Scaling the Hierarchical Topic Modeling Mountain

Neural NMF and Iterative Projection Methods

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IPAM,

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Computational and Applied Mathematics
UCLA

Talk Outline

1. Introduction
2. Neural NMF
3. Iterative Projection Methods
4. Applications
5. Conclusions

Introduction

Motivation

- MyLymeData: large collection of Lyme disease patient survey data collected by LymeDisease.org ($\sim$12,000 patients, 100s of questions)

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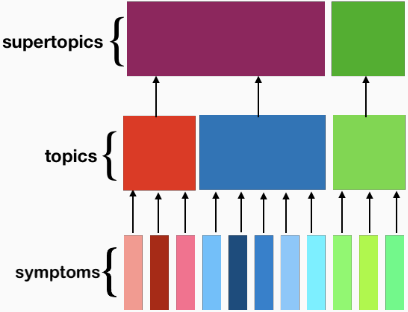

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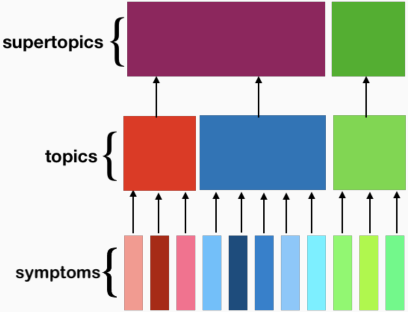

⇒ hypothesis formation about post-treatment/chronic Lyme disease

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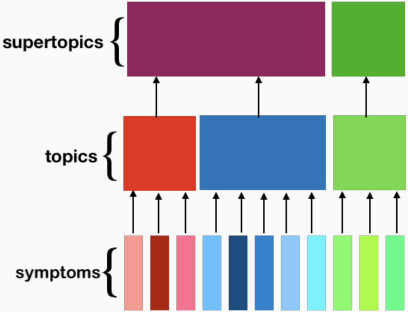

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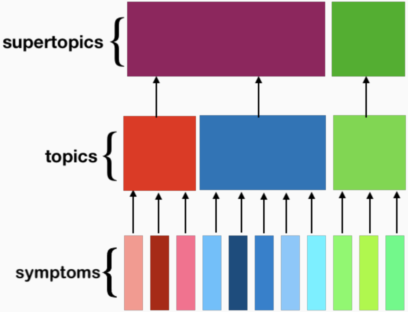

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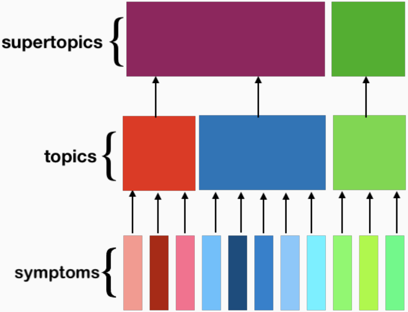

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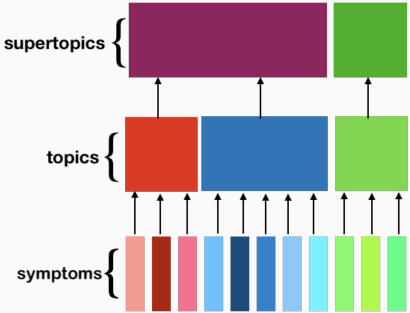

Answer: Neural Nonnegative Matrix Factorization

[Gao, H., Molitor, Needell, Sadovnik, Will, Zhang '19]

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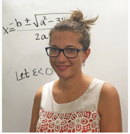
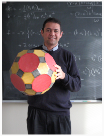
`Sampling Kaczmarz-Motzkin Methods`

[H., Ma '19], [De Loera, H., Needell '17]





Topic Modeling

- principal component analysis (PCA)

  [Pearson 1901]

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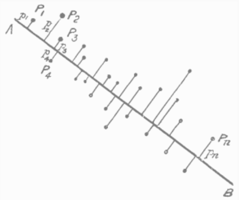

Pearson, K. (1901) *On lines and planes of closest fit to systems of points in space.*

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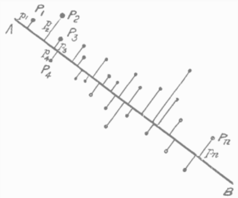

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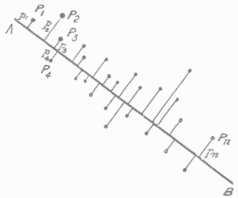

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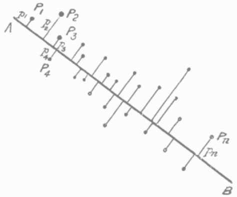
- nonnegative matrix factorization (NMF)
  - [Paatero, Tapper 1994]
  - [Lee, Seung 1999]



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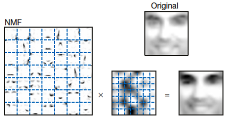
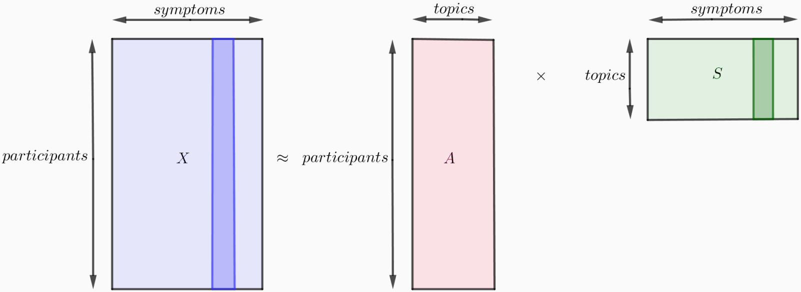


Lee, D., Seung, S. (1999) *Learning the parts of objects by non-negative matrix factorization.*

Nonnegative Matrix Factorization (NMF)

Model: Given nonnegative data X, compute nonnegative A and S of lower rank so that

$$X \approx AS.$$



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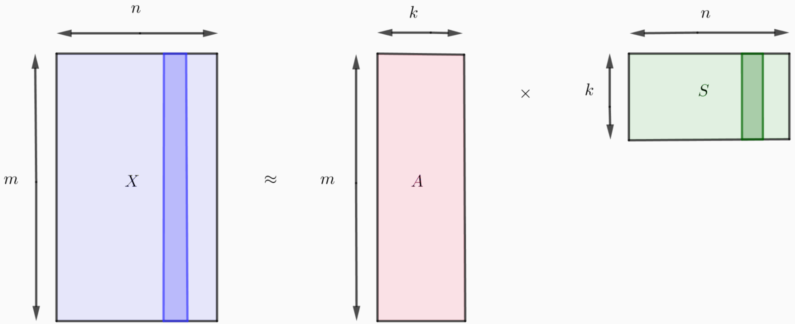

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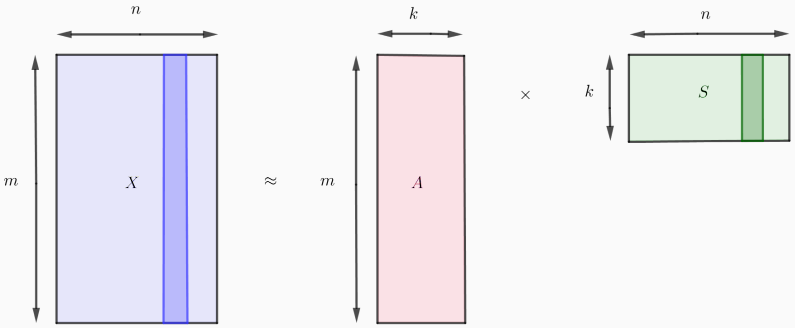

- ▷ Often formulated as optimization problem

$$\min_{A \in \mathbb{R}_{\geq 0}^{m \times k}, S \in \mathbb{R}_{\geq 0}^{k \times n}} \|X - AS\|_F.$$

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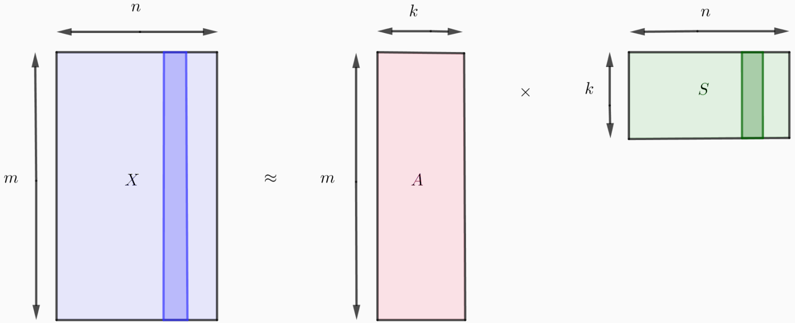

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- Non-convex optimization problem, NP-hard to compute global optimum for fixed k [Vavasis 2008]

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Model: Sequentially factorize

$$X \approx A^{(0)}S^{(0)}, S^{(0)} \approx A^{(1)}S^{(1)}, S^{(1)} \approx A^{(2)}S^{(2)}, ..., S^{(\mathcal{L}-1)} \approx A^{(\mathcal{L})}S^{(\mathcal{L})}.$$

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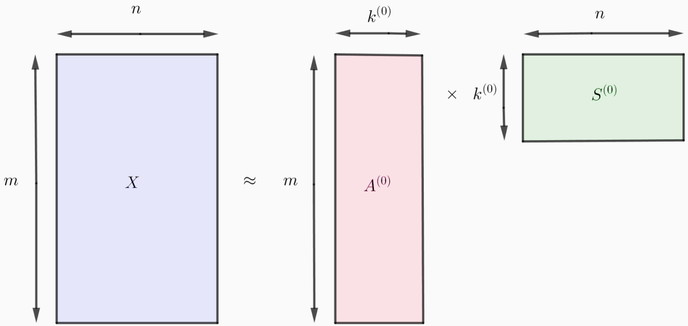

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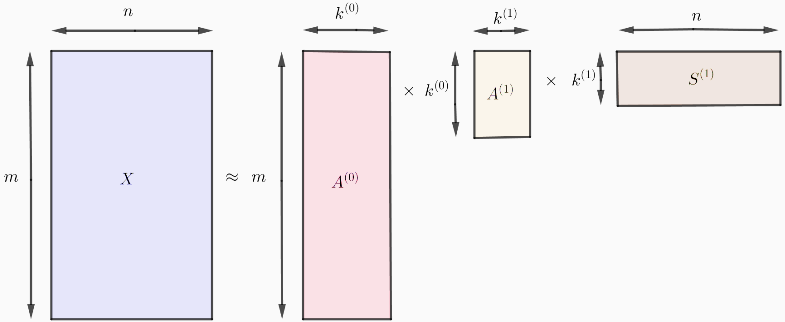

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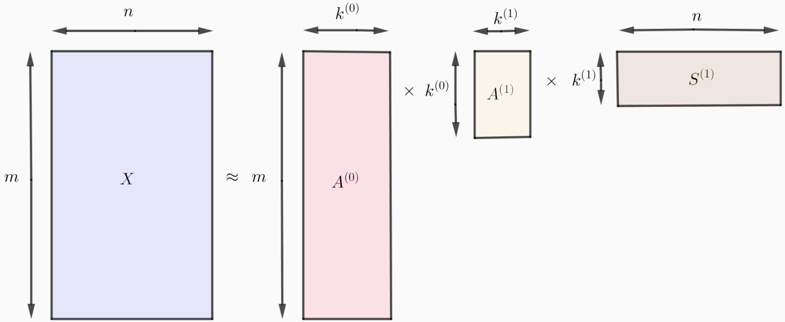

- $k^{(\ell)}$: supertopics collecting $k^{(\ell-1)}$ subtopics

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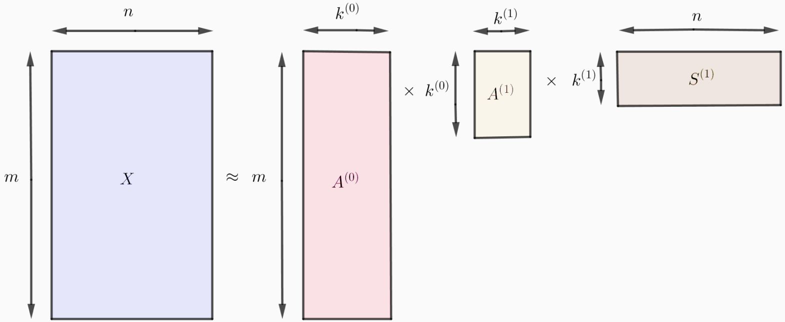
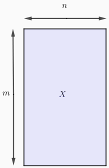


- $k^{(\ell)}$: supertopics collecting $k^{(\ell-1)}$ subtopics
- error propagates through layers

[Cichocki, Zdunek '06]

Neural NMF

Hierarchical NMF



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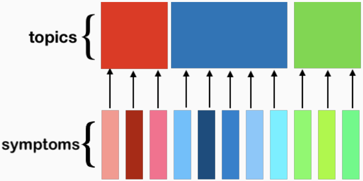

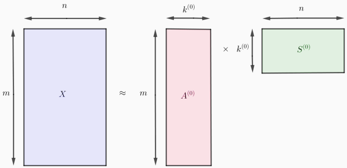

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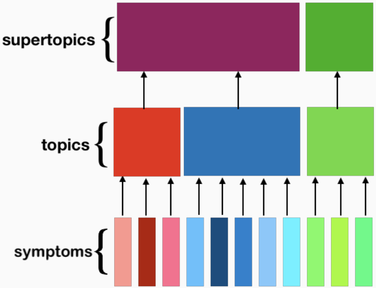

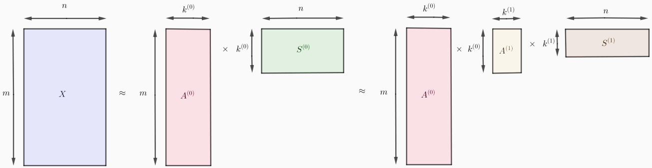

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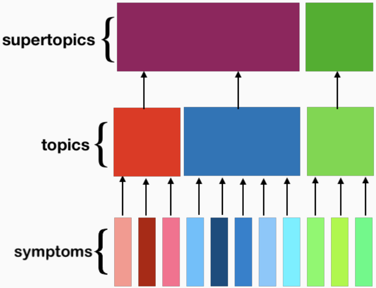
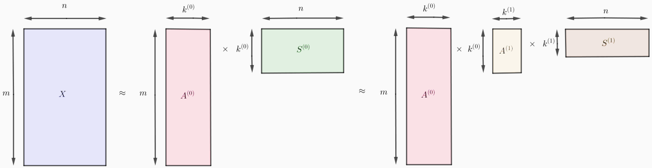
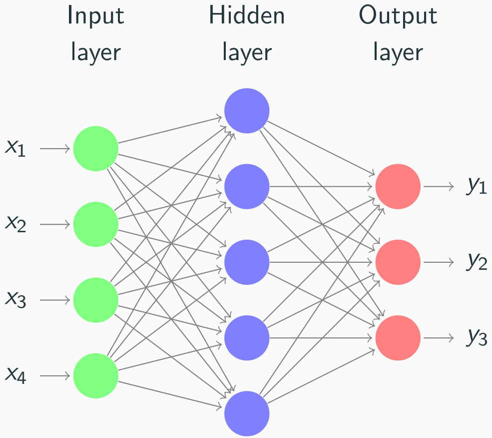


- ▷ hNMF can be implemented in a `feed-forward neural network` structure



Goal: Identify weights $W_1, W_2, ..., W_L$ to minimize model error

$$\sum_{n=1}^{N} E(\{W_i\}) = f(\mathbf{y}(\mathbf{x}_n, \{W_i\}), \mathbf{x}_n, \mathbf{t}_n).$$



Feed-forward Neural Networks

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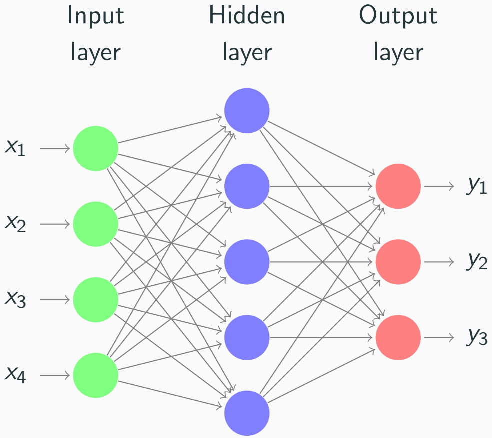

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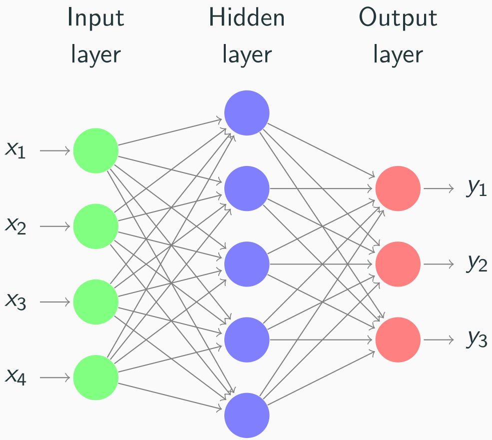

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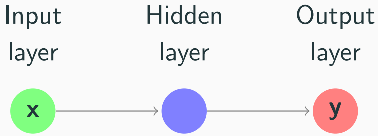

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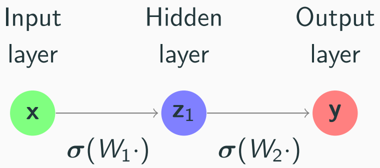

Training:

- forward propagation:
  $\mathbf{z}_1 = \boldsymbol{\sigma}(W_1 \mathbf{x})$,
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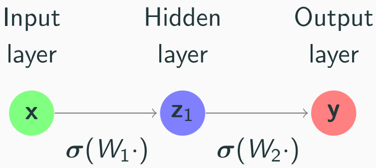

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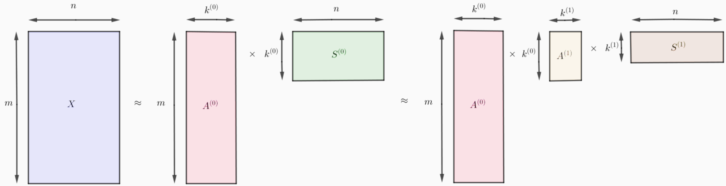
- back propagation: update $\{W_i\}$ with $\nabla E(\{W_i\})$

Our method: Neural NMF

Goal: Develop true forward and back propagation algorithms for hNMF.



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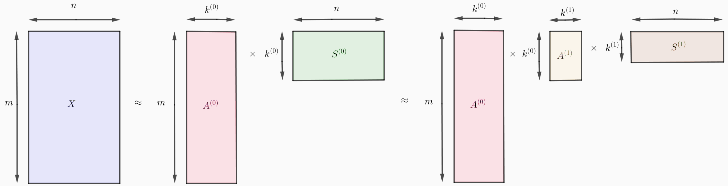

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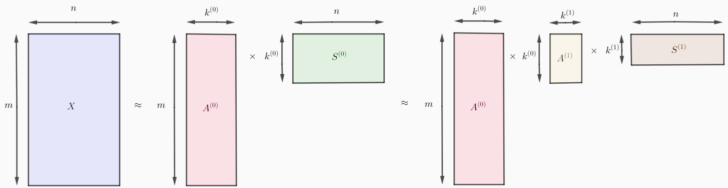

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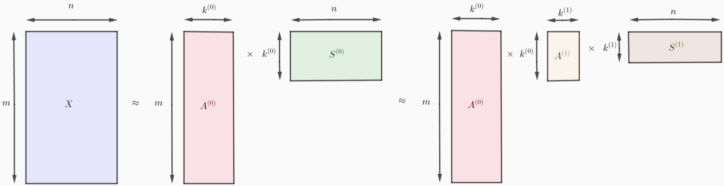

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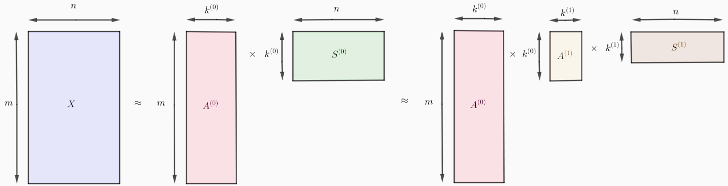

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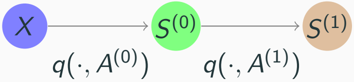
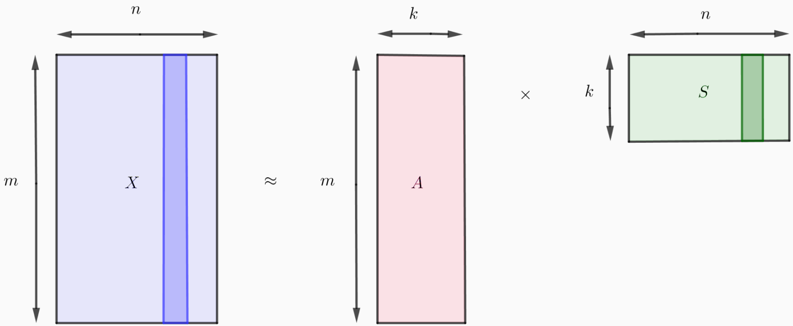


Least-squares Subroutine

- ▷ least-squares is a fundamental subroutine in forward-propagation



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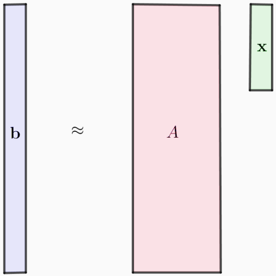

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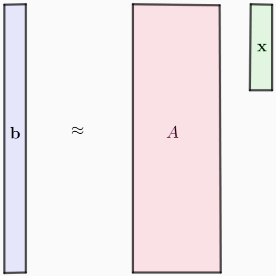
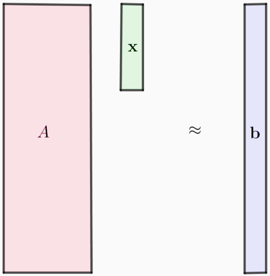


- iterative projection methods can solve these problems

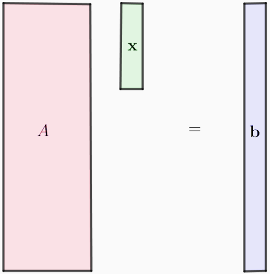
Iterative Projection Methods

General Setup



General Setup

We are interested in solving highly overdetermined systems of equations, $A\mathbf{x} = \mathbf{b}$, where $A \in \mathbb{R}^{m \times n}$, $\mathbf{b} \in \mathbb{R}^m$ and $m \gg n$. Rows are denoted $\mathbf{a}_i^T$.



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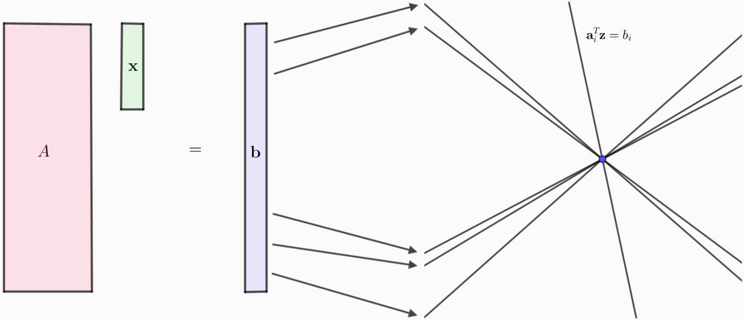

Iterative Projection Methods

If $\{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} = \mathbf{b}\}$ is nonempty, these methods construct an `approximation` to a solution:

1. Randomized Kaczmarz Method

Applications:

1. Tomography (Algebraic Reconstruction Technique)

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Applications:

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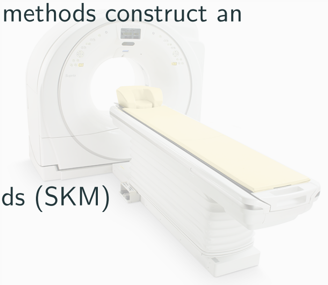

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3. Sampling Kaczmarz-Motzkin Methods (SKM)

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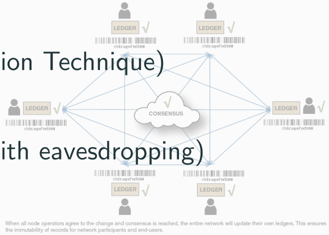
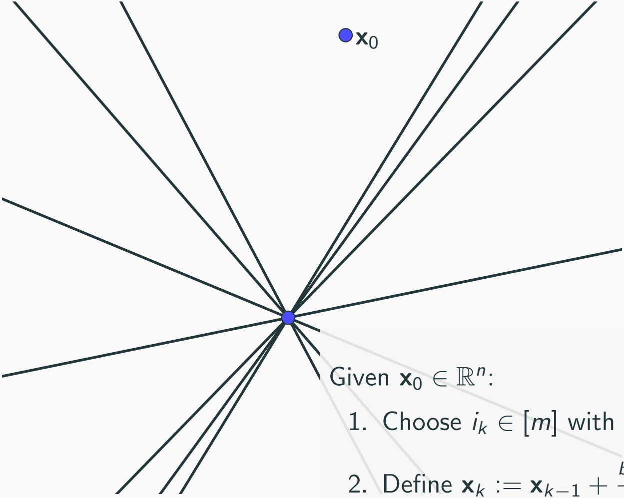


1. Tomography (Algebraic Reconstruction Technique)
2. Linear programming
3. Average consensus (greedy gossip with eavesdropping)



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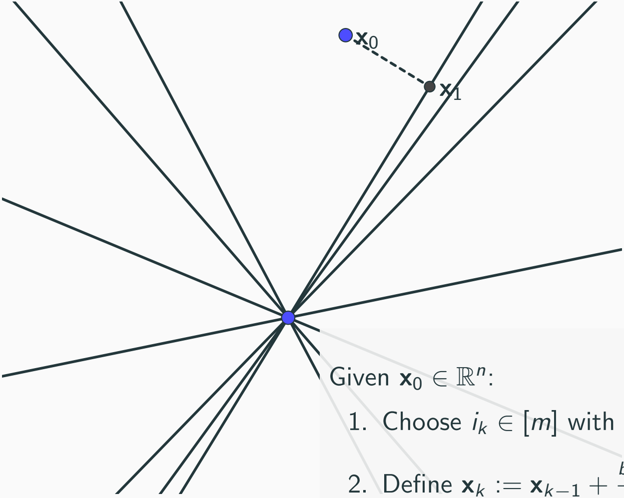
3. Repeat.

[Kaczmarz 1937], [Strohmer, Vershynin 2009]

Kaczmarz Method



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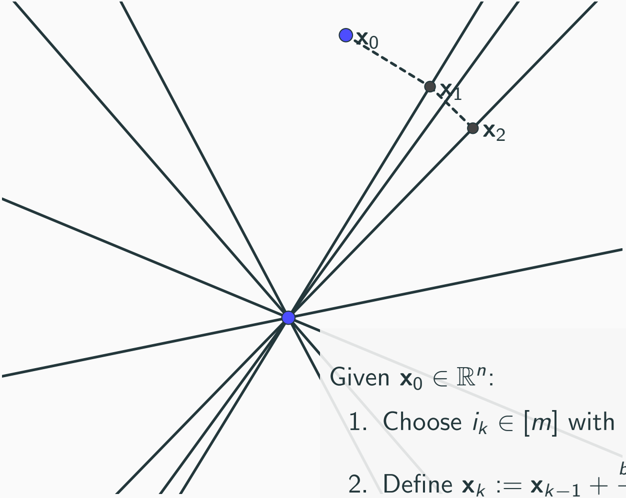

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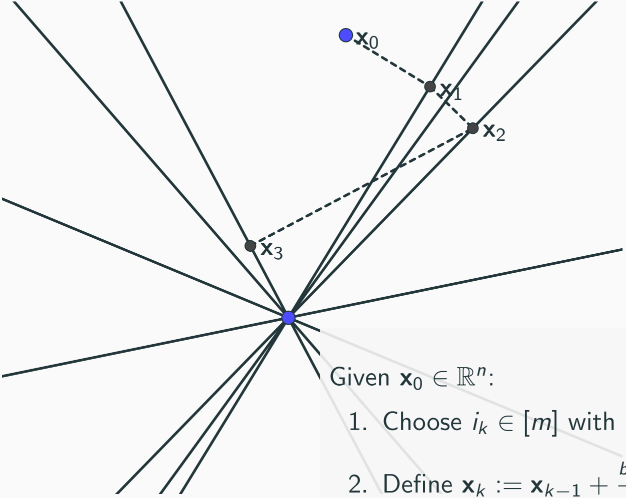

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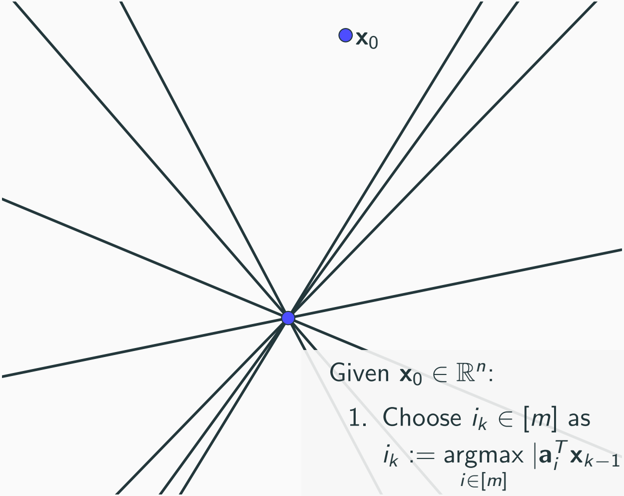

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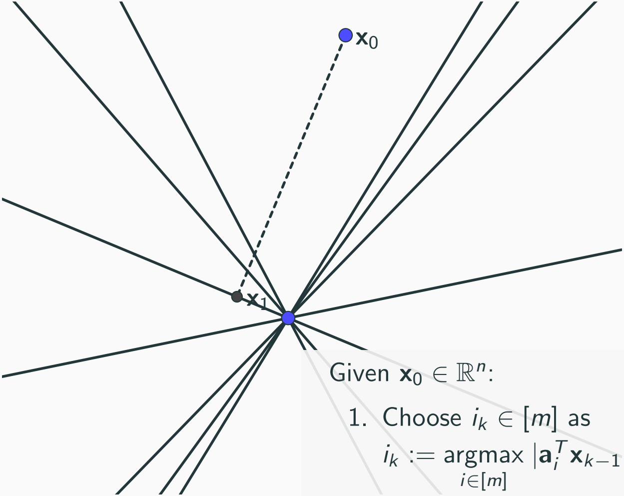

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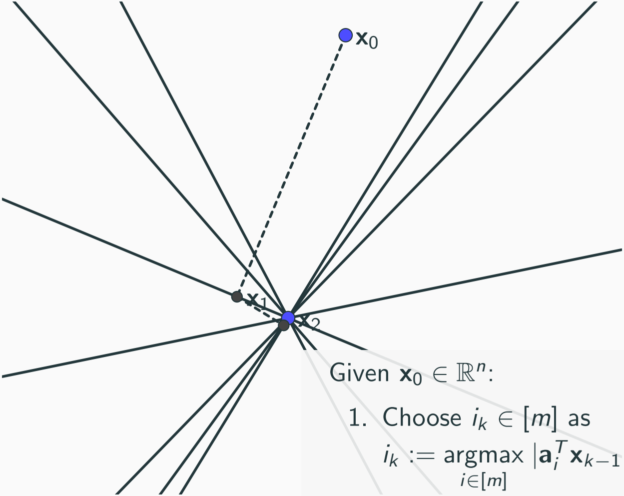

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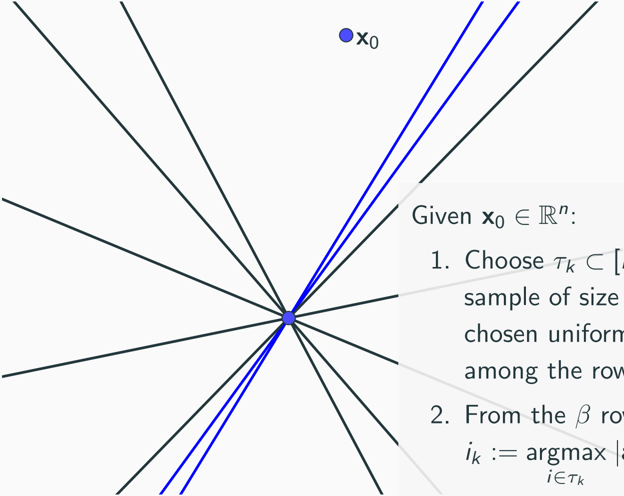
Our Hybrid Method (SKM)



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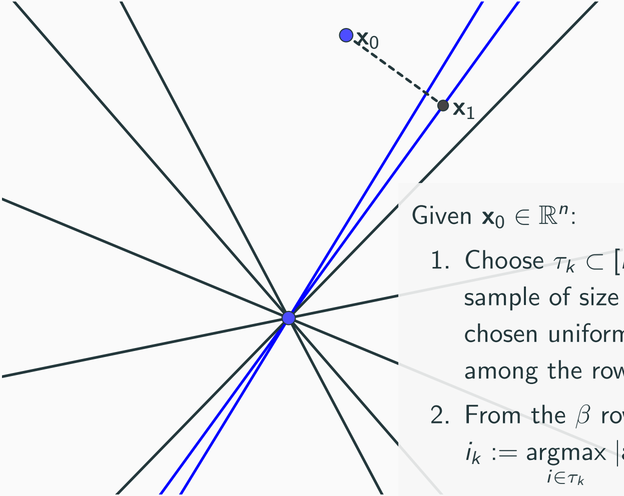

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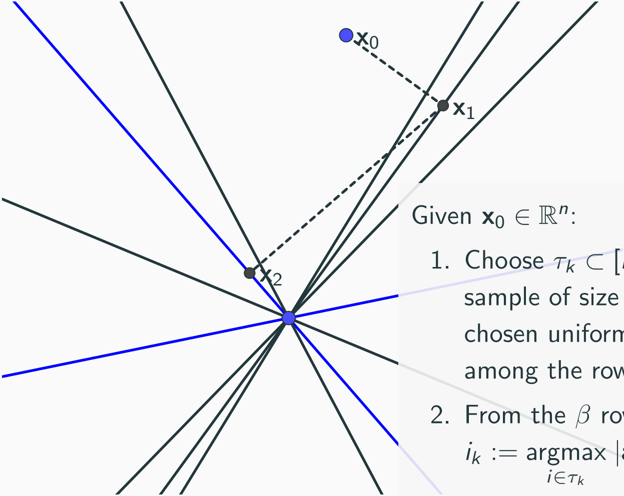

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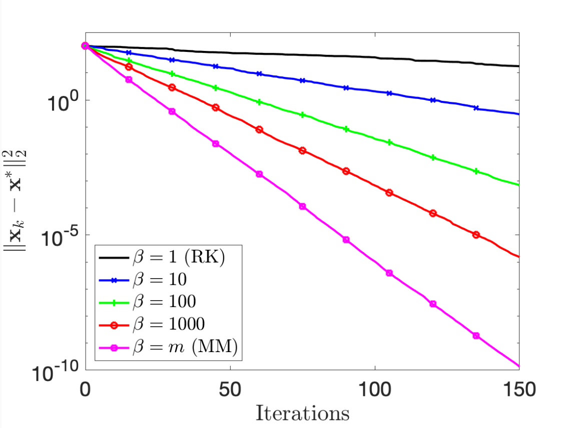

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- A is 50000×100 Gaussian matrix, consistent system
- 'faster' convergence for larger sample size

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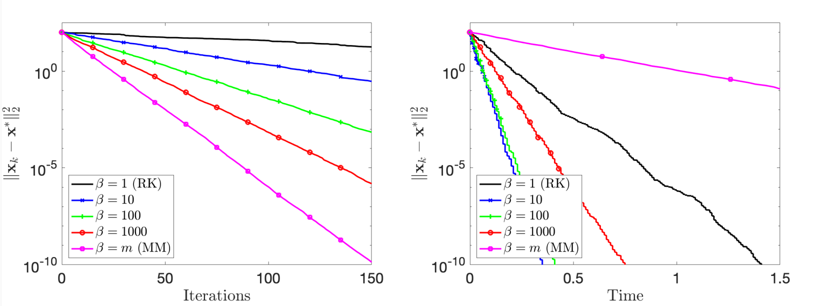

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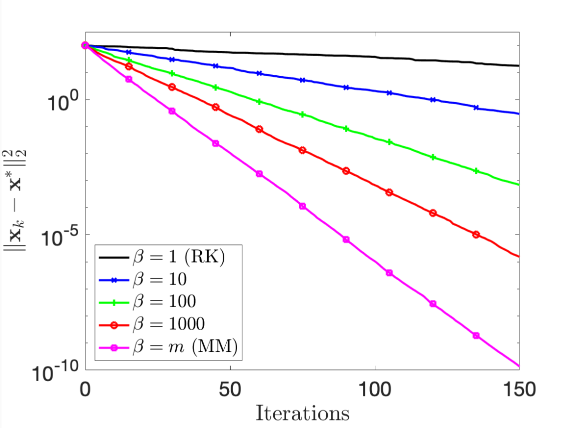

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Convergence Rates

Below are the convergence rates for the methods on a system, $A\mathbf{x} = \mathbf{b}$, which is consistent with unique solution $\mathbf{x}$, whose rows have been normalized to have unit norm.

- RK (Strohmer, Vershynin '09):

$$\mathbb{E}||\mathbf{x}_k - \mathbf{x}||_2^2 \leq \left(1 - \frac{\sigma_{\min}^2(A)}{m}\right)^k ||\mathbf{x}_0 - \mathbf{x}||_2^2$$

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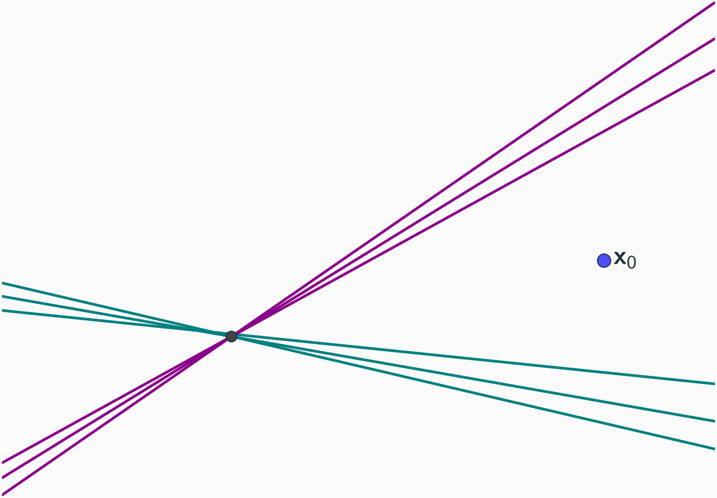
`Why are these all the same?`

A Pathological Example



Structure of the Residual

Several works have used sparsity of the residual to improve the convergence rate of greedy methods.

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However, not much sparsity can be expected in most cases. Instead, we'd like to use dynamic range of the residual to guarantee faster convergence.

$$\gamma_k := \frac{\sum_{\tau \in \binom{[m]}{\beta}} \|A_\tau \mathbf{x}_k - \mathbf{b}_\tau\|_2^2}{\sum_{\tau \in \binom{[m]}{\beta}} \|A_\tau \mathbf{x}_k - \mathbf{b}_\tau\|_\infty^2}$$

Accelerated Convergence Rate

Theorem (H. - Ma 2019)

Let A be normalized so $\|\mathbf{a}_i\|_2 = 1$ for all rows $i = 1, ..., m$. If the system $A\mathbf{x} = \mathbf{b}$ is consistent with the unique solution $\mathbf{x}^*$ then the SKM method converges at least linearly in expectation and the rate depends on the dynamic range of the random sample of rows of A, τ_j. Precisely, in the $j+1$st iteration of SKM, we have

$$\mathbb{E}_{\tau_j}\|\mathbf{x}_{j+1} - \mathbf{x}^*\|_2^2 \leq \left(1 - \frac{\beta\sigma_{\min}^2(A)}{\gamma_j m}\right)\|\mathbf{x}_j - \mathbf{x}^*\|_2^2,$$

where $\gamma_j := \frac{\sum_{\tau \in \binom{[m]}{\beta}} \|A_\tau \mathbf{x}_j - \mathbf{b}_\tau\|_2^2}{\sum_{\tau \in \binom{[m]}{\beta}} \|A_\tau \mathbf{x}_j - \mathbf{b}_\tau\|_\infty^2}$.

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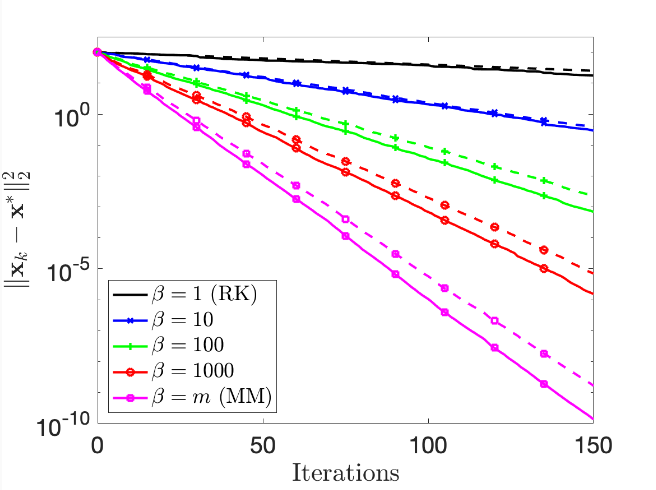

- ▷ A is 50000×100 Gaussian matrix, consistent system
- ▷ bound uses dynamic range of sample of β rows

What can we say about γ_j?

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$$\mathbb{E}_{\tau_k} \|\mathbf{x}_k - \mathbf{x}^*\|_2^2 \leq \alpha \|\mathbf{x}_{k-1} - \mathbf{x}^*\|_2^2$$

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RK	$\alpha = 1 - \frac{\sigma_{\min}^2(A)}{m}$
SKM	$\alpha = 1 - \frac{\sigma_{\min}^2(A)}{m}$
MM	$1 - \frac{\sigma_{\min}^2(A)}{4} \leq \alpha \leq 1 - \frac{\sigma_{\min}^2(A)}{m}$

[H., Needell 2019]

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SKM	$\alpha = 1 - \frac{\sigma_{\min}^2(A)}{m}$	$1 - \frac{\beta\sigma_{\min}^2(A)}{m} \leq \alpha \leq 1 - \frac{\sigma_{\min}^2(A)}{m}$
MM	$1 - \frac{\sigma_{\min}^2(A)}{4} \leq \alpha \leq 1 - \frac{\sigma_{\min}^2(A)}{m}$	$1 - \sigma_{\min}^2(A) \leq \alpha \leq 1 - \frac{\sigma_{\min}^2(A)}{m}$

[H., Needell 2019], [H., Ma 2019]

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▷ nontrivial bounds on γ_k for Gaussian and average consensus systems

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- ▷ provides simple result for MM in case of non-normalized rows (none previously)
- ▷ now can analyze γ_k for systems with unequal row norms

Sketch of Proof

Pythagorean theorem

$$\begin{aligned} \|\mathbf{x}_k - \mathbf{x}^*\|_2^2 &= \|\mathbf{x}_{k-1} - \mathbf{x}^*\|_2^2 - \|\mathbf{x}_{k-1} - \mathbf{x}_k\|_2^2 \\ &= \|\mathbf{x}_{k-1} - \mathbf{x}^*\|_2^2 - \|A_{\tau_k}\mathbf{x}_{k-1} - \mathbf{b}_{\tau_k}\|_\infty^2 \end{aligned}$$

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$$\begin{aligned}\mathbb{E}_{\tau_k}\|A_{\tau_k}\mathbf{x}_{k-1} - \mathbf{b}_{\tau_k}\|_\infty^2 &= \sum_{\tau \in \binom{[m]}{\beta}} \frac{1}{\binom{m}{\beta}} \|A_\tau \mathbf{x}_{k-1} - \mathbf{b}_\tau\|_\infty^2 \\ &= \frac{1}{\binom{m}{\beta}} \sum_{\tau \in \binom{[m]}{\beta}} \|A_\tau \mathbf{x}_{k-1} - \mathbf{b}_\tau\|_\infty^2 \\ &= \frac{1}{\binom{m}{\beta}\gamma_k} \sum_{\tau \in \binom{[m]}{\beta}} \|A_\tau \mathbf{x}_{k-1} - \mathbf{b}_\tau\|_2^2 \\ &= \frac{\beta}{\gamma_k m}\|A\mathbf{x}_{k-1} - \mathbf{b}\|_2^2 \geq \frac{\beta\sigma_{\min}^2(A)}{\gamma_k m}\|\mathbf{x}_{k-1} - \mathbf{x}^*\|_2^2\end{aligned}$$

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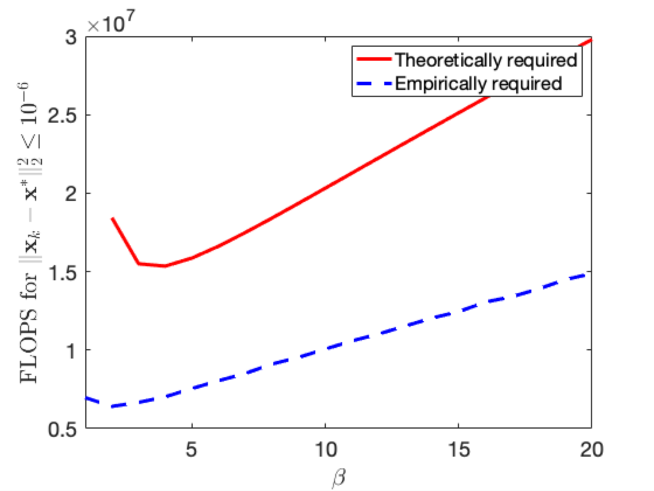
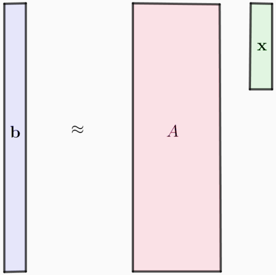


Back to Hierarchical NMF



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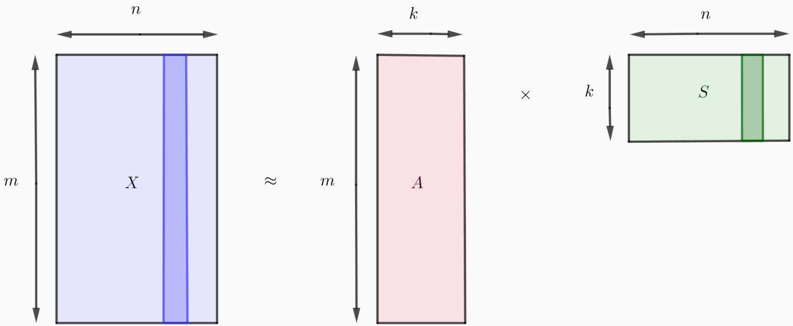

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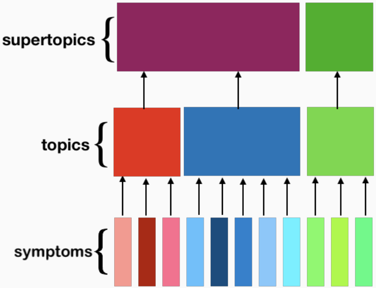

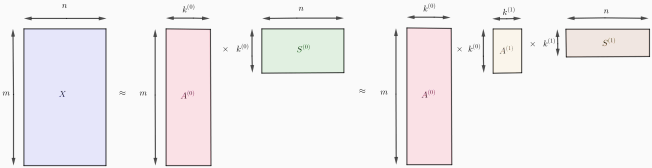

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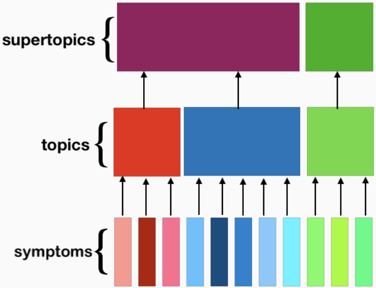
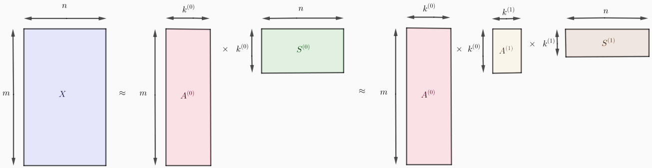


Compare:

- ▷ hNMF (sequential NMF)



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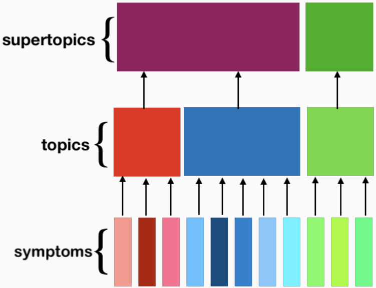

Compare:

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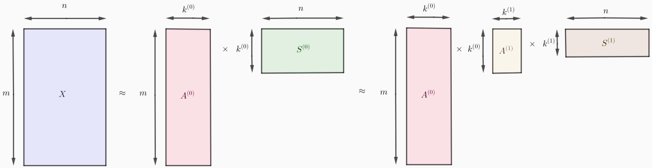
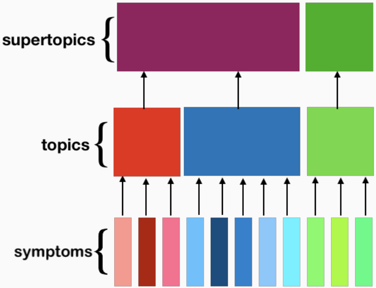
- ▷ Deep NMF [Flenner, Hunter '18]





Compare:

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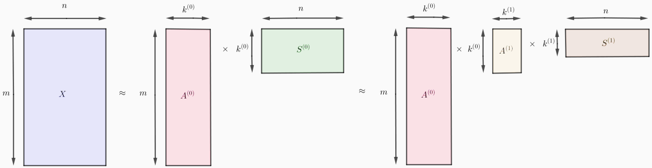
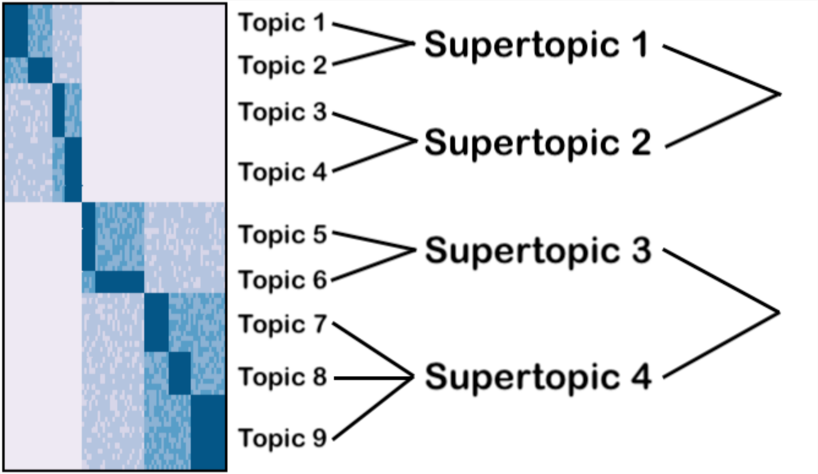
- Neural NMF



Applications

Experimental results: synthetic data



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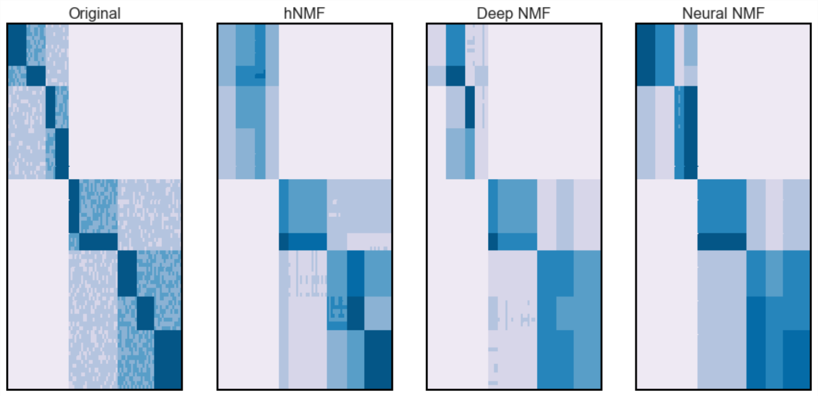

- ▷ unsupervised reconstruction with two-layer structure ($k^{(0)} = 9, k^{(1)} = 4$)

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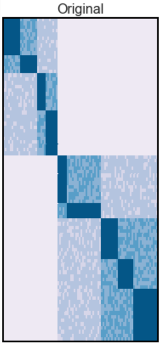

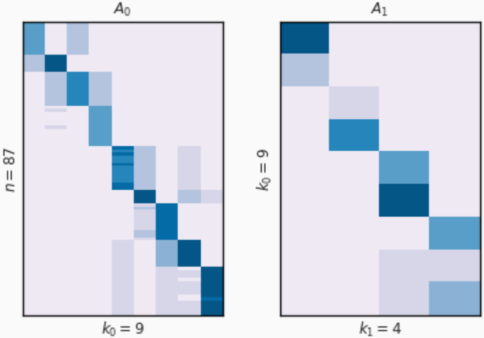

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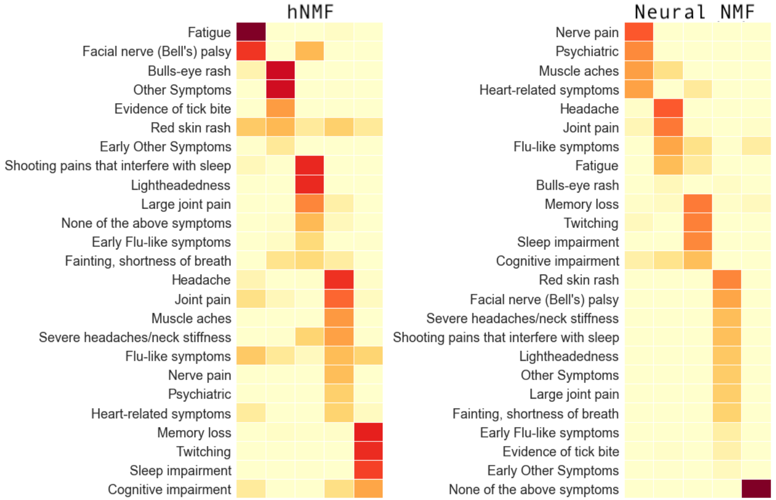
Experimental results: MyLymeData



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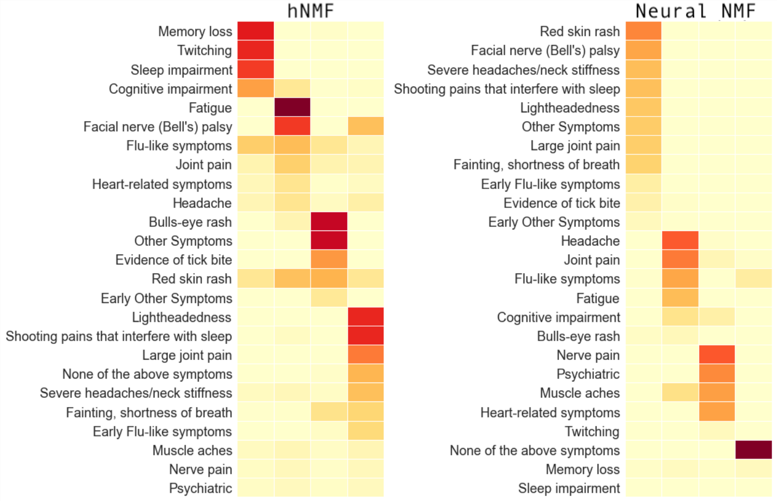

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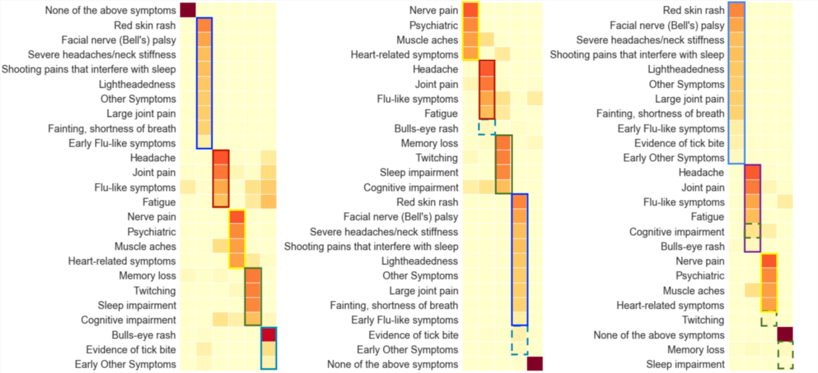

$k^{(0)} = 6$ $k^{(1)} = 5$ $k^{(2)} = 4$

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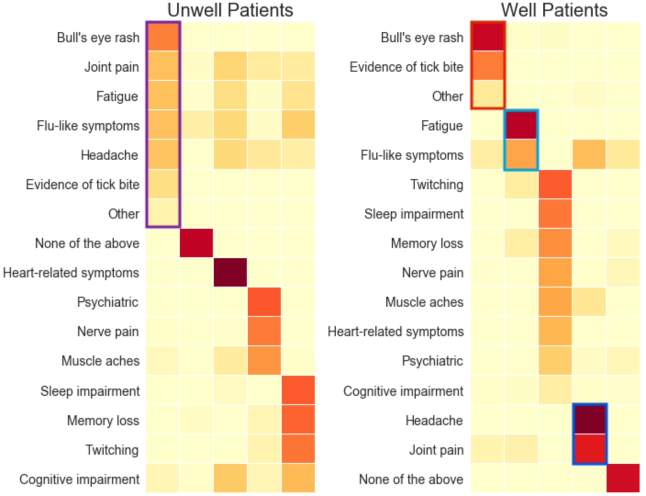

MyLymeData Takeaways

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- unwell and well patients have very different presentation of bulls-eye rash symptom in topics
- patients unwell because lacking bulls-eye rash for diagnosis or indicative of different disease pathway?

Conclusions

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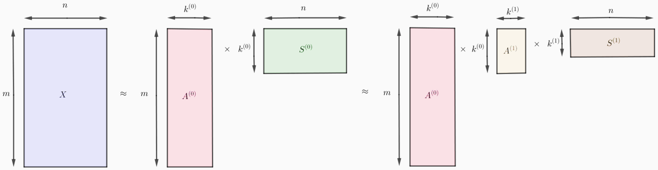
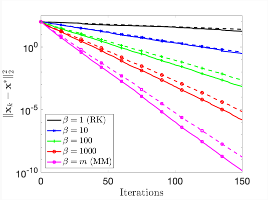
- ▷ hNMF model can be implemented as a feed-forward neural network



- ▷ presented our method `Neural NMF`
- ▷ described family of algorithms which can solve fundamental least-squares subroutine
- ▷ presented accelerated convergence analysis for `SKM`



- ▷ applied Neural NMF to synthetic data and MyLymeData

Thanks for listening!

Questions?

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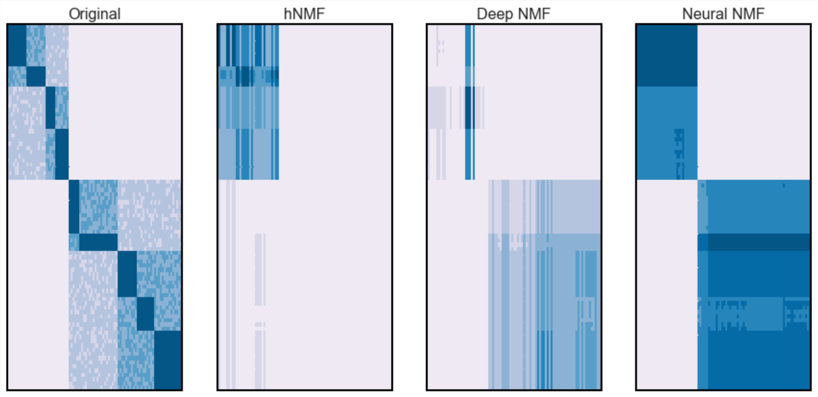
Experimental results: synthetic data



- semisupervised reconstruction (40% labels) with three-layer structure ($k^{(0)} = 9, k^{(1)} = 4, k^{(2)} = 2$)

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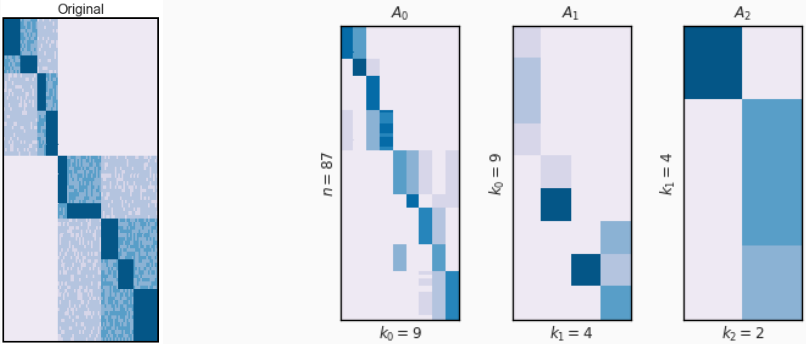

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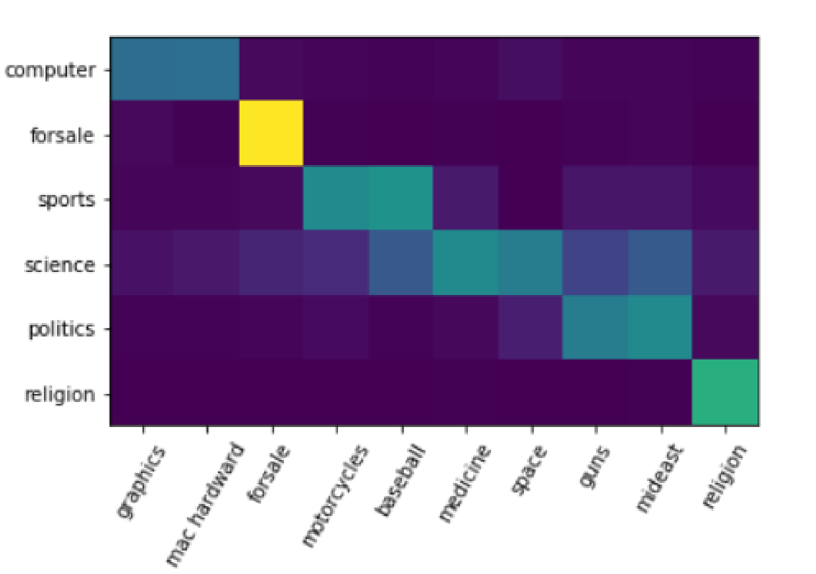
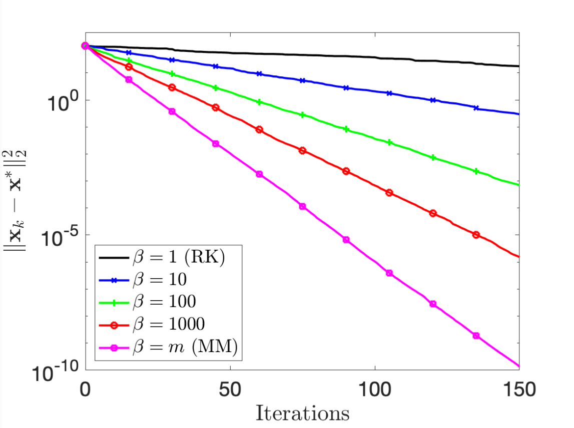
Table 1: Reconstruction error / classification accuracy

	Layers	Hier. NMF	Deep NMF	Neural NMF
Unsuper.	1	0.053	0.031	0.029
	2	0.399	0.414	**0.310**
	3	0.860	0.838	**0.492**
Semisuper.	1	0.049 / 0.933	0.031 / 0.947	0.042 / **1**
	2	0.374 / 0.926	0.394 / 0.911	**0.305** / **1**
	3	0.676 / 0.930	0.733 / 0.930	**0.496** / **0.990**
Supervised	1	0.052 / 0.960	0.042 / 0.962	0.042 / **1**
	2	0.311 / 0.984	0.310 / 0.984	0.307 / 1
	3	0.495 / 1	0.494 / 1	0.498 / 1

Experimental results: 20 Newsgroups data



Experimental Convergence



- β: sample size
- A is 50000×100 Gaussian matrix, consistent system
- ‘faster’ convergence for larger sample size

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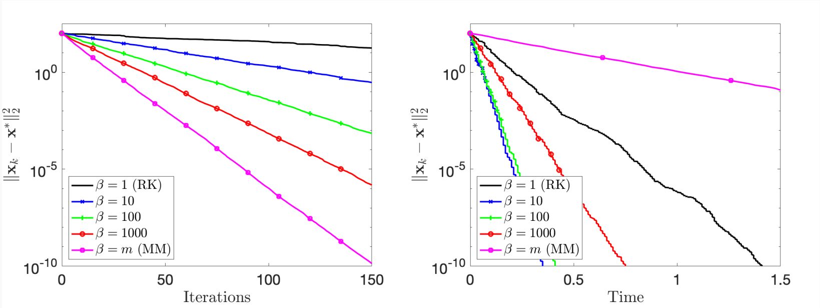

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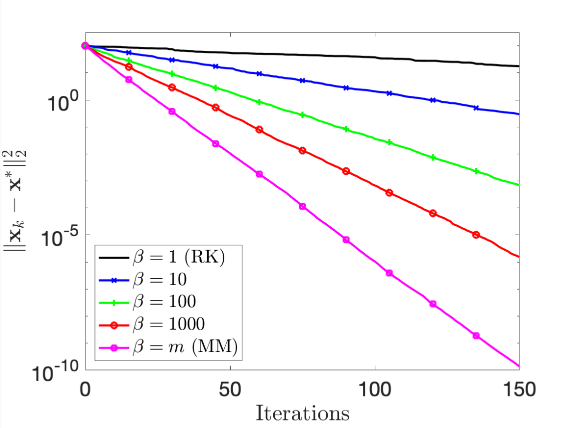

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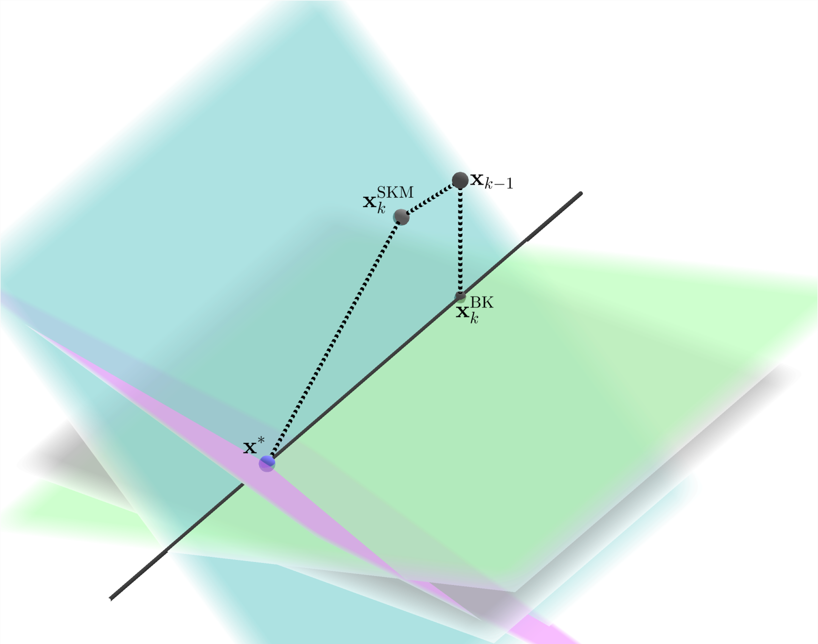
- ▷ [Sun, Nasrabadi, Tran '17]
  - similar method lacking nonnegativity constraints

Block Kaczmarz



Bound on γ_j

$\gamma_k \geq \frac{\beta}{m}\sigma^2_{\min}(A)$ when A is row-normalized