15.095 **Lecture 22b: Sparse PCA Under a Modern Optimization Lens**

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What is Principal Component Analysis?

- Project data onto few orthogonal directions that maximize variance.
- Find leading k principal components by singular value decomposition $\mathbf{\Sigma} = \boldsymbol{U}\Lambda\boldsymbol{U}^\top$, and taking the first k columns of $\boldsymbol{U}$.
- Allows us to compress a data matrix $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ into a smaller matrix $\boldsymbol{X}_{\text{new}} \in \mathbb{R}^{n \times k}$ by setting $\boldsymbol{X}_{\text{new}} \leftarrow \boldsymbol{U}_{[1:k]}\boldsymbol{X}$

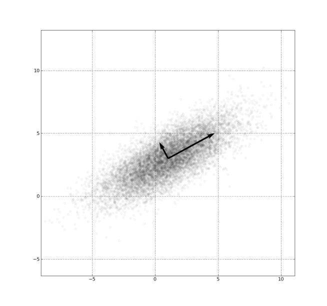

Figure 1: A synthetic data set. Arrows indicate directions of first two principal components.

What's wrong with Principal Component Analysis?

PCs are linear combinations of n original features. Often unacceptable!

- In medicine, decisions taken using PCs must be interpretable.
- In scientific applications, e.g., protein folding, each co-ordinate axis has a physical interpretation. Reduced co-ordinate axes should too.
- In financial applications, e.g., investing across index funds, each non-zero entry in each PC incurs a cost.

How do we fix Principal Component Analysis?

Impose sparsity constraint. Proposed by d'Aspermont et. al. (04, 07).

- Improves interpretability.
- Reduces susceptibility to noise.
- Reduces storage space required for reconstruction.

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Problem Statement (one PC)

$$\underbrace{\max_{\boldsymbol{x} \in \mathbb{R}^n}}_{\text{leading principal component}} \quad \langle \boldsymbol{x}\boldsymbol{x}^\top, \boldsymbol{\Sigma} \rangle \text{ s.t. } \langle \boldsymbol{x}, \boldsymbol{x} \rangle = 1, \ \|\boldsymbol{x}\|_0 \leq k.$$

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What's hard about this problem?

- Non-convex in continuous variables.
- Need binaries to model sparsity constraint.
- Not obvious how to build a mixed-integer conic representation.

Literature Review: A vast literature on sparse PCA

Discrete Optimization

Branch & Bound: Moghaddam, Weiss and Avidan (06), Berk & Bertsimas (19)

Heuristics

Lasso: Zou, Hastie and Tibshirani (06)
Power method: Journeé, Nesterov, Richtárik & Sepulchre (10), Yuan & Zhang (13)

Convex Relaxations

Semidefinite: d'Aspermont et. al. (04, 14).
Sum-of-Squares: Ma & Wigderson (15)
l_1: Dey, Mazumder & Wang: (18)

Statistical Learning Theory

SDO tightness: Amini & Wainwright (08)
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Several fundamental questions remain unanswered:

Does sparse PCA admit a mixed-integer conic formulation?

- Could address sparse PCA using general-purpose decomposition schemes.

Can we obtain high-quality optimality gaps at scale?

Plan for lecture:

Part I: Show sparse PCA exhibits *hidden* mixed-integer conic formulation; propose branch-and-cut method which scales to $n = 100$s, $k = 10$s.

Part II: Propose dual bounds which scale to $n = 1,000$s, $k = 100$s.

Part I: A Mixed-Integer Semidefinite Optimization (MISDO) Reformulation and A Cutting-Plane Method

A MISDO Reformulation I

Model cardinality constraint using binary variables:

$$\max_{\boldsymbol{z}\in\{0,1\}^n} \max_{\boldsymbol{x}\in\mathbb{R}^n} \langle \boldsymbol{x}\boldsymbol{x}^\top, \boldsymbol{\Sigma}\rangle \text{ s.t. } \langle \boldsymbol{x}, \boldsymbol{x}\rangle = 1,\ x_i = 0 \text{ if } z_i = 0, \forall i \in [n], \boldsymbol{e}^\top \boldsymbol{z} \leq k.$$

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Non-convex. Therefore, *lift* by setting $\boldsymbol{X} = \boldsymbol{x}\boldsymbol{x}^\top$ and substituting:

$$\max_{\boldsymbol{z}\in\{0,1\}^n} \max_{\boldsymbol{X}\in S^n_+} \langle \boldsymbol{X}, \boldsymbol{\Sigma}\rangle \text{ s.t. } \mathrm{tr}(\boldsymbol{X}) = 1, X_{i,j} = 0 \text{ if } z_i = 0, \boldsymbol{e}^\top \boldsymbol{z} \leq k, \mathrm{Rank}(\boldsymbol{X}) = 1.$$

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Still hard, due to rank constraint.

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Still hard, due to rank constraint. **Magic trick:** drop constraint w.l.o.g.

A MISDO Reformulation II

Mixed-Integer Conic Reformulation

$$\max_{\boldsymbol{z}\in\{0,1\}^n} \max_{\boldsymbol{X}\in S_+^n} \langle \boldsymbol{X}, \Sigma \rangle \text{ s.t. } \mathrm{tr}(\boldsymbol{X}) = 1, X_{i,j} = 0 \text{ if } z_i = 0, \boldsymbol{e}^\top \boldsymbol{z} \leq k.$$

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Objective linear in $\boldsymbol{X}$. Therefore, for any fixed $\boldsymbol{z}$, some extreme point $\boldsymbol{X}$ is optimal. But all extreme $\boldsymbol{X}$'s are rank-one!

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Sparse PCA exhibits hidden mixed-integer conic representability.

Formal proof of MISDO Reformulation

The following two problems attain the same optimal objective:

$$\max_{\boldsymbol{x}\in\mathbb{R}^n} \quad \boldsymbol{x}^\top \boldsymbol{\Sigma} \boldsymbol{x} \text{ s.t. } \boldsymbol{x}^\top \boldsymbol{x} = 1,\ ||\boldsymbol{x}||_0 \leq k,$$

$$\max_{\boldsymbol{z}\in\{0,1\}^n:\boldsymbol{e}^\top \boldsymbol{z}\leq k} \quad \max_{\boldsymbol{X}\in S^n_+} \quad \langle \boldsymbol{\Sigma}, \boldsymbol{X}\rangle$$

$$\text{s.t.} \quad \mathrm{tr}(\boldsymbol{X}) = 1,\ X_{i,j} = 0 \text{ if } z_i = 0,\ \forall i, j \in [n].$$

Proof: given feasible solution to one, construct feasible solution to other with equal/greater.

- Let $\boldsymbol{x} \in \mathbb{R}^{n\times n}$ be a feasible in first. Immediate that $(\boldsymbol{X} := \boldsymbol{x}\boldsymbol{x}^\top, \boldsymbol{z})$ feasible in second with equal cost, $z_i = 1$ if $|x_i| > 0$, $z_i = 0$ o/w.
- Let $(\boldsymbol{X}, \boldsymbol{z})$ be feasible in second, let $\boldsymbol{X} = \sum_{i=1}^n \lambda_i \boldsymbol{x}_i \boldsymbol{x}_i^\top$ be Cholesky decomposition of $\boldsymbol{X}$, where $\boldsymbol{e}^\top \boldsymbol{\lambda} = 1, \boldsymbol{\lambda} \geq \boldsymbol{0}$. Set $\hat{\boldsymbol{x}} := \arg\max_i [\boldsymbol{x}_i^\top \boldsymbol{\Sigma} \boldsymbol{x}_i]$. Then, $\hat{\boldsymbol{x}}$ is feasible in first with equal or greater payoff.

So what? MISDOs are notoriously hard!

Simplifying the Problem

General MISDOs are **really** hard.

Therefore, solve using **ideas** from SDO, but in **semidefinite-free** fashion.

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$$\text{where } f(\boldsymbol{z}) = \max_{\boldsymbol{X} \in S^n_+} \langle \boldsymbol{X}, \boldsymbol{\Sigma} \rangle \text{ s.t. } \mathrm{tr}(\boldsymbol{X}) = 1, |X_{i,j}| \le M_{i,j} z_i, \boldsymbol{e}^\top \boldsymbol{z} \le k,$$

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where $M_{i,j} = \frac{1}{2}$ if $i \neq j$ and $M_{i,i} = 1$ (why is this a valid M?)

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By strong duality:

Saddle Point Reformulation

$$f(\boldsymbol{z}) = \min_{\boldsymbol{\alpha} \in S^n, \boldsymbol{\lambda}} \lambda - \sum_{i=1}^{n} M_{i,j} z_i \sum_{j=1}^{n} |\alpha_{i,j}| \text{ s.t. } \lambda \mathbb{I} + \alpha \succeq \boldsymbol{\Sigma},$$

which proves $f(\boldsymbol{z})$ is concave in $\boldsymbol{z}$ (why?).

The Outer-Approximation Method

We solve saddle-point reformulation via outer-approximation

$$\max_{\boldsymbol{z}\in\{0,1\}^n:\boldsymbol{e}^\top\boldsymbol{z}\leq k}\ \min_{\boldsymbol{\alpha}\in S^n,\boldsymbol{\lambda}}\ \lambda-\sum_{i=1}^{n} z_i\sum_{j=1}^{n} M_{i,j}|\alpha_{i,j}| \text{ s.t. } \lambda\mathbb{I}+\alpha\succeq\boldsymbol{\Sigma}.$$

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Outer-Approximation Procedure

- Iteratively construct a piece-wise linear upper approximation.
- Implemented using lazy constraint callbacks in CPLEX/Gurobi.
- In practice, tractable. But benefits from warm-starting.

How to solve the subproblem?

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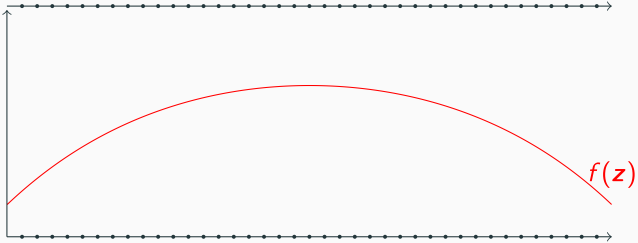
Subproblem Strategy

- For fixed $\boldsymbol{z}$, subproblem easy to solve: $\lambda^\star = \lambda_{\max}(\boldsymbol{\Sigma}_{\boldsymbol{z},\boldsymbol{z}})$, where $\boldsymbol{\Sigma}_{\boldsymbol{z},\boldsymbol{z}}$ is submatrix of $\boldsymbol{\Sigma}$ induced by $\boldsymbol{z}$, $\boldsymbol{\alpha}^\star = (\mathbb{I}-\mathrm{Diag}(\boldsymbol{z}))\boldsymbol{\Sigma}(\mathbb{I}-\mathrm{Diag}(\boldsymbol{z}))$.
- Subproblem solvable in $O(k^2)$ time!

Outer Approximation in 1000 Words



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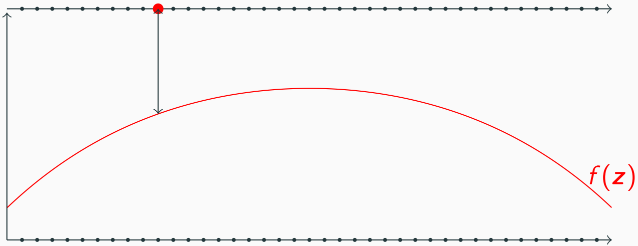

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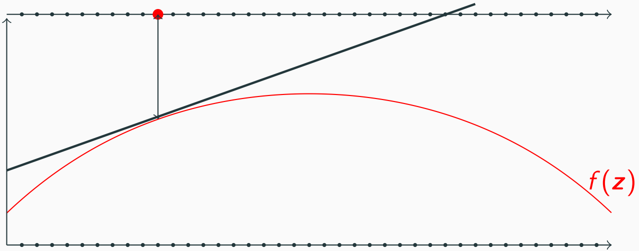

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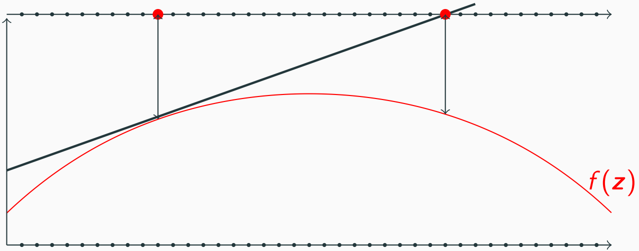

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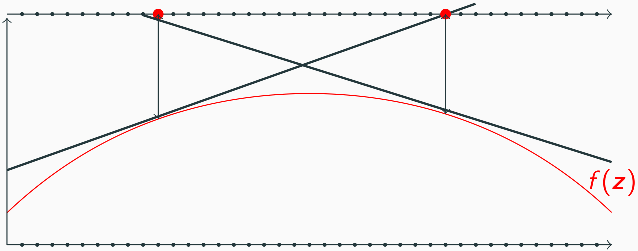

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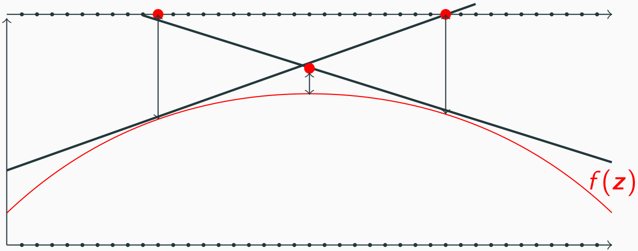

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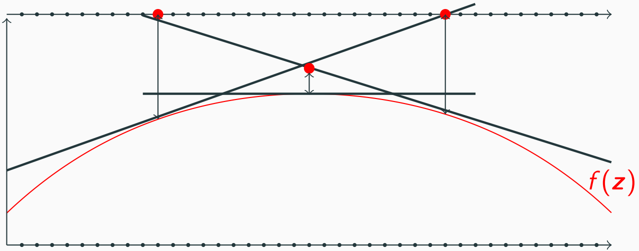


The Gershgorin Circle Theorem

Let A be a positive semidefinite matrix and for each i let $R_i := \sum_{j \neq i} |A_{i,j}|$ be absolute sum of off-diagonal entries in ith column. Then,

- (a) For each eigenvalue λ_i of A, there exists some index j such that $|\lambda_i - A_{j,j}| \leq R_j$.
- (b) If the union of l discs $[R_j - A_{j,j}, R_j + A_{j,j}]$ does not overlap with any of the remaining $n - l$ discs then exactly l eigenvalues of A lie within these discs.

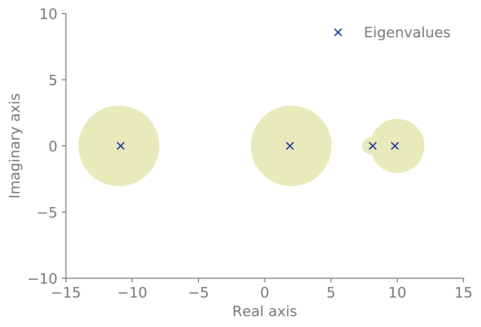
Proof: definition of eigenvalue+triangle inequality, see Wikipedia.

Worked example from Wikipedia: Consider the matrix

$$\begin{pmatrix} 10 & -1 & 0 & 1 \\ 0.2 & 8 & 0.2 & 0.2 \\ 1 & 1 & 2 & 1 \\ -1 & -1 & -1 & -11 \end{pmatrix}.$$

Discs are $D(10, 2)$, $D(8, 0.6)$, $D(2, 3)$, $D(-11, 3)$.

Plot shows discs and actual eigenvalues.



Strengthening the Master Problem

Outer-approximation benefits from strengthening master problem. To strengthen it, invoke Gershgorin circle theorem. We have the bound:

$$f(\boldsymbol{z}) \leq \max_{i \in [n]: z_i = 1} \sum_{j \in [n]} z_j |\Sigma_{i,j}|.$$

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Bound non-convex, but can model using n extra binary variables. Gives:

Gershgorin Circle Theorem Inequalities

$$\exists \boldsymbol{s} \in \{0,1\}^n, t \in \mathbb{R} : f(\boldsymbol{z}) \leq t, t \geq \sum_{i \in [n]} z_i |\Sigma_{i,j}|,$$
$$t \leq \sum_{i \in [n]} z_i |\Sigma_{i,j}| + M(1 - s_i), \boldsymbol{e}^\top \boldsymbol{s} = 1.$$

Strengthens formulation, and give hints about where to branch next.

Performance of Outer-Approximation

Dataset	n	k	Outer-Approx			Outer-Approx+ Circle Theorem		
			Time(s)	Nodes	Cuts	Time(s)	Nodes	Cuts
Pitprops	13	5	0.30	1,608	1,176	**0.06**	38	8
		10	0.14	414	387	**0.02**	18	21
Wine	13	5	0.57	2,313	1,646	**0.02**	46	11
		10	0.17	376	311	**0.03**	54	58
Miniboone	50	5	**0.01**	0	11	**0.01**	0	3
		10	**0.01**	0	16	0.02	0	3
Communities	101	5	> 600	28,462	25,843	**0.20**	201	3
		10	> 600	37,479	36,251	**0.34**	406	39
Arrhythmia	274	5	> 600	42,474	13,595	**6.07**	135	1,233

Solves problems where $n = 100$s, $k = 10$s in seconds or minutes.

Part II: Scalable dual bounds

Scalable Dual Bounds

- Branch-and-bound great, but only **proves** optimality when $n = 100$s.

Scalable Dual Bounds

- Branch-and-bound great, but only **proves** optimality when $n = 100$s.
- We now propose a method which provides (near) optimality guarantees when $n = 1000$s.

Background: Second-order Cone Optimization

A generic second-order cone problem:

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} \quad \boldsymbol{c}^\top \boldsymbol{x}$$
$$\text{s.t.} \quad \|\boldsymbol{A}_i^\top \boldsymbol{x} + b_i\|_2 \leq c_i^\top \boldsymbol{x} + d_i,\ \forall i \in [m],\ \boldsymbol{D}\boldsymbol{x} = \boldsymbol{d}.$$

Modeling power:

- Linear inequalities.
- Convex quadratics.
- Portfolio risk and chance constraints.

Why is this useful?

- Most general continuous problem can solve to optimality at scale.

How to solve?

- Mosek or Gurobi (interior point method).

Modeling Power: Rotated Second-order Cone Constraints

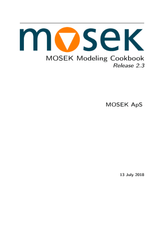
A large class of problems can be cast as second-order cone problems since

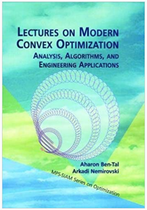
$$\text{(a)} \quad x^2 \le yz, y, z \ge 0 \iff \left\| \begin{pmatrix} 2x \\ y - z \end{pmatrix} \right\|_2 \le y + z,$$

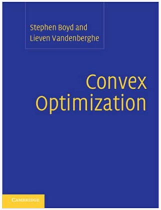
$$\text{(b)} \quad \boldsymbol{x}_i^\top \boldsymbol{P}_i \boldsymbol{x} + 2q_i^\top \boldsymbol{x} + r_i \le 0 \iff \left\| \boldsymbol{P}_i^{\frac{1}{2}} \boldsymbol{x} + \boldsymbol{P}_i^{\frac{-1}{2}} \boldsymbol{q}_i \right\|_2 \le \left(q_i^\top \boldsymbol{P}_i^{-1} q_i - r_i \right)^{\frac{1}{2}}$$

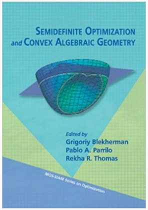
$$\text{(c)} \quad t \ge x^{\frac{3}{2}}, x \ge 0 \iff \exists s : 2st \ge x^2, \frac{1}{4}x \ge s^2$$

And many other problems! Good places to look are:









Preamble to Part II: An Outer Approximation of the PSD Cone

The constraint $\boldsymbol{X} \succeq \mathbf{0}$ can be expensive. Therefore, relax. Recall: $\boldsymbol{X} \succeq \mathbf{0}$ if and only if

$$\boldsymbol{x}^\top \boldsymbol{X} \boldsymbol{x} \geq 0, \forall \boldsymbol{x} : \ \|\boldsymbol{x}\|_2 = 1,$$

and only considering $\boldsymbol{x} = \frac{\sqrt{2}}{2}(\boldsymbol{e}_i + \boldsymbol{e}_j)$, i.e.,

$$\boldsymbol{x}^\top \boldsymbol{X} \boldsymbol{x} \geq 0, \forall \boldsymbol{x} = \frac{\sqrt{2}}{2}(\boldsymbol{e}_i + \boldsymbol{e}_j)$$

i.e., $X_{i,i} X_{j,j} \geq X_{i,j}^2 \ \forall i, j$ is a valid outer approximation.

Our Convex Relaxation

Obtain scalability by relaxing and rounding.

Start by relaxing $\boldsymbol{z} \in \{0,1\}^p$ to $\boldsymbol{z} \in [0,1]^p$. Gives:

$$\max_{\boldsymbol{z} \in [0,1]^p : \boldsymbol{e}^\top \boldsymbol{z} \leq k} \ \max_{\boldsymbol{X} \succeq \boldsymbol{0}} \quad \langle \boldsymbol{\Sigma}, \boldsymbol{X} \rangle \quad \text{s.t.} \quad \mathrm{tr}(\boldsymbol{X}) = 1, \quad |X_{i,j}| \leq M_{i,j} z_i \ \forall i, j.$$

Our Convex Relaxation

Obtain scalability by relaxing and rounding.

Start by relaxing $\boldsymbol{z} \in \{0,1\}^p$ to $\boldsymbol{z} \in [0,1]^p$. Gives:

$$\max_{\boldsymbol{z} \in [0,1]^p : \boldsymbol{e}^\top \boldsymbol{z} \leq k} \max_{\boldsymbol{X} \succeq \mathbf{0}} \quad \langle \boldsymbol{\Sigma}, \boldsymbol{X} \rangle \quad \text{s.t.} \quad \mathrm{tr}(\boldsymbol{X}) = 1, \quad |X_{i,j}| \leq M_{i,j} z_i \ \forall i, j.$$

Remaining expensive bit is $\boldsymbol{X} \succeq \mathbf{0}$, holds if principal minors non-negative.

Our Convex Relaxation

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Remaining expensive bit is $\boldsymbol{X} \succeq \mathbf{0}$, holds if principal minors non-negative.

Relax, by only enforcing non-negativity on 2×2 minors, and impose some extra valid inequalities. Gives:

A Scalable Second-Order Cone Relaxation

$$\max_{\substack{\boldsymbol{z}\in[0,1]^p:\\ \boldsymbol{e}^\top \boldsymbol{z}\leq k}} \max_{\boldsymbol{X}\in\mathcal{S}^n} \langle \boldsymbol{\Sigma}, \boldsymbol{X}\rangle \text{ s.t. } \mathrm{tr}(\boldsymbol{X}) = 1,\ |X_{i,j}| \leq M_{i,j} z_i, X_{i,j}^2 \leq X_{i,i} X_{j,j}.$$

Strengthening the Relaxation

Two valid inequalities:

- From Cauchy-Schwarz, $\|\boldsymbol{x}\|_0 \leq k$ and $\|\boldsymbol{x}\|_2 \leq 1$ imply $\|\boldsymbol{x}\|_1 \leq \sqrt{k}$. Therefore, since $\boldsymbol{X}$ models $\boldsymbol{x}\boldsymbol{x}^\top$, we have $\|\boldsymbol{X}\|_1 \leq k$.
- Since $z_i = x_i z_i$ and $\|\boldsymbol{x}\|_2 = 1$, we have $\sum_{i=1}^n X_{i,j}^2 = \sum_{i=1}^n x_i^2 x_j^2 = x_i^2 = x_i^2 z_i = X_{i,i} z_i$. This gives the valid inequality:

$$\sum_{i=1}^n X_{i,j}^2 \leq X_{i,i} z_i, \ \forall i \in [n]$$

Putting it all together

A Strong and Scalable Second-Order Cone Relaxation

$$\max_{\substack{\boldsymbol{z}\in[0,1]^p:\\ \boldsymbol{e}^\top \boldsymbol{z}\leq k}} \max_{\boldsymbol{X}\in\mathcal{S}^n} \langle \boldsymbol{\Sigma}, \boldsymbol{X}\rangle \text{ s.t. } \mathrm{tr}(\boldsymbol{X})=1,\ |X_{i,j}|\leq M_{i,j}z_i, X_{i,j}^2\leq X_{i,i}X_{j,j}\ \forall i,j,$$

$$\underbrace{\|\boldsymbol{X}\|_1\leq k, \sum_{i=1}^n X_{i,j}^2\leq X_{i,i}z_i}_{\text{Valid Inequalities}}.$$

How to get feasible solutions?

Putting it all together

A Strong and Scalable Second-Order Cone Relaxation

$$\max_{\substack{\boldsymbol{z}\in[0,1]^p:\\ \boldsymbol{e}^\top \boldsymbol{z}\leq k}} \max_{\boldsymbol{X}\in\mathcal{S}^n} \langle \boldsymbol{\Sigma}, \boldsymbol{X}\rangle \text{ s.t. } \mathrm{tr}(\boldsymbol{X})=1,\ |X_{i,j}|\leq M_{i,j}z_i, X_{i,j}^2 \leq X_{i,i}X_{j,j}\ \forall i,j,$$

$$\underbrace{\|\boldsymbol{X}\|_1 \leq k, \sum_{i=1}^n X_{i,j}^2 \leq X_{i,i}z_i}_{\text{Valid Inequalities}}.$$

How to get feasible solutions?

Solve relaxation, round $\boldsymbol{z}^\star$ solution to relaxation greedily, resolve for $\boldsymbol{X}$.

Performance of Relax and Round

Dataset	p	k	Relative Gap (%)	Time (s)
Pitprops	13	5	1.51%	0.02
		10	5.29%	0.02
Miniboone	50	5	0.00%	0.11
		10	0.00%	0.12
		20	0.00%	0.39
Communities	101	5	0.07%	0.67
		10	0.66%	0.68
		20	3.32%	1.84
Arrhythmia	274	5	3.37%	27.2
		10	3.01%	25.6
		20	8.87%	21.8
Micromass	1300	5	0.04%	239.4
		10	0.63%	232.6
		20	13.1%	983.5

Solves problems where $n = 1000$s, $k = 100$s in minutes or hours.

Instances we can't solve via exact methods highlighted in blue.

Improving relax and round

In relaxation, optimal $\boldsymbol{X}^\star$ is not, in general, positive semidefinite.

Therefore, impose constraint $\boldsymbol{x}^\top \boldsymbol{X}\boldsymbol{x} \geq \mathbf{0}$ for a most violated $\boldsymbol{x}$ in $\boldsymbol{x}^\top \boldsymbol{X}^\star \boldsymbol{x} \geq 0$, and resolve.

Iteratively imposing inequality 20 times halves remaining gap.

Performance of Relax and Round With and Without 20 cuts

Dataset	p	k	Rel Gap (%)	T (s)	Rel Gap 20 cuts (%)	T (s)
Pitprops	13	5	1.51%	0.02	0.72%	0.36
		10	5.29%	0.02	1.12%	0.36
Miniboone	50	5	0.00%	0.11	0.00%	0.11
		10	0.00%	0.12	0.00%	0.12
		20	0.00%	0.39	0.00	0.39
Communities	101	5	0.07%	0.67	0.07%	14.8
		10	0.66%	0.68	0.66%	14.4
		20	3.32%	1.84	2.23%	33.5
Arrhythmia	274	5	3.37%	27.2	1.39%	203.6
		10	3.01%	25.6	1.33%	184.0
		20	8.87%	21.8	4.48%	426.8
Micromass	1300	5	0.04%	239.4	0.01%	$4,639$
		10	0.63%	232.6	0.32%	$6,392$
		20	13.1%	983.5	5.88%	$16,350$

Solves problems where $n = 1000$s, $k = 100$s in minutes or hours.

Instances we can't solve via exact methods highlighted in blue.

Does this translate to better out-of-sample performance?

Performance on Synthetic Data

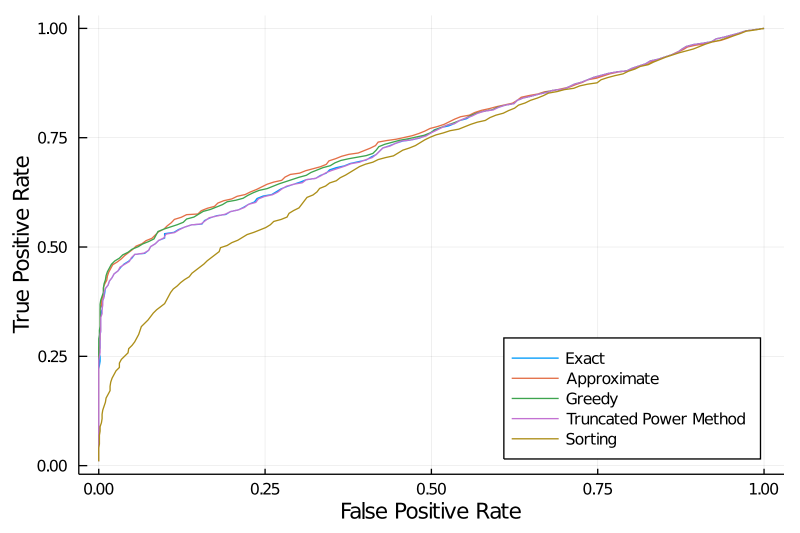
Set $p = 150$, $k = 100$, recover leading PC of $\boldsymbol{\Sigma} = \frac{1}{n}\boldsymbol{U}^\top \boldsymbol{U} + \frac{\sigma}{\|\boldsymbol{v}\|_2^2}\boldsymbol{v}\boldsymbol{v}^\top$ where $\boldsymbol{U}$ is i.i.d. uniform noise,

$$v_i = \begin{cases} 1 \text{ if } i \leq 50, \\ \frac{1}{i-50} \text{ if } 51 \leq i \leq 100 \\ 0 \text{ otherwise} \end{cases}$$

is signal, compute true positive and false positive rate as we vary k

Approximate method yields better AUC than exact at scale!

Performance on Synthetic Data: Results



Thanks for listening!

Questions?

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