$A \approx BC$

Matrix Approximation Problems

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EU Regional School, RWTH Aachen
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(MPI für biologische Kybernetik, Tübingen)

MAX-PLANCK-GESELLSCHAFT

MPI FOR BIOLOGICAL CYBERNETICS

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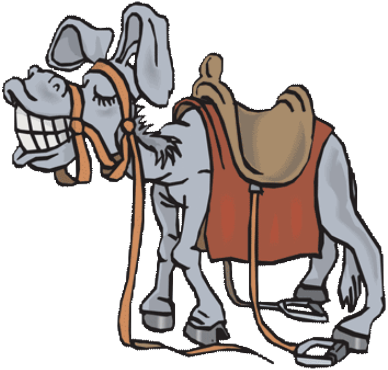

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Given an input matrix $\boldsymbol{A}$ compute a matrix $\hat{\boldsymbol{A}}$ that satisfies certain desired properties, e.g.,

- symmetry, $\hat{\boldsymbol{A}}^T = \hat{\boldsymbol{A}}$
- sparsity, # nnz($\hat{\boldsymbol{A}}$) is small
- positive definiteness, $\hat{\boldsymbol{A}} \succeq 0$
- low-rank, $\hat{\boldsymbol{A}} = \boldsymbol{BC}$
- constraints, $\hat{\boldsymbol{A}} \in \mathcal{A}$
- ...

Today's lecture touches

1. Matrix Analysis
2. Numerical linear algebra
3. Computer Science
4. High-performance computing
5. Numerical optimization
6. Statistics
7. Data mining & machine learning
8. Image Processing, Astronomy, etc.

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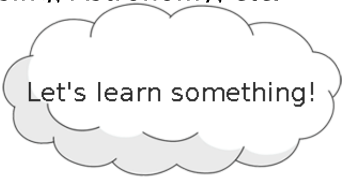

Introduction – matrices all over

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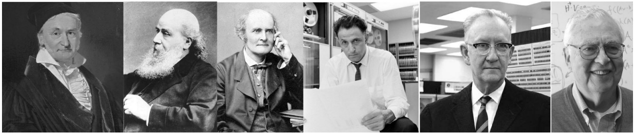

Matrix Collage made from images on Wikipedia; Sci. Comp. images take from Tim Davis' website; Internet graph from Wikipedia;[1]

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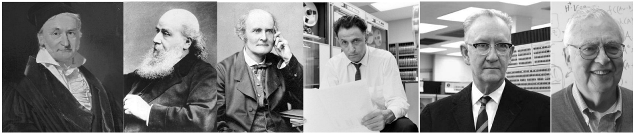

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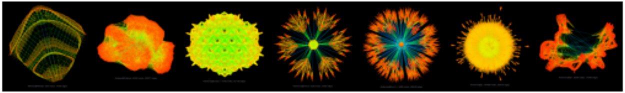

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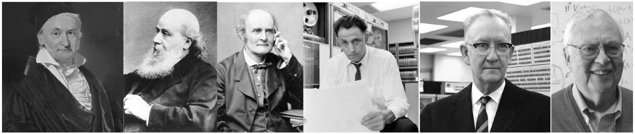

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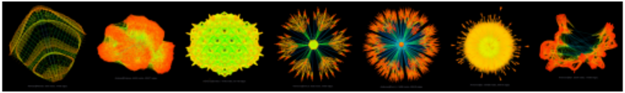

- Statistics

IV:	Ziel: >90	97,3 %	100 %	65,8 %	93,8 %	90,5 %	100 %	87,5 %	98,5 %
Darstellung der hirnversorg. Arterien	Auffälligkeit: <80	n=185	n=79	n=76	n=128	n=74	n=190	n=56	n=130
V:	Ziel: n. b.	21,3 %	21,0 %	23,4 %	32,8 %	30,2 %	25,2 %	17,9 %	16,1 %
Schluck-störungen	Auffälligkeit: <20	n=183	n=62	n=64	n=119	n=53	n=147	n=39	n=87
VI:	Ziel: >80	38,6 %	94,5 %	82,8 %	97,1 %	81,0 %	87,3 %	68,0 %	30,6 %
Logopädie	Auffälligkeit: <60	n=83	n=39	n=29	n=68	n=21	n=79	n=25	n=36
VII:	Ziel: >90	97,7 %	98,0 %	89,8 %	100 %	97,4 %	98,4 %	100 %	95,5%
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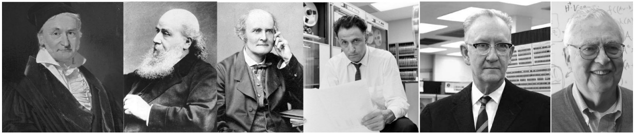

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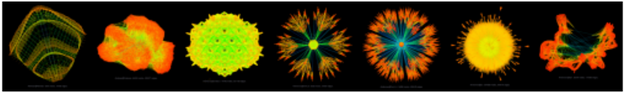

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The Internet Graph[1]

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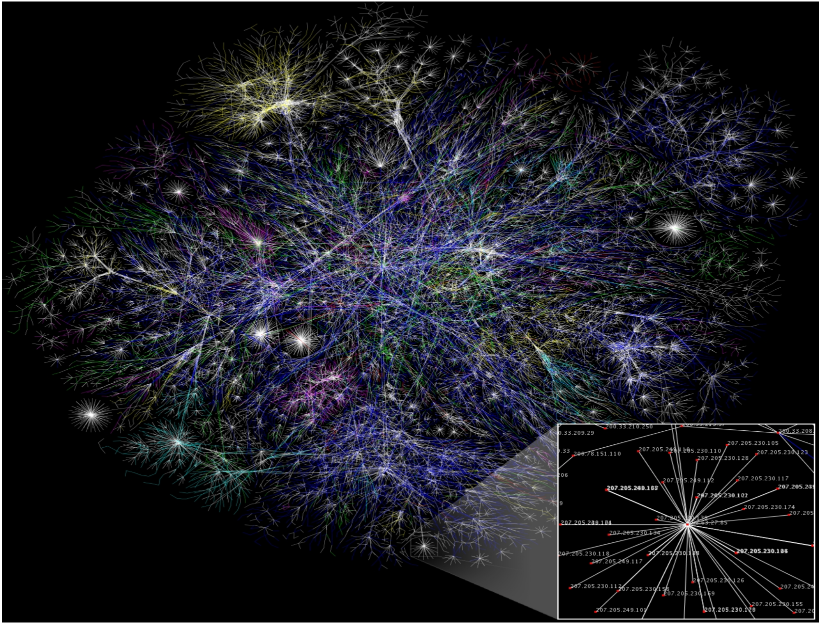
0.33.209.29
200.33.210.250
200.78.151.110
207.205.230.105
207.205.230.128
207.205.230.123
207.205.230.117
207.205.230.174
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207.205.230.118
207.205.249.117
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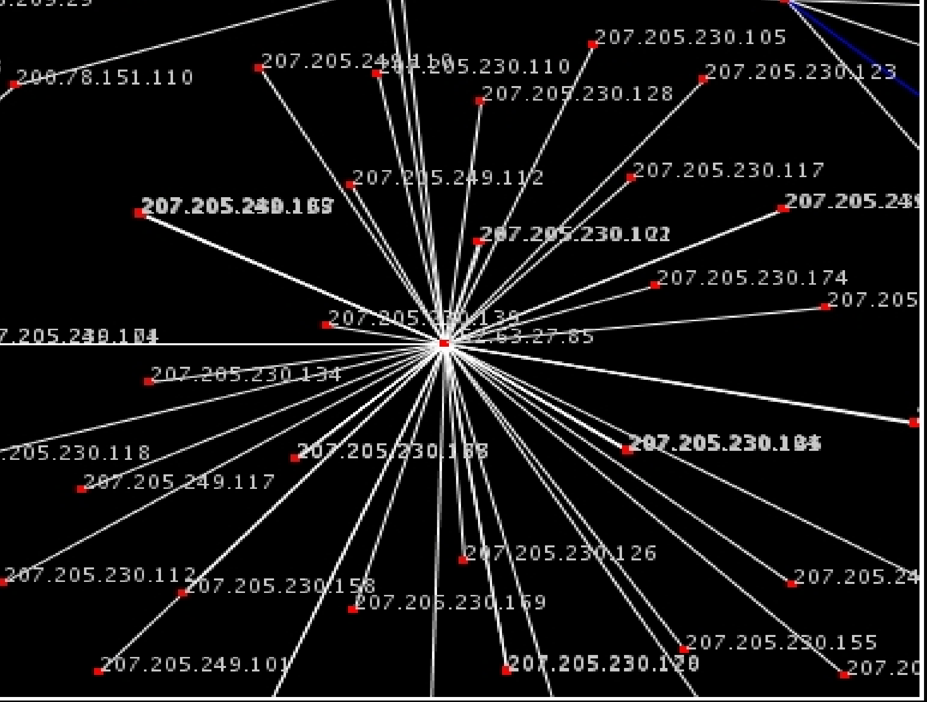

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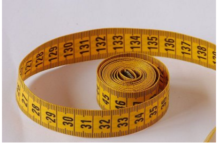

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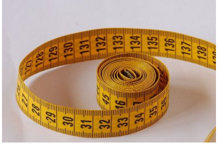

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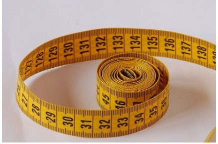

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$AC \neq CA$ and $AC > AB + BC$!

Rounding errors, noise confound:

Expected symmetric, orthogonal, real, posdef, etc., but obtained something else!

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Algorithm requires input to satisfy a property

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Dimensionality reduction:

- Reduce storage
- Numerical benefits
- Expose structure
- Enable visualization
- Easier analysis
- E.g., for face recognition

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Dimensionality reduction:

Hires (3MB)

Lores (3KB!)

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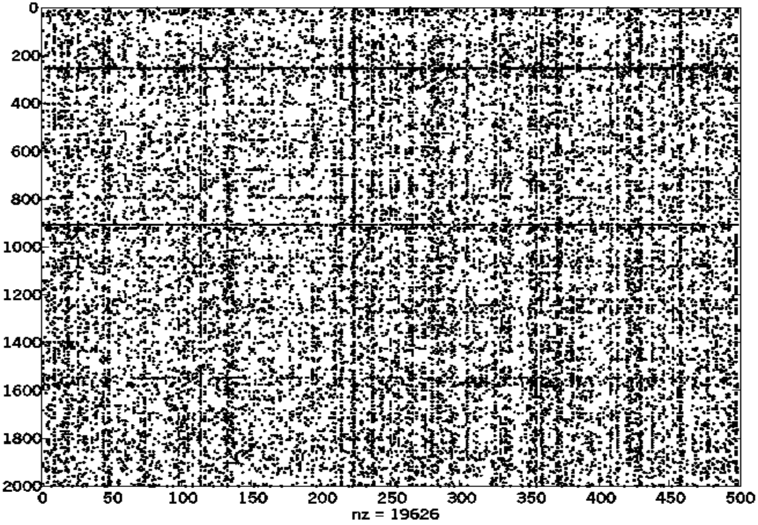

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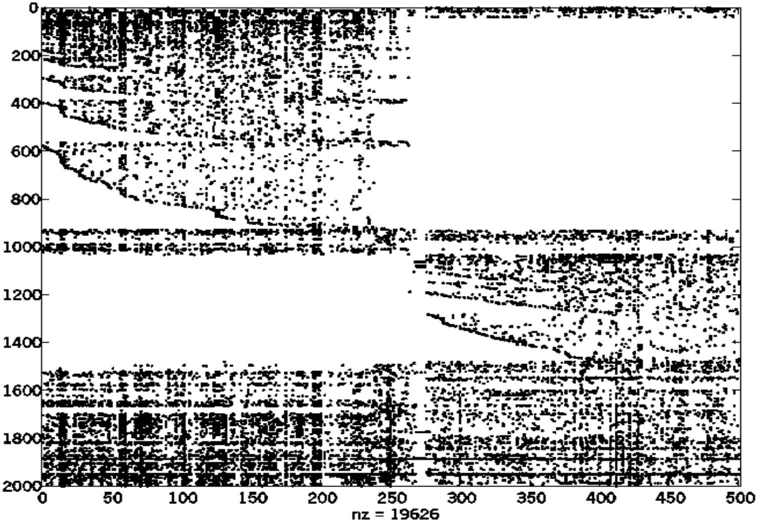

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- Winners, and most top-performing methods: ultimately based on *matrix approximation* ideas!

Preliminaries

Introduction – preliminary concepts

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Commonly used: $\Delta(\boldsymbol{A}, \widehat{\boldsymbol{A}}) = \|\boldsymbol{A} - \widehat{\boldsymbol{A}}\|$

Digression: Matrix Norms

An (operator) *norm* of a matrix $\boldsymbol{A}$ is defined as

$$\boxed{\|\boldsymbol{A}\| = \max_{\|\boldsymbol{x}\|=1} \|\boldsymbol{A}\boldsymbol{x}\|}$$

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We will mostly use the Frobenius norm for convenience

Warmup example

Suppose $\boldsymbol{A} \in \mathbb{R}^{n \times n}$. What is the nearest symmetric matrix?

$$\boxed{\min \quad \|\boldsymbol{A} - \widehat{\boldsymbol{A}}\|_F \quad \text{s.t.} \quad \widehat{\boldsymbol{A}}^T = \widehat{\boldsymbol{A}}}$$

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Solution: FaHo55

$\widehat{\boldsymbol{A}} = (\boldsymbol{A} + \boldsymbol{A}^T)/2$. To verify, do the following:

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since $\|\boldsymbol{X}\|_{\mathrm{F}} = \|\boldsymbol{X}^T\|_{\mathrm{F}}$.

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Let $\boldsymbol{B} \in \mathbb{R}^{m \times k}$ and $\boldsymbol{C} \in \mathbb{R}^{k \times n}$. Then, $\operatorname{rank}(\boldsymbol{BC}) \leq k$. And we have the formula from the title slide:

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"Factors" $\boldsymbol{B}$, $\boldsymbol{C}$ can be computed by solving

$$\boxed{\min \tfrac{1}{2} \|\boldsymbol{A} - \boldsymbol{BC}\|_F^2}$$

But How??

The SVD

Recall fundamental matrix *factorization*:

$$\boxed{\text{Singular Value Decomposition}}$$

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SVD (Thm. 2.5.2 [GoLo96])

Let $\boldsymbol{A} \in \mathbb{R}^{m \times n}$. There exist *orthogonal* matrices $\boldsymbol{U}$ and $\boldsymbol{V}$

$$\boldsymbol{U}^T \boldsymbol{A} \boldsymbol{V} = \mathrm{Diag}(\sigma_1, \ldots, \sigma_p), \quad p = \min(m, n),$$

where $\sigma_1 \geq \sigma_2 \geq \cdots \geq 0$.

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$$\boldsymbol{A}_{m \times n} = \boldsymbol{U}_{m \times m} \begin{bmatrix} \Sigma_{n \times n} \\ 0 \end{bmatrix} \boldsymbol{V}_{n \times n}^T$$

Exercise: $\boldsymbol{A} = \sum_i \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T$ $\quad (\boldsymbol{U} = [\boldsymbol{u}_i]$ and $\boldsymbol{V} = [\boldsymbol{v}_i])$

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Theorem (Optimality of SVD)

Let $\boldsymbol{A}$ *have the SVD* $\boldsymbol{U\Sigma V}^T$. *If* $k < \operatorname{rank}(\boldsymbol{A})$ *and*

$$\boldsymbol{A}_k = \sum_{i=1}^{k} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T, \qquad \textit{then,}$$

$$\|\boldsymbol{A} - \boldsymbol{A}_k\|_2 \le \|\boldsymbol{A} - \boldsymbol{B}\|_2, \quad \textit{s.t.} \quad \operatorname{rank}(\boldsymbol{B}) \le k$$
$$\|\boldsymbol{A} - \boldsymbol{A}_k\|_F \le \|\boldsymbol{A} - \boldsymbol{B}\|_F, \quad \textit{s.t.} \quad \operatorname{rank}(\boldsymbol{B}) \le k.$$

Truncated SVD (TSVD) – Proof Sketch

Prove: TSVD yields "best" Rank-k approximation to matrix $\boldsymbol{A}$

Proof: (2-norm).

1. First verify that $\|\boldsymbol{A} - \boldsymbol{A}_k\|_2 = \sigma_{k+1}$

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Prove: TSVD yields "best" Rank-k approximation to matrix $\boldsymbol{A}$

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We used: $\|\boldsymbol{Az}\|_2 \leq \|\boldsymbol{A}\|_2 \|\boldsymbol{z}\|_2$ $\square$

TSVD – Message

If we are seeking a rank-k approximation to $\boldsymbol{A}$

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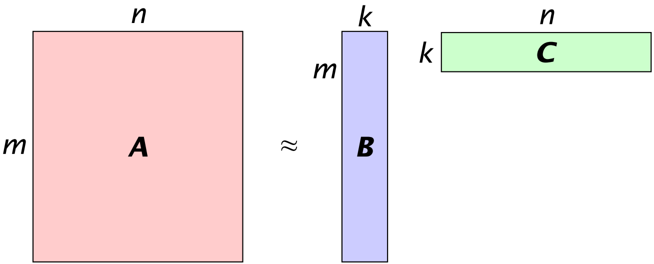

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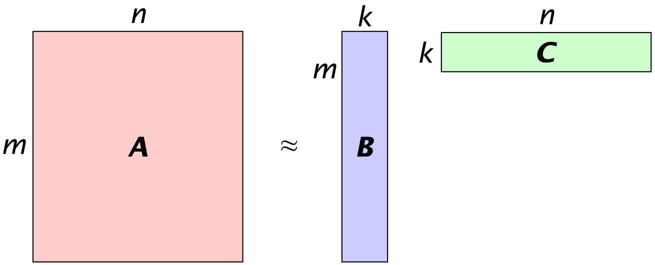

$$\boxed{\text{TSVD yields: } \boldsymbol{B} = \boldsymbol{U}_k\Sigma_k, \text{ and } \boldsymbol{C} = \boldsymbol{V}_k^T}$$

Example Problems

1. Truncated SVD, PCA

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2. Nonnegative matrix approximation (aka NMF)

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TSVD, PCA

Principal component analysis, aka PCA based on TSVD

PCA computes top-k eigenvectors (*principal components*)

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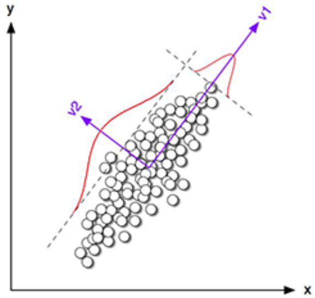
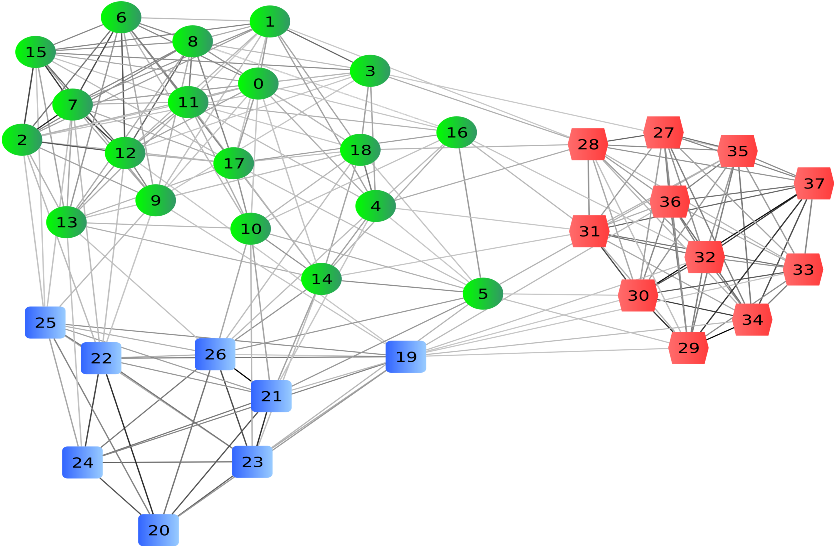
Dimensionality reduction; exploratory data analysis;



Principal components account for variance (spread)

Clustering, Co-clustering



Clustering, Co-clustering

Original matrix

a	+	a	+	+
z	∘	z	∘	∘
a	+	a	+	+
–	*	–	*	*
–	*	–	*	*
z	∘	z	∘	∘

Clustering, Co-clustering

Clustered matrix

a	a	+	+	+
z	z	∘	∘	∘
a	a	+	+	+
–	–	*	*	*
–	–	*	*	*
z	z	∘	∘	∘

After clustering and permutation

Clustering, Co-clustering

Co-clustered matrix

a	a	+	+	+
a	a	+	+	+
z	z	∘	∘	∘
z	z	∘	∘	∘
–	–	*	*	*
–	–	*	*	*

After co-clustering and permutation

Clustering, Co-clustering

Let $\boldsymbol{X} \in \mathbb{R}^{m \times n}$ be the input matrix.

We cluster *columns* of $\boldsymbol{X}$

Well-known *k-means* clustering problem can be written as

$$\min_{\boldsymbol{B},\boldsymbol{C}} \quad \frac{1}{2}\|\boldsymbol{X} - \boldsymbol{B}\boldsymbol{C}\|_{\mathrm{F}}^2 \quad \text{s.t.} \quad \boldsymbol{C}^T\boldsymbol{C} = \mathrm{Diag}(\text{sizes})$$

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Teaser: How would you write a co-clustering problem?

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Recall the Netflix example.

The general *matrix completion* task is:

Recover a matrix from a sampling of its entries!

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One recent result:

> Can perfectly recover most low-rank matrices!

Nearest positive definite

Sometimes one needs to find for a *symmetric* $\boldsymbol{A}$

$$\boxed{\min \quad \|\boldsymbol{A} - \hat{\boldsymbol{A}}\|_F \quad \text{s.t.} \quad \hat{\boldsymbol{A}} \succeq 0}$$

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Solution: BoXi06

$\boldsymbol{A} = \boldsymbol{A}_+ - \boldsymbol{A}_-$, $\boldsymbol{A}_+ = \boldsymbol{A}_+^T \succeq 0$, $\boldsymbol{A}_- = \boldsymbol{A}_-^T \succeq 0$, $\boldsymbol{A}_+\boldsymbol{A}_- = 0$. Moreover

$$\|\boldsymbol{A} - \boldsymbol{A}_+\|_{\mathrm{F}} = \|\boldsymbol{A}_-\|_{\mathrm{F}} \leq \|\boldsymbol{A} - \boldsymbol{X}\|_{\mathrm{F}}$$

for *any* $\boldsymbol{X} \succeq 0$. (Observe, computing $\boldsymbol{A}_-$ enough)

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$$\boxed{\text{Modified Cholesky: } \boldsymbol{A} + \boldsymbol{E} \text{ with } \|\boldsymbol{E}\|_2 = O(n)}$$

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So why not impose $\boldsymbol{B} \geq 0$, $\boldsymbol{C} \geq 0$?

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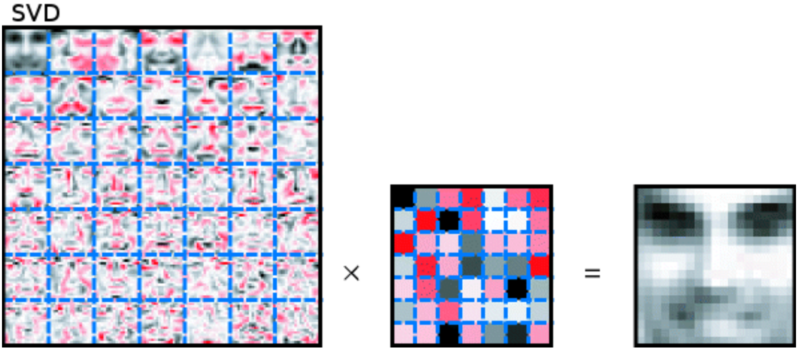

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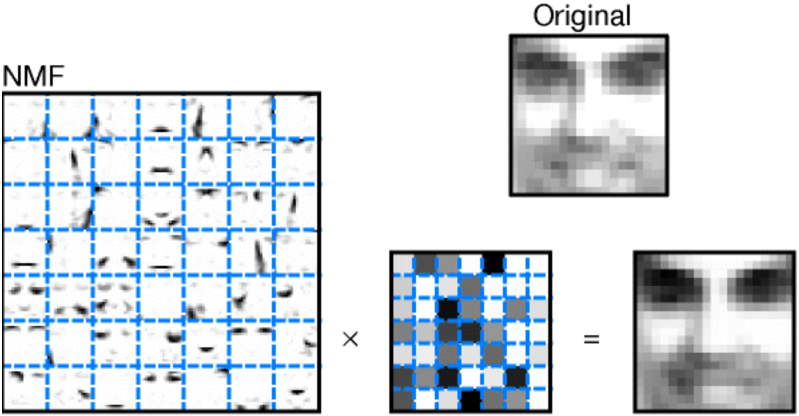

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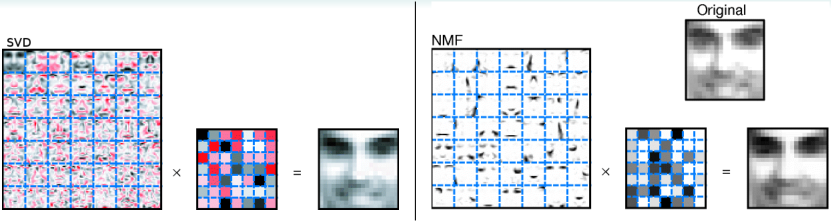

Examples from original Lee/Seung paper on NMA

Other Variants of NMA

- KL-NMA – very interesting variant – more popular for modeling "co-occurrence" data
- Bregman NMA – examples from literature – spam filtering
- Sparsity constrained NMA (Hoyer, etc.)
- Local NMA
- Numerous other variations

Sparsity Constrained Versions

- Sparse PCA
- Semi-discrete decomposition
- Discrete basis problem
- Lasso for variable selection
- Sparse generalized eigenvalue problem
- Other variants

Algorithms & Theory

Algorithms: NMA

We consider the *NMA* problem:

$$\boxed{\boldsymbol{A} \approx \boldsymbol{B}\boldsymbol{C} \quad \text{s.t.} \quad \boldsymbol{B}, \boldsymbol{C} \geq 0.}$$

Algorithms: NMA

Measure quality of approximation using Δ:

$$\boxed{\text{minimize} \quad \Delta(\boldsymbol{A}, \boldsymbol{BC}) \quad \text{s.t.} \quad \boldsymbol{B}, \boldsymbol{C} \geq 0}$$

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Instantiations: where Δ is

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- Even that cannot be found easily!

NMA Algorithms

- Hack: “Zero-out” TSVD
- Alternating methods
- Directly optimizing (won’t cover)
- Online algorithms (won’t cover)

NMA Algorithm: Zero-out SVD

Input: $\boldsymbol{A}$, k

1. $[\boldsymbol{U}, \Sigma, \boldsymbol{V}] = \mathrm{SVD}(\boldsymbol{A}, k)$
2. $\boldsymbol{B} \leftarrow \boldsymbol{U}_k \Sigma_k$, $\boldsymbol{C} \leftarrow \boldsymbol{V}_k^T$
3. $\boldsymbol{B} \leftarrow \max(0, \boldsymbol{B})$, $\boldsymbol{C} \leftarrow \max(0, \boldsymbol{C})$

Advantages: Simple, deterministic

Disadvantages: could be slow, no theoretical guarantees, solution can be really bad!

NMA Algorithm: Alternating Methods

Generic Iterative Alternating Descent

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4. $t \leftarrow t + 1$, and repeat until stopping criteria met.

For least-squares NMA

$$\|\boldsymbol{A} - \boldsymbol{B}^{t+1}\boldsymbol{C}^{t+1}\|_F^2 \leq \|\boldsymbol{A} - \boldsymbol{B}^{t}\boldsymbol{C}^{t+1}\|_F^2 \leq \|\boldsymbol{A} - \boldsymbol{B}^{t}\boldsymbol{C}^{t}\|_F^2$$

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Bad News!

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$$C = \underset{C}{\operatorname{argmin}} \; \|A - B^t C\|_F^2; \qquad C^{t+1} \leftarrow \max(0, C)$$

$$B = \underset{B}{\operatorname{argmin}} \; \|A - BC^{t+1}\|_F^2; \qquad B^{t+1} \leftarrow \max(0, B)$$

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$$\|A - B^{t+1}C^{t+1}\|_F^2 \le \|A - B^t C^{t+1}\|_F^2 \le \|A - B^t C^t\|_F^2$$

is NOT guaranteed!

Alternating NNLS

"Simple" fix is to instead compute

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How to solve the "argmin"??

Alternating NNLS – subproblem

The *nonnegative least squares* (NNLS) subproblem is

$$\boxed{\min_{\boldsymbol{C}\geq 0} \quad \frac{1}{2}\|\boldsymbol{A}-\boldsymbol{BC}\|_F^2}$$

Essentially the same as solving

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- Nice, convex optimization problem
- Numerous algorithms for solving
- Let us look at the simplest

Background – Gradient Methods

Consider first the *unconstrained* problem

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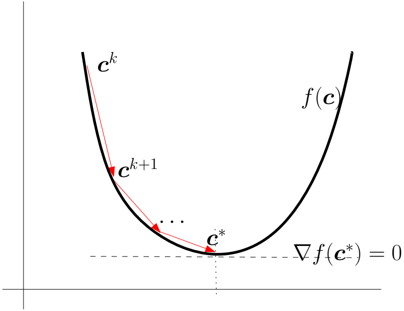

Familiar gradient descent

Background – Gradient Methods

Gradient descent: Vector $\boldsymbol{c}^{k+1}$ is chosen as

$$\boxed{\boldsymbol{c}^{k+1} = \boldsymbol{c}^k - \alpha_k \nabla f(\boldsymbol{c}^k), \quad k = 0, 1, \ldots}$$

- **Step-size** $\alpha_k \geq 0$
- **Descent direction** $-\nabla f(\boldsymbol{c}^k)$

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More generally, *Gradient methods* iterate as

$$\boxed{\boldsymbol{c}^{k+1} = \boldsymbol{c}^k + \alpha_k \boldsymbol{d}^k, \quad k = 0, 1, \ldots}$$

where the descent direction is

$$\boxed{\boldsymbol{d}^k \text{ such that } \langle \boldsymbol{d}^k, \nabla f(\boldsymbol{c}^k) \rangle < 0}$$

Gradient Methods

Gradient methods

$$\boxed{\boldsymbol{c}^{k+1} = \boldsymbol{c}^k + \alpha_k \boldsymbol{d}^k, \quad k = 0, 1, \dots}$$

- Different choices of $\boldsymbol{d}^k$
  - Scaled gradient $\boldsymbol{d}^k = -\boldsymbol{D}^k \nabla f(\boldsymbol{c}^k)$, $\boldsymbol{D}^k \succ 0$
  - Note: $\boldsymbol{D}^k = \boldsymbol{I}$ gives *steepest descent*
  - Newton's method, conjugate gradients, etc.

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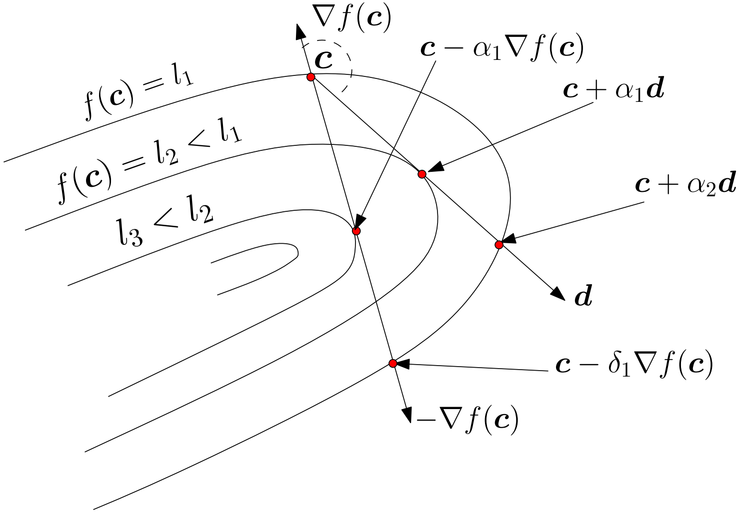
Step-sizes α_k chosen to ensure *descent*

$$f(\boldsymbol{c}^{k+1}) < f(\boldsymbol{c}^k)$$

Gradient Methods – Illustration



(adapted from Bertsekas, Nonlinear Programming)

Gradient Methods – Handling constraints

Our problem is **constrained**

$$\boxed{\min_{\mathbf{c}\geq 0} \quad f(\mathbf{c}) = \frac{1}{2}\|\mathbf{a} - \mathbf{B}\mathbf{c}\|_F^2}$$

Recall gradient-descent iteration

$$\boxed{\mathbf{c}^{k+1} = \quad \mathbf{c}^k - \alpha_k \nabla f(\mathbf{c}^k) \ , \quad k = 0, 1, \ldots}$$

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Replace it with *Gradient-Projection*!

$$\boxed{\boldsymbol{c}^{k+1} = P_+(\boldsymbol{c}^k - \alpha_k \nabla f(\boldsymbol{c}^k)), \quad k = 0, 1, \ldots}$$

$P_+\boldsymbol{x} = \max(0, \boldsymbol{x})$: projection to ensure *non-negativity*

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$$\boxed{\text{minimize} \quad \tfrac{1}{2}\|\boldsymbol{A} - \boldsymbol{B}\boldsymbol{C}\|_F^2 \quad \text{s.t.} \quad \boldsymbol{B}, \boldsymbol{C} \geq 0.}$$

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by alternating

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So are we ready to implement this?

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So are we ready to implement this?
How to compute $\nabla F(\boldsymbol{C}^k)$?

Background – Matrix Derivatives

Derivative of $f : \mathbb{R}^{m \times n} \to \mathbb{R}$ is defined as

$$\frac{\partial f(\boldsymbol{X})}{\partial \boldsymbol{X}} \triangleq \left[\frac{\partial f(\boldsymbol{X})}{\partial x_{pq}} \right]$$

I. Compute $\partial \mathrm{Tr}(\boldsymbol{X}\boldsymbol{Y}) / \partial \boldsymbol{X}$

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Recall $\mathrm{Tr}(\boldsymbol{X}\boldsymbol{Y}) = \sum_{ij} x_{ij} y_{ji}$. Hence, $\partial \mathrm{Tr}(\boldsymbol{X}\boldsymbol{Y})/\partial \boldsymbol{X} = \boldsymbol{Y}^T$.

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II. Verify that: $\partial \|\boldsymbol{X}\|_F^2 / \partial \boldsymbol{X} = 2\boldsymbol{X}$

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Solution:

Recall that $\|\boldsymbol{X}\|_F^2 = \mathrm{Tr}(\boldsymbol{X}^T\boldsymbol{X})$. So,

$$\frac{\partial \|\boldsymbol{X}\|_F^2}{\partial \boldsymbol{X}} = \frac{\partial \mathrm{Tr}(\boldsymbol{X}^T\boldsymbol{X})}{\partial x_{pq}} = \frac{\partial (\sum_{ij} x_{ij}^2)}{\partial x_{pq}} = 2x_{pq}.$$

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Solution: Brute force

$$\mathrm{Tr}(\boldsymbol{X}^T \boldsymbol{A}\boldsymbol{X}) = \sum_{ij} x_{ij} (\boldsymbol{A}\boldsymbol{X})_{ji} = \sum_{ijk} x_{ij} a_{jk} x_{ki}$$

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Solution:

$F(\boldsymbol{C}) = \|\boldsymbol{A}\|_{\mathrm{F}}^2 - 2\,\mathrm{Tr}(\boldsymbol{C}\boldsymbol{A}^T\boldsymbol{B}) + \mathrm{Tr}(\boldsymbol{C}^T\boldsymbol{B}^T\boldsymbol{B}\boldsymbol{C})$

$$\frac{\partial F(\boldsymbol{C})}{\partial \boldsymbol{C}} = -2\boldsymbol{B}^T\boldsymbol{A} + 2\boldsymbol{B}^T\boldsymbol{B}\boldsymbol{C}.$$

In passing: The Fréchet derivative

Given $f : V \to W$, the *Fréchet differential* at point $\boldsymbol{X}$ is the linear-mapping L that satisfies for all $\boldsymbol{E} \in V$ the relation

$$\boxed{f(\boldsymbol{X} + \boldsymbol{E}) - f(\boldsymbol{X}) - L(\boldsymbol{X}, \boldsymbol{E}) = o(\|\boldsymbol{E}\|)}$$

The *Fréchet derivative* $D_f(\boldsymbol{X})$ (of f at point $\boldsymbol{X}$) identified via:

$$\boxed{L(\boldsymbol{X}, \boldsymbol{E}) = D_f(\boldsymbol{X})(\boldsymbol{E})}$$

Can be used to develop matrix calculus formally.

Implementation

Exercise: LSNMA

Implement the gradient-projection NMA algorithm

Exercise: Complexity

What is the computational complexity per (major) iteration?

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Exercise: LSNMA

Implement the gradient-projection NMA algorithm

Exercise: Complexity

What is the computational complexity per (major) iteration?

Solution:

A lot! Especially since there might be many (inner) gradient projection iterations for each major iteration.

What to do?

Alternating descent

Idea! Do not insist on minimization

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Recall that we originally wanted *descent*

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There exists a more popular alternating-descent algorithm!

Multiplicative Updates

The Lee & Seung Algorithm

Lee & Seung (2000) proposed the following "algorithm"

$$\boldsymbol{C}' \leftarrow \boldsymbol{C} \odot \frac{\boldsymbol{B}^T \boldsymbol{A}}{\boldsymbol{B}^T \boldsymbol{B} \boldsymbol{C}}$$
$$\boldsymbol{B}' \leftarrow \boldsymbol{B} \odot \frac{\boldsymbol{A} \boldsymbol{C}'^T}{\boldsymbol{B} \boldsymbol{C}' \boldsymbol{C}'^T}.$$

This algorithm's simplicity made NMA popular.

Note: $\boldsymbol{A} \odot \boldsymbol{B} = [a_{ij} b_{ij}]$ – *elementwise multiplication*

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- Easy to see that nonnegativity respected
- Somewhat harder to prove descent

$$\|\boldsymbol{A} - \boldsymbol{B}'\boldsymbol{C}'\|_F^2 \le \|\boldsymbol{A} - \boldsymbol{B}\boldsymbol{C}'\|_F^2 \le \|\boldsymbol{A} - \boldsymbol{B}\boldsymbol{C}\|_F^2$$

Multiplicative updates – preliminaries

Let $\boldsymbol{c}$ be an arbitrary column of $\boldsymbol{C}$. Consider the subproblem:

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Constructing g

- Main difficulty for $f(\boldsymbol{c}) = \frac{1}{2}\|\boldsymbol{a} - \boldsymbol{B}\boldsymbol{c}\|_2^2$ due to $\boldsymbol{B}\boldsymbol{c}$
- We need to decouple $\boldsymbol{B}\boldsymbol{c}$ — let's see how.

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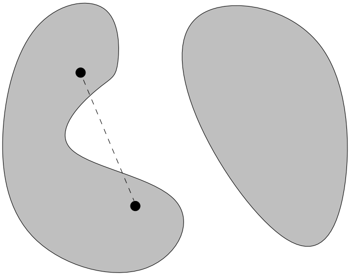

Non-convex, and a convex set

Constructing g

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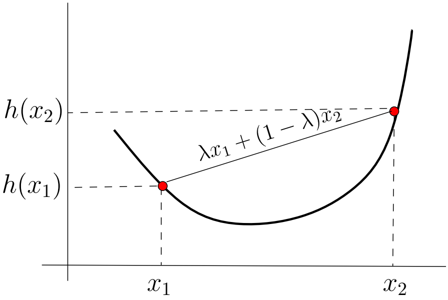

A convex function

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&= g(\boldsymbol{c}, \tilde{\boldsymbol{c}}), \quad \text{where} \quad \lambda_{ij} \quad \text{are convex coeffts}
\end{aligned}$$

Constructing g

In summary:

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Exercise: Richardson-Lucy

Let $f(\boldsymbol{c}) = \sum_i a_i \log(a_i/(\boldsymbol{B}\boldsymbol{c})_i) - a_i + (\boldsymbol{B}\boldsymbol{c})_i$.
Derive an auxiliary function $g(\boldsymbol{c}, \tilde{\boldsymbol{c}})$ for this $f(\boldsymbol{c})$

Minimizing g

Recall,core step: $\boldsymbol{c}^{t+1} = \operatorname{argmin} g(\boldsymbol{c}, \boldsymbol{c}^t)$

Solve $\partial g(\boldsymbol{c}, \boldsymbol{c}^t)/\partial c_p = 0$

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Extending to matrices, we obtain Lee & Seung's update

$$\boldsymbol{C}^{t+1} = \boldsymbol{C}^t \odot \frac{\boldsymbol{B}^T \boldsymbol{A}}{\boldsymbol{B}^T \boldsymbol{B} \boldsymbol{C}^t}$$

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- MM algorithms subject of a separate lecture!

Summary

- We looked at least-squares NMA

$$\min \quad \frac{1}{2}\|\boldsymbol{A} - \boldsymbol{B}\boldsymbol{C}\|_F^2, \quad \text{s.t.} \quad \boldsymbol{B}, \boldsymbol{C} \geq 0.$$

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Take home message: The methods, techniques that we saw, are general. You can use them for many other problems!

Applications & Practical Concerns

Applications – example areas

1. Statistics
2. Data mining, Machine learning
3. Signal processing (images, speech, music, etc.)
4. Computer graphics
5. Chemometrics
6. Remote Sensing
7. Scientific computing
8. …

TSVD

- Statistics
- Psychometrics
- Data Mining, Machine learning
- Information Retrieval
- Biology, Bioinformatics
- In general, exploratory data analysis

Bioinformatics – gene microarray analysis

Biologists measure *activity* (aka gene-expression) of different genes under various conditions (time, temperature, etc.).

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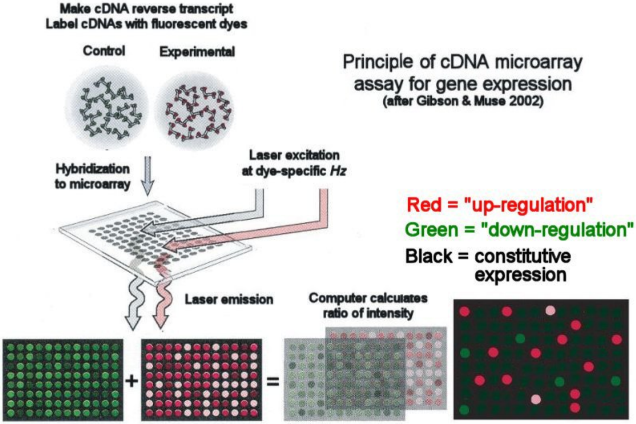

Bioinformatics – gene microarray analysis

Biologists measure *activity* (aka gene-expression) of different genes under various conditions (time, temperature, etc.).
Activity recorded using *gene microarray*
Activities across numerous "conditions" or experiments

We measure an $m \times n$ ($m \gg n$) *genes* $\times$ *array* matrix.

Some "cleaning" (pre-processing) etc. needed.

Truncated SVD on this gene-expression matrix is performed.

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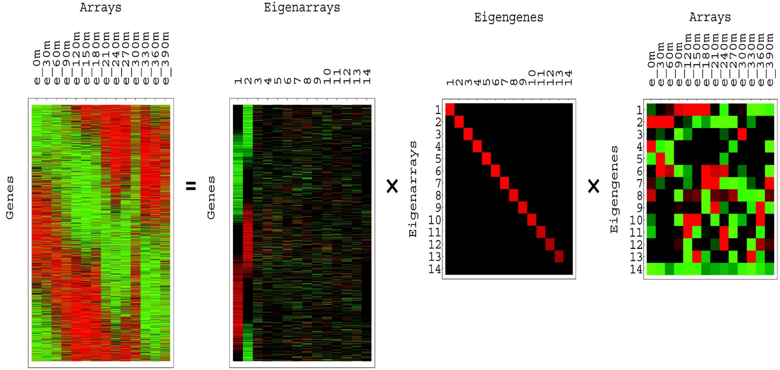

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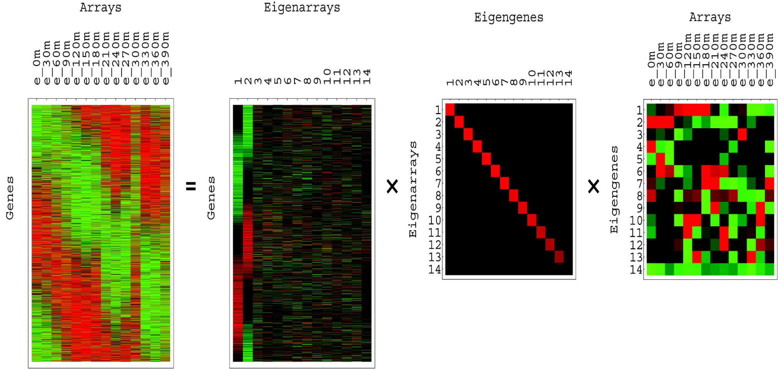

Significant "eigengenes" $\Longrightarrow$ independent biological processes and experimental artifacts.

Figure taken from: http://www.bme.utexas.edu/research/orly/teaching/BME341

NMA

- Chemometrics
- Document modeling, text-analysis
- Spam modeling
- Bioinformatics
- Music analysis
- Computer Vision
- Image processing
- Remote sensing (hyperspectral imaging)
- Dimensionality reduction
- Computer graphics
- Collaborative filtering
- Multiframe blind deconvolution

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CISI	CRAN	MED
retrieval	wing	patients
system	pressure	cells
systems	mach	growth
indexing	supersonic	hormone
scientific	shock	cancer
science	jet	treatment
index	lift	buckling
search	wings	blood
computer	body	cases
document	theory	cell

Image analysis – toy example

"Swimmer" database – 256, 32 x 32 images [DoSt03]

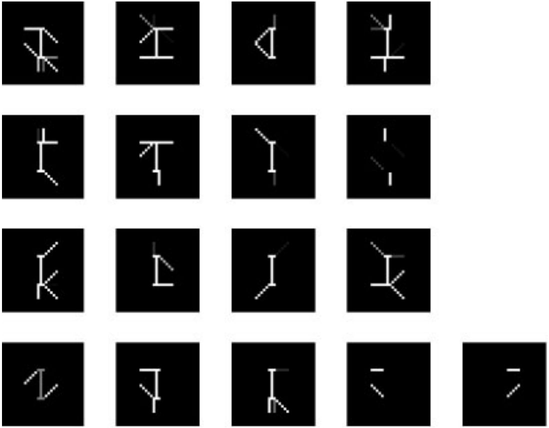
- Stick figures showing different configurations of the limbs of a swimmer
- Data matrix of size 1024×256

Image analysis – toy example

"Swimmer" database – 256, 32 x 32 images [DoSt03]

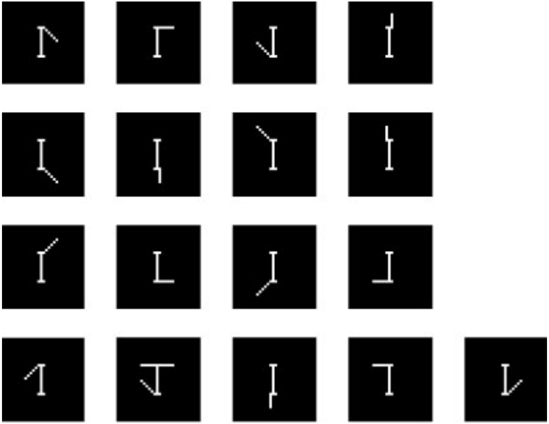
- Stick figures showing different configurations of the limbs of a swimmer
- Data matrix of size 1024×256
- Decompose the matrix into 1024×17 (17 seemed to be the "true" nonnegative rank)

Image analysis – toy example



Rank-17 decomposition via Lee/Seung's algo
Time: 182.4 seconds, Objective: 2.41×10^7

Image analysis – toy example



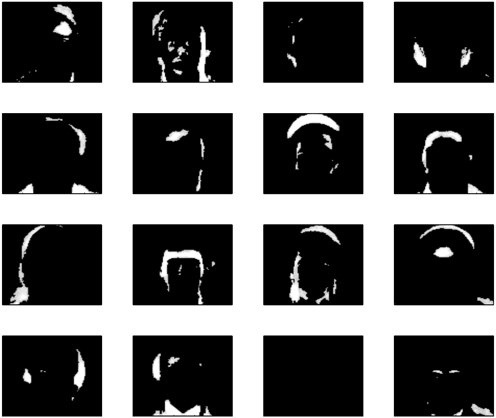
Via more advanced projection algorithm

Time: *62.3* seconds, Objective: 6.85×10^{-4}

Part of a face recognition system

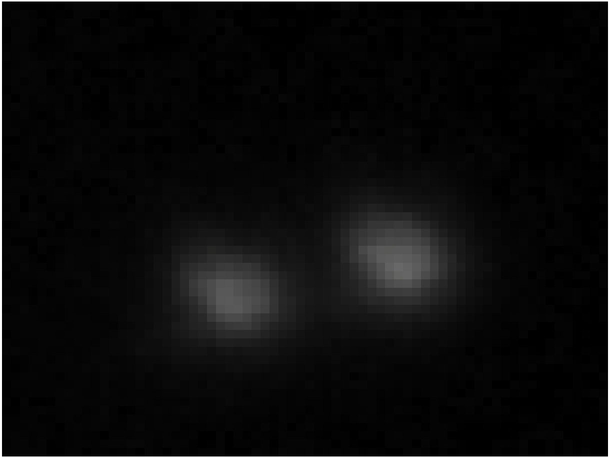
- 143 images from MIT face image database
- Input matrix $\boldsymbol{A} \in \mathbb{R}_{+}^{9216 \times 143}$

Part of a face recognition system



- A rank-20 approximation to the input
- The basis vectors (columns of $\boldsymbol{B}$) approximately correspond to important "*parts*" describing the faces.

Multiframe blind deconvolution – astronomy

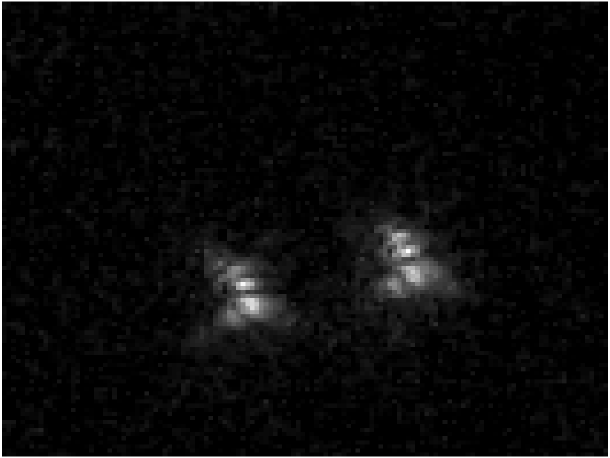


long-time exposure (approx. 1 s)

Problem: Atmospheric turbulence

Courtesy of Karl-Ludwig Bath, IAS, Hakos, Namibia

Multiframe blind deconvolution – astronomy



short-time exposure (approx. 10ms)

Problem: Atmospheric turbulence

Courtesy of Karl-Ludwig Bath, IAS, Hakos, Namibia

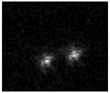
Multiframe blind deconvolution – astronomy

real-time video (15 fps)

Problem: Atmospheric turbulences

Courtesy of Karl-Ludwig Bath, IAS, Hakos, Namibia

Our model of the video

time t	$\boldsymbol{y}_t$	$=$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}$	$+$	$\boldsymbol{n}_t$
0		$=$		$\star$		$+$	$\boldsymbol{n}_0$

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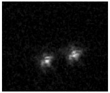
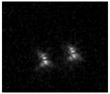
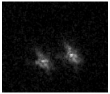
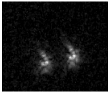
time t	$\boldsymbol{y}_t$	$=$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}$	$+$	$\boldsymbol{n}_t$
0		$=$		$\star$		$+$	$\boldsymbol{n}_0$
1		$=$		$\star$		$+$	$\boldsymbol{n}_1$
2		$=$		$\star$		$+$	$\boldsymbol{n}_2$
k		$=$		$\star$		$+$	$\boldsymbol{n}_k$

$$\begin{bmatrix} | & \vdots & | \\ \boldsymbol{y}_1 & | & \boldsymbol{y}_n \\ | & \vdots & | \end{bmatrix} \approx \begin{bmatrix} | & \vdots & | \\ \boldsymbol{a}_1 & | & \boldsymbol{a}_t \\ | & \vdots & | \end{bmatrix} \star \boldsymbol{x}$$

Convolution operation may be written as

$$\boxed{\boldsymbol{a} \star \boldsymbol{x} = \boldsymbol{A}\boldsymbol{x} = \boldsymbol{X}\boldsymbol{a}}$$

$$\begin{bmatrix} | & \vdots & | \\ \mathbf{y}_1 & | & \mathbf{y}_n \\ | & \vdots & | \end{bmatrix} \approx \begin{bmatrix} | & \vdots & | \\ \mathbf{a}_1 & | & \mathbf{a}_t \\ | & \vdots & | \end{bmatrix} \star \mathbf{x}$$

Convolution operation may be written as

$$\boxed{\mathbf{a} \star \mathbf{x} = \mathbf{A}\mathbf{x} = \mathbf{X}\mathbf{a}}$$

$$\begin{bmatrix} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_t \end{bmatrix} \approx \begin{bmatrix} \mathbf{A}_1 \\ \cdots \\ \mathbf{A}_t \end{bmatrix} \mathbf{x}$$

$$\begin{bmatrix} \mathbf{y}_1 & \mathbf{y}_2 & \cdots & \mathbf{y}_t \end{bmatrix} \approx \mathbf{X} \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_t \end{bmatrix}$$

$$\boxed{\mathbf{Y} \approx \mathbf{X}\mathbf{A}}$$

Multiframe blind deconvolution

We seek to minimize

$$\frac{1}{2}\|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|_F^2 \quad \text{s.t.} \quad \boldsymbol{X}, \boldsymbol{A} \geq 0$$

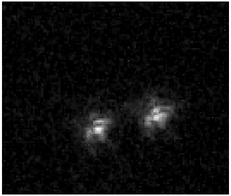
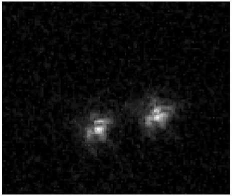
Multiframe blind deconvolution

We seek to minimize

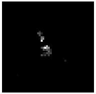
$$\frac{1}{2}\|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{A}\|_F^2 \quad \text{s.t.} \quad \boldsymbol{X}, \boldsymbol{A} \geq 0$$

Note 1: $\boldsymbol{X}$ and $\boldsymbol{A}$ are the *unknowns*
Note 2: Additional constraints may be present on $\boldsymbol{X}$ or $\boldsymbol{A}$
Note 3: Looks like an NMA problem (except $\boldsymbol{X}$ or $\boldsymbol{A}$ have special structure due to the convolution $\boldsymbol{a} \star \boldsymbol{x}$)

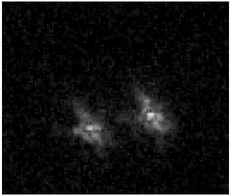
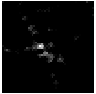
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$=$	$\boldsymbol{x}_t$
1		$=$	

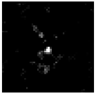
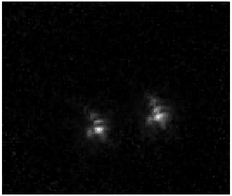
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
2		$\approx$		$\star$	

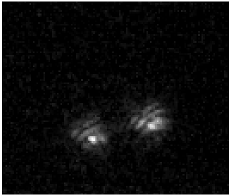
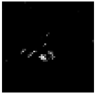
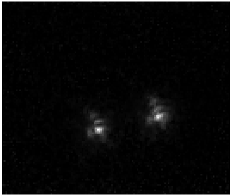
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
3		$\approx$		$\star$	

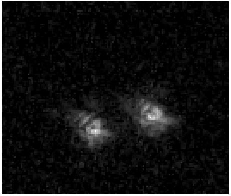
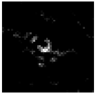
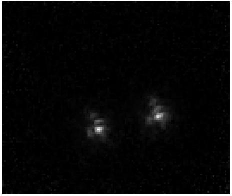
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
4		$\approx$		$\star$	

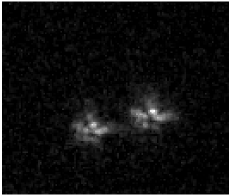
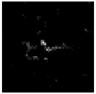
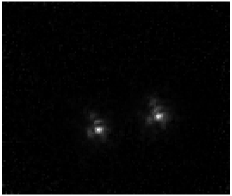
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
5		$\approx$		$\star$	

Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
6		$\approx$		$\star$	

Double star epsilon lyrae

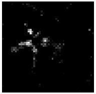
time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
7		$\approx$		$\star$	

Double star epsilon lyrae

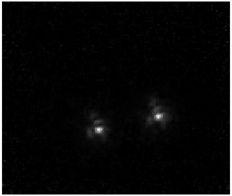
time t $\quad \boldsymbol{y}_t \approx \boldsymbol{a}_t \star \boldsymbol{x}_t$

8

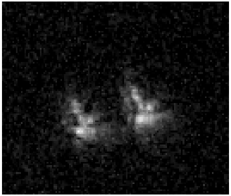
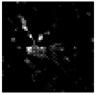
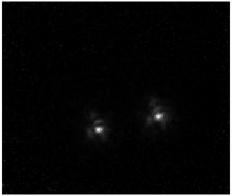
$\approx$



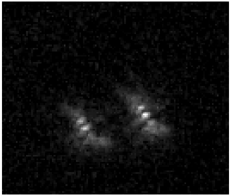
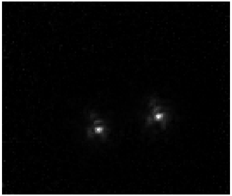
$\star$



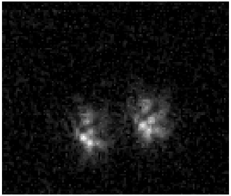
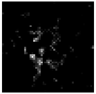
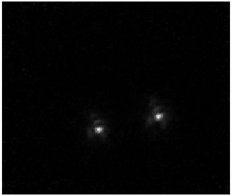
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
9		$\approx$		$\star$	

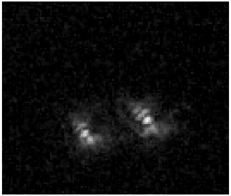
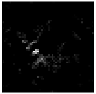
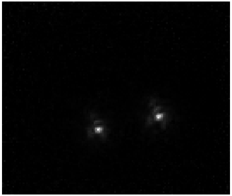
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
10		$\approx$		$\star$	

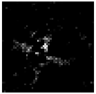
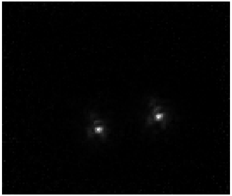
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
11		$\approx$		$\star$	

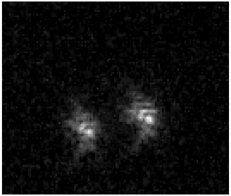
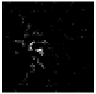
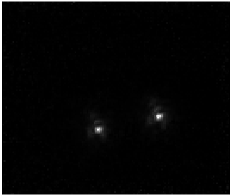
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
12		$\approx$		$\star$	

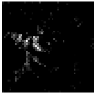
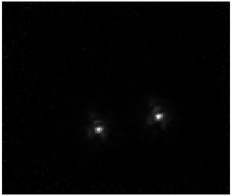
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
13		$\approx$		$\star$	

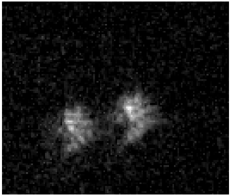
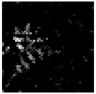
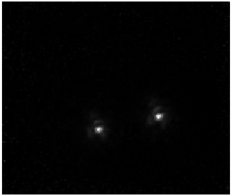
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
14		$\approx$		$\star$	

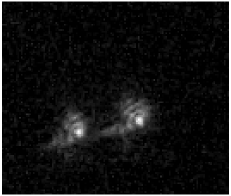
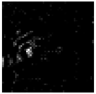
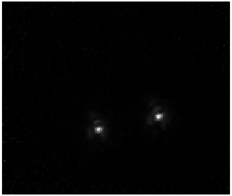
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
15		$\approx$		$\star$	

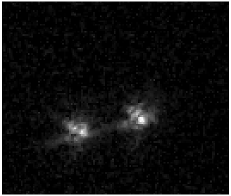
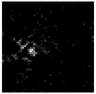
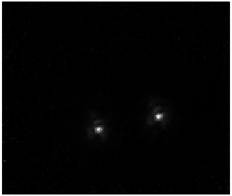
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
16		$\approx$		$\star$	

Double star epsilon lyrae

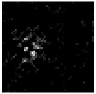
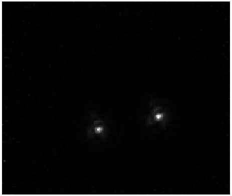
time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
17		$\approx$		$\star$	

Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
18		$\approx$		$\star$	

Double star epsilon lyrae

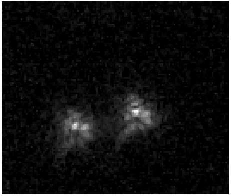
time t $\quad \boldsymbol{y}_t \approx \boldsymbol{a}_t \star \boldsymbol{x}_t$

19  $\approx$  $\star$ 

Double star epsilon lyrae

time t $\quad \boldsymbol{y}_t \approx \boldsymbol{a}_t \star \boldsymbol{x}_t$

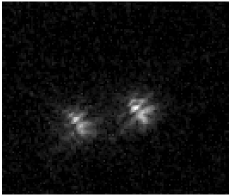
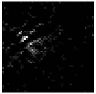
20



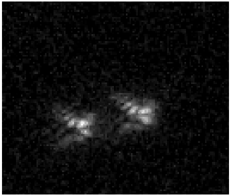
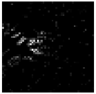
$\approx$

$\star$

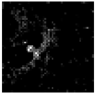
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
21		$\approx$		$\star$	

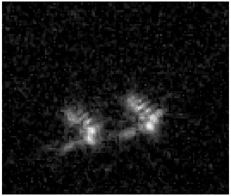
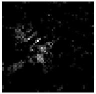
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
22		$\approx$		$\star$	

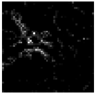
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
23		$\approx$		$\star$	

Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
24		$\approx$		$\star$	

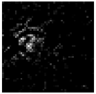
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
25		$\approx$		$\star$	

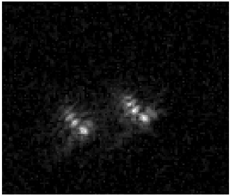
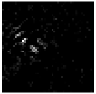
Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
26		$\approx$		$\star$	

Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
27		$\approx$		$\star$	

Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
28		$\approx$		$\star$	

Double star epsilon lyrae

time t $\quad \boldsymbol{y}_t \approx \boldsymbol{a}_t \star \boldsymbol{x}_t$

29

$\approx$

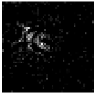
$\star$

Double star epsilon lyrae

time t $\quad \boldsymbol{y}_t \approx \boldsymbol{a}_t \star \boldsymbol{x}_t$

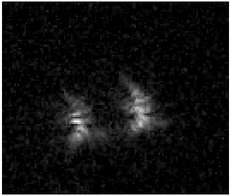
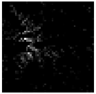
30

$\approx$

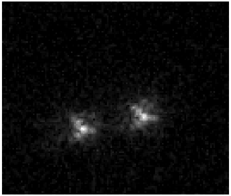
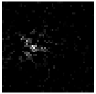


$\star$

Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
31		$\approx$		$\star$	

Double star epsilon lyrae

time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
32		$\approx$		$\star$	

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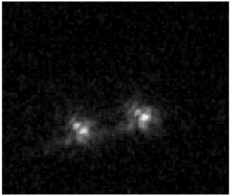
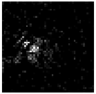
time t	$\boldsymbol{y}_t$	$\approx$	$\boldsymbol{a}_t$	$\star$	$\boldsymbol{x}_t$
33		$\approx$		$\star$	

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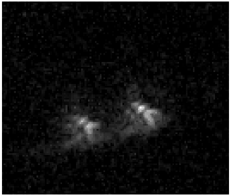
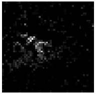
34		$\approx$		$\star$	

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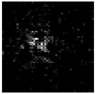
35		$\approx$		$\star$	

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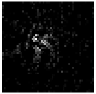
36		$\approx$		$\star$	

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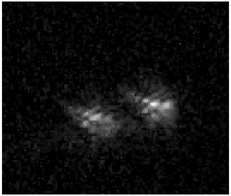
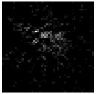
37		$\approx$		$\star$	

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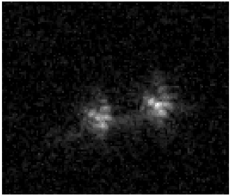
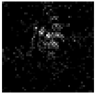
38  $\approx$  $\star$ 

Double star epsilon lyrae

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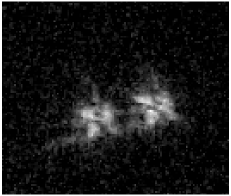
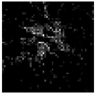
39		$\approx$		$\star$	

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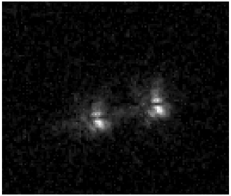
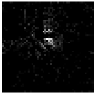
40		$\approx$		$\star$	

MFBD Video

Video example

Discussion & Wrap-up

Summary

1. Introduction to matrix approximation problems
   - Background, motivation
   - Truncated SVD; its properties
   - List of some popular problems, e.g., NMA
2. Algorithms for NMA
   - Alternating minimization
   - Alternating descent
   - Gradient Projection
   - Multiplicative updates
3. Applications
   - Bioinformatics app of SVD
   - Image processing, astronomy, etc. of NMA

Challenges, other stuff

- Theoretical: Non-convex optimization
- Analysis, new algorithms, new problems
- Practical: Large-scale, sparse data
- Cluster, multi-core, GPU, etc.
- Efficient SVD (PROPACK, SLEPc, etc.)
- Methods based on random projections
- Numerous other *matrix nearness* problems exist
- Tensor approximations

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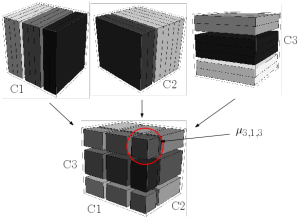

Closing: Huge Matrix Problems

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- Input matrix $\boldsymbol{A}$ of size $43.9M \times 769M$; total 4.38×10^9 nonzeros (1.2×10^{-7} - density)
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I think YOU can do better!