Tucker Compression, Parallel Factor Analysis and Block Term Decompositions: New Results

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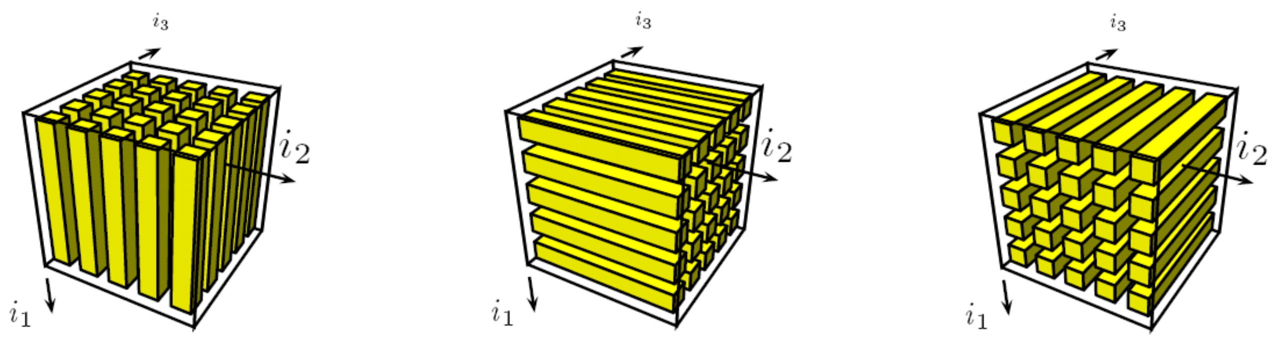
Overview

- Preliminaries
- Tucker decomposition / Multilinear SVD
- Parallel Factor Decomposition
- Block Term Decomposition

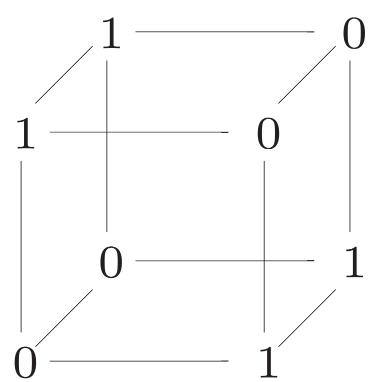
Columns, rows and mode-n vectors

Mode-n vectors of a tensor: generalization of column/row vectors of a matrix



Multilinear rank of a tensor

- The column (row) rank of a matrix $\mathbf{A}$ is equal to the maximal number of columns (rows) of $\mathbf{A}$ that form a linearly independent set
- Mode-n rank of a tensor: dimension of the vector space generated by mode-n vectors
- Mode-n ranks can be mutually different
- Rank-(R_1, R_2, R_3) tensor: $\text{rank}_1(\mathcal{A}) = R_1$, $\text{rank}_2(\mathcal{A}) = R_2$, $\text{rank}_3(\mathcal{A}) = R_3$
- Multilinear rank: (R_1, R_2, R_3)



$R_1 = R_2 = 2 \quad R_3 = 1$

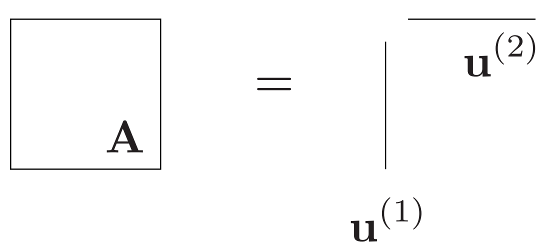
Rank-1 tensor

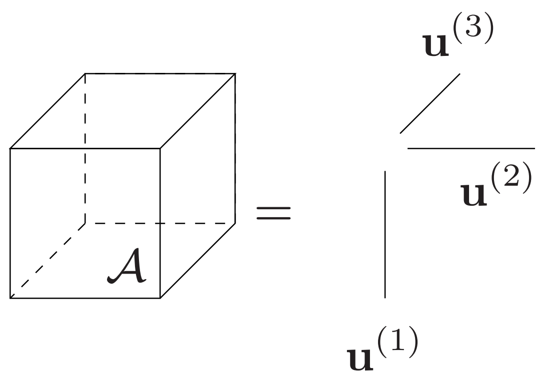
- Rank-1 matrix: outer product of 2 vectors $\mathbf{u}^{(1)}$, $\mathbf{u}^{(2)}$:

$$\begin{aligned} a_{i_1 i_2} &= u^{(1)}_{i_1} u^{(2)}_{i_2} \\ \mathbf{A} &= \mathbf{u}^{(1)} \cdot \mathbf{u}^{(2)^T} \equiv \mathbf{u}^{(1)} \circ \mathbf{u}^{(2)} \end{aligned}$$

- Rank-1 tensor: outer product of N vectors $\mathbf{u}^{(1)}$, $\mathbf{u}^{(2)}$, . . . , $\mathbf{u}^{(N)}$:

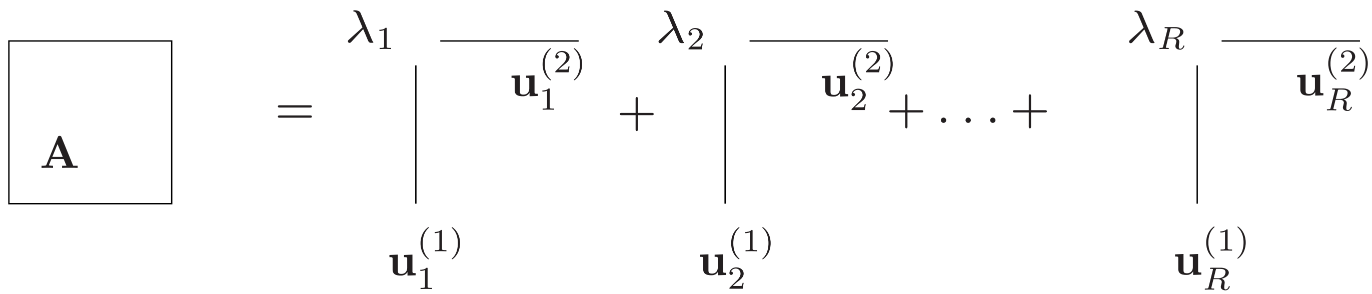
$$\begin{aligned} a_{i_1 i_2 \dots i_N} &= u^{(1)}_{i_1} u^{(2)}_{i_2} \dots u^{(N)}_{i_N} \\ \mathcal{A} &= \mathbf{u}^{(1)} \circ \mathbf{u}^{(2)} \circ \dots \circ \mathbf{u}^{(N)} \end{aligned}$$



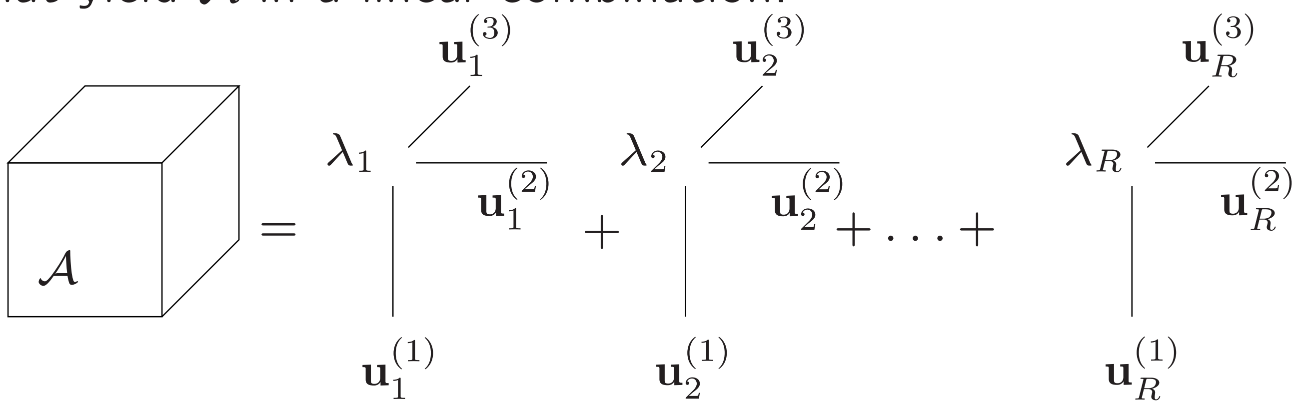


Rank of a tensor

- The rank R of a matrix $\mathbf{A}$ is minimal number of rank-1 matrices that yield $\mathbf{A}$ in a linear combination.



- The rank R of an Nth-order tensor $\mathcal{A}$ is the minimal number of rank-1 tensors that yield $\mathcal{A}$ in a linear combination.



[*Hitchcock, 1927*]

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  - Multilinear rank and associated decomposition
  - Best rank-(R_1, R_2, R_3) approximation
  - Numerical algorithms
  - Local optima
  - Hierarchical Tucker compression
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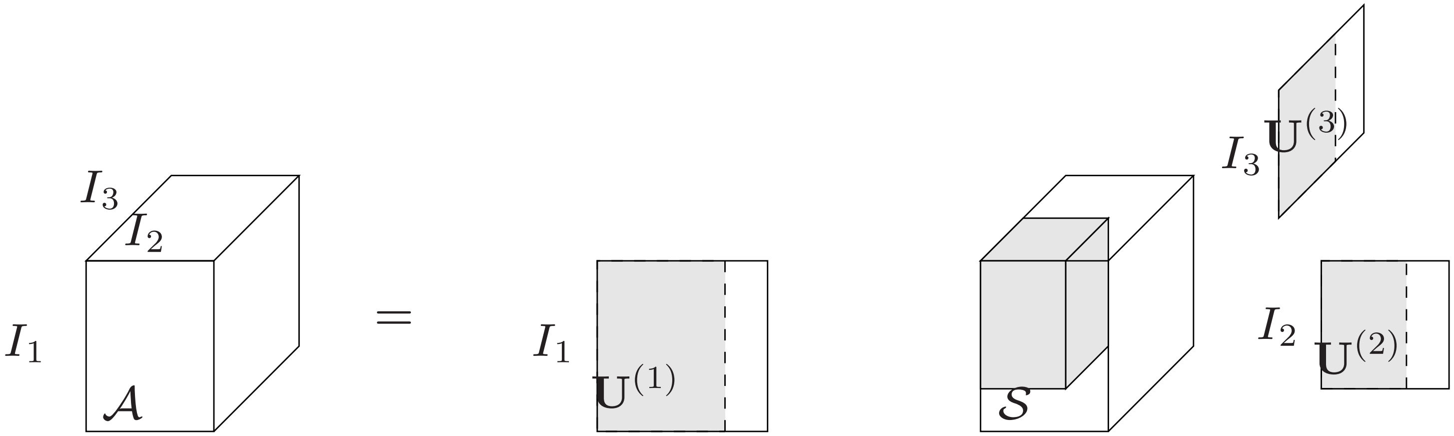
Multilinear rank and associated decomposition

Definition:

$$\mathcal{A} = \mathcal{S} \bullet_1 \mathbf{U}^{(1)} \bullet_2 \mathbf{U}^{(2)} \bullet_3 \ldots \bullet_N \mathbf{U}^{(N)}$$

in which $\mathcal{S}$ is all-orthogonal and ordered
$\mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \ldots, \mathbf{U}^{(N)}$ are orthogonal



[*Tucker '64*], [*De Lathauwer '00*]

Computation

$$\mathcal{A} = \mathcal{S} \bullet_1 \mathbf{U}^{(1)} \bullet_2 \mathbf{U}^{(2)} \bullet_3 \mathbf{U}^{(3)}$$

- $(I_1 \times I_2 I_3)$ matrix $\mathbf{A}^{(1)}$ in which all the columns are stacked

  SVD: $\mathbf{A}^{(1)} = \mathbf{U}^{(1)} \cdot \mathbf{\Sigma}^{(1)} \cdot \mathbf{U}^{(1)^T}$

- $(I_2 \times I_3 I_1)$ matrix $\mathbf{A}^{(2)}$ in which all the row vectors are stacked

  SVD: $\mathbf{A}^{(2)} = \mathbf{U}^{(2)} \cdot \mathbf{\Sigma}^{(2)} \cdot \mathbf{U}^{(2)^T}$

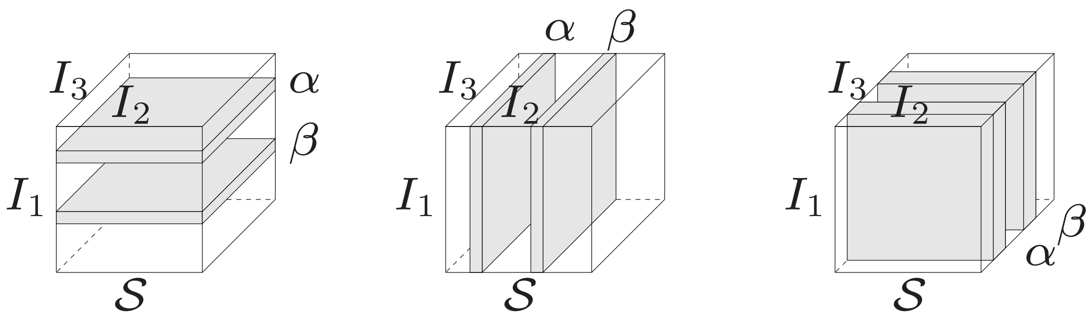
- $(I_3 \times I_1 I_2)$ matrix $\mathbf{A}^{(3)}$ in which all the mode-3 vectors are stacked

  SVD: $\mathbf{A}^{(3)} = \mathbf{U}^{(3)} \cdot \mathbf{\Sigma}^{(3)} \cdot \mathbf{U}^{(3)^T}$

- Compute $\mathcal{S}$:

$$\mathcal{S} = \mathcal{A} \bullet_1 \mathbf{U}^{(1)^T} \bullet_2 \mathbf{U}^{(2)^T} \bullet_3 \mathbf{U}^{(3)^T}$$

All-orthogonality:

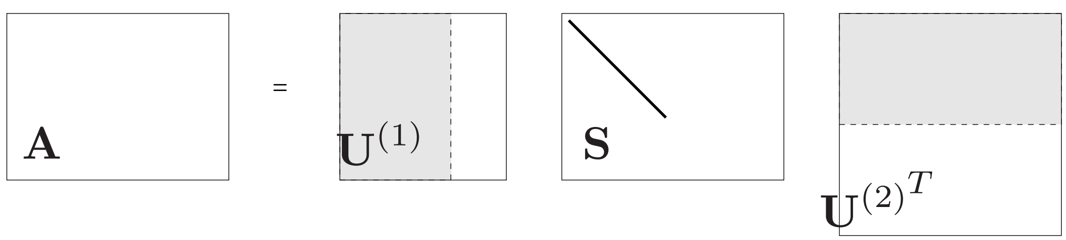


All-orthogonality is a generalization of diagonality

Ordering: slices have decreasing Frobenius norm

Norms of slices = mode-n singular values

Matrix SVD:



Definition:

$$\mathcal{A} = \mathcal{S} \bullet_1 \mathbf{U}^{(1)} \bullet_2 \mathbf{U}^{(2)} \bullet_3 \ldots \bullet_N \mathbf{U}^{(N)}$$

Properties:

- Mode-n singular values = norms of slices = singular values of $\mathbf{A}_{(n)}$
- N sets of singular values
- Mode-n rank revealing
- Number of significant $\sigma_i^{(n)}$ = numerical mode-n rank
- Similar uniqueness properties as matrix SVD
- Decomposition of 2nd order tensor = matrix SVD
- Link with matrix EVD:

$$\mathbf{A}_{(n)} \cdot {\mathbf{A}_{(n)}}^T = \mathbf{U}^{(n)} \cdot \mathrm{diag}((\sigma_1^{(n)})^2, \ldots, (\sigma_{I_n}^{(n)})^2) \cdot {\mathbf{U}^{(n)}}^T$$

Massive datasets:

[*Mahoney et al. '06*], [*Tyrtyshnikov et al. '06*], [*Oseledets et al. '08*]

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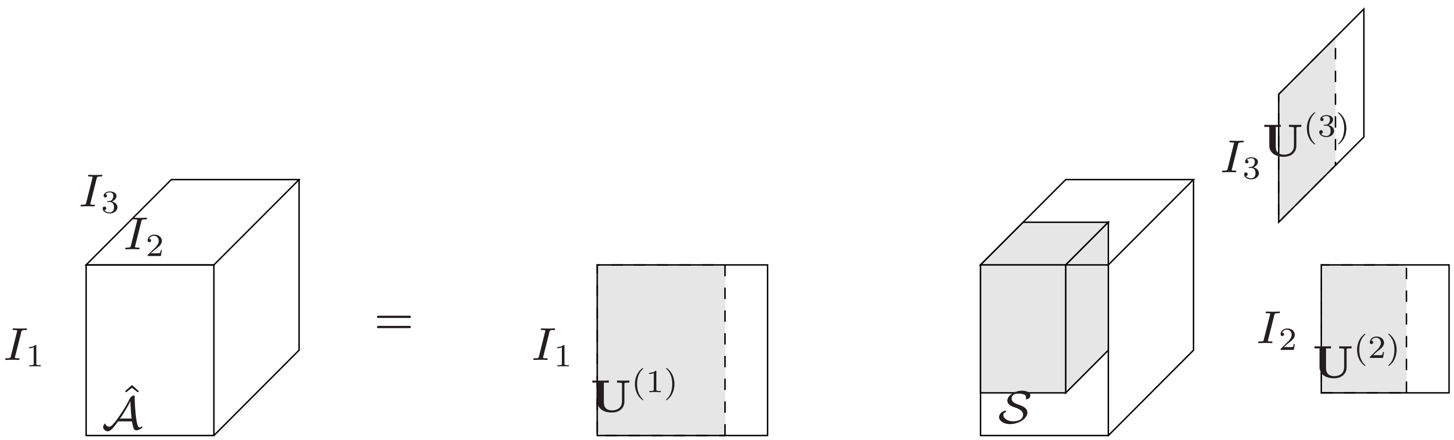
Best Multilinear Rank-$(R_1, R_2, \ldots, R_N)$ Approximation

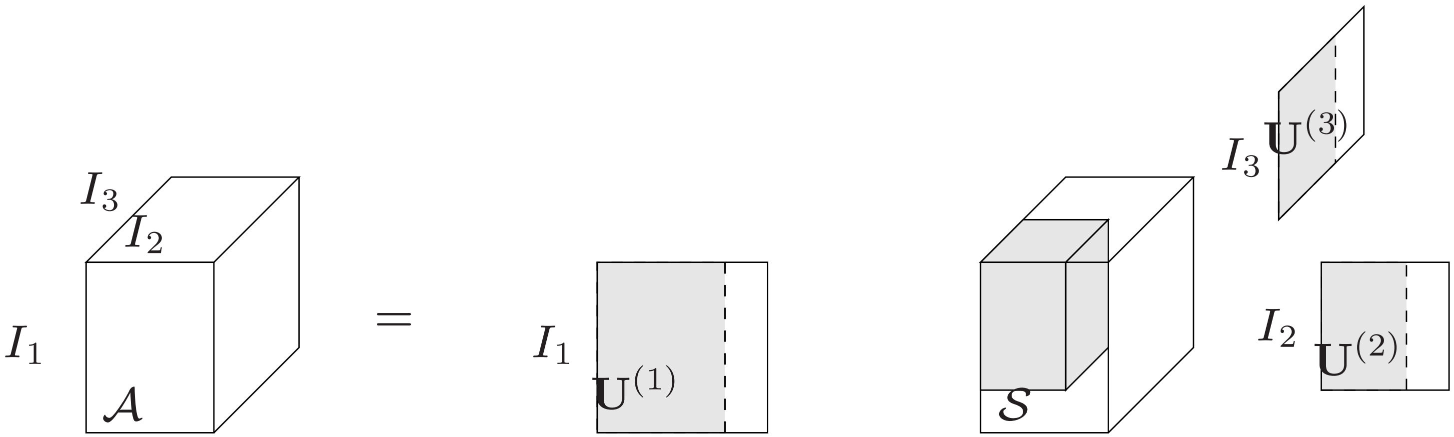
Problem: minimize $\|\mathcal{A} - \hat{\mathcal{A}}\|$ subject to

$$\text{rank}_1(\hat{\mathcal{A}}) \leqslant R_1 \qquad \text{rank}_2(\hat{\mathcal{A}}) \leqslant R_2 \qquad \text{rank}_3(\hat{\mathcal{A}}) \leqslant R_3$$

Parameterization: $\mathcal{A} = \mathcal{S} \bullet_1 \mathbf{U}^{(1)} \bullet_2 \mathbf{U}^{(2)} \bullet_3 \mathbf{U}^{(3)}$



Truncation of multilinear SVD



Gives good but not optimal approximation

Further optimization required

Error bound:

$$\|\mathcal{A} - \hat{\mathcal{A}}\|^2 \leqslant \sum_{i_1=R_1+1}^{I_1} \sigma_{i_1}^{(1)^2} + \sum_{i_2=R_2+1}^{I_2} \sigma_{i_2}^{(2)^2} + \sum_{i_3=R_3+1}^{I_3} \sigma_{i_3}^{(3)^2}$$

Problem reformulation

Matrix case:

$$\min \|\mathbf{A} - \mathbf{U}^{(1)} \cdot \mathbf{\Sigma} \cdot \mathbf{U}^{(2)^T}\|$$

is equivalent with

$$\max \|\mathbf{U}^{(1)^T} \cdot \mathbf{A} \cdot \mathbf{U}^{(2)}\|$$

Tensor case:

$$\min \|\mathcal{A} - \mathcal{S} \bullet_1 \mathbf{U}^{(1)} \bullet_2 \mathbf{U}^{(2)} \bullet_3 \mathbf{U}^{(3)}\|$$

is equivalent with

$$\max \|\mathcal{A} \bullet_1 \mathbf{U}^{(1)^T} \bullet_2 \mathbf{U}^{(2)^T} \bullet_3 \mathbf{U}^{(3)^T}\|$$

$$= \max \|\mathbf{U}^{(1)^T} \cdot \mathbf{A}^{(1)} \cdot (\mathbf{U}^{(2)} \otimes \mathbf{U}^{(3)})^T\|$$

$$= \max \|\mathbf{U}^{(2)^T} \cdot \mathbf{A}^{(2)} \cdot (\mathbf{U}^{(3)} \otimes \mathbf{U}^{(1)})^T\|$$

$$= \max \|\mathbf{U}^{(3)^T} \cdot \mathbf{A}^{(3)} \cdot (\mathbf{U}^{(1)} \otimes \mathbf{U}^{(2)})^T\|$$

Suggests alternating least squares algorithm

(Higher-order) orthogonal iteration

Matrix case: Iterate over:

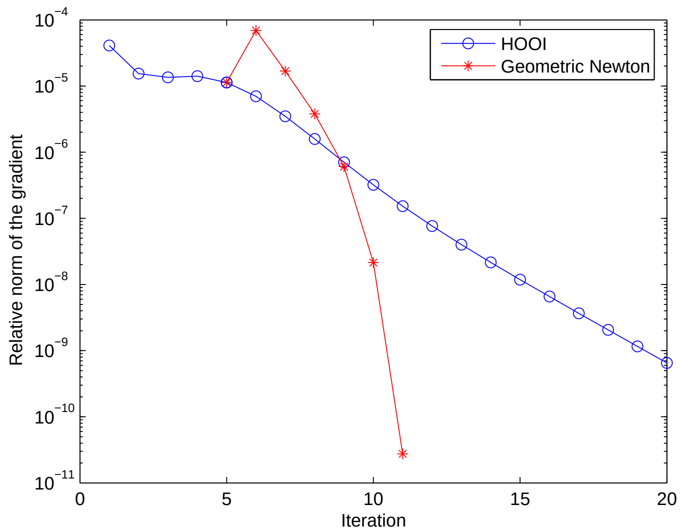
1. Compute $\mathbf{B}^{(1)} = \mathbf{A} \cdot \mathbf{U}^{(2)}$; $\mathbf{U}^{(1)} = \text{qf}(\mathbf{B}^{(1)})$
2. Compute $\mathbf{B}^{(2)} = \mathbf{A}^T \cdot \mathbf{U}^{(1)}$; $\mathbf{U}^{(2)} = \text{qf}(\mathbf{B}^{(2)})$

Tensor case: Iterate over:

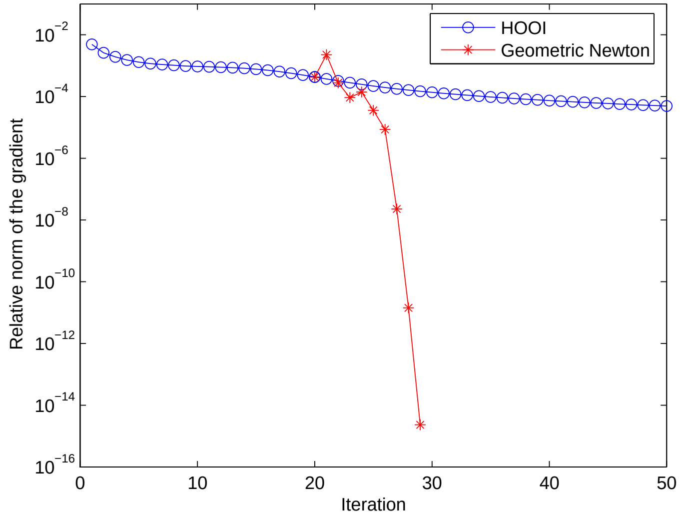
1. Compute $\mathbf{B}^{(1)} = \mathbf{A}^{(1)} \cdot (\mathbf{U}^{(2)} \otimes \mathbf{U}^{(3)})^T$; $\mathbf{U}^{(1)}$ maximizes $\|\mathbf{U}^{(1)^T} \cdot \mathbf{B}^{(1)}\|$
2. Compute $\mathbf{B}^{(2)} = \mathbf{A}^{(2)} \cdot (\mathbf{U}^{(3)} \otimes \mathbf{U}^{(1)})^T$; $\mathbf{U}^{(2)}$ maximizes $\|\mathbf{U}^{(2)^T} \cdot \mathbf{B}^{(2)}\|$
3. Compute $\mathbf{B}^{(3)} = \mathbf{A}^{(3)} \cdot (\mathbf{U}^{(1)} \otimes \mathbf{U}^{(2)})^T$; $\mathbf{U}^{(3)}$ maximizes $\|\mathbf{U}^{(3)^T} \cdot \mathbf{B}^{(3)}\|$

[*Kroonenberg '83*], [*De Lathauwer '00*]

Orthogonal iterations can be slow [*Zhang and Golub '01*], [*Eldén and Savas '06*]



dominant rank-(R_1, R_2, R_3) part



random tensor

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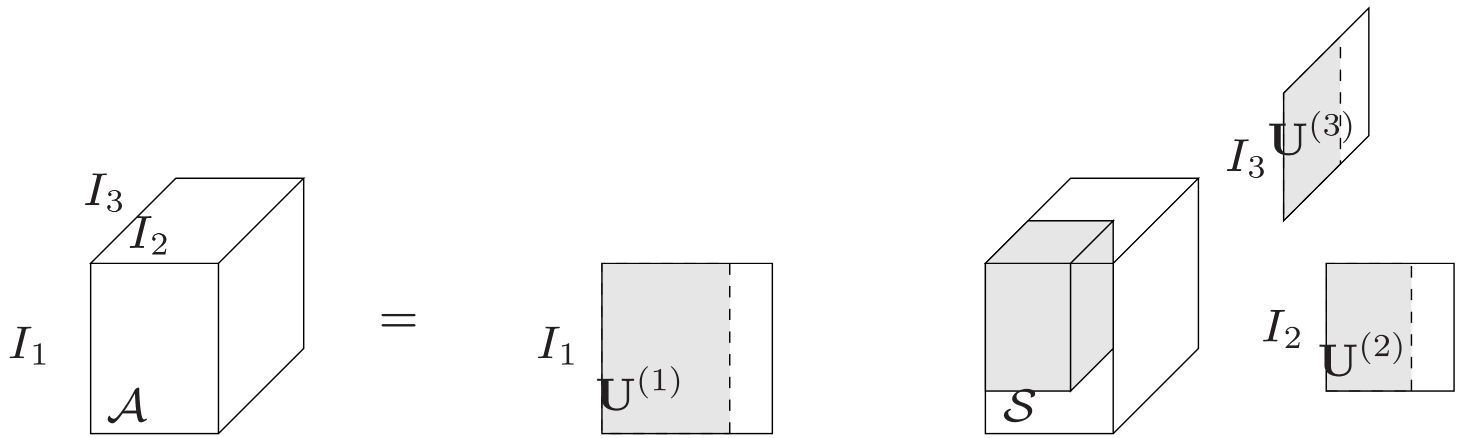
Only subspaces are of interest

$\longrightarrow$ work on products of quotient spaces (Grassmann)



$\longrightarrow$ Optimization on manifolds

[*Edelman, Arias and Smith '98*], [*Absil, Mahoney and Sepulchre '08*]

Faster solutions

Optimization on manifolds:

- Newton [*Eldén and Savas '06*], [*Ishteva et al. '08*]
- Quasi-Newton [*Savas and Lim '08*]
- Trust region [*Ishteva et al. '09*] (→ poster)
- Conjugate gradient [*Ishteva et al. '09*]

Krylov method: [*Savas '08*]

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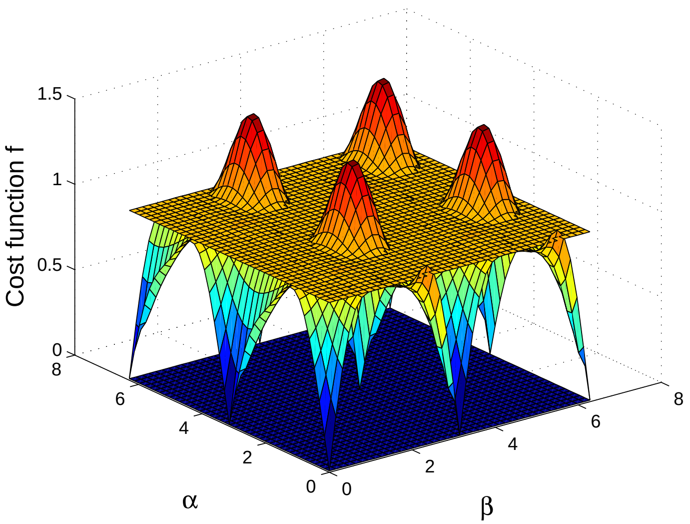
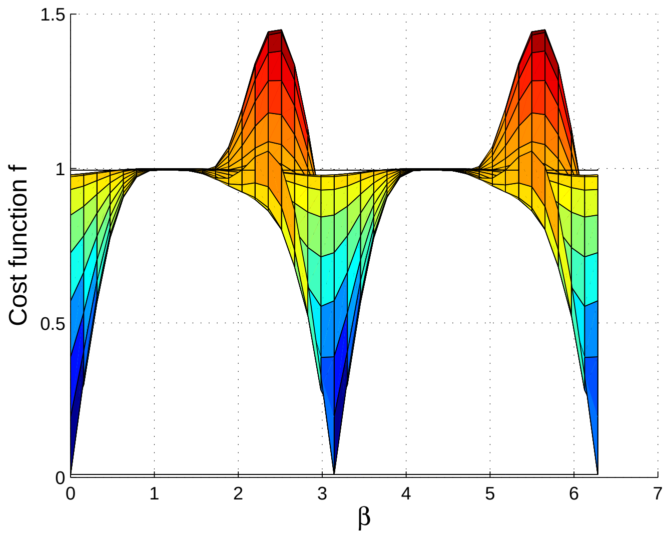
Local optima (1)

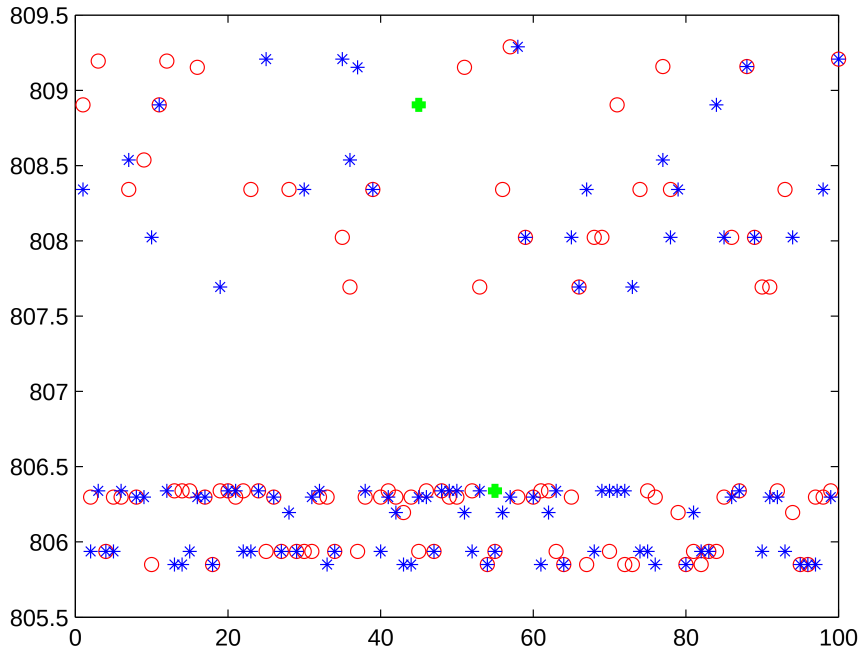
Tensor with dominant rank-(R_1, R_2, R_3) part:

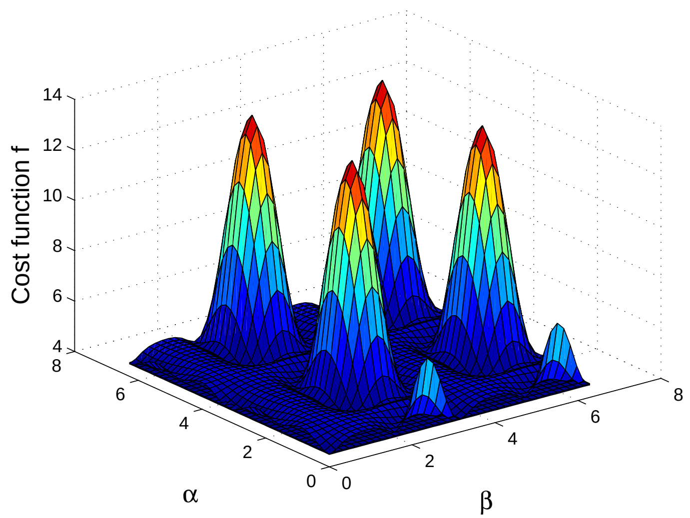


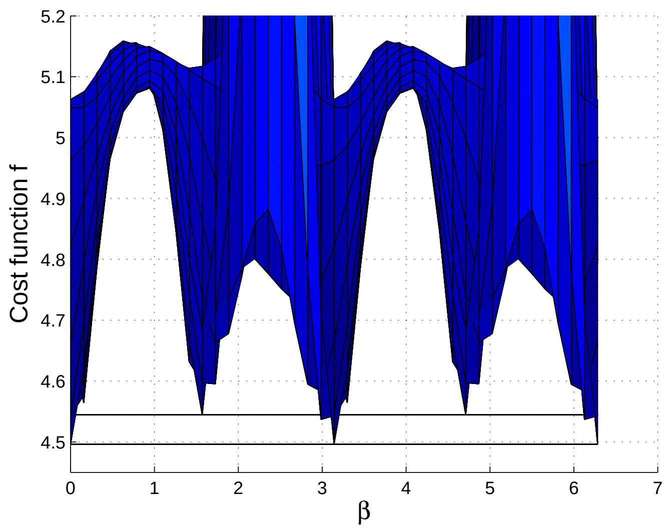


Local optima (2)

Random tensor:







→ inspection of multilinear singular values is important

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Hierarchical Tucker compression

Work in several steps:

- Computation multilinear singular values and vectors
- Standard Tucker compression. Compression ratio dictated by

$$\|\mathcal{A} - \hat{\mathcal{A}}\|^2 \leqslant \sum_{i_1=R_1+1}^{I_1} {\sigma_{i_1}^{(1)}}^2 + \sum_{i_2=R_2+1}^{I_2} {\sigma_{i_2}^{(2)}}^2 + \sum_{i_3=R_3+1}^{I_3} {\sigma_{i_3}^{(3)}}^2$$

- Best rank-$(\tilde{R}_1, \tilde{R}_2, \tilde{R}_3)$ approximation

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  - Applications: dimensionality reduction
    estimation dominant subspace
- Parallel Factor Decomposition
- Block Term Decomposition

Preprocessing for CANDECOMP/PARAFAC decomposition

General principle:

- reduce dimensionality by means of multilinear approximation
- separate the signals in low-dimensional space
- dimensions do not have to be minimal
- transformation matrices are important
- inspection of multilinear singular values

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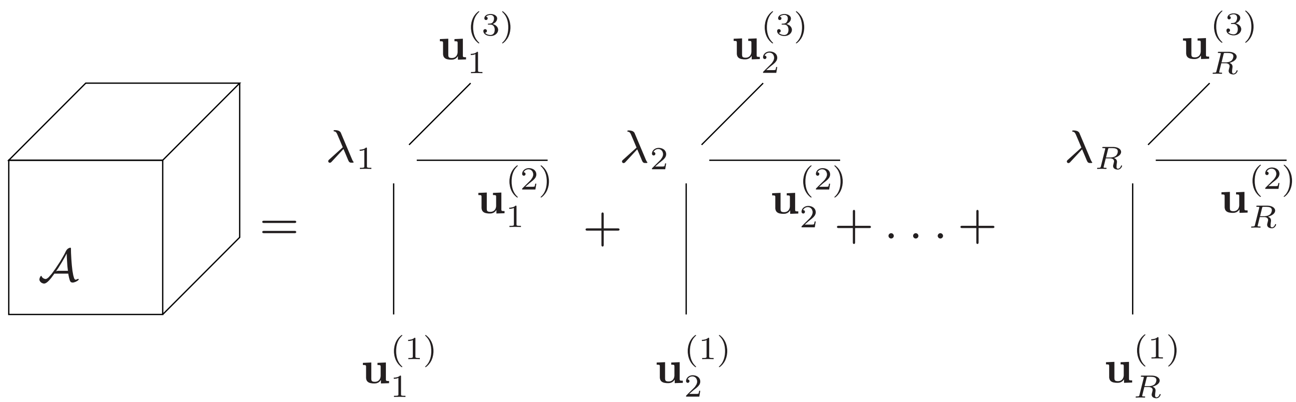
CANDECOMP/PARAFAC

Canonical Decomposition / Parallel Factor Decomposition of a tensor $\mathcal{A}$ is its decomposition in a minimal sum of rank-1 tensors



Matrix formulation:

$$\mathbf{A}_{I_1 I_2 \times I_3} = (\mathbf{U}^{(1)} \odot \mathbf{U}^{(2)}) \cdot \mathbf{\Lambda} \cdot \mathbf{U}^{(3)^T}$$

[*Harshman '70*], [*Carroll and Chang '70*]

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Uniqueness (1)

The k-rank of a matrix $\mathbf{A}$ is the maximal number such that any set of k columns of $\mathbf{A}$ is linearly independent.

Deterministic bound: For $\mathcal{A} \in \mathbb{C}^{I \times J \times K}$ uniqueness if

$$k(\mathbf{U}^{(1)}) + k(\mathbf{U}^{(2)}) + k(\mathbf{U}^{(3)}) \geqslant 2R + 2$$

[*Kruskal '77*], [*Sidiropoulos '00*], [*Stegeman and Sidiropoulos '06*]

Generic bound:

$$\text{min}(I, R) + \text{min}(J, R) + \text{min}(K, R) \geqslant 2R + 2$$

If $K \geqslant R$:

$$R \leqslant \text{min}(I, R) + \text{min}(J, R) - 2 \leqslant I + J - 2$$

Uniqueness (2)

Theorem 1. For $\mathcal{A} \in \mathbb{C}^{I \times J \times K}$ uniqueness if

$$\min(I, R) + \min(J, R) + \min(K, R) \geqslant 2(R + 1)$$

[*Kruskal '77*], [*Sidiropoulos '00*], [*Stegeman and Sidiropoulos '06*]

Theorem 2. For $\mathcal{A} \in \mathbb{C}^{I \times J \times K}$, with $K \geqslant R$, uniqueness if

$$2R(R-1) \leqslant I(I-1)J(J-1)$$

[*De Lathauwer '06*]

(Compare to $R \leqslant \min(I, R) + \min(J, R) - 2 \leqslant I + J - 2$)

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Algorithms (1)

Classical approach: ALS

- Minimize
$$f(\mathbf{A},\mathbf{B},\mathbf{C}) = \|\mathcal{T} - \sum_{r=1}^{R} A_r \circ B_r \circ C_r\|^2$$
by means of Alternating Least Squares (ALS)
- Estimation of R: trial-and-error

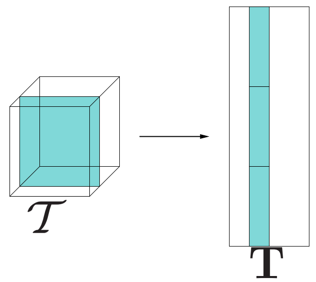
Algorithms (2)

$$f(\mathbf{U}^{(1)}, \mathbf{U}^{(2)}, \mathbf{U}^{(3)}) = \|\mathcal{A} - \sum_{r=1}^{R} \mathbf{u}_r^{(1)} \circ \mathbf{u}_r^{(2)} \circ \mathbf{u}_r^{(3)}\|^2$$

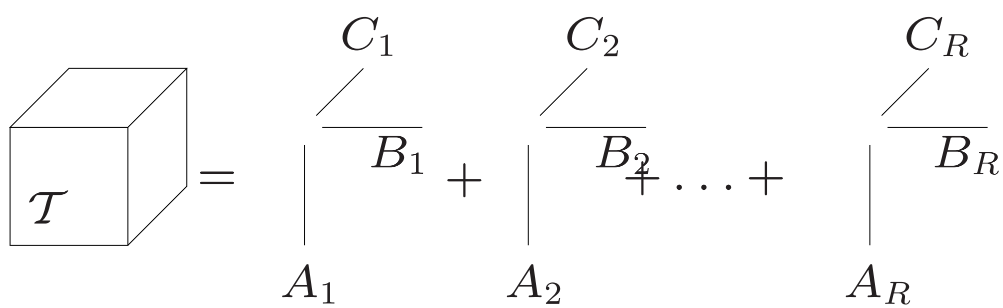
- ALS with Exact Line Search [*Rajih et al. '08*], [*Nion and De Lathauwer '08*]
- ALS with regularization [*Navasca et al. '08*]
- general-purpose optimization:
  - Levenberg-Marquardt
  - conjugate gradient [*Acar et al. '09*]
  - ...
- EVD [*Leurgans et al. '93*], ...
- simultaneous generalized Schur [*De Lathauwer et al. '04*]
- simultaneous matrix diagonalization [*De Lathauwer '06*]
- ...

Simultaneous matrix diagonalization ($K \geqslant R$)

- Matrix representation $\mathbf{T} \in \mathbb{C}^{IJ \times K}$ of $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$:



$$\mathbf{T} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^T = [A_1 \otimes B_1 \ldots A_R \otimes B_R] \cdot \mathbf{C}^T$$



- Matrix representation $\mathbf{T} \in \mathbb{C}^{IJ \times K}$ of $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$:

$$\mathbf{T} = (\mathbf{A} \odot \mathbf{B}) \cdot \mathbf{C}^T = [A_1 \otimes B_1 \ldots A_R \otimes B_R] \cdot \mathbf{C}^T$$

- Determination of tensor rank as matrix rank:
  $R = \text{rank}(\mathbf{T})$ if $\mathbf{A} \odot \mathbf{B}$ and $\mathbf{C}$ full rank
- Other rank-revealing decomposition (e.g. SVD):

$$\mathbf{T} = \mathbf{U} \cdot \mathbf{S} \cdot \mathbf{V}^H$$

$$\mathbf{U} \in \mathbb{C}^{IJ \times R}, \mathbf{S} \in \mathbb{C}^{R \times R}, \mathbf{V} \in \mathbb{C}^{K \times R}$$

- Find $(R \times R)$ nonsingular matrix **W** such that

$$\mathbf{A} \odot \mathbf{B} = (\mathbf{U} \cdot \mathbf{S}) \cdot \mathbf{W} \qquad \mathbf{C}^T = \mathbf{W}^{-1} \cdot \mathbf{V}^H$$

  by imposing rank-1 structure

- Exact data:
  - computation kernel
  - matrix EVD
- Noisy data:
  - computation kernel
  - simultaneous approximate matrix decomposition

[*De Lathauwer '06*]

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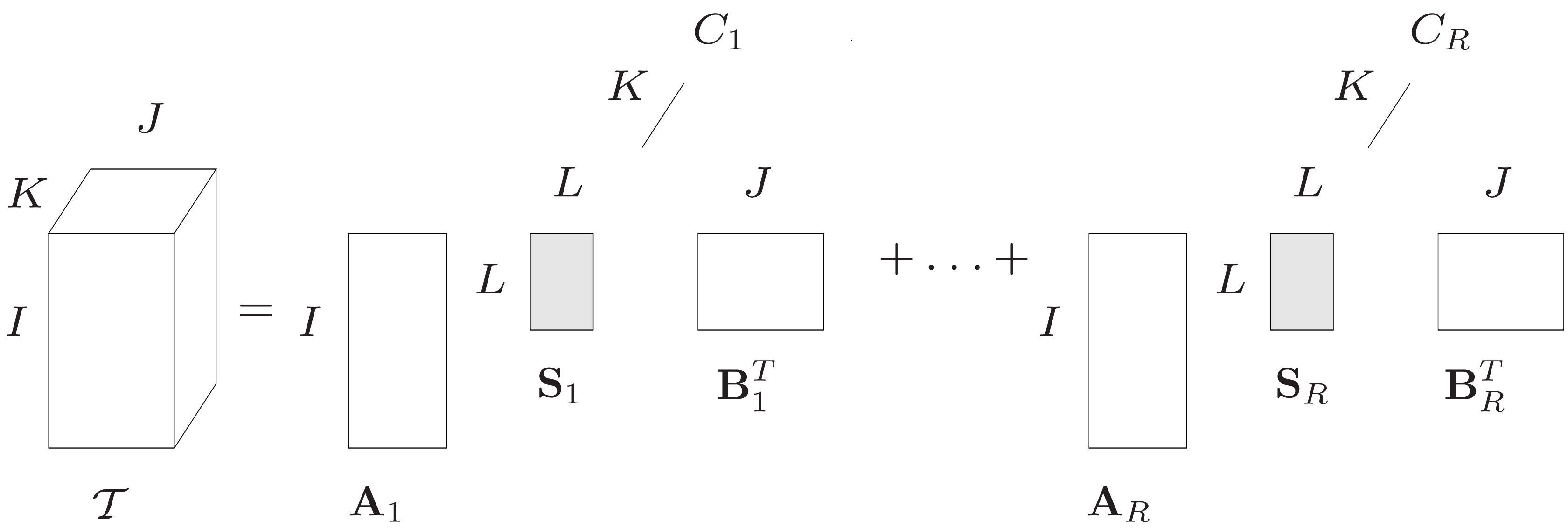
  - Uniqueness
  - Algorithms

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



Uniqueness

$$\min\left(\left\lfloor \frac{I}{L} \right\rfloor, R\right) + \min\left(\left\lfloor \frac{J}{L} \right\rfloor, R\right) + \min(K, R) \geqslant 2R + 2$$

cf. $\min(I, R) + \min(J, R) + \min(K, R) \geqslant 2R + 2$ (PARAFAC)

[*De Lathauwer '08*]

Computation

ALS:

- Minimize
$$f(\mathbf{A}, \mathbf{B}, \mathbf{C}) = \|\mathcal{T} - \sum_{r=1}^{R} (\mathbf{A}_r \cdot \mathbf{B}_r^T) \circ C_r\|^2$$
by means of Alternating Least Squares (ALS)
- Estimation of R, L: trial-and-error

[*De Lathauwer and Nion'08*]

Other algorithms:

- ALS with Exact Line Search [*Nion and De Lathauwer '08*]
- Levenberg-Marquardt [*Nion and De Lathauwer '08*]

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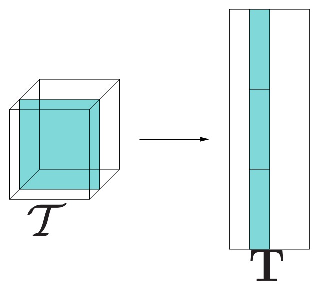
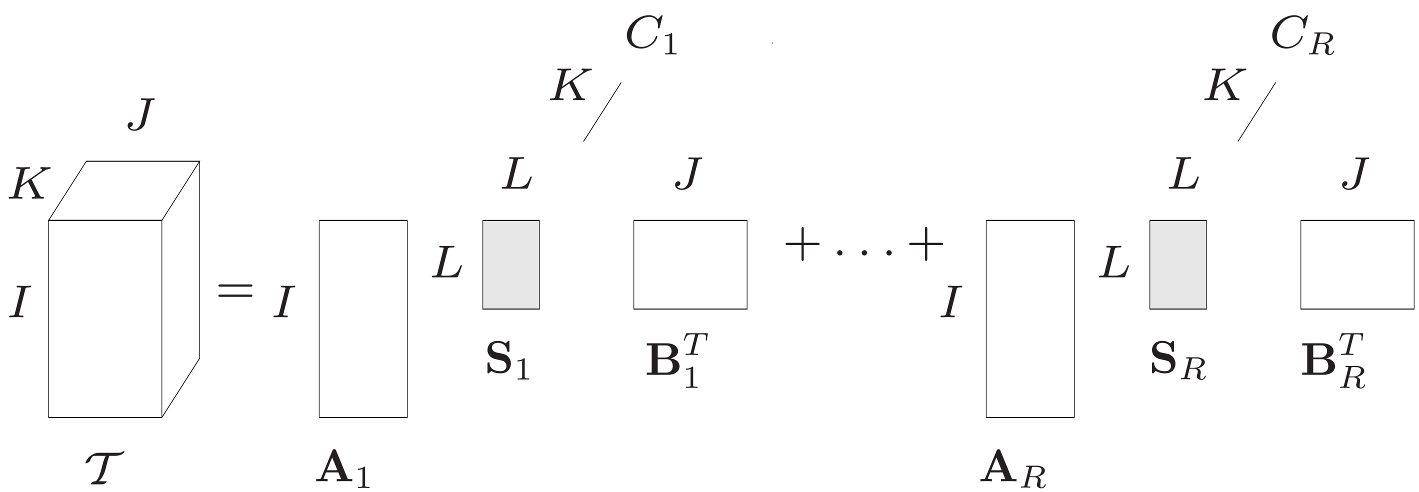


$$\mathbf{T} = \left[\text{vec}(\mathbf{A}_1\mathbf{B}_1^T) \ldots \text{vec}(\mathbf{A}_R\mathbf{B}_R^T)\right] \cdot \mathbf{C}^T$$



- Matrix representation $\mathbf{T} \in \mathbb{C}^{IJ \times K}$ of $\mathcal{T} \in \mathbb{C}^{I \times J \times K}$:

$$\mathbf{T} = \left[\text{vec}(\mathbf{A}_1 \mathbf{B}_1^T) \dots \text{vec}(\mathbf{A}_R \mathbf{B}_R^T) \right] \cdot \mathbf{C}^T$$

- Determination of tensor rank as matrix rank:
$R = \text{rank}(\mathbf{T})$ if $\left[\text{vec}(\mathbf{A}_1 \mathbf{B}_1^T) \dots \text{vec}(\mathbf{A}_R \mathbf{B}_R^T) \right]$ and $\mathbf{C}$ full rank
- Other rank-revealing decomposition (e.g. SVD):

$$\mathbf{T} = \mathbf{U} \cdot \mathbf{S} \cdot \mathbf{V}^H$$

$$\mathbf{U} \in \mathbb{C}^{IJ \times R}, \mathbf{S} \in \mathbb{C}^{R \times R}, \mathbf{V} \in \mathbb{C}^{K \times R}$$

- Find $(R \times R)$ nonsingular matrix $\mathbf{W}$ such that

$$\left[\text{vec}(\mathbf{A}_1 \mathbf{B}_1^T) \dots \text{vec}(\mathbf{A}_R \mathbf{B}_R^T) \right] = (\mathbf{U} \cdot \mathbf{S}) \cdot \mathbf{W} \qquad \mathbf{C}^T = \mathbf{W}^{-1} \cdot \mathbf{V}^H$$

by imposing rank-L structure

- Exact data:
  - computation kernel
  - matrix EVD
- Noisy data:
  - computation kernel
  - simultaneous approximate matrix decomposition

Uniqueness ($K \geqslant R$)

Deterministic conditions:

[• $\left[\text{vec}(\mathbf{A}_1\mathbf{B}_1^T)\ldots\text{vec}(\mathbf{A}_R\mathbf{B}_R^T)\right]$ is full rank]

- $\mathbf{C}$ is full rank
- $\{\Phi\left(\mathbf{A}_t\mathbf{B}_t^T, \mathbf{A}_u\mathbf{B}_u^T, \mathbf{A}_v\mathbf{B}_v^T\right)\}$ linearly independent

Generic condition:

$$R(R-1)(R-2) \leqslant \frac{1}{6}I(I-1)(I-2)J(J-1)(J-2) \qquad K \geqslant R$$

Conclusion

- Tucker decomposition or multilinear SVD
  - Local optima
  - Inspection of multilinear singular values
  - Hierarchical Tucker compression
  - Numerical algorithms
- Parallel factor decomposition
  - Relaxed uniqueness condition
  - Determination of tensor rank as matrix rank
  - Exact data: computation based on standard linear algebra
  - Noisy data: computation based on simultaneous approximate matrix decomposition

- Decomposition in rank-$(L, L, 1)$ terms
  - Definition
  - Uniqueness conditions
  - Determination of R as matrix rank
  - Exact data: computation based on standard linear algebra
  - Noisy data: computation based on simultaneous approximate matrix decomposition

Announcement

International Conference on
Tensor Decompositions and Applications (TDA 2010)
Sept. 13–17, 2010
Monopoli (Bari), Italy