# Tensor methods: An introduction

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L. De Lathauwer, "Tensor methods: An introduction," slides presented at a STADIUS colloquium seminar, Leuven, February 23, 2026 (71 p.)

## Overview


Introduction

Dimensionality reduction - Principal Component Analysis

Denoising

Blind source separation - Latent Variable analysis

Blind similarity assessment

Polynomial equations

Regression and classification

Structured data fusion

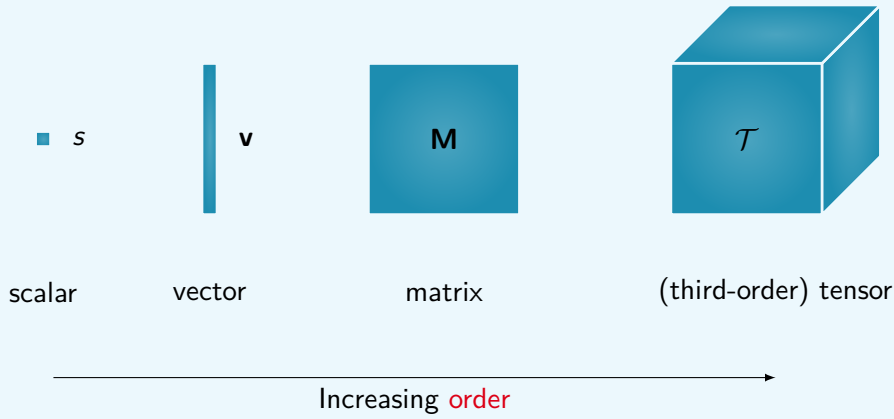
Large-scale data analysis and curse of dimensionality

Completion

Harmonic retrieval

Tensorlab and Tensorlab+

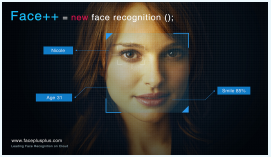
Higher-order tensors are a generalization of scalars, vectors, and matrices.



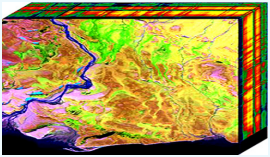
# Examples of tensors



- Color images, video, ...
- Hyperspectral images
- Text mining: term $\times$ document $\times$ author
- (Social) networks: score $\times$ object $\times$ referee $\times$ criterion
- Event Related Potential (ERP): subject $\times$ time $\times$ frequency $\times$ channel $\times$ ...
- Face recognition: people $\times$ pose $\times$ illumination $\times$ angle
- Multi-way data acquisition (intentional)





# From matrix to tensor: tensorization

- Set of data matrices, recorded at different $t$, under different conditions...
- Sets of covariance matrices
- Higher-order statistics
- Deliberate tensorization of data matrix
  time-frequency, wavelet, Hankel, Löwner, derivatives, decimation/segmentation...
- ...



## Exponentials as rank-1 matrices and tensors

- Consider an exponential signal $f(k) = az^k$, sampled uniformly:

$$\begin{bmatrix} a & az & az^2 & az^3 & \cdots \end{bmatrix}$$

- Let's arrange it in a Hankel matrix $\mathbf{H}$ — which has rank 1!

$$\mathbf{H} = \begin{bmatrix} a & az & az^2 & \cdots \\ az & az^2 & az^3 & \cdots \\ az^2 & az^3 & az^4 & \cdots \\ \vdots & \vdots & \vdots & \end{bmatrix} = a \begin{bmatrix} 1 \\ z \\ z^2 \\ \vdots \end{bmatrix} \begin{bmatrix} 1 & z & z^2 & \cdots \end{bmatrix}$$

- Row $\begin{bmatrix} 1 & z & z^2 & \cdots \end{bmatrix}$ can by itself be mapped to Hankel matrix. Also column can be mapped to Hankel matrix. Etc.
- Leads to ... a symmetric $(2 \times 2 \times \ldots \times 2)$ tensor $\mathcal{H}$ that has rank 1!

$$\mathcal{H} = a \begin{bmatrix} 1 \\ z \end{bmatrix} \otimes \begin{bmatrix} 1 \\ z \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 1 \\ z \end{bmatrix}$$

$a$ : amplitude
$z$ : base

- Tensor recognition

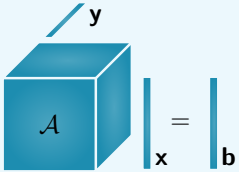
# Tensor recognition: example (1)

## Linear transformation



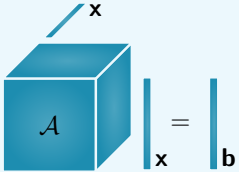

$\sum_j a_{ij} x_j = b_i$ matrix $\mathbf{A}$ (order 2)

## Bilinear transformation




$\sum_{jk} a_{ijk} x_j y_k = b_i$ tensor $\mathcal{A}$ (order 3)

## Quadratic transformation




$\sum_{jk} a_{ijk} x_j x_k = b_i$ tensor $\mathcal{A}$ (order 3)

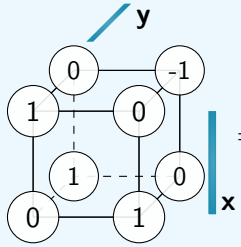
# Tensor recognition: example (2)

## Complex number multiplication

$$(a+bi)(c+di) = (ac-bd) + (bc+ad)i$$

$$ac - bd = \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} 1 & \\ & -1 \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}$$

$$bc + ad = \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} & 1 \\ 1 & \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}$$




$$= \begin{bmatrix} ac-bd \\ bc+ad \end{bmatrix} \quad \text{with } \mathbf{x} = \begin{bmatrix} a \\ b \end{bmatrix}, \mathbf{y} = \begin{bmatrix} c \\ d \end{bmatrix}$$

## Matrix multiplication

$\mathbf{C} = \mathbf{A}\mathbf{B}^{\mathsf{T}}$ e.g. $(2 \times 2)$ $\mathbf{A}, \mathbf{B}, \mathbf{C} \rightarrow (4 \times 4 \times 4)$ tensor

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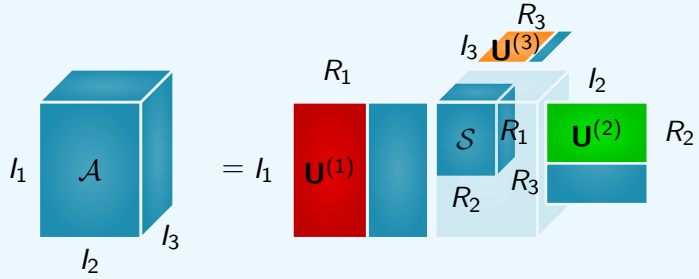
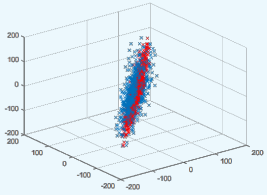
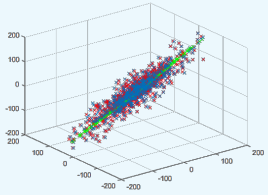
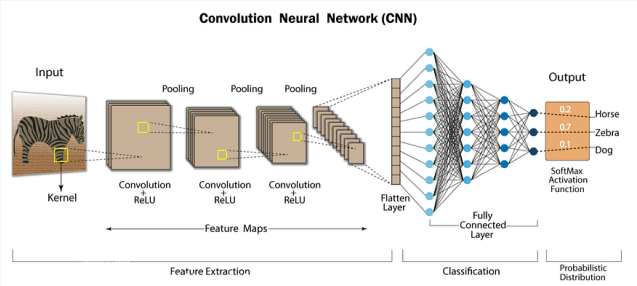
# From linear to multilinear PCA: dominant subspaces and compression





# Application example: efficient evaluation of CNNs




[Shahriar 2023]

1D convolution: $\mathbf{y}[n] = \mathbf{f}[n] * \mathbf{x}[n] = \sum_{n'=1}^{N'} \mathbf{f}[n']\mathbf{x}[n-n']$

2D SISO convolution: $\mathbf{Y}[m,n] = \mathbf{F}[m,n] *_2 \mathbf{X}[m,n]$
$= \sum_{m'=1}^{M'} \sum_{n'=1}^{N'} \mathbf{F}[m',n']\mathbf{X}[m-m',n-n']$

2D MIMO convolution: $\mathbf{Y}_i[m,n] = \mathbf{F}_{ij}[m,n] *_2 \mathbf{X}_j[m,n]$
$\rightarrow$ compression $\mathcal{F} \in \mathbb{R}^{I \times J \times M' \times N'}$

[Denton, Zaremba, et al. 2014; Kim, Par, et al. 2016]

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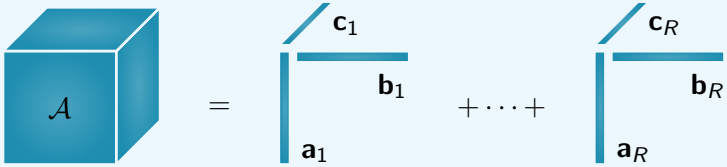
# From dyadic to polyadic decomposition: signal separation and data analysis








# Factor Analysis and Blind Source Separation

- Decompose a data matrix in rank-1 terms that can be interpreted

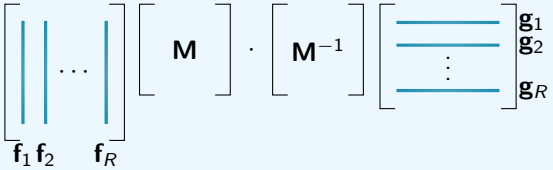
  E.g. statistics, telecommunication, biomedical applications, chemometrics, data analysis, ...

$$\mathbf{A} = \mathbf{F} \cdot \mathbf{G}^{\mathsf{T}}$$

$$\mathbf{A} = \mathbf{f}_1 \mathbf{g}_1 + \mathbf{f}_2 \mathbf{g}_2 + \cdots + \mathbf{f}_R \mathbf{g}_R$$

- $\mathbf{F}$: mixing matrix  $\mathbf{G}$: source signals
- Matrix decomposition in rank-1 terms is not unique!

$$\mathbf{A} = (\mathbf{FM}) \cdot (\mathbf{M}^{-1}\mathbf{G}^{\mathsf{T}}) = \tilde{\mathbf{F}} \cdot \tilde{\mathbf{G}}^{\mathsf{T}}$$



## What about SVD?

The SVD is unique . . . thanks to orthogonality constraints!

$$\mathbf{A} = \mathbf{U}^{(1)} \cdot \mathbf{S} \cdot \mathbf{U}^{(2)^\mathsf{T}} = \sum_{r=1}^{R} s_{rr} \mathbf{u}_r^{(1)} \mathbf{u}_r^{(2)^\mathsf{T}}$$

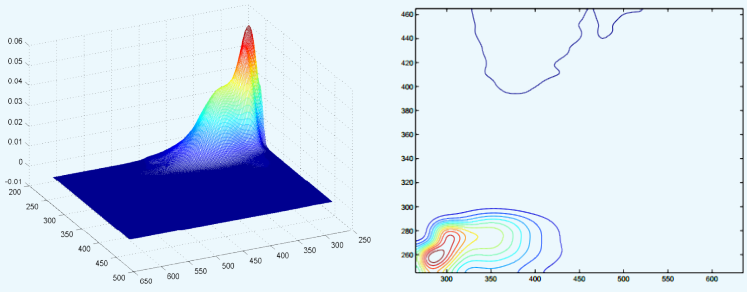
with $\mathbf{U}^{(1)}$, $\mathbf{U}^{(2)}$ orthogonal, $\mathbf{S}$ diagonal.

- Whether these constraints make sense, depends on the application
- SVD is great for dimensionality reduction/numerical compression
  best rank-$R$ approximation $\leftarrow$ truncated SVD



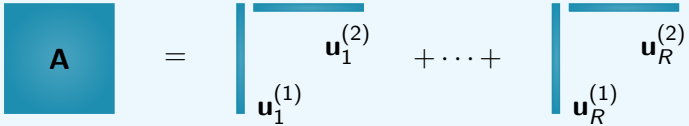
# An example where matrices fail

## Excitation-emission spectroscopy



# Excitation-emission spectroscopy

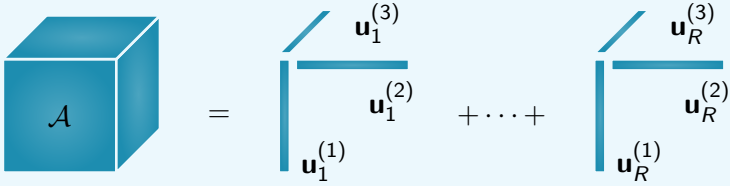
row vector $\sim$ excitation spectrum
column vector $\sim$ emission spectrum
coefficients $\sim$ concentrations




Spectra are nonnegative (and not orthogonal)
Nonnegative Matrix Factorization (NMF) not unique in general

## Tensor approach

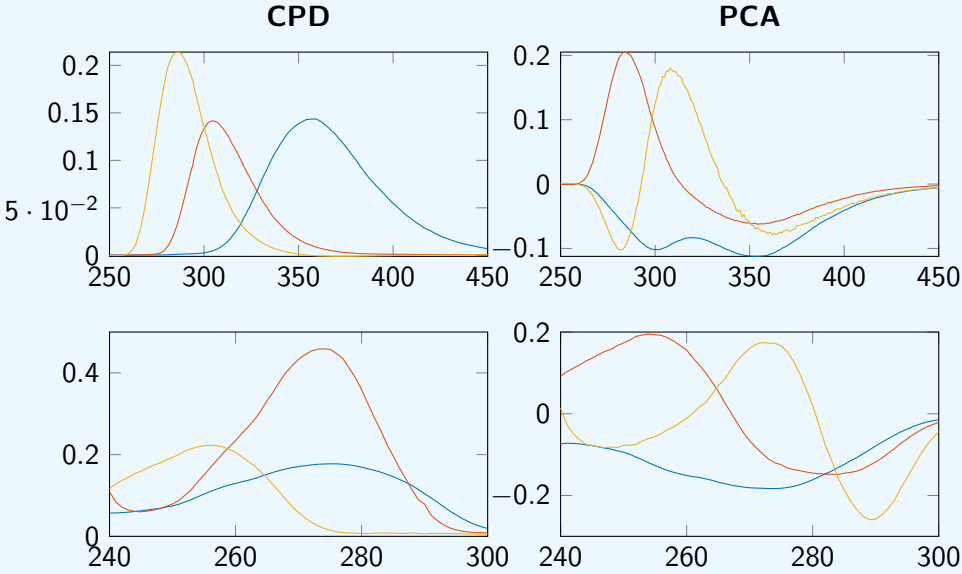
row vector $\sim$ excitation spectrum
column vector $\sim$ emission spectrum
coefficients $\sim$ concentrations



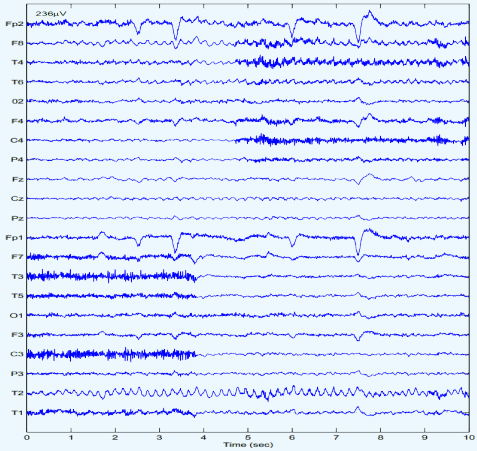

- Surprising fact: unique under mild conditions on number of terms and differences between terms
- Orthogonality (triangularity, ...) not required (but may be imposed)

[Smilde, Bro, et al. 2004]

# Example: amino acids

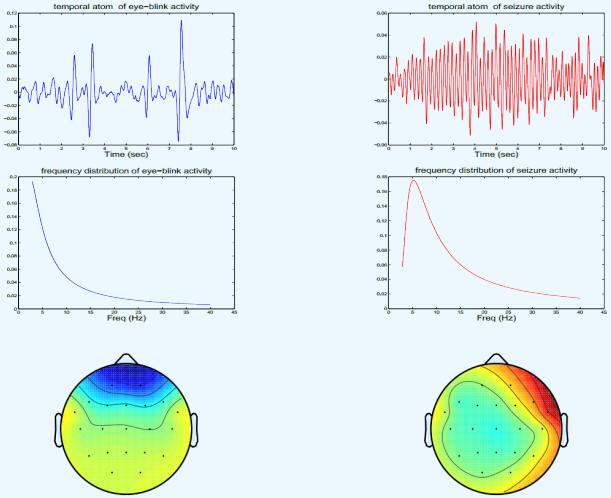


# Application: detection epileptic seizure in EEG




Tensorization: biorthogonal wavelet

# Components: eye blink and epileptic activity

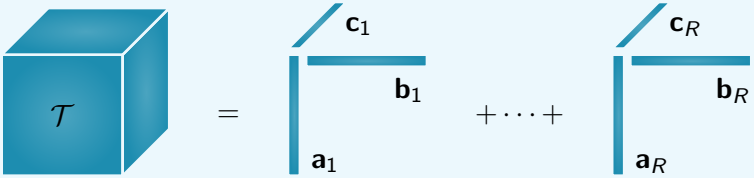



[De Vos, Vergult, et al. 2007; Acar, Aykut-Bingol, et al. 2007]

# Canonical polyadic decomposition

Rank: minimal number of rank-1 terms [Hitchcock 1927]

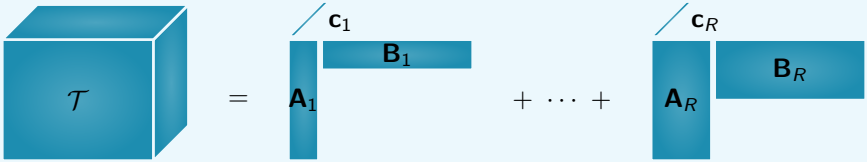
Canonical Polyadic Decomposition (CPD): decomposition in minimal number of rank-1 terms [Harshman 1970; Carrol and Chang 1970]




Unique under mild conditions on number of terms and differences between terms

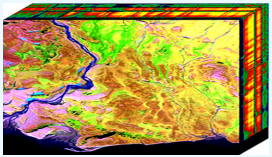
Additional constraints such as orthogonality, triangularity, ... are not required, but may be imposed.

# Decomposition in multilinear rank-$(L, L, 1)$ terms

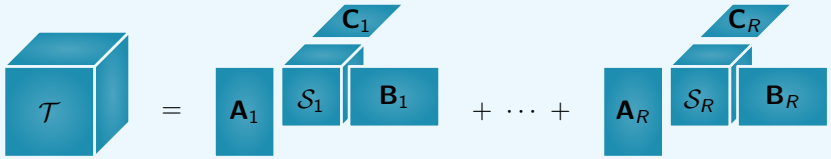



Surprising fact: unique under mild conditions

[De Lathauwer 2008; De Lathauwer 2011; Sørensen and De Lathauwer 2015; Sørensen, Domanov, et al. 2015; Domanov and De Lathauwer 2020]



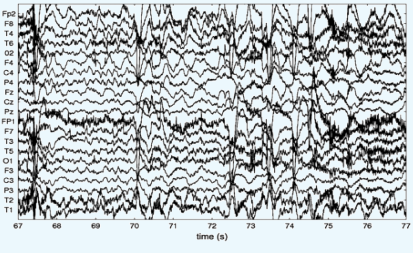
# Decomposition in ML rank-$(R_1, R_2, R_3)$ terms



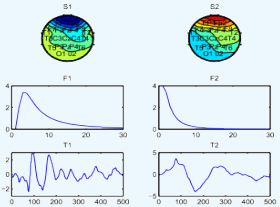

Unique under mild conditions
Rank $\leftrightarrow$ multilinear rank
Atoms (rank-1) $\leftrightarrow$ molecules (low ML rank)

[De Lathauwer 2008]

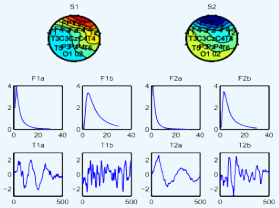
# Application: detection epileptic seizure in EEG



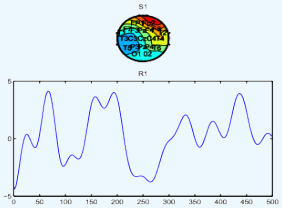

(a) Raw EEG




(b) CPD




(c) CWT-BTD




(d) H-BTD

[Hunyadi, Camps, et al. 2014]

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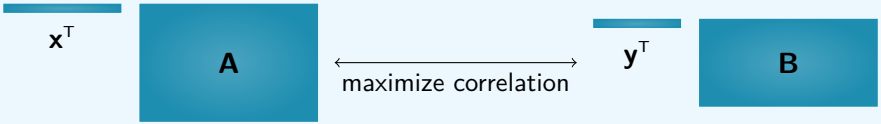
# What about CCA/GSVD?

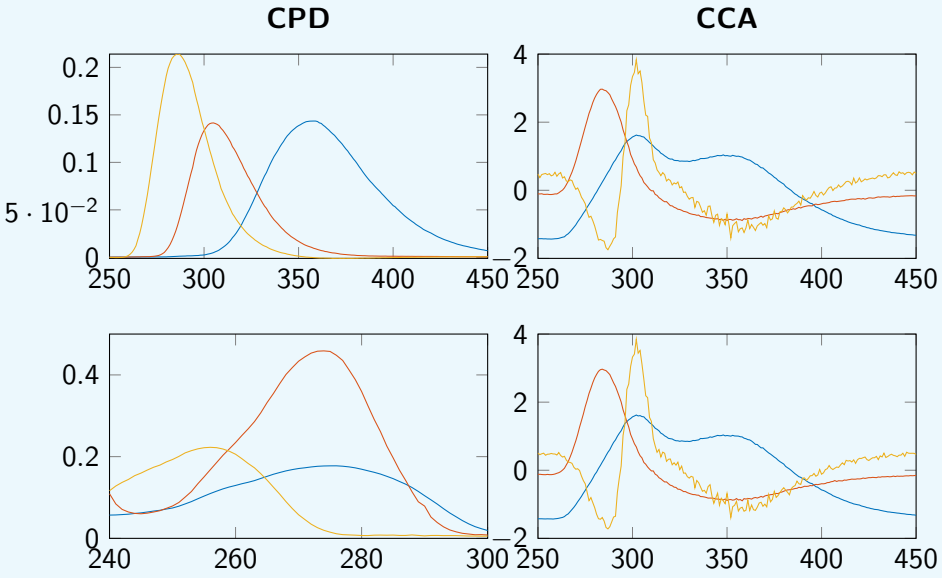
Step 1
$$\mathbf{A} = \mathbf{U}_A \cdot \mathbf{\Sigma}_A \cdot \mathbf{V}_A^\top \quad \text{SVD}$$
$$\mathbf{B} = \mathbf{U}_B \cdot \mathbf{\Sigma}_B \cdot \mathbf{V}_B^\top \quad \text{SVD}$$

Step 2
$$\mathbf{W} = \mathbf{V}_A^\top \cdot \mathbf{V}_B$$

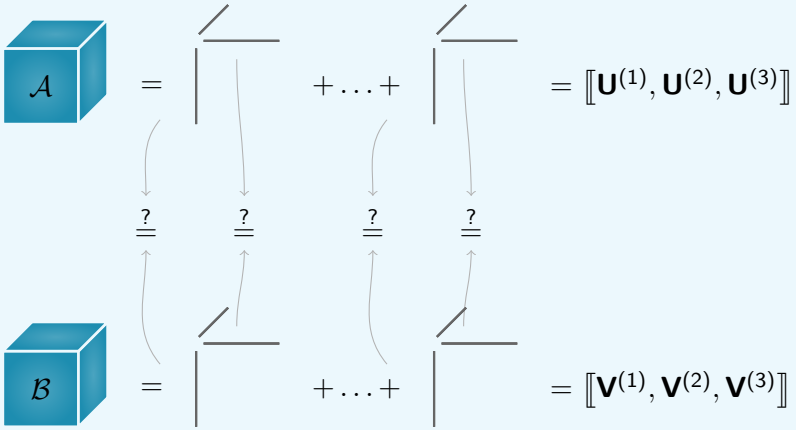
Step 3
Singular values of $\mathbf{W}$ = cosines of principal angles between subspaces row $(\mathbf{A})$ and row $(\mathbf{B})$.



# Example: amino acids



## Graphical representation of comparing factor matrices




$$\mathbf{A}_{[1;2,3]} = \mathbf{U}^{(1)} \left(\mathbf{U}^{(2)} \odot \mathbf{U}^{(3)}\right)^{\mathsf{T}} \rightarrow \quad \text{Tucker: } \operatorname{col}\left(\mathbf{A}_{[1;2,3]}\right) \simeq \operatorname{col}\left(\mathbf{U}^{(1)}\right)$$

$$\overset{\text{SVD}}{=} \mathbf{U} \cdot \mathbf{\Sigma} \cdot \mathbf{V}^{\mathsf{T}} \qquad \text{Here: } \operatorname{row}\left(\mathbf{A}_{[1;2,3]}\right) \simeq \operatorname{row}\left(\left(\mathbf{U}^{(2)} \odot \mathbf{U}^{(3)}\right)^{\mathsf{T}}\right)$$

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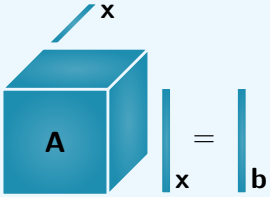
# From linear to multilinear/polynomial

## Linear




$$\sum_j a_{ij} x_j = b_i$$

## Bilinear/quadratic




$$\sum_{jk} a_{ijk} x_j y_k = b_i$$
$$\sum_{jk} a_{ijk} x_j x_k = b_i$$

## Multilinear/polynomial

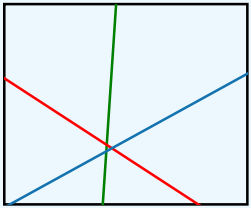
Tensor higher-order

$$\sum_{j_1 j_2 \ldots j_D} a_{i j_1 j_2 \ldots j_D} x_{j_1} y_{j_2} \ldots z_{j_D} = b_i$$
$$\sum_{j_1 j_2 \ldots j_D} a_{i j_1 j_2 \ldots j_D} x_{j_1} x_{j_2} \ldots x_{j_D} = b_i$$

# Overdetermined linear and polynomial systems of equations

Overdetermined *linear* systems:

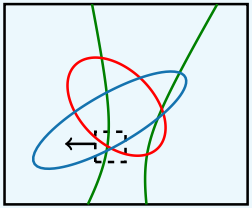
*local*, *simple* models, *one* solution



$$
\begin{aligned}
a_{11}x + a_{12}y &= b_1 \\
a_{21}x + a_{22}y &= b_2 \\
a_{31}x + a_{32}y &= b_3
\end{aligned}
$$

Overdetermined *polynomial* systems:

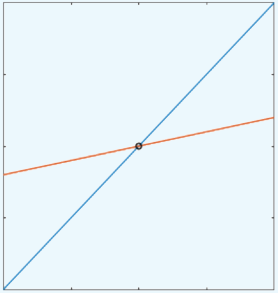
*global*, *rich* models, *multiple* solutions

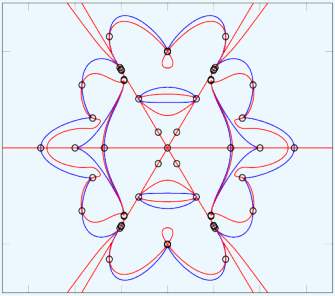


$$
\begin{aligned}
a_{11}x + a_{12}y + a_{13}x^2 + a_{14}xy + a_{15}y^2 &= b_1 \\
a_{21}x + a_{22}y + a_{23}x^2 + a_{24}xy + a_{25}y^2 &= b_2 \\
a_{31}x + a_{32}y + a_{33}x^2 + a_{34}xy + a_{35}y^2 &= b_3
\end{aligned}
$$

Nonlinearities are essential in AI

# From linear to multilinear/polynomial





Linear equations

$$\begin{cases} a_{11}x_1 + a_{12}x_2 - b_1 = 0 \\ a_{21}x_1 + a_{22}x_2 - b_2 = 0 \end{cases}$$

Polynomial equations

$$\begin{cases} p_1(x_1, x_2) = 0 \\ p_2(x_1, x_2) = 0 \end{cases}$$

[Sorber, Van Barel, et al. 2014]

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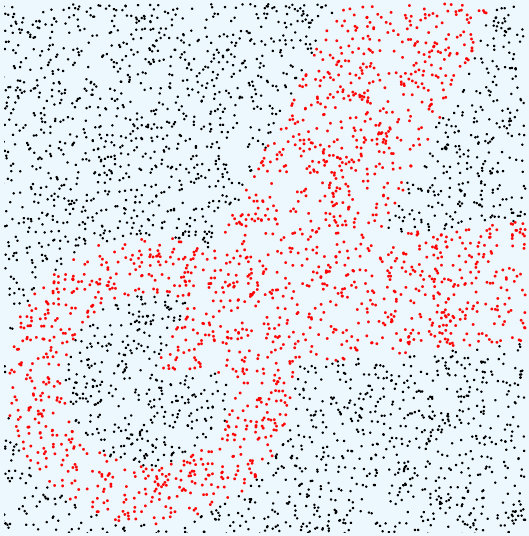
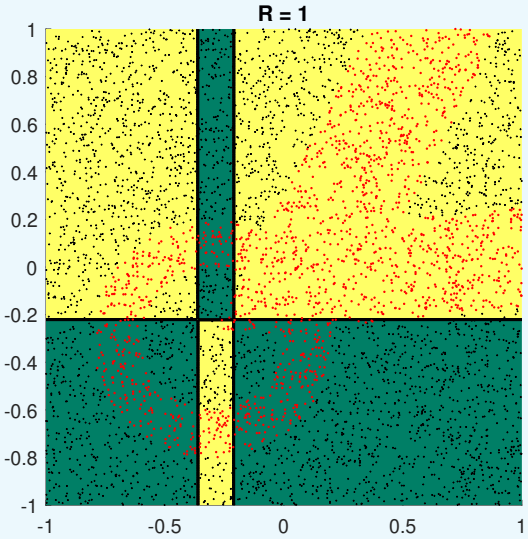
# Nonlinear decision boundary modelled using splines

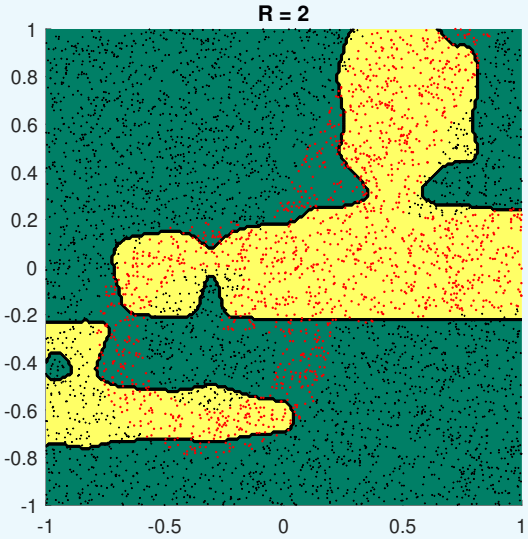
**Consider the labeled dataset:**



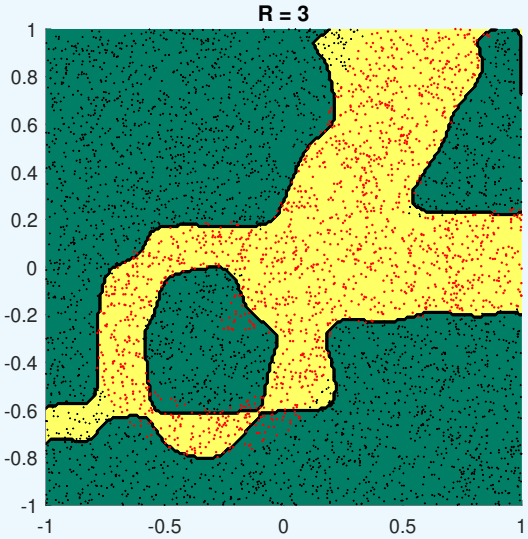
# The separable rank can be increased to account for complexity of the classification sets



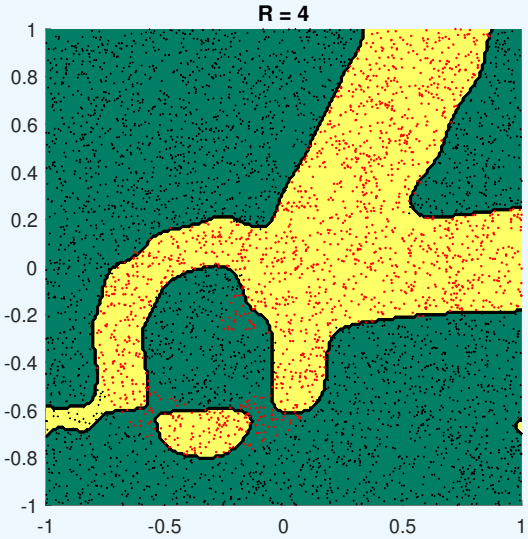
# The separable rank can be increased to account for complexity of the classification sets



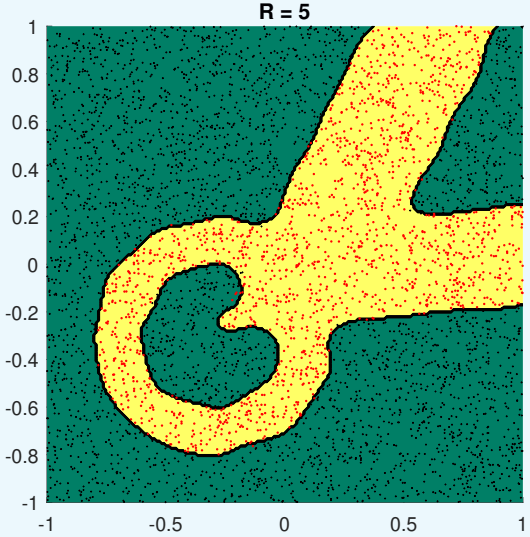
# The separable rank can be increased to account for complexity of the classification sets



# The separable rank can be increased to account for complexity of the classification sets



# The separable rank can be increased to account for complexity of the classification sets




Possibility to impose constraints

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- Harmonic retrieval
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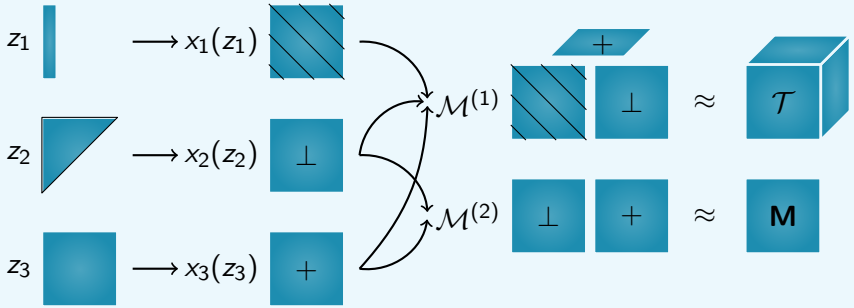
# Coupled matrix/tensor decompositions




Multiview data analysis / data fusion — e.g. EEG-fMRI

Divide-and-conquer data analysis / data fission — e.g. structured arrays

# Application: data fusion for completion/prediction/collaborative filtering

**Five coupled data sets:** *user-location-activity*, *user-user*, *location-feature*, *activity-activity* and *user-location*
**Challenge:** predict user participation in activities
**Solution with SDF:** compute coupled tensor factorization

$$\underset{\mathbf{U},\mathbf{L},\mathbf{A},\mathbf{F},\mathbf{d}_{\mathsf{uu}},\mathbf{d}_{\mathsf{aa}},\mathbf{d}_{\mathsf{ul}}}{\text{minimize}} \quad \frac{\omega_1}{2}\,||\mathcal{T} - [\![\mathbf{U},\mathbf{L},\mathbf{A}]\!]||_{\mathcal{W}}^2 + \frac{\omega_2}{2}\,||\mathbf{M}_{\mathsf{uu}} - \mathbf{U}\mathbf{D}_{\mathsf{uu}}\mathbf{U}^{\mathsf{T}}||_{\mathsf{F}}^2 +$$
$$\frac{\omega_3}{2}\,||\mathbf{M}_{\mathsf{ul}} - \mathbf{U}\mathbf{D}_{\mathsf{ul}}\mathbf{L}^{\mathsf{T}}||_{\mathsf{F}}^2 + \frac{\omega_4}{2}\,||\mathbf{M}_{\mathsf{lf}} - \mathbf{L}\mathbf{F}^{\mathsf{T}}||_{\mathsf{F}}^2 + \frac{\omega_5}{2}\,||\mathbf{M}_{\mathsf{aa}} - \mathbf{A}\mathbf{D}_{\mathsf{aa}}\mathbf{A}^{\mathsf{T}}||_{\mathsf{F}}^2 +$$
$$\frac{\omega_6}{2}\left(||\mathbf{U}||_{\mathsf{F}}^2 + ||\mathbf{L}||_{\mathsf{F}}^2 + ||\mathbf{A}||_{\mathsf{F}}^2 + ||\mathbf{F}||_{\mathsf{F}}^2 + ||\mathbf{d}_{\mathsf{uu}}||_{\mathsf{F}}^2 + ||\mathbf{d}_{\mathsf{aa}}||_{\mathsf{F}}^2 + ||\mathbf{d}_{\mathsf{ul}}||_{\mathsf{F}}^2\right)$$

Exploratory data analysis / fast prototyping
Incomplete large-scale data

[Sorber, Van Barel, et al. 2015]

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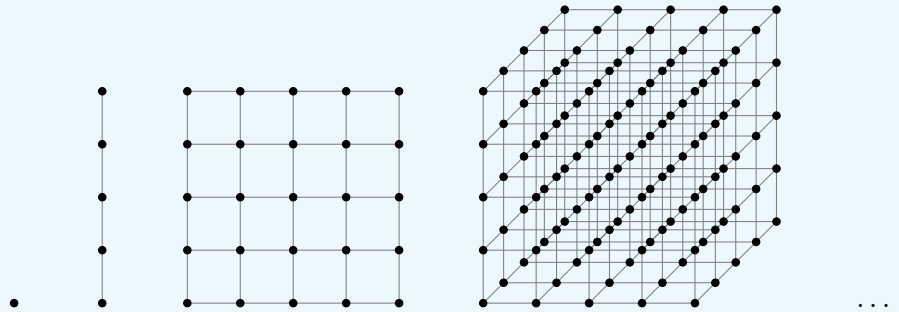
## Tensors and scientific computing

Scientific computing: discretization of functions in many variables: "curse of dimensionality"



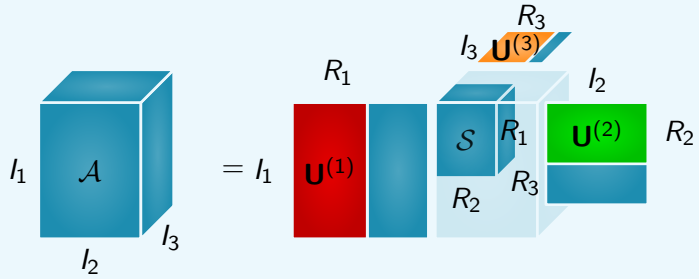

Exponential increase of entries: $I^N$

Computation: in terms of parameterized approximation

Parallel computation: cannot break the curse

# MLSVD / low ML rank approximation: numerical pros and cons

- Well-posed
- (Approximate) computation via matrix SVD
- Error bounds
- Curse not broken
- Numerically reliable but limited to modest order

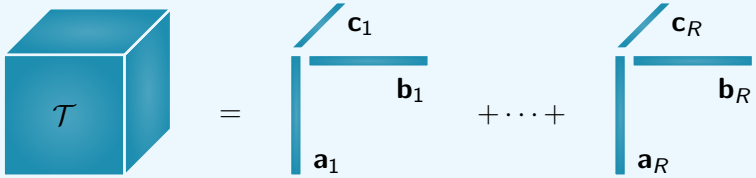



Order 3 $= I^3 \rightarrow \mathcal{O}\left(3IR + R^3\right)$

Order N $= I^N \rightarrow \mathcal{O}\left(IR + R^N\right)$

# CPD / low rank approximation: numerical pros and cons

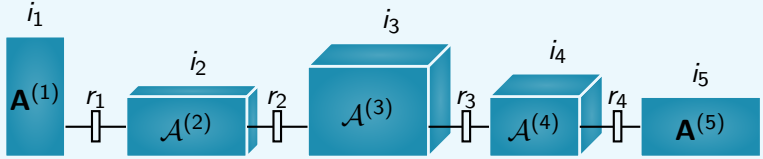
- Possibly ill-posed
- Possibly ill-conditioned
- Curse broken
- Powerful tool but not always numerically reliable




Order 3 $= I^3 \rightarrow \mathcal{O}(3IR)$
Order N $= I^N \rightarrow \mathcal{O}(NIR)$

# Tensor Trains or Matrix Product States

- Write tensor as a train of matrix -. . . third-order tensors . . . - matrix [Oseledets 2011]




- Mathematically, for a general $N$th order tensor $\mathcal{T} \in \mathbb{C}^{I_1 \times \cdots \times I_N}$

$$t_{i_1 i_2 \cdots i_N} = \sum_{r_1, r_2, \ldots, r_{N-1}} a^{(1)}_{i_1 r_1} a^{(2)}_{r_1 i_2 r_2} a^{(3)}_{r_2 i_3 r_3} \cdots a^{(N-1)}_{r_{N-2} i_{N-1} r_{N-1}} a^{(N)}_{r_{N-1} i_N}$$

- Total number of entries: $I^N \leftrightarrow$ number of variables: $\mathcal{O}\left(2IR + (N-2)IR^2\right)$
- Curse broken and can be computed via QR/SVD
- Truncation error bound

$$\|\mathcal{T} - \hat{\mathcal{T}}_{\mathrm{TT,\ trunc}}\|_{\mathrm{F}}^2 \leqslant (N-1) \min_{\mathrm{rank_{TT}}(\hat{\mathcal{T}}) \leqslant (R_1, R_2, \ldots, R_{N-1})} \|\mathcal{T} - \hat{\mathcal{T}}\|_{\mathrm{F}}^2$$

- hTucker [Hackbusch 2012]

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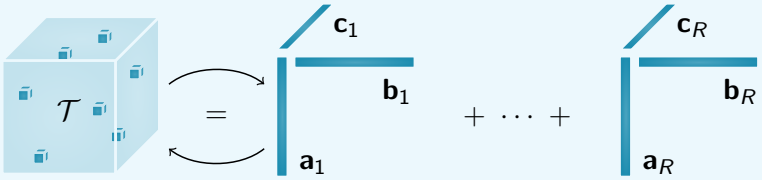
# Canonical polyadic decomposition




- Mathematically, for a general $N$th order tensor $\mathcal{T} \in \mathbb{C}^{I \times \cdots \times I}$

$$\mathcal{T} = \sum_{r=1}^{R} \mathbf{a}_r^{(1)} \otimes \mathbf{a}_r^{(2)} \otimes \cdots \otimes \mathbf{a}_r^{(N)} = \left[\!\left[ \mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \ldots, \mathbf{A}^{(N)} \right]\!\right]$$

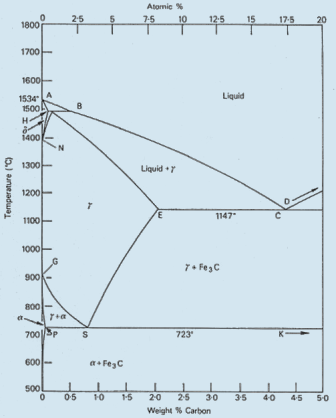
- Total number of entries: $I^N \leftrightarrow$ number of variables: $\mathcal{O}(NIR)$
- Curse broken, but possibly ill-conditioned/ill-posed problem

# Modeling multiway thermodynamic data

Modes: fraction atom/molecule $n$ in a multi-component material

Value: Gibbs free energy, chemical potential, melting temperature (e.g., computed using thermodynamic software)

## First-order example



Modes: fraction atom/molecule $n$ in a multi-component material
Value: Gibbs free energy, chemical potential, melting temperature (e.g., computed using thermodynamic software)

## Second-order example

- Alloy with $c_1$ % iron, $c_2$ % carbon and $100 - c_1 - c_2$ % nickel
- Discretize $c_1$ and $c_2$ in 100 steps
- Grid of size $100^2$

[Vervliet, Debals, Sorber, and De Lathauwer 2014]

## Multiway dataset

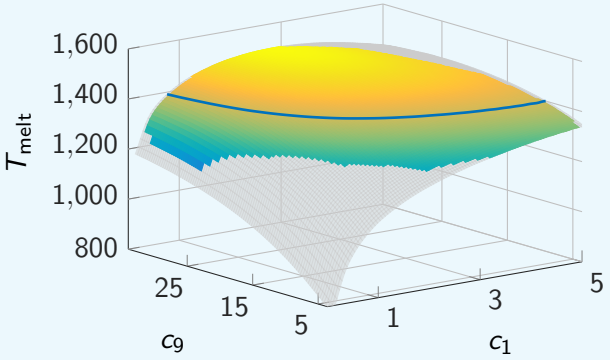
- # constituent materials: 10 (thus $N = 9$)
- Size: $100 \times 100 \times \cdots \times 100 \approx 10^{18}$ elements
- # Samples: 130 000 of which 30 000 are validation samples
- Undersampling rate $= 10^{13}$
- Model:

$$\mathcal{T} = \sum_{r=1}^{R} \mathbf{a}_r^{(1)} \otimes \mathbf{a}_r^{(2)} \otimes \cdots \otimes \mathbf{a}_r^{(N)}$$

### Algorithm

- Tensorlab 3.0 with `cpd_nls` and `UseCPDI` option [Vervliet, Debals, Sorber, and De Lathauwer 2014; Vervliet, Debals, Sorber, Van Barel, et al. 2016]
- Initialization: optimally scaled best-out-of-five strategy

# Visualization



## Recap

- From a ninth order tensor with $10^{18}$ elements...
- we took 100 000 samples...
- to get a rank-5 model with $5 \times 9 \times 100 = 4\,500$ parameters...
- to get a continuous model with $\mathcal{O}(100)$ parameters...
- in 3 min

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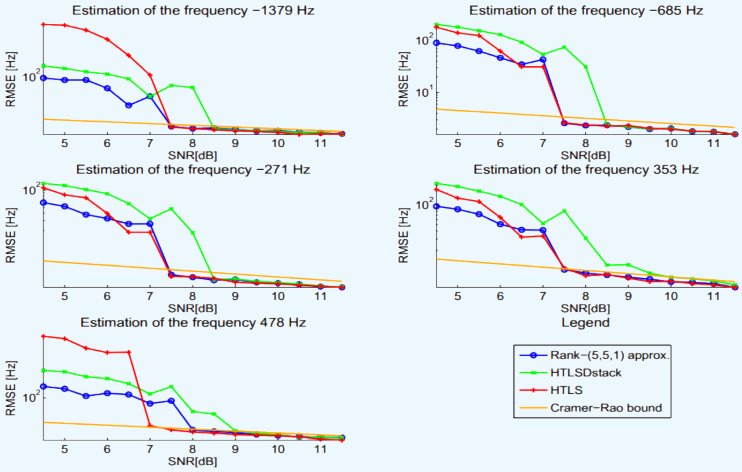
# Low ML rank approximation: illustration (NMR)

Harmonic retrieval: Hankel matrix $\rightarrow$ tensor: signal subspace

Five-peak signal, decreasing $R_3$ from 5 to 1 [Papy, De Lathauwer, et al. 2009]



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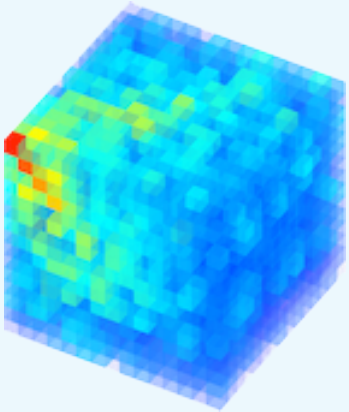
# Tensorlab

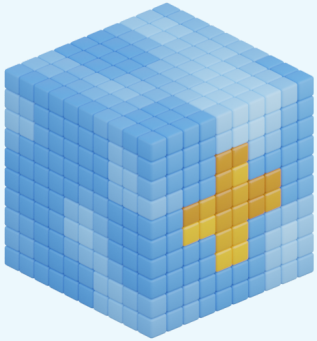
- Tensorlab 1: Tensor decompositions
- Complex Optimization Toolbox
  `www.esat.kuleuven.be/sista/cot`
- Tensorlab 2: Structured Data Fusion
- Tensorlab 3: Large-scale algorithms, tensorization
- Extensive documentation and demos

`www.tensorlab.net`



# Tensorlab+

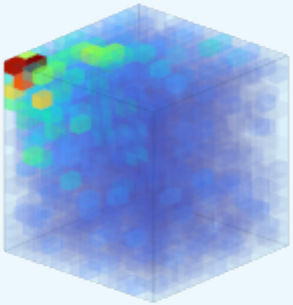
- code supporting 44 papers
- 200+ experiments
- reproducing 250+ figures and table
- 40 tutorials and demos



`www.tensorlab.net`
`www.tensorlabplus.net`

# pyTensorlab: a Python package for tensor computations and complex optimization

- Advanced algorithms for tensor decompositions
- New efficient tensor types built on top of NumPy
- Practical visualization tools
- Support for complex optimization
- Fully typed code for faster development
- Extensive documentation, detailed API, and demos



See `www.pytensorlab.net` or `pip install pytensorlab`.

# Getting started

N. Sidiropoulos, L. De Lathauwer, et al. [July 2017]. "Tensor Decomposition for Signal Processing and Machine Learning". In: *IEEE Transactions on Signal Processing* 65.13, pp. 3551–3582

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T. G. Kolda and B. W. Bader [Aug. 2009]. "Tensor decompositions and applications". In: *SIAM Review* 51.3, pp. 455–500

N. Vervliet and L. De Lathauwer [2019]. "Numerical optimization based algorithms for data fusion". In: *Data Fusion Methodology and Applications*. Ed. by M. Cocchi. Vol. 31. Elsevier. Chap. 4, pp. 81–128

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# References VII




Vervliet, N., Debals, O., Sorber, L., Van Barel, M., et al. (Mar. 2016). *Tensorlab 3.0*. Available online at `https://www.tensorlab.net`.