MANIFOLD OPTIMIZATION IN DATA SCIENCE

Max Pfeffer

Networks Seminar

IISc Bangalore

March 3, 2026

MATRIX FACTORIZATIONS

MATRIX FACTORIZATIONS

- Dimensionality Reduction

MATRIX FACTORIZATIONS

- Dimensionality Reduction
- Feature Extraction

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  - ↳ PCA

MATRIX FACTORIZATIONS

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- Clustering

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  - ↳ Unsupervised Learning

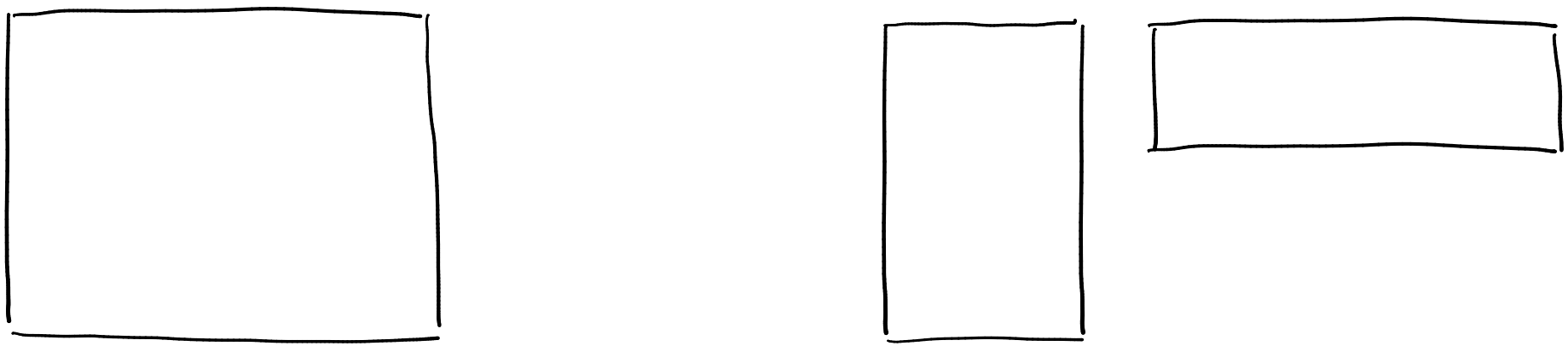
MATRIX FACTORIZATIONS

$$M \in \mathbb{R}^{m \times n}$$

MATRIX FACTORIZATIONS

$M \in \mathbb{R}^{m \times n}$ $X \in \mathbb{R}^{m \times r}$ $Y \in \mathbb{R}^{n \times r}$

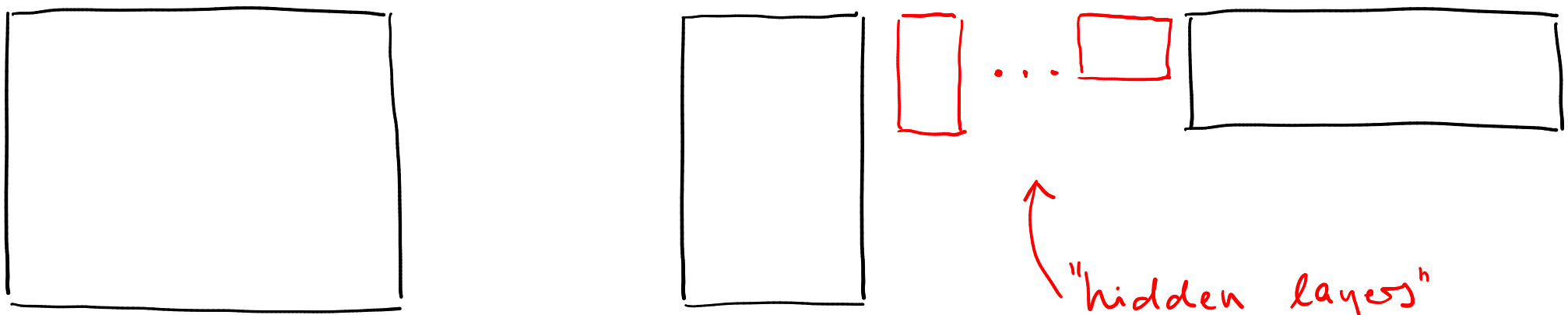
$M = X Y^T$



MATRIX FACTORIZATIONS

$M \in \mathbb{R}^{m \times n}$ $\quad X \in \mathbb{R}^{m \times r_1}$ $\quad A_i \in \mathbb{R}^{r_i \times r_{i+1}}$ $\quad Y \in \mathbb{R}^{n \times r_\ell}$

$M = X A_1 \cdots A_\ell Y^T$



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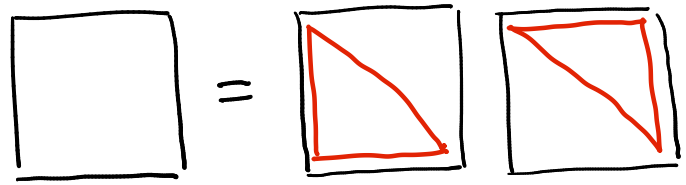
- Cholesky decomposition: $M = CC^T$, $M = M^T$



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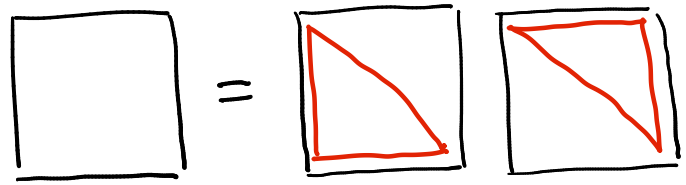
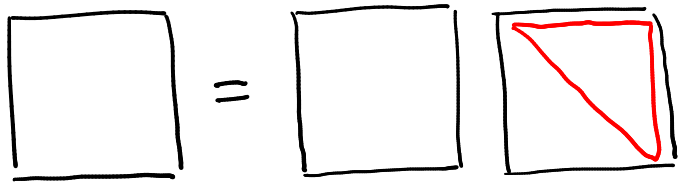


- QR-decomposition: $M = QR$, $Q^TQ = I$

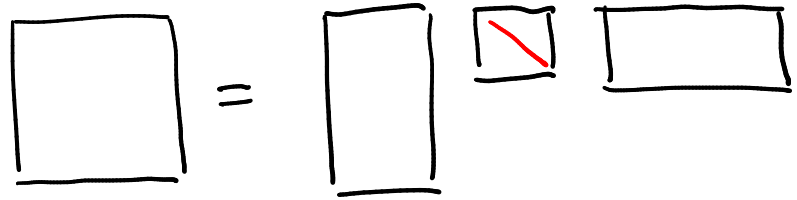


MATRIX FACTORIZATIONS

Examples:

- Singular-value-decomposition: (SVD)

$M = U \Sigma V^T, \quad U^T U = V^T V = I$



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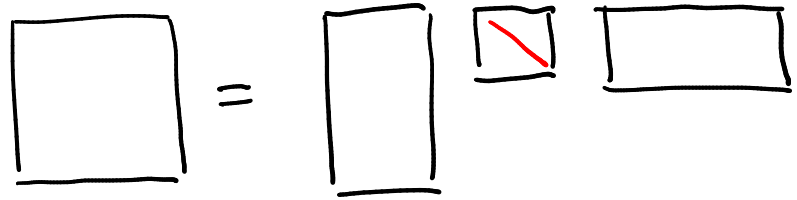
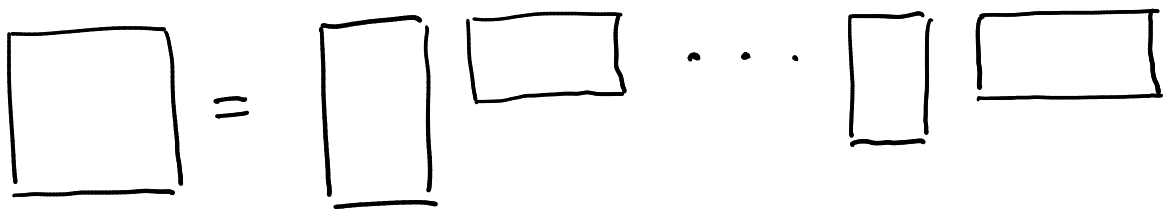


- Linear neural network: $M = A_1 \cdots A_\ell$



TENSOR FACTORIZATIONS

$$T \in \mathbb{R}^{n_1 \times \dots n_d}$$

TENSOR FACTORIZATIONS

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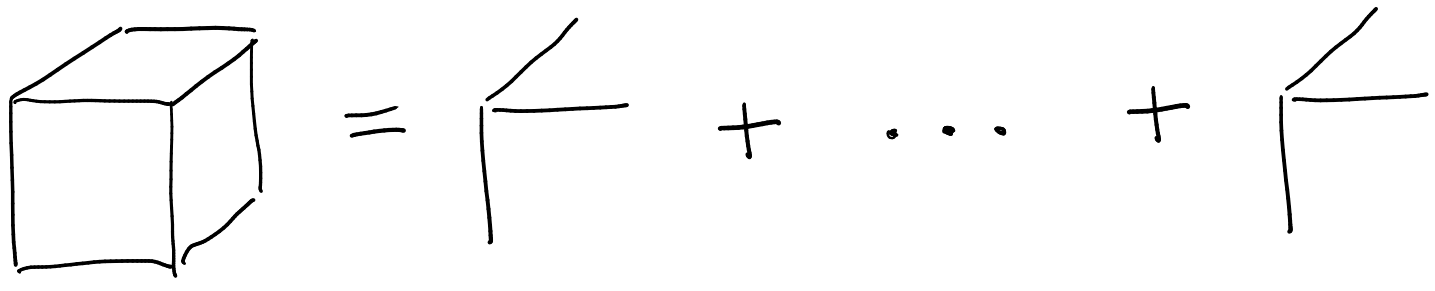
- Canonical Polyadic (CP) decomposition:

$$T = \sum_{i=1}^{R} u_1^{(i)} \otimes \cdots \otimes u_d^{(i)} \quad , \quad u_j^{(i)} \in \mathbb{R}^{n_j}$$



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  − difficult to compute
  − not closed

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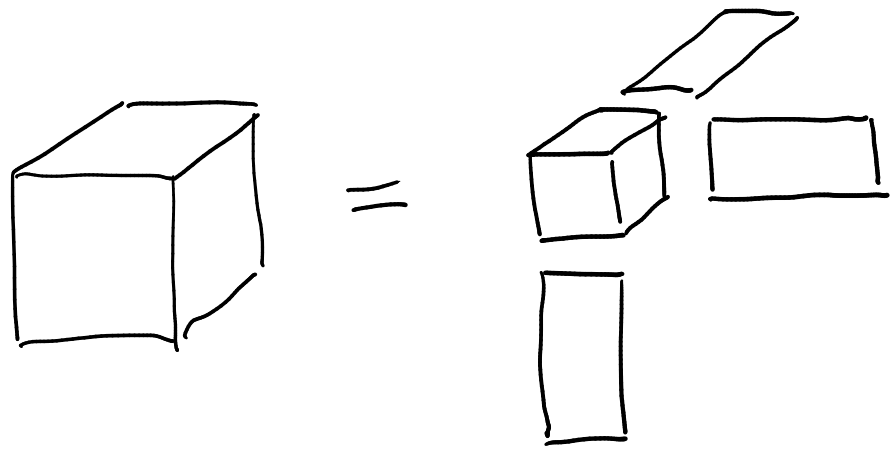
Formats:

- Tuckers decomposition:

$$T = C \circ_1 U_1 \circ_2 U_2 \cdots \circ_d U_d \quad , \quad C \in \mathbb{R}^{r_1 \times \dots \times r_d}$$

$$U_i \in \mathbb{R}^{n_i \times r_i}$$



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  - still exponential in d

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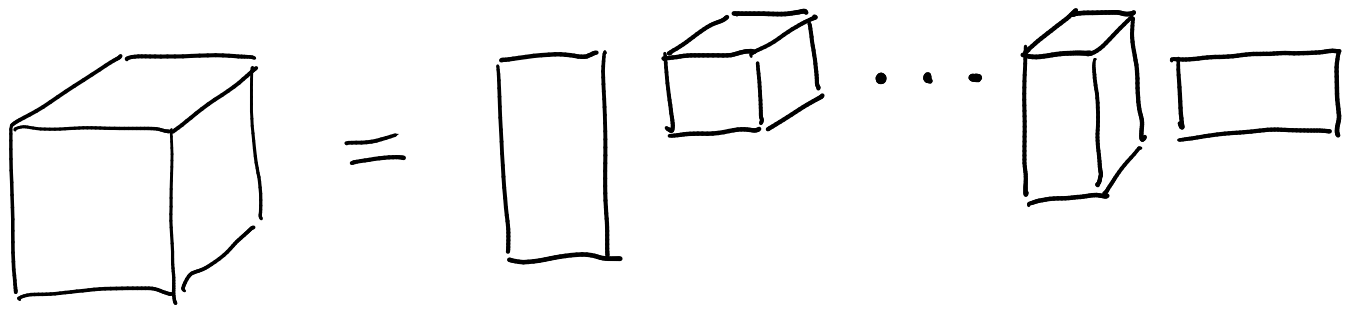
Formats:

- Tensor Train (TT) decomposition:

$$T = U_1 \bullet U_2 \bullet \cdots \bullet U_d \quad , \quad U_i \in \mathbb{R}^{r_{i-1} \times n_i \times r_i}$$

$$r_0 = r_d = 1$$



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+ better storage than Tucker
+ easy to compute
+ can be made unique
- interpretation not straightforward

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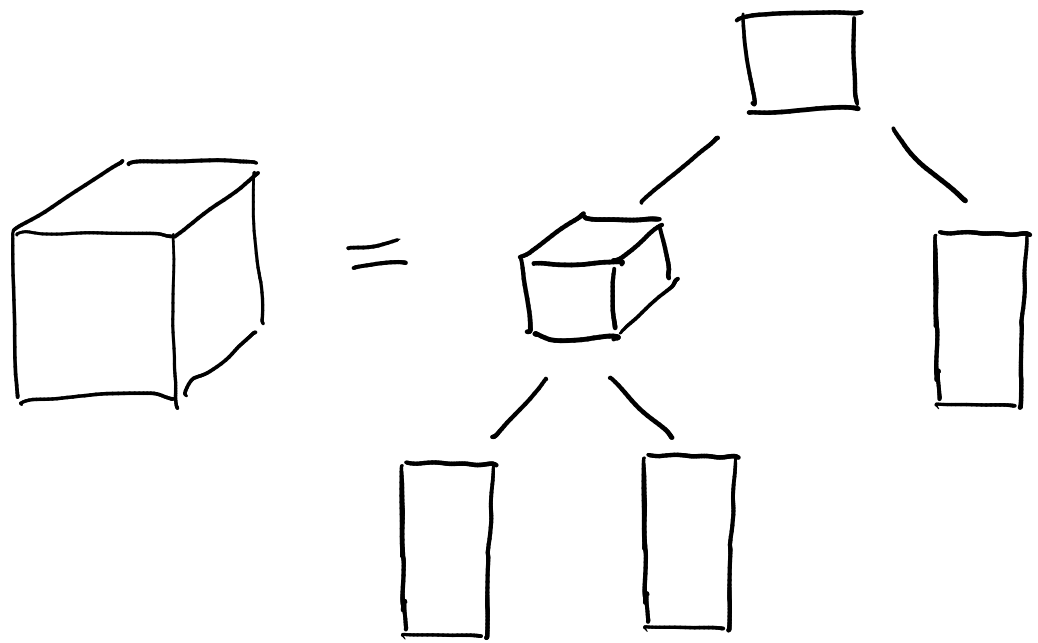
Formats:

- General tree tensor networks:



JOINT FACTORIZATIONS

Take collection of matrices $M_1, \ldots, M_K$

and/or tensors $\mathcal{T}_1, \ldots, \mathcal{T}_L$.

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Decompose them with some shared factors.

Example: $X = [x_1 \cdots x_R]$

$$M = X Y^T \quad , \quad T = \sum_{i=1}^{R} x_i \otimes u_1^{(i)} \otimes \cdots \otimes u_{d-1}^{(i)}$$

CONSTRAINTS

It is often beneficial to impose the factors with constraints.

CONSTRAINTS

Some examples:

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  - is a form of independence

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  - when orthogonality is too much to ask

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  - when the data is also nonnegative

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- many more

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- rank $M \leq$ constrained rank M

ALGORITHMS

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- LU-decomposition can be computed exactly using the Gauss-algorithm.
- QR can be computed using Householder transformations.
- SVD can be computed to arbitrary accuracy in polynomial time.

ALGORITHMS

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for each matrix / tensor

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format of the decomposition

ALGORITHMS

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General form:

$$\min_{X,Y \in S} \|M - XY^T\|_F^2$$

↖ subset constraints

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General form:

$$\min_{X,Y} \|M - XY^T\|_F^2 + \lambda g(X,Y)$$

penalty for constraints

ALGORITHMS

Otherwise, we need optimization algorithms.

General form:

$$\min_{X, Y_1, Y_2} \| M_1 - X Y_1^T \|_F^2 + \| M_2 - X Y_2^T \|$$

joint factorization

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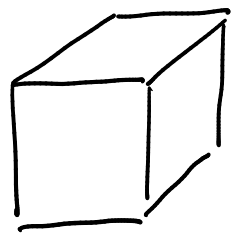

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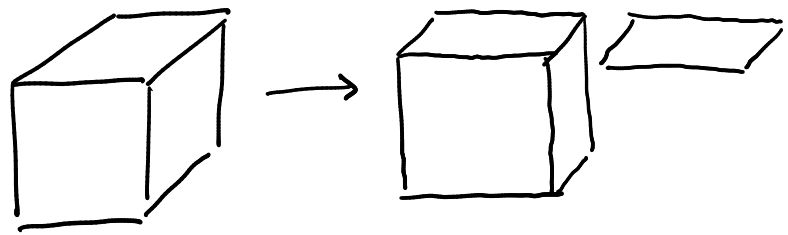

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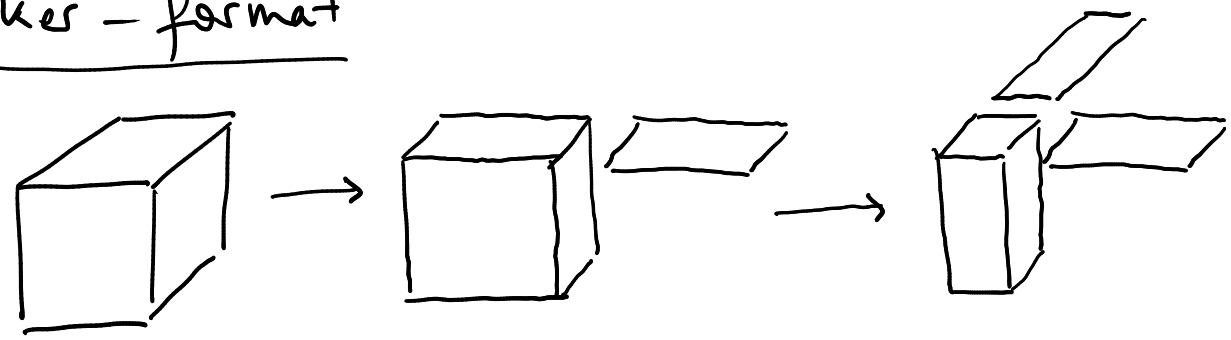

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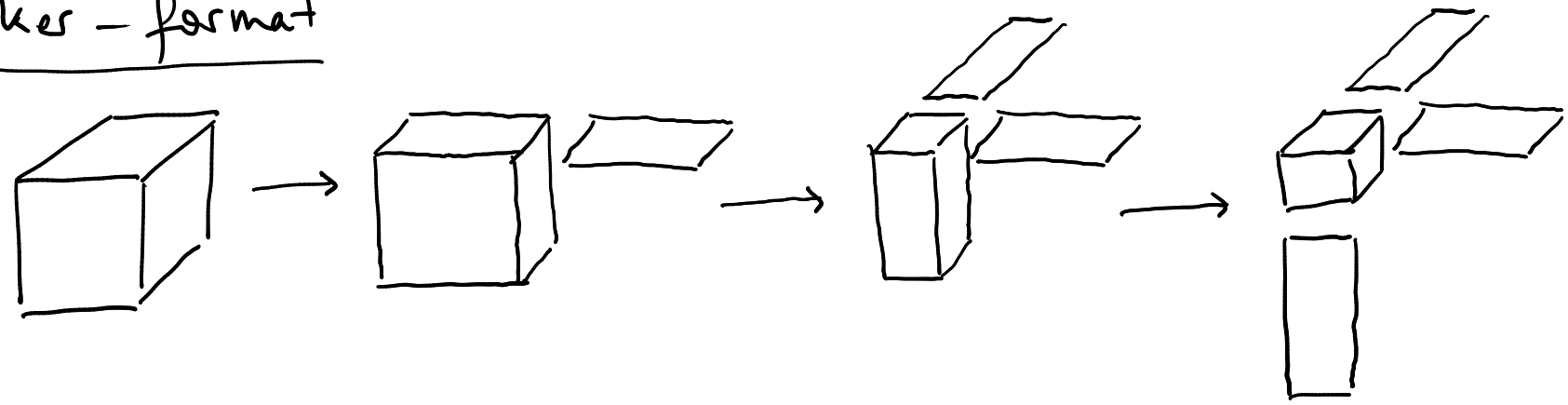

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↻ repeat

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- Alternating least squares (ALS):
  - cost will always decrease
  - convergence to critical point not always guaranteed
  - often fast but can be slow

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- Alternating least squares (ALS):
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  → Riemannian optimization

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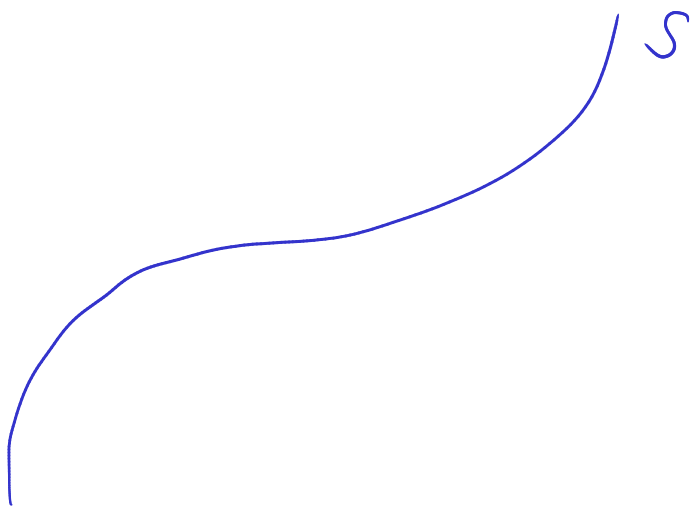

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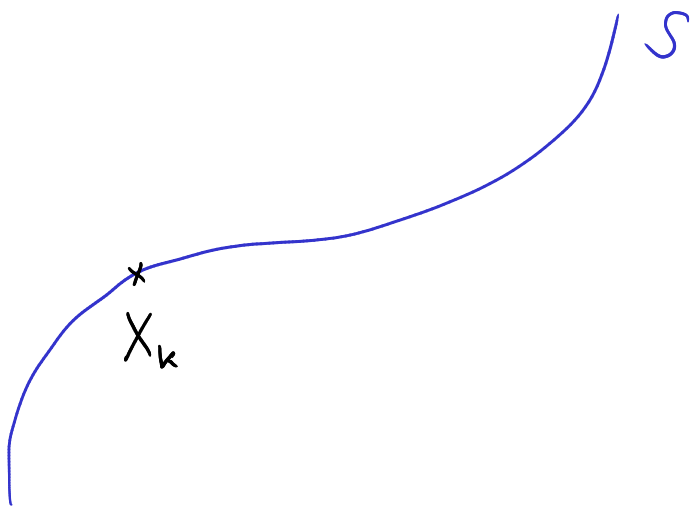

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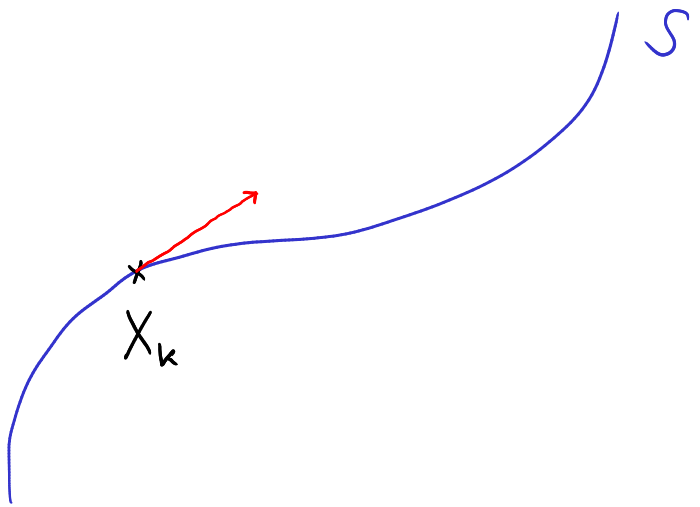

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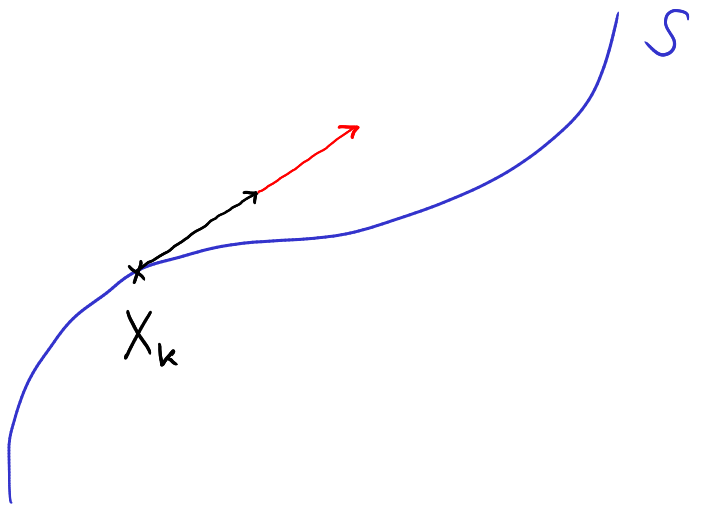

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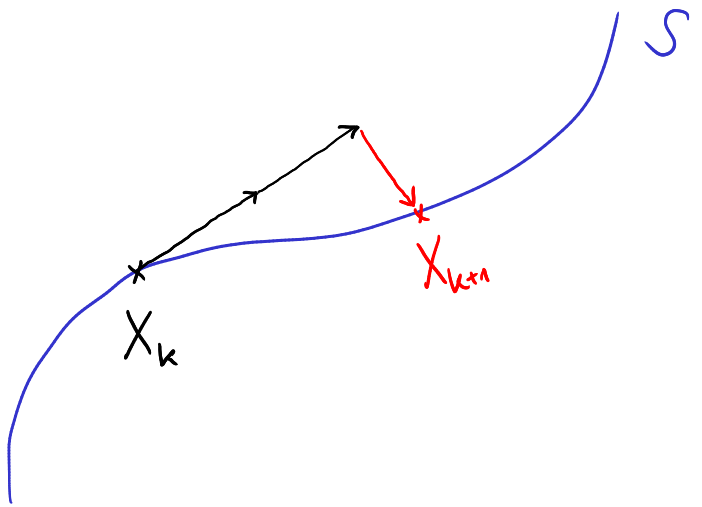

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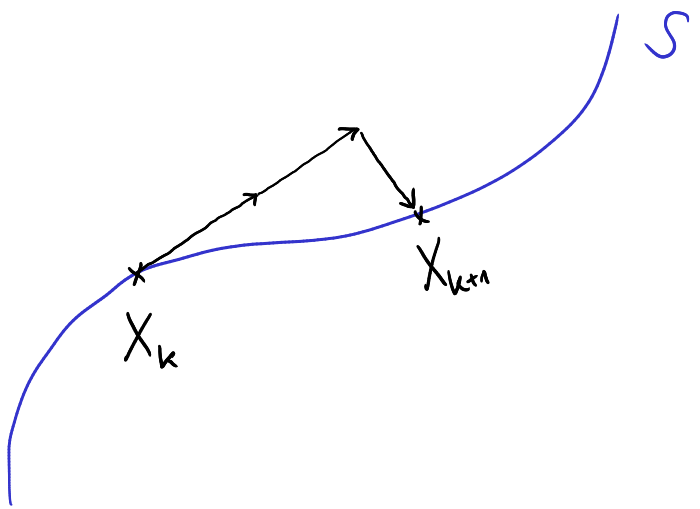
} many improvements possible!



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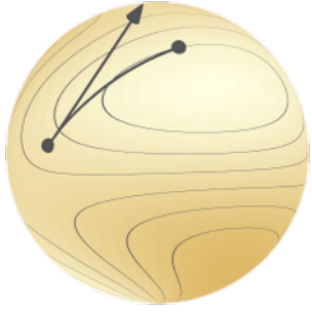

Manopt

PyManopt

Manopt.jl

RIEMANNIAN OPTIMIZATION

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  $\longrightarrow$ nonsmooth optimization on Riemannian manifolds

APPLICATIONS

CANCER CLASSIFICATION

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Minimization problem:

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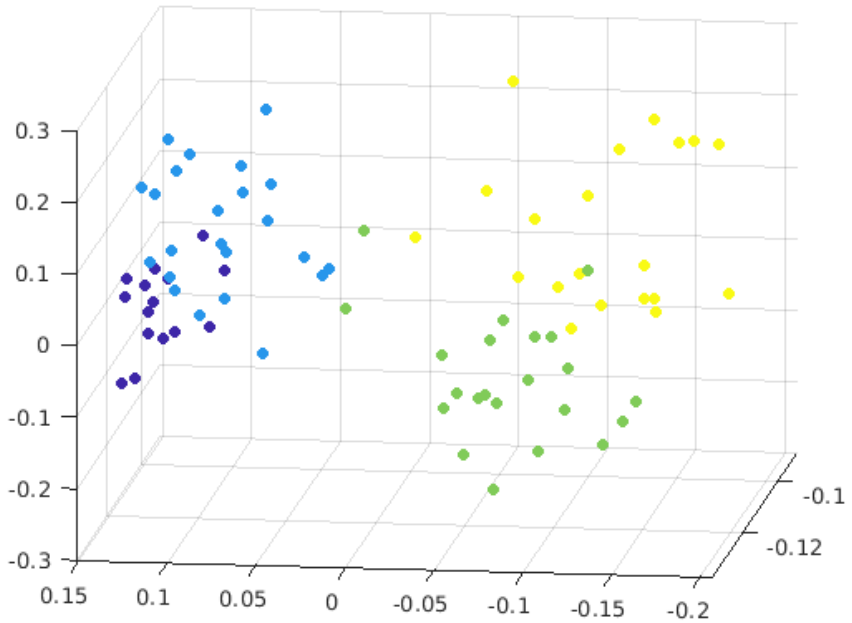
$U = Z \circ Z$, $V_1 = W_1 \circ W_1$, $V_2 = W_2 \circ W_2$

$V_3 \in Ob(n_3, r)$, $W_1 \in Ob^4(n_1, r)$, $W_2 \in Ob^4(n_2, r)$

CANCER CLASSIFICATION

For uveal melanoma data (TCGA):



First 3 principal components of U matrix

M. Pfeffer, A. Uschmajew, A. Amaro, U. Pfeffer:
Data fusion techniques for the integration of multi-domain genomic data from uveal melanoma.
Cancers, 11 (2019) 10, 1434

A. Amaro, **M. Pfeffer**, U. Pfeffer, F. Reggiani:
Evaluation and Comparison of Multi-Omics Data Integration Methods for Subtyping of Cutaneous Melanoma.
Biomedicines 10(12) (2022)

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- Solution optimal only in Frobenius norm and not in "norm" given by A

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Alternative approach:

Minimize $f(X) = \text{trace}\left(X^T A(X)\right)$

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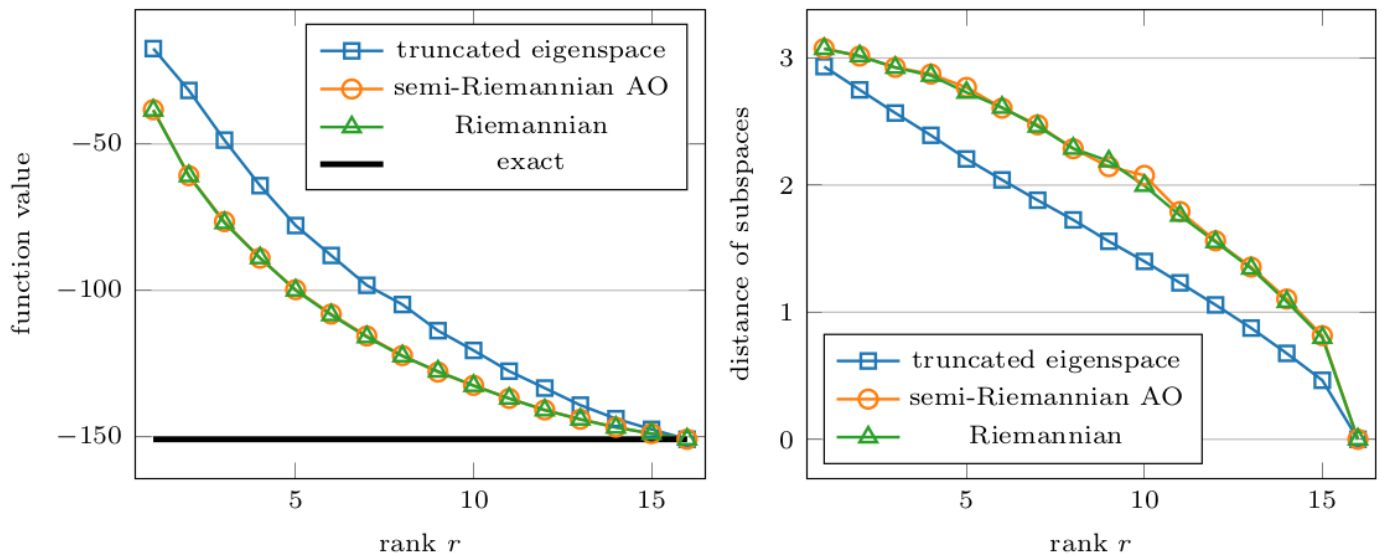

C. Krumnow, **M. Pfeffer**, A. Uschmajew:
Computing eigenspaces with low rank constraints.
SIAM Journal on Scientific Computing, 43 (2021) 1, p. 586-608

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Measurement operator

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↖ Rank-r manifold

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λ: penalty parameter

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Application:

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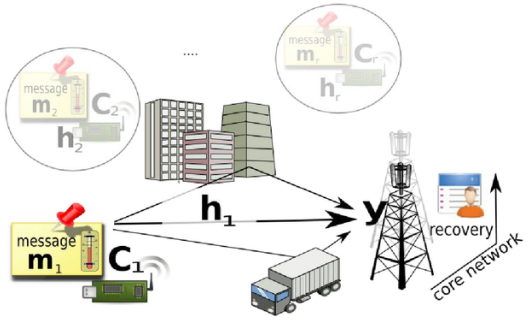

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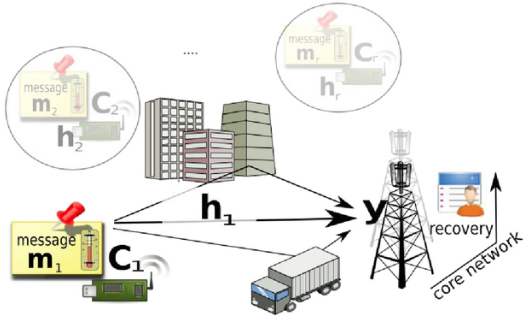

$\longrightarrow$ rank $(X) = 1$

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Proximal map for $g(X) = \lambda \|X\|_{1,2}$ on the low-rank manifold!

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↑ row-soft thresholding

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− slow (so far)

LOW-RANK & ROW-SPARSE RECOVERY

	Adaptive IHT		Adaptive RIHT		RPG	
ε	Iterations	CPU time	Iterations	CPU time	Iterations	CPU time
Random Rank One Measurements						
10^{-1}	196	0.4131s	196	0.2586s	6691	9.5539s
10^{-3}	831	1.7495s	831	1.1103s	11490	16.675s
10^{-5}	1583	3.3613s	1582	2.0928s	16095	23.931s
Fourier Measurements						
10^{-1}	8	0.1455s	10	0.0691s	4211	25.331s
10^{-3}	25	0.4592s	30	0.2189s	8941	58.069s
10^{-5}	45	0.8268s	46	0.3392s	13545	91.412s

H. Eisenmann, F. Krahmer, **M. Pfeffer**, A. Uschmajew:
Riemannian thresholding methods for row-sparse and low-rank matrix recovery.
Numerical Algorithms (2022)

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Facts:
- Finding X is a co-NP-complete problem.
- For $M \in \partial\mathcal{CP}_5$, X is unique.
- The polynomial equations describing $\partial\mathcal{CP}_5$ have very high degree.

COMPLETELY POSITIVE MATRICES

Minimize

$$f(B) = \| M - (B \circ B)(B \circ B)^T \|_F^2$$

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$$A = \begin{pmatrix} 163 & 108 & 27 & 4 & 4 & 27 & 108 \\ 108 & 163 & 108 & 27 & 4 & 4 & 27 \\ 27 & 108 & 163 & 108 & 27 & 4 & 4 \\ 4 & 27 & 108 & 163 & 108 & 27 & 4 \\ 4 & 4 & 27 & 108 & 163 & 108 & 27 \\ 27 & 4 & 4 & 27 & 108 & 163 & 108 \\ 108 & 27 & 4 & 4 & 27 & 108 & 163 \end{pmatrix}$$

COMPLETELY POSITIVE MATRICES

$$B = \begin{pmatrix}
\sqrt{27} & \frac{51}{\sqrt{27}} & \sqrt{27} & 0 & 0 & 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & \sqrt{6} & \sqrt{6} & 0 & 0 \\
0 & \sqrt{27} & \frac{51}{\sqrt{27}} & \sqrt{27} & 0 & 0 & 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & \sqrt{6} & \sqrt{6} & 0 \\
0 & 0 & \sqrt{27} & \frac{51}{\sqrt{27}} & \sqrt{27} & 0 & 0 & 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & \sqrt{6} & \sqrt{6} \\
0 & 0 & 0 & \sqrt{27} & \frac{51}{\sqrt{27}} & \sqrt{27} & 0 & \sqrt{6} & 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 & \sqrt{6} \\
0 & 0 & 0 & 0 & \sqrt{27} & \frac{51}{\sqrt{27}} & \sqrt{27} & \sqrt{6} & \sqrt{6} & 0 & 0 & \sqrt{\frac{2}{3}} & 0 & 0 \\
\sqrt{27} & 0 & 0 & 0 & 0 & \sqrt{27} & \frac{51}{\sqrt{27}} & 0 & \sqrt{6} & \sqrt{6} & 0 & 0 & \sqrt{\frac{2}{3}} & 0 \\
\frac{51}{\sqrt{27}} & \sqrt{27} & 0 & 0 & 0 & 0 & \sqrt{27} & 0 & 0 & \sqrt{6} & \sqrt{6} & 0 & 0 & \sqrt{\frac{2}{3}}
\end{pmatrix}.$$

M. Pfeffer, J. Samper: **The cone of 5×5 completely positive matrices.** (2021)

THANK YOU !