# Estimation low rank matrices with sparse factors



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

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

# Dictionary Learning

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

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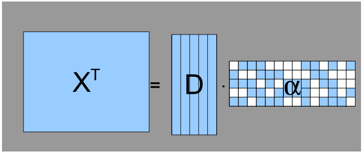

- e.g. overcomplete dictionaries for natural images
- sparse decomposition
- (Elad and Aharon, 2006)

# Dictionary Learning /Sparse PCA

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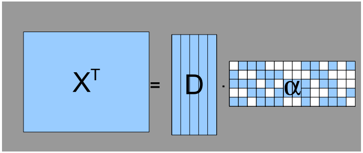

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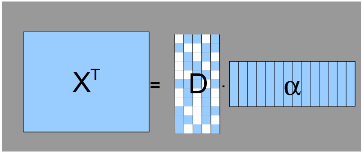
## Sparse PCA



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

**Sparsity of the loadings vs sparsity of the dictionary elements**

# Applications

## 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, $X^\top = \begin{bmatrix} X_1^\top & \dots & X_K^\top \end{bmatrix}$ with $X_k$ low rank, so that there exists a low rank matrix $Z_k$ such that $X_k = Z_k X_k$. Finally,

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

## Sparse PCA from $\hat{\Sigma}_n$

## Sparse bilinear regression

$$y = x^\top M x' + \varepsilon$$

# Existing approaches

## Bi-convex formulations

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

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

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## 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.

# Rank one case with square loss

$$\min_{u,v,\sigma} \|X - \sigma u v^\top\|_2 \qquad \text{s.t.} \qquad \begin{aligned} &\sigma \in \mathbb{R}_+, \\ &u \in \mathcal{U} \subset \mathbb{R}^n, \quad v \in \mathcal{V} \subset \mathbb{R}^p, \\ &\|u\|_2 = \|v\|_2 = 1. \end{aligned}$$

is equivalent to solving

$$\max_{u,v} \quad u^\top X v \qquad \text{s.t.} \qquad \begin{aligned} &u \in \mathcal{U} \subset \mathbb{R}^n, \quad v \in \mathcal{V} \subset \mathbb{R}^p, \\ &\|u\|_2 = \|v\|_2 = 1. \end{aligned}$$

- Corresponds to sparse PCA when $u = v$.

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## Approaches differ according to view

- analysis view → build sequences of rank 1 approximations,
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## Analysis SPCA focusses on solving rank-1 sparse PCA

- convex formulations: d'Aspremont et al. (2007, 2008); Amini and Wainwright (2009)
- modified power methods: Journée et al. (2010); Luss and Teboulle (2013); Yuan and Zhang (2013)

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## Synthesis SPCA focusses on finding several complementary sparse factors

Essentially based on nuclear norms (Jameson, 1987; Bach et al., 2008; Bach, 2013).

# A new formulation for sparse matrix factorization and a new matrix norm

# 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 $k$.
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Propose a convex formulation for sparse matrix factorization that

- is able to handle multiple sparse factors
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Propose algorithms based on this formulation.

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a $(k, q)$-decomposition of $Z$ any optimal solution $(a_i^\star, b_i^\star, c_i^\star)_{1 \leq i \leq r}$

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- Can we define a principled relaxation of the $(k,q)$-rank?

# Atomic Norm (Chandrasekaran et al., 2012)

### Definition (Atomic norm of the set of atoms $\mathcal{A}$)

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

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so that

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

Call $\Omega_{k,q}$ the $(k, q)$-trace norm and solutions the $(k, q)$-sparse SVDs.

# Properties of the $(k, q)$-trace norm

## Nesting property

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## Dual norm and reformulation

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

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# The (k,q)-CUT-norm: an $\ell_\infty$ counterpart

With the following subset of $\mathcal{A}_k^m$:

$$\widetilde{\mathcal{A}}_k^m = \left\{ a \in \mathbb{R}^m, \ \|a\|_0 = k \ , \ \forall i \in \mathrm{supp}(a), \ |a_i| = \frac{1}{\sqrt{k}} \right\},$$

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- When $k = m_1$ and $q = m_2$, $\widetilde{\Omega}_{n,n}$ is the gauge function of the CUT-polytope of a bipartite graph (Deza and Laurent, 1997).

# Vector case

When $q = m_2 = 1$, we retrieve vector norms:

- $\Omega_{k,1} = \theta_k$ is the $k$-support norm of Argyriou et al. (2012).
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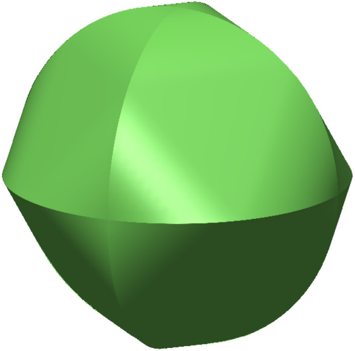

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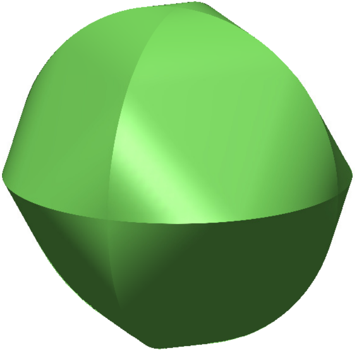
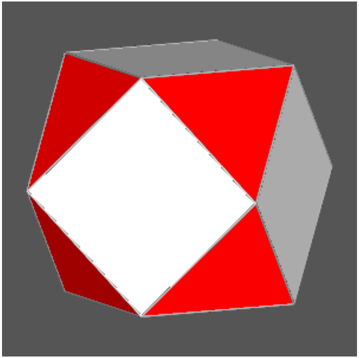
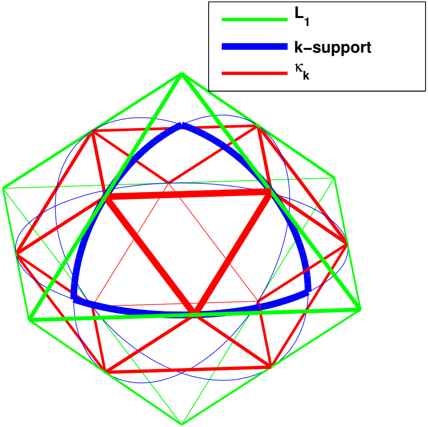
$$\kappa_j(w) = \frac{1}{\sqrt{j}} \max\left(\|w\|_\infty, \frac{1}{j}\|w\|_1\right).$$





# Relation between unit balls



$\theta_k$, $\kappa_k$ and $\frac{1}{\sqrt{k}}\|\cdot\|_1$ for $k = 2$ in $\mathbb{R}^3$.

# Learning matrices with sparse factors

## Sparse bilinear regression

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## Subspace clustering

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## Rank $r$ sparse PCA

$$\min_Z \frac{1}{2}\|\hat{\Sigma}_n - Z\|_F^2 \quad + \quad \lambda\,\Omega_{k,k}(Z) \quad \text{s.t.} \quad Z \succeq 0\,, \qquad \text{or}$$

$$\min_Z \frac{1}{2}\|\hat{\Sigma}_n - Z\|_F^2 \quad + \quad \lambda\,\Omega_{k,\succeq}(Z)\,,$$

with $\Omega_{k,\succeq}$ the atomic norm for the set $\mathcal{A}_{k,\succeq} = \{aa^\top, a \in \mathcal{A}_k\}$.

# Statistical guarantees

# Statistical dimension (Amelunxen et al., 2013)

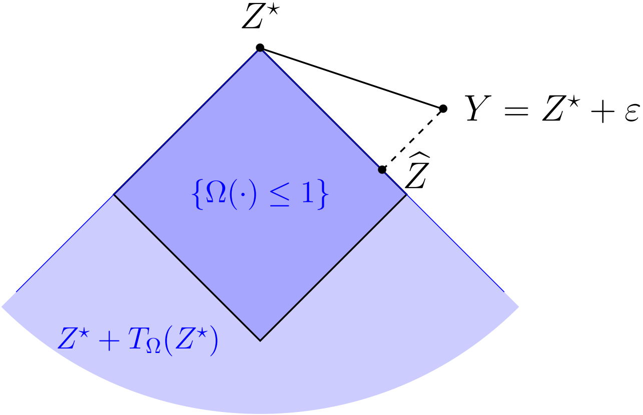
$Z^\star$
$Y = Z^\star + \varepsilon$
$\widehat{Z}$
$\{\Omega(\cdot) \leq 1\}$
$Z^\star + T_\Omega(Z^\star)$

figure inspired by Amelunxen et al. (2013)

# Statistical dimension (Amelunxen et al., 2013)

Tangent cone:

$$T_{\Omega}(Z) := \overline{\bigcup_{\tau>0} \left\{ H \in \mathbb{R}^{m_1 \times m_2} \ : \ \Omega(Z + \tau H) \leq \Omega(Z) \right\}} .$$

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The statistical dimension $\mathfrak{S}(Z, \Omega)$ of $\Omega$ at $Z$ can then be formally defined as

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

where

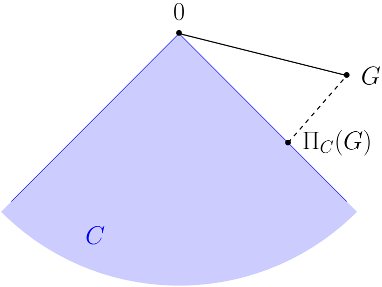
- $G$ is a matrix with i.i.d. standard normal entries
- $\Pi_{T_\Omega(Z)}(G)$ is the orthogonal projection of $G$ onto $T_\Omega(Z)$.

"The statistical dimension $\delta$ is the unique continuous, rotation-invariant localization valuation on the set of convex cones that satisfies $\delta(L) = \dim(L)$ for any subspace $L$."

# Relation between Gaussian width and statistical dimension

Gaussian width of intersection of the cone with a Euclidean ball:

$$
\begin{aligned}
w(C) &= \max_{U \in T_\Omega(Z) \cap \mathbb{S}^{d-1}} \langle U, G \rangle \\
&= \mathbb{E}\big[\, \|\Pi_C(G)\|_{\mathrm{Fro}} \,\big].
\end{aligned}
$$



Amelunxen et al. (2013) show that

$$w(C)^2 \le \mathfrak{S}(C) \le w(C)^2 + 1.$$

# General Null Space property

Consider the optimization problem

$$\min_{Z} \Omega(Z) \qquad \text{s.t.} \qquad y = \mathcal{X}(Z) \tag{1}$$

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### Theorem (NSP)

*$Z^*$ is the unique optimal solution of (1) if and only if*

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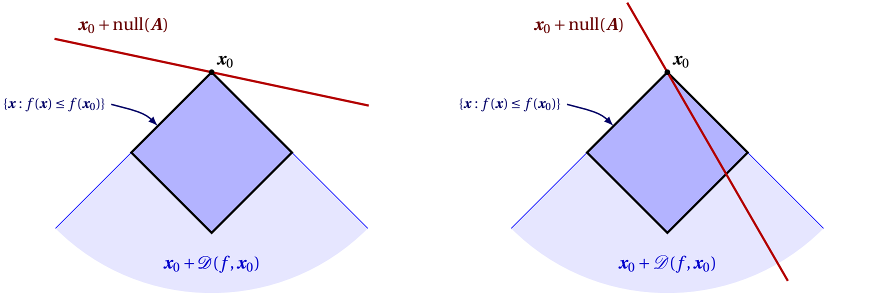
Note: this motivates a posteriori the construction of atomic norms.

# Nullspace property and $\mathfrak{S}$ (Chandrasekaran et al., 2012)


$x_0 + \mathrm{null}(A)$
$x_0$
$\{x : f(x) \leq f(x_0)\}$
$x_0 + \mathscr{D}(f, x_0)$
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$x_0 + \mathscr{D}(f, x_0)$

Figure from Amelunxen et al. (2013)

## Exact recovery from random measurements

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

$$\widehat{Z} = \arg\min_{Z} \Omega(Z) \quad \text{s.th.} \quad \mathcal{X}(Z) = y$$

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

# Denoising with an atomic norm

If

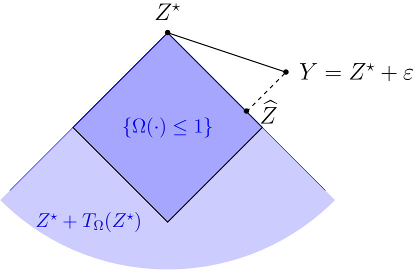
- $Y = Z^\star + \frac{\sigma}{\sqrt{n}}\epsilon$
- with $\epsilon$ standard Gaussian,

then

$$\widehat{Z} = \arg\min_{Z} \|Z - Y\|_{\mathrm{Fro}} \quad \text{s.t.} \quad \Omega(Z) \le \Omega(Z^\star)$$

satisfies

$$\boxed{\mathbb{E}\|\widehat{Z} - Z^\star\|^2 \le \frac{\sigma^2}{n}\mathfrak{S}(Z^\star, \Omega).}$$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# Statistical dimension at elements of $\widetilde{\mathcal{A}}_{k,q}$

- Consider an element $ab^\top \in \widetilde{\mathcal{A}}_{k,q}$.
- We have $\|ab^\top\|_0 = kq$.

So

| Matrix norm | $\mathfrak{S}$ |
|---|---|
| $\ell_1$ | $\Theta(kq \ \log \frac{m_1 m_2}{kq})$ |
| trace-norm | $\Theta(m_1 + m_2)$ |
| $\ell_1$ + trace-norm | **?** |
| $(k, q)$-trace | **?** |
| $(k, q)$-cut | **?** |

# Theoretical results

Proposition (UB on $\mathfrak{S}(A, \widetilde{\Omega}_{k,q})$)

*For any* $A \in \widetilde{\mathcal{A}}_{k,q}$, *we have that*

$$\mathfrak{S}(A, \widetilde{\Omega}_{k,q}) \;\leq\; 16(k+q) + 9\left(k \log \frac{m_1}{k} + q \log \frac{m_2}{q}\right) .$$

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## Proposition (UB on $\mathfrak{S}(A, \Omega_{k,q})$)

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

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

*we have*

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

# Summary of results for statistical dimension

| Matrix norm | $\mathfrak{S}$ | Vector norm | $\mathfrak{S}$ |
|---|---|---|---|
| $\ell_1$ | $\Theta(kq\ \log \frac{m_1 m_2}{kq})$ | $\ell_1$ | $\Theta(k \log \frac{p}{k})$ |
| trace-norm | $\Theta(m_1 + m_2)$ | $\ell_2$ | $p$ |
| $\ell_1 +$ trace-n. | $\Omega\big(kq \wedge (m_1 + m_2)\big)$[1] | elastic net | $\Theta(k \log \frac{p}{k})$ |
| $(k, q)$-trace | $\mathcal{O}((k \vee q) \log (m_1 \vee m_2))$ | $k$-support | $\Theta(k \log \frac{p}{k})$ |
| $(k, q)$-cut | $\mathcal{O}(k \log \frac{m_1}{k} + q \log \frac{m_2}{q})$ | $\kappa_k$ | $\Theta(k \log \frac{p}{k})$ |
| "cut-norm" | $\mathcal{O}(m_1 + m_2)$ | $\ell_\infty$ | $p$ |

[1] Proof relying on a result of Oymak et al. (2012)

# Algorithm

# Working set algorithm

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

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

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

## Proposition

*The global problem is solved by a solution $Z_{\mathcal{S}}$ of the restricted problem if and only if*

$$\forall (I, J) \in \mathcal{G}_{k,q}, \quad \left\|\left[\nabla\mathcal{L}(Z_{\mathcal{S}})\right]_{I,J}\right\|_{\mathrm{op}} \leq \lambda. \qquad (\star)$$

# Working set algorithm

## Active set algorithm

Iterate:

1. Solve the restricted problem
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 → NP-hard

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

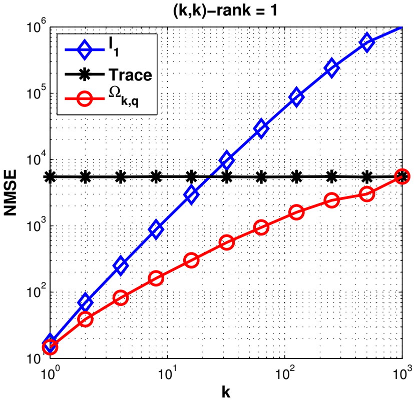
- convex relaxations,
- truncated power iteration method

to heuristically find blocks potentially violating the constraint.

# Experiments

# Denoising results

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



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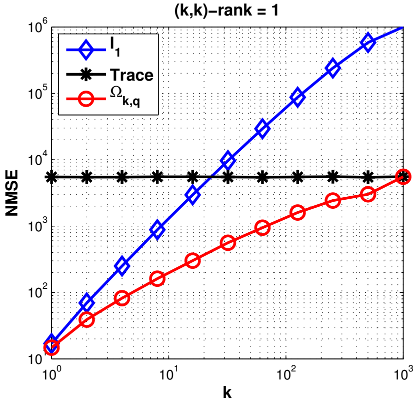
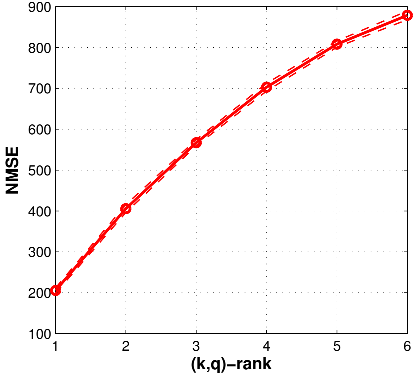
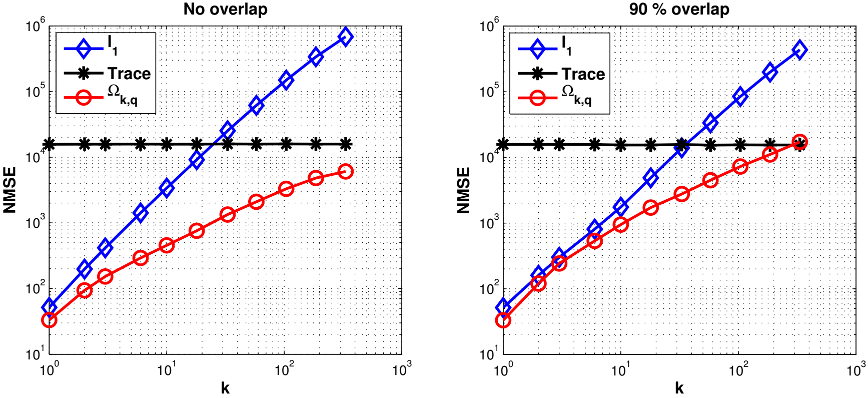
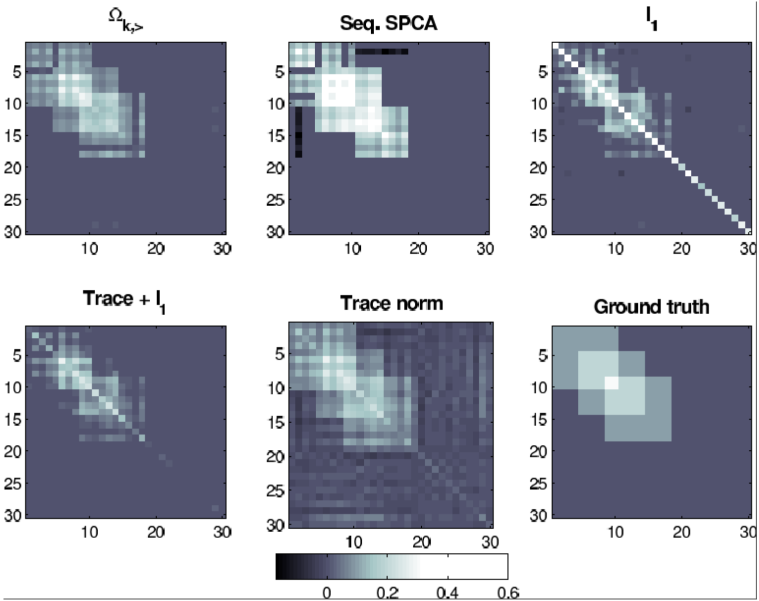




# Denoising results $[Z \in \mathbb{R}^{300\times 300}$ and $\sigma^2$ small $\Rightarrow$ MSE $\propto \mathfrak{S}(ab^\top, \Omega_{k,q})\,\sigma^2]$



# Empirical results for sparse PCA



# Conclusions

## Summary

- Gain in statistical performance at the expense of theoretical tractability.
- Even though the problem is NP-hard the structure of the convex problem can be exploited to devise efficient heuristics.

## Not discussed

- slow rate analysis
- purely geometric results

## Open questions and future work

- Generalization to the case where $(k, q)$ can be different for each pair of factors and not known a priori.

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