# Less is More: <br> Sparsity in Principal Component Analysis and in Linear Systems 

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## Goals

- Examine linear algebra problems with cardinality constraints
- Develop new formulations, and corresponding convex relaxations
- New formulations may offer insights into problem
- Ultimate objective is to derive estimates of the quality of the convex relaxations


## Outline

- Principal component analysis
- The sparse PCA problem
- New formulation and SDP relaxation
- Quality estimate
- Sparsity in linear systems


## Principal component analysis

PCA is a classic tool in multivariate data analysis

- Input: a $n \times n$ covariance matrix $\Sigma$
- Output: a sequence of factors ranked by variance
- Each factor is a linear combination of the problem variables

Typical use: reduce the number of dimensions of a model while maximizing the information (variance) contained in the simplified model

## Solving the PCA problem

- The PCA problem can be solved via the eigenvalue decomposition of the covariance matrix:

$$
\Sigma=\sum_{i=1}^{n} \lambda_{i} x_{i} x_{i}^{T}
$$

- $\lambda_{1} \geq \ldots \geq \lambda_{n} \geq 0$ are the eigenvalues of $\Sigma$
- The corresponding eigenvectors $x_{i}$ are called the principal components, or factors.


## PCA and rank-one approximation

- The first principal component, $x_{1}$, can be obtained via the solution to the rank-one approximation problem:

$$
\min _{z}\left\|\Sigma-z z^{T}\right\|_{F}
$$

the solution of which is $z=\lambda_{1} x_{1} x_{1}^{T}$.

$$
\text { (Here, }\|A\|_{F}^{2}=\operatorname{Tr} A^{T} A \text { denotes the Frobenius norm of a matrix } A \text {.) }
$$

- Above problem can be reduced to the variational problem:

$$
\max _{x} x^{T} \Sigma x:\|x\|_{2}=1
$$

the solution of which is $x=x_{1}$.

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## Looking for sparse factors

Gene expression data analysis: "explaining data with a few genes"

- PCA is used for clustering and visualizing data (gene responses vs. drugs)
- principal axes represent a combination of genes that are important in explaining data
- the sparser the axes, the less genes are involved
- ultimately, a short list of genes that explain data could yield a universal diagnostic chip


## PCA vs. sparse PCA: example

## PCA



Sparse PCA


Clustering of gene expression data in the PCA versus sparse PCA basis with 500 genes. The factors $f$ on the left are dense and each use all 500 genes while the sparse factors $g_{1}, g_{2}$ and $g_{3}$ on the right involve 6,4 and 4 genes respectively. (Data source: Iconix Pharmaceuticals, Inc.)

## Some previous work

- Vines (2000): restrict the factors' coefficients in a small set of integers, such as 0,1 , and -1
- Cadima and Jolliffe (1995): simple threshold approach
- Jolliffe and Udin (2003): SCoTLASS
- Zou, Hastie and Tibshirani (2004): write PCA as a regression problem, and add a $l_{1}$-norm penalty to it
- d'Aspremont, EI Ghaoui, Jordan, Lanckriet (2004): Direct sparse PCA


## Direct Sparse PCA

- Cardinality-penalized variational problem:

$$
\max _{x} x^{T} \Sigma x-\rho\|x\|_{0}:\|x\|_{2}=1
$$

where $\rho>0$, and $\|x\|_{0}$ denotes the number of non-zero elements in $x$

- Let $X=x x^{T}$, and approximate problem by

$$
\max _{X} \operatorname{Tr} \Sigma X-\rho\|X\|_{1}: X \succeq 0, \quad \operatorname{Tr} X=1, \quad \operatorname{Rank}(X)=1
$$

( $\|\cdot\|_{1}$ denotes sum of absolute values)

- Dropping the rank constraint leads to an SDP


## Solving direct sparse PCA

- The direct sparse PCA problem

$$
\max _{X} \operatorname{Tr} \Sigma X-\rho\|X\|_{1}: X \succeq 0, \quad \operatorname{Tr} X=1
$$

can be solved as an SDP, via general-purpose interior-point methods Complexity: $O\left(n^{6} \log (1 / \epsilon)\right)$

- For large-scale problems, first-order methods (Nesterov, 2005) can be used Complexity: $O\left(n^{4} \sqrt{\log n} / \epsilon\right)$


## Problems with direct sparse PCA

- Direct sparse PCA relies on two relaxation steps:
- Lower bound on $\|\cdot\|_{0}$-norm: via Cauchy-Schwartz inequality,

$$
\forall x,\|x\|_{2}=1:\|x\|_{0} \geq\|x\|_{1}^{2}
$$

- Rank relaxation: lift $x x^{T} \rightarrow X$, and drop rank constraint on $X$
- Analysis of the quality of the approximation seems to be difficult


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## Equality vs. inequality model

Sparse PCA problem:

$$
\phi:=\max _{x} x^{T} \Sigma x-\rho\|x\|_{0}:\|x\|_{2}=1
$$

We will develop SDP bounds for the related quantity:

$$
\tilde{\phi}:=\max _{x} x^{T} \Sigma x-\rho\|x\|_{0}:\|x\|_{2} \leq 1
$$

Fact: (assume WLOG $\Sigma_{11} \geq \ldots \geq \Sigma_{n n}$ )

- If $\rho \geq \Sigma_{11}$, then $\tilde{\phi}=0, \phi=\Sigma_{11}-\rho$ (with optimizer $x^{*}=e_{1}$ )
- If $\rho<\Sigma_{11}$, then $\tilde{\phi}=\phi>0$

In the sequel, assume $\rho<\Sigma_{11}$

## Towards a new formulation

Our problem:

$$
\begin{equation*}
\phi:=\max _{x} x^{T} \Sigma x-\rho\|x\|_{0}:\|x\|_{2} \leq 1 \tag{1}
\end{equation*}
$$

We have

$$
\begin{equation*}
\phi=\max _{u \in\{0,1\}^{n}} \max _{y^{T} y \leq 1} y^{T} D(u) \Sigma D(u) y-\rho \cdot \mathbf{1}^{T} u \tag{2}
\end{equation*}
$$

where $D(u):=\operatorname{diag}(u)$

- The boolean vector $u$ represents the sparsity pattern of an optimal solution
- Optimal $(y, u)$ in (2) related to optimal $x$ in (1) by

$$
x=D(u) y
$$

## Towards a new formulation (cont'd)

Eliminating $y$ in (2), obtain

$$
\begin{aligned}
\phi & =\max _{x} x^{T} \Sigma x-\rho\|x\|_{0}:\|x\|_{2} \leq 1 \\
& =\max _{u \in\{0,1\}^{n}} \max _{y^{T} y \leq 1} y^{T} D(u) \Sigma D(u) y-\rho \cdot \mathbf{1}^{T} u \\
& =\max _{u \in\{0,1\}^{n}} \lambda_{\max }(D(u) \Sigma D(u))-\rho \cdot \mathbf{1}^{T} u
\end{aligned}
$$

- Optimal $y$ is an eigenvector corresponding to $\lambda_{\text {max }}$ above
- Optimal $x$ is $x=D(u) y$


## Towards a new formulation (cont'd)

- Cholesky decomposition: Let $\Sigma=A^{T} A$, where $A=\left[a_{1} \ldots a_{n}\right]$, with $a_{i} \in \mathbb{R}^{m}, i=1, \ldots, n$, and $m=\operatorname{Rank}(\Sigma)$
- Our previous formulation leads to a formulation based on eigenvalue maximization:

$$
\phi=\max _{u \in\{0,1\}^{n}} \lambda_{\max }\left(D(u) A^{T} A D(u)\right)-\rho \cdot \mathbf{1}^{T} u
$$

## Towards a new formulation (cont'd)

- Cholesky decomposition: Let $\Sigma=A^{T} A$, where $A=\left[a_{1} \ldots a_{n}\right]$, with $a_{i} \in \mathbb{R}^{m}, i=1, \ldots, n$, and $m=\operatorname{Rank}(\Sigma)$
- Our previous formulation leads to a formulation based on eigenvalue maximization:

$$
\begin{aligned}
\phi & =\max _{u \in\{0,1\}^{n}} \lambda_{\max }\left(D(u) A^{T} A D(u)\right)-\rho \cdot \mathbf{1}^{T} u \\
& =\max _{u \in\{0,1\}^{n}} \lambda_{\max }\left(A D(u)^{2} A^{T}\right)-\rho \cdot \mathbf{1}^{T} u
\end{aligned}
$$

## Towards a new formulation (cont'd)

- Cholesky decomposition: Let $\Sigma=A^{T} A$, where $A=\left[a_{1} \ldots a_{n}\right]$, with $a_{i} \in \mathbb{R}^{m}, i=1, \ldots, n$, and $m=\operatorname{Rank}(\Sigma)$
- Our previous formulation leads to a formulation based on eigenvalue maximization:

$$
\begin{aligned}
\phi & =\max _{u \in\{0,1\}^{n}} \lambda_{\max }\left(D(u) A^{T} A D(u)\right)-\rho \cdot \mathbf{1}^{T} u \\
& =\max _{u \in\{0,1\}^{n}} \lambda_{\max }\left(A D(u)^{2} A^{T}\right)-\rho \cdot \mathbf{1}^{T} u \\
& =\max _{u \in\{0,1\}^{n}} \lambda_{\max }\left(A D(u) A^{T}\right)-\rho \cdot \mathbf{1}^{T} u
\end{aligned}
$$

## Eigenvalue maximization problem

- Using the convexity of the largest eigenvalue function, we obtain the representation

$$
\phi=\max _{u \in[0,1]^{n}} \lambda_{\max }\left(\sum_{i=1}^{n} u_{i} a_{i} a_{i}^{T}\right)-\rho \cdot \mathbf{1}^{T} u
$$

- Set $B_{i}:=a_{i} a_{i}^{T}-\rho \cdot I_{m}, i=1, \ldots, n$, and express $\phi$ as

$$
\phi=\max _{u \in[0,1]^{n}} \lambda_{\max }\left(\sum_{i=1}^{n} u_{i} B_{i}\right)
$$

- The computation of $\phi$ can be interpreted as a eigenvalue maximization problem, where the sparsity pattern $u$ is the decision variable


## An alternate expression

We have

$$
\begin{aligned}
\phi & =\max _{u \in[0,1]^{n}} \lambda_{\max }\left(\sum_{i=1}^{n} u_{i} B_{i}\right) \\
& =\max _{u \in[0,1]^{n}} \max _{\xi^{T} \xi \leq 1} \xi^{T}\left(\sum_{i=1}^{n} u_{i} a_{i} a_{i}^{T}\right) \xi-\rho \cdot \mathbf{1}^{T} u \\
& =\max _{\xi^{T} \xi \leq 1} \sum_{i=1}^{n}\left(\left(a_{i}^{T} \xi\right)^{2}-\rho \xi^{T} \xi\right)_{+} \\
& =\max _{\xi^{T} \xi=1} \sum_{i=1}^{n}\left(\left(a_{i}^{T} \xi\right)^{2}-\rho\right)_{+}
\end{aligned}
$$

## Try rank relaxation?

$$
\begin{aligned}
\phi & =\max _{\xi^{T} \xi=1} \sum_{i=1}^{n}\left(\left(a_{i}^{T} \xi\right)^{2}-\rho\right)_{+} \\
& =\max _{X} \sum_{i=1}^{n}\left(a_{i}^{T} X a_{i}-\rho\right)_{+}: X \succeq 0, \operatorname{Tr} X=1, \quad \operatorname{Rank}(X)=1 \\
& \leq \max _{X} \sum_{i=1}^{n}\left(a_{i}^{T} X a_{i}-\rho\right)_{+}: X \succeq 0, \operatorname{Tr} X=1
\end{aligned}
$$

- Rank relaxation is actually exact ( $\leq$ is an equality) ...
- .. Unfortunately, it is useless as the rank-relaxed problem is still not convex!


## Recovering the sparsity pattern

We have obtained

$$
\phi=\max _{\xi^{T} \xi=1} \sum_{i=1}^{n}\left(\left(a_{i}^{T} \xi\right)^{2}-\rho\right)_{+}
$$

- An optimal sparsity pattern $u$ is obtained from an optimal solution $\xi$ to the above problem by setting

$$
u_{i}= \begin{cases}1 & \text { if }\left(a_{i}^{T} \xi\right)^{2}>\rho, \\ 0 & \text { otherwise }\end{cases}
$$

Thus, for every $i$ such that $\rho \geq a_{i}^{T} a_{i}$, we can always assume that the optimal sparsity pattern satisfies $u_{i}=0$ (ignore $a_{i}$ )

- In the sequel, we assume WLOG $a_{i}^{T} a_{i}>\rho$ for every $i$


## SDP relaxation

Our new formulation is (having set $B_{i}=a_{i} a_{i}^{T}-\rho \cdot I_{m}$ ):

$$
\phi=\max _{u \in[0,1]^{n}} \lambda_{\max }\left(\sum_{i=1}^{n} u_{i} B_{i}\right)
$$

SDP relaxation:

$$
\phi \leq \psi:=\min _{\left(Y_{i}\right)_{i=1}^{n}} \lambda_{\max }\left(\sum_{i=1}^{n} Y_{i}\right): Y_{i} \succeq B_{i}, \quad Y_{i} \succeq 0, \quad i=1, \ldots, n
$$

## SDP relaxation

Our new formulation is (having set $B_{i}=a_{i} a_{i}^{T}-\rho \cdot I_{m}$ ):

$$
\phi=\max _{u \in[0,1]^{n}} \lambda_{\max }\left(\sum_{i=1}^{n} u_{i} B_{i}\right)
$$

SDP relaxation:

$$
\phi \leq \psi:=\min _{\left(Y_{i}\right)_{i=1}^{n}} \lambda_{\max }\left(\sum_{i=1}^{n} Y_{i}\right): Y_{i} \succeq B_{i}, \quad Y_{i} \succeq 0, \quad i=1, \ldots, n
$$

Proof: if $\left(Y_{i}\right)_{i=1}^{n}$ is feasible for the above SDP, then for every $\xi \in \mathbb{R}^{m}$, $\xi^{T} \xi \leq 1$, and $u \in[0,1]^{n}$, we have

$$
\xi^{T}\left(\sum_{i=1}^{n} u_{i} B_{i}\right) \xi \leq \sum_{i=1}^{n}\left(\xi^{T} B_{i} \xi\right)_{+} \leq \xi^{T}\left(\sum_{i=1}^{n} Y_{i}\right) \xi \leq \psi
$$

## Dual of SDP relaxation

Dual problem is

$$
\begin{aligned}
\psi & =\max _{X,\left(P_{i}\right)_{i=1}^{n}} \sum_{i=1}^{n} \operatorname{Tr} P_{i} B_{i}: X \succeq P_{i} \succeq 0, \quad i=1, \ldots, n, \quad \operatorname{Tr} X=1 \\
& =\max _{X} \sum_{i=1}^{n} \operatorname{Tr}\left(X^{1 / 2} a_{i} a_{i}^{T} X^{1 / 2}-\rho X\right)_{+} \quad: X \succeq 0, \quad \operatorname{Tr} X=1
\end{aligned}
$$

where $\operatorname{Tr} B_{+}=$sum of non-negative eigenvalues of symmetric matrix $B$

## Dual of SDP relaxation (cont'd)

The bound $\phi \leq \psi$ can also be inferred directly from the dual:

$$
\begin{aligned}
\phi & =\max _{\xi^{T} \xi=1} \sum_{i=1}^{n}\left(\left(a_{i}^{T} \xi\right)^{2}-\rho\right)_{+} \\
& =\max _{X} \sum_{i=1}^{n}\left(a_{i}^{T} X a_{i}-\rho\right)_{+}: X \succeq 0, \quad \operatorname{Tr} X=1, \quad \operatorname{Rank}(X)=1 \\
& =\max _{X} \sum_{i=1}^{n} \operatorname{Tr}\left(X^{1 / 2} a_{i} a_{i}^{T} X^{1 / 2}-\rho X\right)_{+}: X \succeq 0, \quad \operatorname{Tr} X=1, \quad \operatorname{Rank}(X)= \\
& \leq \max _{X}\left\{\sum_{i=1}^{n} \operatorname{Tr}\left(X^{1 / 2} a_{i} a_{i}^{T} X^{1 / 2}-\rho X\right)_{+}: X \succeq 0, \quad \operatorname{Tr} X=1\right\}=\psi
\end{aligned}
$$

If $\operatorname{Rank}(X)=1$ at the optimum of the dual problem, then $\leq$ becomes an equality, and $\phi=\psi$

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## Quality of SDP relaxation (1)

(Inspired by Ben-Tal \& Nemirovski, 2002)
Upper bound: $\phi \leq \psi=\max _{X \succeq 0, \operatorname{Tr} X=1} \sum_{i=1}^{n} \operatorname{Tr}\left(X^{1 / 2} a_{i} a_{i}^{T} X^{1 / 2}-\rho X\right)_{+}$

- Let $X \succeq 0, \operatorname{Tr} X=1$, be optimal for $\psi$, so that

$$
\psi=\sum_{i=1}^{n} \alpha_{i}
$$

where

$$
B_{i}(X):=X^{1 / 2} B_{i} X^{1 / 2}=X^{1 / 2}\left(a_{i} a_{i}^{T}-\rho I\right) X^{1 / 2}, \quad \alpha_{i}:=\operatorname{Tr}\left(B_{i}(X)_{+}\right)
$$

- Let $k:=\boldsymbol{\operatorname { R a n k }}(X)$, assume $k>1$


## Quality of SDP relaxation (2)

(Fix $i \in\{1, \ldots, n\}$, drop subscript on $\alpha_{i}, B_{i}(X)=X^{1 / 2}\left(a_{i} a_{i}^{T}-\rho I\right) X^{1 / 2}$ )

- In view of our assumption $\min _{i} a_{i}^{T} a_{i}>\rho, B(X)$ has exactly one positive eigenvalue, equal to $\alpha=\operatorname{Tr} B_{+}$
- Denote by $-\beta_{j}\left(\beta_{j}>0\right)$ the remaining non-zero eigenvalues; one can show that

$$
\sum_{j=1}^{k-1} \beta_{j} \leq \rho
$$

- Assume $\xi \sim \mathcal{N}\left(0, I_{m}\right)$; by rotational invariance of the normal distribution:

$$
\mathbf{E}\left(\xi^{T} B(X) \xi\right)_{+}=\mathbf{E}\left(\alpha \xi_{1}^{2}-\sum_{j=1}^{k-1} \beta_{j} \xi_{j-1}^{2}\right)_{+}
$$

## Quality of SDP relaxation (3)

Thus

$$
\begin{aligned}
\mathbf{E}\left(\xi^{T} B(X) \xi\right)_{+} & \geq \min _{\beta \geq 0, \sum_{j} \beta_{j} \leq \rho} \mathbf{E}\left(\alpha \xi_{1}^{2}-\sum_{j=1}^{k-1} \beta_{j} \xi_{j+1}^{2}\right) \\
& =\mathbf{E}\left(\alpha \xi_{1}^{2}-\frac{\rho}{k-1} \sum_{j=1}^{k-1} \xi_{j+1}^{2}\right) \\
& \geq\left(\alpha-\rho+\frac{2}{\pi} \sqrt{\alpha^{2}+\frac{\rho^{2}}{k-1}}\right)_{+}^{+}
\end{aligned}
$$

Here we have used a result in Ben-Tal \& Nemirovski (2002):

$$
\forall \gamma \in \mathbb{R}^{d}: \quad \mathbf{E}\left|\sum_{i=1}^{d} \gamma_{i} \xi_{i}^{2}\right| \geq \frac{2}{\pi}\|\gamma\|_{2}
$$

## Quality of SDP relaxation (4)

Summing over $i$, and with $\alpha_{i}:=\operatorname{Tr}\left(B_{i}(X)_{+}\right), \psi=\sum_{i=1}^{n} \alpha_{i}$, we get:

$$
\begin{aligned}
\mathbf{E} \sum_{i=1}^{n}\left(\xi^{T} B_{i}(X) \xi\right)_{+} & \geq \sum_{i=1}^{n}\left(\alpha_{i}-\rho+\frac{2}{\pi} \sqrt{\alpha_{i}^{2}+\frac{\rho^{2}}{k-1}}\right)_{+} \\
& \geq \frac{1}{2}\left(\psi-n \rho+\frac{2}{\pi} \sqrt{\psi^{2}+\frac{n^{2} \rho^{2}}{k-1}}\right)_{+} \\
& \geq \frac{1}{\pi} \psi \quad\left(=\frac{1}{\pi} \psi \mathbf{E}\left(\xi^{T} X \xi\right)\right),
\end{aligned}
$$

provided $\psi \geq n \rho$.

## Quality of SDP relaxation (5)

## Assuming $\psi \geq n \rho$ :

- The previous bound implies that there exist $\xi \in \mathbb{R}^{m}$ such that

$$
\sum_{i=1}^{n}\left(\xi^{T} B_{i}(X) \xi\right)_{+} \geq \frac{\psi}{\pi}\left(\xi^{T} X \xi\right)
$$

- Thus, with $u_{i}=1$ if $\xi^{T} B_{i}(X) \xi>0, u_{i}=0$ otherwise, we obtain that there exist $\xi \in \mathbb{R}^{m}$ and $u \in[0,1]^{n}$ such that

$$
\xi^{T}\left(\sum_{i=1}^{n} u_{i} B_{i}(X)\right) \xi \geq \frac{\psi}{\pi}\left(\xi^{T} X \xi\right)
$$

## Quality of SDP relaxation (5)

- With $z=X^{1 / 2} \xi$ :

$$
z^{T}\left(\sum_{i=1}^{n} u_{i} B_{i}\right) z \geq \frac{\psi}{\pi} \cdot\left(z^{T} z\right)
$$

- We conclude that there exist $u \in[0,1]^{n}$ such that

$$
(\psi \geq \phi \geq) \lambda_{\max }\left(\sum_{i=1}^{n} u_{i} B_{i}\right) \geq \frac{1}{\pi} \psi
$$

## Quality of SDP relaxation (6)

When is condition $\psi \geq n \rho$ met?

Find a lower bound on $\psi$ :

$$
\begin{aligned}
(\psi \geq) \phi & =\max _{X} \sum_{i=1}^{n}\left(a_{i}^{T} X a_{i}-\rho\right)_{+}: X \succeq 0, \quad \operatorname{Tr} X=1 \\
& \geq \max _{i} a_{i}^{T} a_{i}-\rho \quad\left(\text { choose } X=a_{j} a_{j}^{T} /\left(a_{j}^{T} a_{j}\right), \text { where } j:=\arg \max _{i} a_{i}^{T} a_{i}\right)
\end{aligned}
$$

Thus, condition $\psi \geq n \rho$ is met when $\rho \leq \frac{1}{n+1} \max _{i} a_{i}^{T} a_{i} \ldots$
... Don't forget we assumed $\rho<a_{i}^{T} a_{i}$ for every $i$. . .

## Quality of SDP relaxation: summary

Theorem: Assume

$$
\rho<\min \left(\min _{1 \leq i \leq n} \Sigma_{i i}, \frac{1}{n+1} \max _{1 \leq i \leq n} \Sigma_{i i}\right) .
$$

Then,

$$
\begin{equation*}
\frac{1}{\pi} \psi \leq \phi \leq \psi . \tag{3}
\end{equation*}
$$

## Quality of SDP relaxation: summary

Theorem: Assume

$$
\rho<\min \left(\min _{1 \leq i \leq n} \Sigma_{i i}, \frac{1}{n+1} \max _{1 \leq i \leq n} \Sigma_{i i}\right) .
$$

Then,

$$
\begin{equation*}
\frac{1}{\pi} \psi \leq \phi \leq \psi . \tag{4}
\end{equation*}
$$

Corollary: Assume (WLOG) $\Sigma_{11} \geq \ldots \geq \Sigma_{n n}$. If $\Sigma$ satisfies

$$
\forall p \in\{2, \ldots, n\}: \Sigma_{p p}<\frac{1}{p} \max _{i} \Sigma_{i i}
$$

Then (4) holds for every $\rho<\Sigma_{22}$.

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## Sparse solutions of linear equations

Minimum cardinality problem:

$$
\phi:=\min \|x\|_{0}: A x=b
$$

where

- $m \leq n, A=\left[a_{1}, \ldots, a_{n}\right] \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^{m}$
- $\|x\|_{0}$ denotes the number of non-zero elements of $x$


## The minimum cardinality problem

- Problem arises in a number of fields (compression, signal processing, etc)
- Problem is NP-hard
- A vast body of literature is attached to it

A classical approach: obtain a suboptimal solution by solving the LP

$$
\min \|x\|_{1}: A x=b
$$

In signal processing, approach is called "basis pursuit"

## Some previous approaches

- Convex approximation methods:
- Chen, Donoho (1994): basis pursuit
- Tropp (2004-5): analyze $l_{1}$-norm approximation using QP duality
- Bayesian methods: Lewicki \& Sejnowski (2000), Miller (2002)
- Greedy methods: e.g. Orthogonal Matching Pursuit, see Miller (2002)
- Global optimization: see Miller (2002)
- Nonlinear optimization: Rao, Kreutz-Delgado (1999)


## A modified problem

We consider a slightly modified problem:

$$
\phi(\sigma):=\min _{x}\|x\|_{0}: A x=b, \quad\|x\|_{2} \leq \sigma
$$

where $\sigma>0$ is given.

- $\phi=\lim _{\sigma \rightarrow+\infty} \phi(\sigma)$
- Assume that $A$ is full row rank, and that the above problem is feasible,i.e.

$$
b^{T}\left(A A^{T}\right)^{-1} b \leq \sigma^{2}
$$

- Norm constraint often makes sense from a practical point of view


## A boolean SDP formulation

The problem can be formulated as

$$
\phi(\sigma)=\min _{u, x} 1^{T} u: A D(u) y=b, \quad\|y\|_{2} \leq \sigma, \quad u \in\{0,1\}^{n}
$$

where $D(u):=\boldsymbol{\operatorname { d i a g }}(u)$, and $x=D(u) y$

$$
\text { Lemma: } \exists y \in \mathbb{R}^{n},\|y\|_{2} \leq 1, B y=b \Longleftrightarrow B B^{T} \succeq b b^{T}
$$

Thus

$$
\begin{aligned}
\phi(\sigma) & =\min _{u} 1^{T} u: \sigma^{2} A D(u)^{2} A^{T} \succeq b b^{T}, u \in\{0,1\}^{n} \\
& =\min _{u} \mathbf{1}^{T} u: \sigma^{2} \sum_{i=1}^{n} u_{i} a_{i} a_{i}^{T} \succeq b b^{T}, u \in\{0,1\}^{n}
\end{aligned}
$$

## SDP bound

Relax the boolean constraint and obtain the lower bound

$$
\phi(\sigma) \geq \psi(\sigma):=\min _{u} \mathbf{1}^{T} u: \sigma^{2} \sum_{i=1}^{n} u_{i} a_{i} a_{i}^{T} \succeq b b^{T}, u \in[0,1]^{n}
$$

This an SDP, with dual:

$$
\psi(\sigma)=\max _{X \succeq 0}\left(b^{T} X b\right) / \sigma^{2}-\sum_{i=1}^{n}\left(a_{i}^{T} X a_{i}-1\right)_{+}
$$

## An SOCP representation of the bound

The SDP bound can be expressed as

$$
\psi(\sigma)=\psi(\sigma):=\min _{u} \mathbf{1}^{T} u: b^{T}\left(\sum_{i=1}^{n} u_{i} a_{i} a_{i}^{T}\right)^{-1} b \leq \sigma^{2}, u \in[0,1]^{n}
$$

Usign QCQP duality, we obtain the equivalent representation

$$
\psi(\sigma)=\max _{z, \mu \geq 0} 2 b^{T} z-\mu \sigma^{2}-\sum_{i=1}^{n}\left(\left(a_{i}^{T} z\right)^{2} / \mu-1\right)_{+}
$$

- Above problem can be expressed as a (rotated cone) SOCP
- As such, can be efficiently solved


## Link with the $l_{1}$-norm approximation

We can also express the previous SOCP as the (non-convex) QCQP

$$
\psi(\sigma)=\max _{\xi}\left(b^{T} \xi\right)^{2} / \sigma^{2}-\sum_{i=1}^{n}\left(\left(a_{i}^{T} \xi\right)^{2}-1\right)_{+}
$$

For $\sigma \rightarrow \infty$, the solution set to above problem converges to that of the LP

$$
\psi=\max _{y} b^{T} \xi:\left|a_{i}^{T} \xi\right| \leq 1, \quad i=1, \ldots, n
$$

which is the (dual of) the classical LP relaxation

## Extensions

New formulations and bounds can be extended to other problems:

- sparse solutions to linear inequalities:

$$
\phi:=\min \|x\|_{0}: A x \leq b
$$

(Hint: previous formulation is convex in b...)

- penalized versions, such as

$$
\phi:=\min _{x}\|A x-b\|_{2}^{2}+\rho\|x\|_{0}
$$

## Challenges

- Evaluate the quality of the SOCP bound
- Investigate the results for $\sigma \rightarrow \infty$


## Wrap-up

- We investigated problems involving sparsity and linear systems
- We devised new formulations and corresponding SDP relaxations
- For the sparse PCA problem we obtained a quality estimate valid for small penalty $\rho$
- Refined results in
L. El Ghaoui, Eigenvalue Maximization in Sparse PCA, http://arxiv.org/abs/math.0C/0601448

