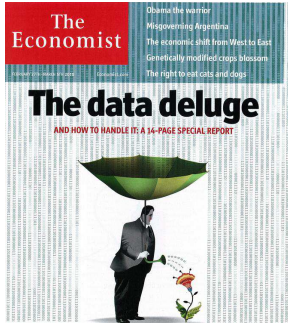


Guaranteed Non-Convex Optimization in Machine Learning

Anima Anandkumar

U.C. Irvine

Learning with Big Data



Data vs. Information

Data vs. Information



SEE, THEY ASKED HOW MUCH MONEY I SPEND ON GUM EACH WEEK, SO I WROTE, "\$500." FOR MY AGE, I PUT "43," AND WHEN THEY ASKED WHAT MY FAVORITE FLAVOR IS, I WROTE "GARLIC / CURRY."



Data vs. Information



- Missing observations, gross corruptions, outliers.

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- High dimensional regime: as data grows, more variables !

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- High dimensional regime: as data grows, more variables !

Data deluge also a data desert!

Learning in High Dimensional Regime

- Useful information: low-dimensional structures.
- Learning with big data: ill-posed problem.

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Learning is finding needle in a haystack



Learning in High Dimensional Regime

- Useful information: **low-dimensional structures**.
- Learning with big data: **ill-posed problem**.

Learning is finding needle in a haystack



- Learning with big data: **computationally challenging!**

Principled approaches for finding low dimensional structures?

How to model information structures?

Latent variable models

- Incorporate **hidden** or **latent** variables.
- Information structures: **Relationships** between latent variables and observed data.

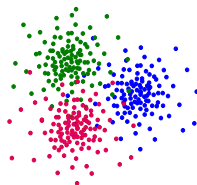
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Basic Approach: mixtures/clusters

- Hidden variable is **categorical**.



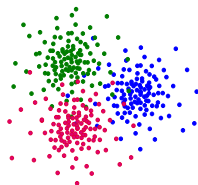
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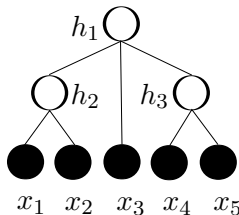
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Advanced: Probabilistic models

- Hidden variables have more general distributions.
- Can model mixed membership/hierarchical groups.



Latent Variable Models (LVMs)

Document modeling

- Observed: words.
- Hidden: topics.



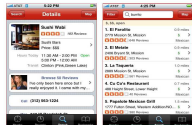
Social Network Modeling

- Observed: social interactions.
- Hidden: communities, relationships.



Recommendation Systems

- Observed: recommendations (e.g., reviews).
- Hidden: User and business attributes



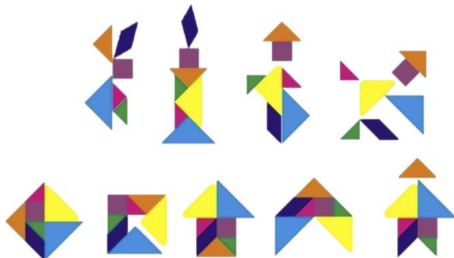
Unsupervised Learning: Learn LVM without labeled examples.

LVM for Feature Engineering

- Learn good features/representations for classification tasks, e.g., computer vision and NLP.

Sparse Coding/Dictionary Learning

- **Sparse** representations, low dimensional hidden structures.
- A few **dictionary** elements make complicated shapes.



Challenges in Learning LVMs

Computational Challenges

- **Maximum likelihood** is NP-hard in most scenarios: non-convex optimization.
- Practice: Local search approaches such as **gradient descent**, **EM**, **Variational Bayes** have no consistency guarantees.

Sample Complexity

- Sample complexity is exponential (w.r.t hidden variable dimension) for many learning methods.

Guaranteed and efficient learning through non-convex methods?

Outline

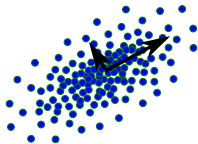
- 1 Introduction
- 2 Spectral Methods**
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Classical Spectral Methods: Matrix PCA and CCA

Single-view Setting: PCA

For centered samples $\{x_i\}$, find projection P with $\text{Rank}(P) = k$ s.t.

$$\min_P \frac{1}{n} \sum_{i \in [n]} \|x_i - Px_i\|^2.$$

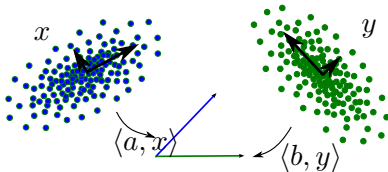


Result: Eigen-decomposition of $S = \text{Cov}(X)$.

Multiview Setting: CCA

For centered samples $\{x_i, y_i\}$, find

$$\max_{a,b} \frac{a^\top \hat{\mathbb{E}}[xy^\top] b}{\sqrt{a^\top \hat{\mathbb{E}}[xx^\top] a \ b^\top \hat{\mathbb{E}}[yy^\top] b}}.$$



Result: Generalized eigen decomposition.

Beyond SVD: Spectral Methods on Tensors

- How to learn the mixture models without separation constraints?
 - ▶ PCA uses **covariance matrix** of data. Are **higher order moments** helpful?
- Unified framework?
 - ▶ **Moment-based estimation** of probabilistic latent variable models?
- SVD gives **spectral decomposition** of matrices.
 - ▶ What are the analogues for tensors?

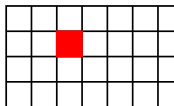
Moment Matrices and Tensors

Multivariate Moments

$$M_1 := \mathbb{E}[x], \quad M_2 := \mathbb{E}[x \otimes x], \quad M_3 := \mathbb{E}[x \otimes x \otimes x].$$

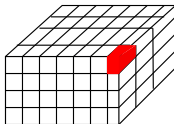
Matrix

- $\mathbb{E}[x \otimes x] \in \mathbb{R}^{d \times d}$ is a second order tensor.
- $\mathbb{E}[x \otimes x]_{i_1, i_2} = \mathbb{E}[x_{i_1} x_{i_2}]$.
- For matrices: $\mathbb{E}[x \otimes x] = \mathbb{E}[xx^\top]$.



Tensor

- $\mathbb{E}[x \otimes x \otimes x] \in \mathbb{R}^{d \times d \times d}$ is a third order tensor.
- $\mathbb{E}[x \otimes x \otimes x]_{i_1, i_2, i_3} = \mathbb{E}[x_{i_1} x_{i_2} x_{i_3}]$.



Spectral Decomposition of Tensors

$$M_2 = \sum_i \lambda_i u_i \otimes v_i$$

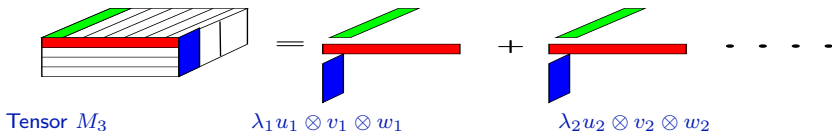


Spectral Decomposition of Tensors

$$M_2 = \sum_i \lambda_i u_i \otimes v_i$$



$$M_3 = \sum_i \lambda_i u_i \otimes v_i \otimes w_i$$



- $u \otimes v \otimes w$ is a rank-1 tensor since its $(i_1, i_2, i_3)^{\text{th}}$ entry is $u_{i_1} v_{i_2} w_{i_3}$.

How to solve this non-convex problem?

Decomposition of Orthogonal Tensors

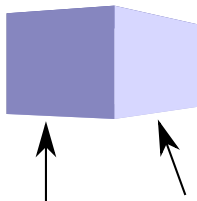
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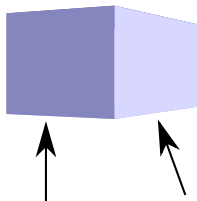
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- $M_3(I, a_1, a_1) = \sum_i w_i \langle a_i, a_1 \rangle^2 a_i = w_1 a_1.$



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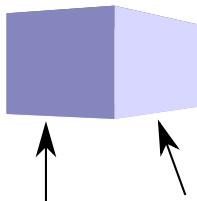
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- Analogous to matrix eigenvectors:
 $Mv = M(I, v) = \lambda v.$



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Two Problems

- How to find eigenvectors of a tensor?
- A is not orthogonal in general.

Orthogonal Tensor Power Method

Symmetric **orthogonal** tensor $T \in \mathbb{R}^{d \times d \times d}$:

$$T = \sum_{i \in [k]} \lambda_i v_i \otimes v_i \otimes v_i.$$

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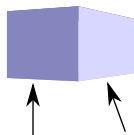
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Algorithm:

tensor power method:

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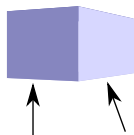
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How do we avoid **spurious** solutions (not part of decomposition)?

- $\{v_i\}$'s are the only robust fixed points.



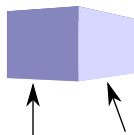
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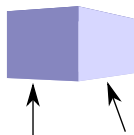
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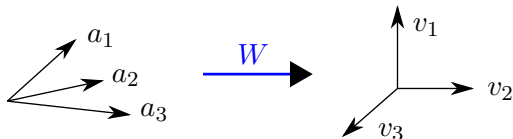


For an **orthogonal** tensor, no spurious local optima!

Whitening: Conversion to Orthogonal Tensor

$$M_3 = \sum_i w_i a_i \otimes a_i \otimes a_i, \quad M_2 = \sum_i w_i a_i \otimes a_i.$$

- Find whitening matrix W s.t. $W^\top A = V$ is an orthogonal matrix.
- When $A \in \mathbb{R}^{d \times k}$ has **full column rank**, it is an **invertible** transformation.

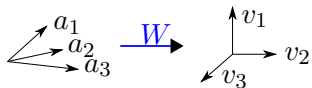


- Use pairwise moments M_2 to find W .
- SVD** of M_2 is needed.

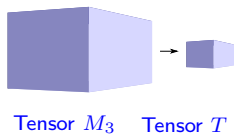
Putting it together

Non-orthogonal tensor $M_3 = \sum_i w_i a_i \otimes a_i \otimes a_i$, $M_2 = \sum_i w_i a_i \otimes a_i$.

- Whitening matrix W :



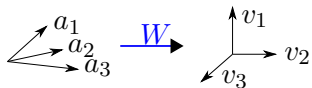
- Multilinear transform: $T = M_3(W, W, W)$



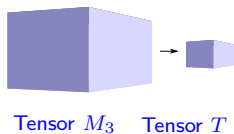
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Tensor Decomposition: Guaranteed Non-Convex Optimization!

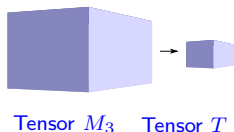
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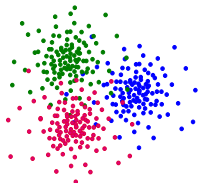


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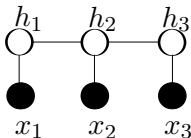
For what latent variable models can we obtain M_2 and M_3 forms?

Tractable Learning for LVMs

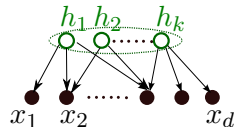
GMM



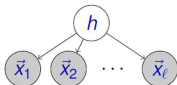
HMM



ICA



Multiview and Topic Models



$$h \in [k],$$

$$\vec{x}_1 \in \mathbb{R}^{d_1}, \vec{x}_2 \in \mathbb{R}^{d_2}, \dots, \vec{x}_\ell \in \mathbb{R}^{d_\ell}.$$

$k = \# \text{ components}$, $\ell = \# \text{ views (e.g., audio, video, text)}$.



View 1: $\vec{x}_1 \in \mathbb{R}^{d_1}$



View 2: $\vec{x}_2 \in \mathbb{R}^{d_2}$



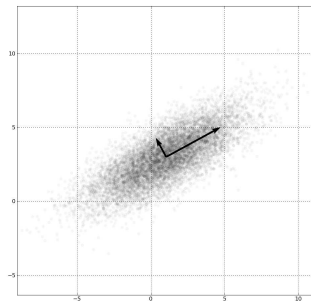
View 3: $\vec{x}_3 \in \mathbb{R}^{d_3}$

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- 2 Spectral Methods
- 3 Robust PCA**
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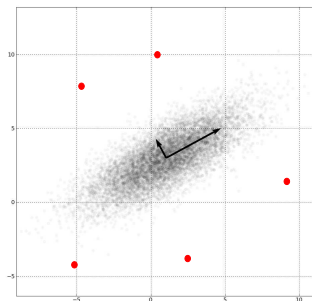
PCA: Classical Method

- Denoising: find hidden low rank structures in data.
- Efficient computation, perturbation analysis.



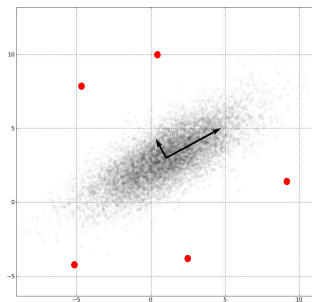
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Not robust to even a few outliers

Robust PCA Problem

- Find **low rank** structure after removing **sparse corruptions**.
- Decompose input matrix as low rank + sparse matrices.

$$\begin{array}{c} \left[\begin{array}{c} \\ \\ \\ \end{array} \right] \\ M \end{array} = \begin{array}{c} \left[\begin{array}{cc} \text{red block} & \text{blue block} \end{array} \right] \\ L^* \end{array} + \begin{array}{c} \left[\begin{array}{ccc} \text{blue blocks} \end{array} \right] \\ S^* \end{array}$$

- $M \in \mathbb{R}^{n \times n}$, L^* is low rank and S^* is sparse.
- Applications in computer vision, topic and community modeling.

Convex Relaxation Techniques

(Hard) Optimization Problem, given $M \in \mathbb{R}^{n \times n}$

$$\min_{L, S} \text{Rank}(L) + \gamma \|S\|_0, \quad M = L + S.$$

- $\text{Rank}(L) = \{\#\sigma_i(L) : \sigma_i(L) \neq 0\}$, $\|S\|_0 = \{\#S(i, j) : S(i, j) \neq 0\}$ are not tractable.

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Convex Relaxation

$$\min_{L, S} \|L\|_* + \gamma \|S\|_1, \quad M = L + S.$$

- $\|L\|_* = \sum_i \sigma_i(L)$, $\|S\|_1 = \sum_{i,j} |S(i, j)|$ are convex sets.
- Chandrasekharan et. al, Candes et. al '11: seminal works.

Other Alternatives for Robust PCA?

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Shortcomings of convex methods

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- Computational cost: $O(n^3/\epsilon)$ to achieve error of ϵ
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- Analysis: requires **dual witness** style arguments.
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Non-convex alternatives?

Proposal for Non-convex Robust PCA

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A non-convex heuristic (AltProj)

- Initialize $L, S = 0$ and iterate:
- $L \leftarrow P_r(M - S)$ and $S \leftarrow H_\zeta(M - L)$.
- $P_r(\cdot)$: rank- r projection. $H_\zeta(\cdot)$: thresholding with ζ .
- Computationally efficient: each operation is just a rank- r SVD or thresholding.

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Any hope for proving guarantees?

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Observations regarding Robust PCA

- Projection on to rank and sparse subspaces: non-convex but tractable: **SVD** and **hard thresholding**.
- But alternating projections: challenging to analyze

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- **Match** the bounds for convex methods (deterministic sparsity).
- Reduced computation: only require **low rank SVDs**!

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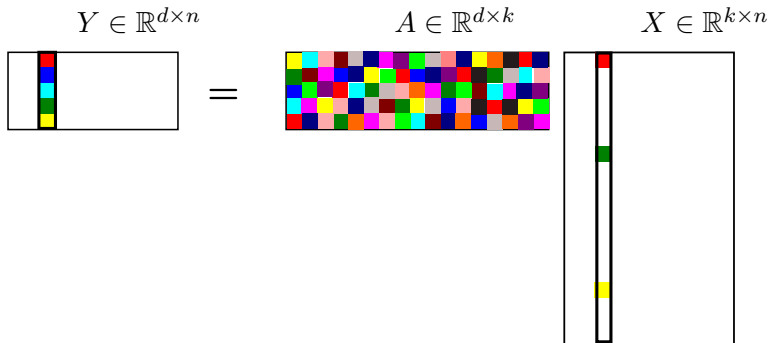
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Best of both worlds: reduced computation with guarantees!

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Dictionary Learning or Sparse Coding



- Each sample is a **sparse** combination of dictionary atoms.

Learning Overcomplete Dictionaries

- No. of dictionary elements $k >$ observed dimensionality n .
- $A = [a_1, \dots, a_k]$: dictionary elements
- $y \in \mathbb{R}^n$: Observation. $Y = [y_1, \dots, y_m] \in \mathbb{R}^{n \times m}$: Observation matrix.
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Intuitions: how incoherence helps

- Each sample is a combination of dictionary atoms: $y_i = \sum_j x_{i,j} a_j$.
- Consider y_i and y_j s.t. they have **no common dictionary atoms**.
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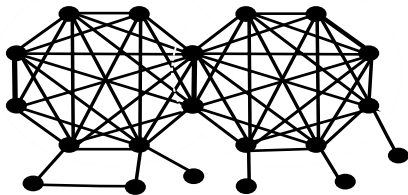
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Construction of Correlation Graph

- Nodes: Samples y_1, \dots, y_n .
- Edges: $|\langle y_i, y_j \rangle| > \tau$ for some threshold τ .

How does the correlation graph help in dictionary learning?

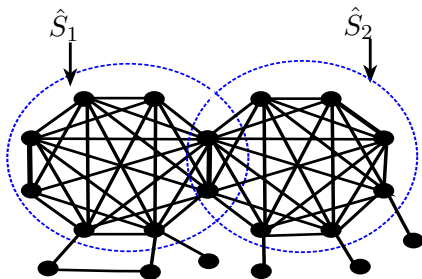
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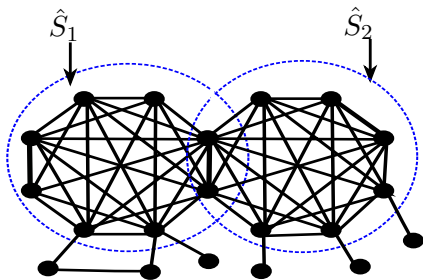
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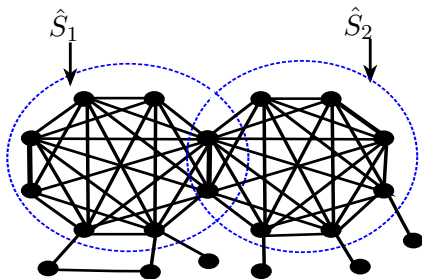
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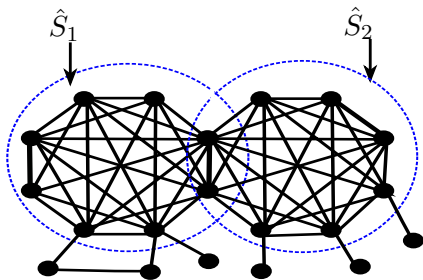
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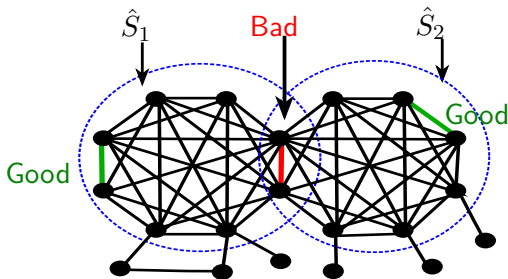
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Result on Approximate Dictionary Estimation

Procedure

- Start with a random edge (y_{i^*}, y_{j^*}) .
- \hat{S} = common nbd. of y_{i^*} and y_{j^*} . If \hat{S} is close to a **clique**, accept.
- Estimate a dictionary element via **top singular vector** of $\sum_{i \in \hat{S}} y_i y_i^\top$.

Theorem

The dictionary A can be estimated with **bounded error** w.h.p. when $s = o(k^{1/3})$ and number of samples $m = \omega(k)$.

- Exact estimation when X is **discrete**, e.g. Bernoulli.

A. Agarwal, A., P. Netrapalli. "Exact Recovery of Sparsely Used Overcomplete Dictionaries," Preprint, Sept. 2013.

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Theorem

The above method converges to the **true solution** (A, X) at a **linear rate** w.h.p. when $s < \min(k^{1/8}, n^{1/9})$ and number of samples $m = \Omega(k^2)$.

Outline

- 1 Introduction
- 2 Spectral Methods
- 3 Robust PCA
- 4 Dictionary Learning
- 5 Conclusion**

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Non-convex Projections vs. Convex Projections

- Projections on to non-convex sets: **NP-hard** in general.
 - ▶ Projections on to **rank** and **sparse sets**: tractable.
- Less information than convex projections: zero-order conditions.

$$\|P(M) - M\| \leq \|Y - M\|, \quad \forall Y \in C(\text{Non-convex}),$$

$$\|P(M) - M\|^2 \leq \langle Y - M, P(M) - M \rangle, \quad \forall Y \in C(\text{Convex}).$$

Non-convex success stories

- **Spectral Methods:** PCA, Tensor methods.
- **Robust PCA:** Alternating projections.
- **Dictionary learning:** Initialize using a “clustering style” method.

Advantages

- **Iterative** methods, **global** convergence guarantees.
- Efficient **sample** and **computational** complexities
- Competitive performance, easily parallelizable and scalable.

(Somewhat) common theme

- Characterize **basin of attraction** for global optimum.
- Obtain a good **initialization** to “land in the ball”: usually also a non-convex method!

My Research Group and Resources

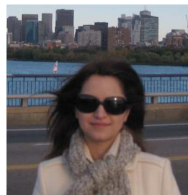
Furong Huang



Majid Janzamin



Hanie Sedghi



Niranjan UN



Forough Arabshahi



- ML summer school lectures available at <http://newport.eecs.uci.edu/anandkumar/MLSS.html>