A new truncation strategy for the higher-order singular value decomposition

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Workshop on Matrix Equations and Tensor Techniques
RWTH Aachen, Germany

November 21, 2011

Joint work with Raf Vandebril and Karl Meerbergen

1. Introduction
   - Context
   - Notation
2. Orthogonal Tucker approximation
3. Truncated HOSVD
4. Sequentially truncated HOSVD
   - Definition
   - Operation count
   - Approximation error
5. Numerical examples
   - Compression of images
   - Handwritten digit classification
   - Compression of simulation results
6. Conclusions

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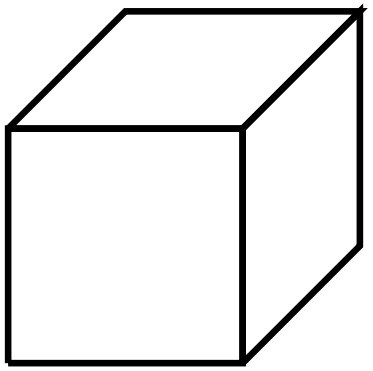
Context I — Everything is a tensor

$d = 0$ Scalar $a =$

$d = 1$ Vector $\mathbf{a} =$

$d = 2$ Matrix $A =$

$d \geq 3$ Tensor $\mathcal{A} =$



Context II – Everything is a tensor

Multidimensional data appears in many applications:

- image and signal processing,
- pattern recognition, data mining and machine learning,
- chemometrics,
- biomedicine,
- psychometrics, ...

Two major problems associated with this data:

1. Storage cost is very high, and
2. analysis and interpretation of patterns and phenomena in data.

Context III — Tensor decompositions for compression

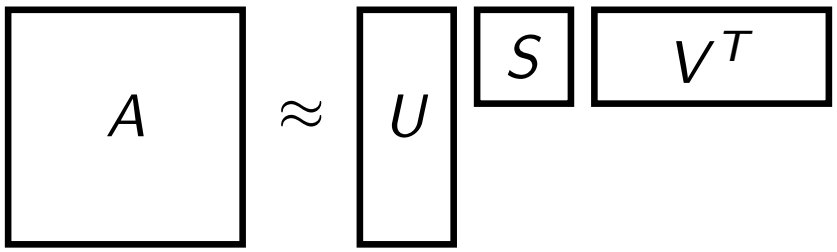
Stable tensor decompositions suitable for **compression** in the

- Low-dimensional case:
  - Tucker (Tucker 1966),
  - Higher-Order SVD (De Lathauwer *et al* 2000),
  - Cross-approximation (Oseledets *et al.* 2008),
  - Sequentially Truncated HOSVD (Vannieuwenhoven *et al.* 2011).
- High-dimensional case:
  - Hierarchical Tucker (Hackbusch and Kühn 2009, Grasedyck 2010),
  - Tensor-Train (Oseledets 2011).

Context IV — Compression

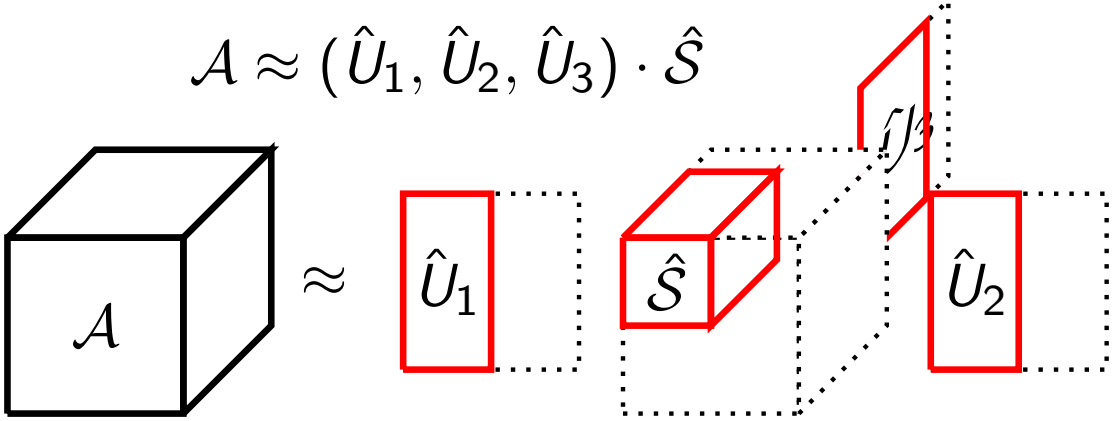
Low-rank representation of matrices by SVD:

$$A \approx USV^T := (U, V) \cdot S$$



Low-rank representation of tensors by Tucker:

$$\mathcal{A} \approx (\hat{U}_1, \hat{U}_2, \hat{U}_3) \cdot \hat{\mathcal{S}}$$



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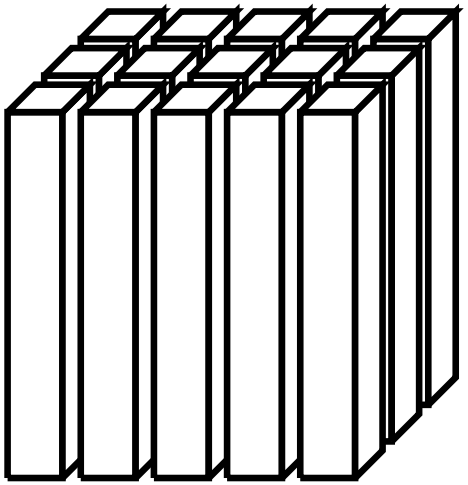
Notation I — Mode k vector space

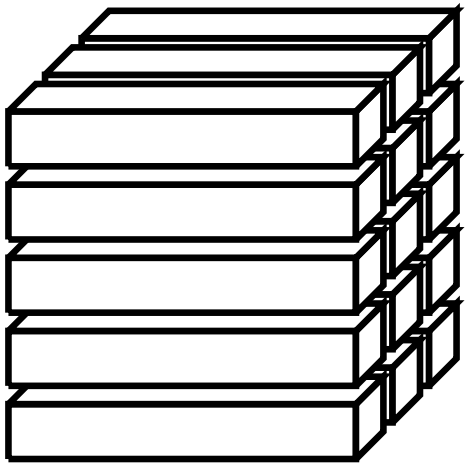
A *tensor* $\mathcal{A}$ of order d is an object in the tensor product of d vector spaces:

$$\mathcal{A} \in \mathbb{R}^{n_1} \otimes \mathbb{R}^{n_2} \otimes \cdots \otimes \mathbb{R}^{n_d} \sim \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$$

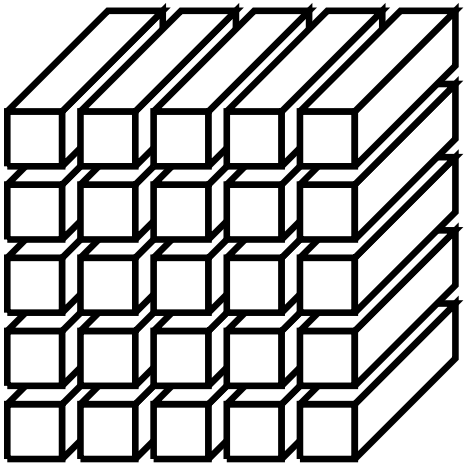
A 3rd order tensor has 3 associated vector spaces:



Mode 1 vectors ($\mathbb{R}^{n_1}$)



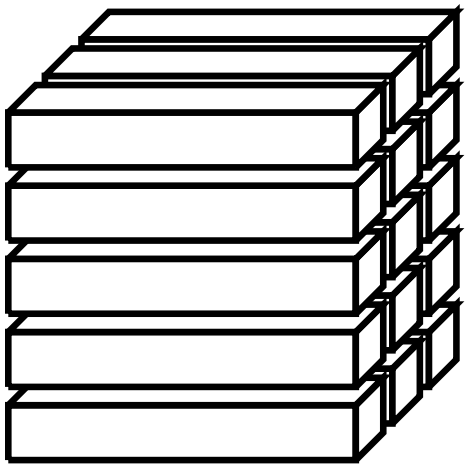
Mode 2 vectors ($\mathbb{R}^{n_2}$)



Mode 3 vectors ($\mathbb{R}^{n_3}$)

Notation II — Unfolding

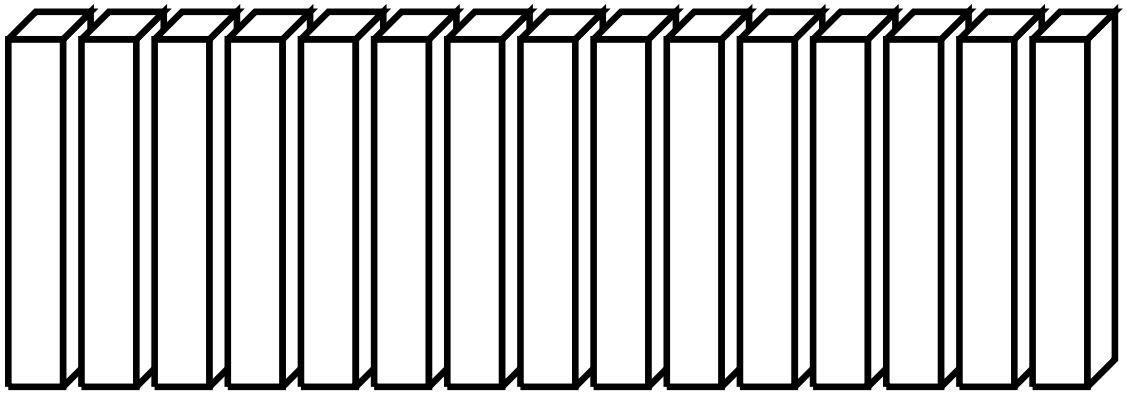
$\mathcal{A} =$



$\in \mathbb{R}^{n_1 \times n_2 \times n_3}$

Mode 2 unfolding

$\mathcal{A}_{(2)} =$



$\in \mathbb{R}^{n_2 \times n_1 n_3}$

Notation III

Frobenius norm:

$$\|\mathcal{A}\|^2 := \sum_{i_1,i_2,i_3} \mathcal{A}^2_{i_1,i_2,i_3}.$$

Multilinear multiplication:

$$[(I, M_2, I) \cdot \mathcal{A}]_{(2)} := M_2 \mathcal{A}_{(2)}.$$
$$(M_1, M_2, M_3) \cdot \mathcal{A} := (M_1, I, I) \cdot (I, M_2, I) \cdot (I, I, M_3) \cdot \mathcal{A}.$$

Projection of mode 2 vectors on span of U_2 (orthogonal columns):

$$\pi_2 \mathcal{A} := (I, U_2 U_2^T, I) \cdot \mathcal{A}$$

Projection of mode 2 vectors on complement of U_2:

$$\pi_2^{\perp} \mathcal{A} := \mathcal{A} - \pi_2 \mathcal{A}$$

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Orthogonal Tucker approximation problem

Best rank-(r_1, r_2, r_3) approximation problem:

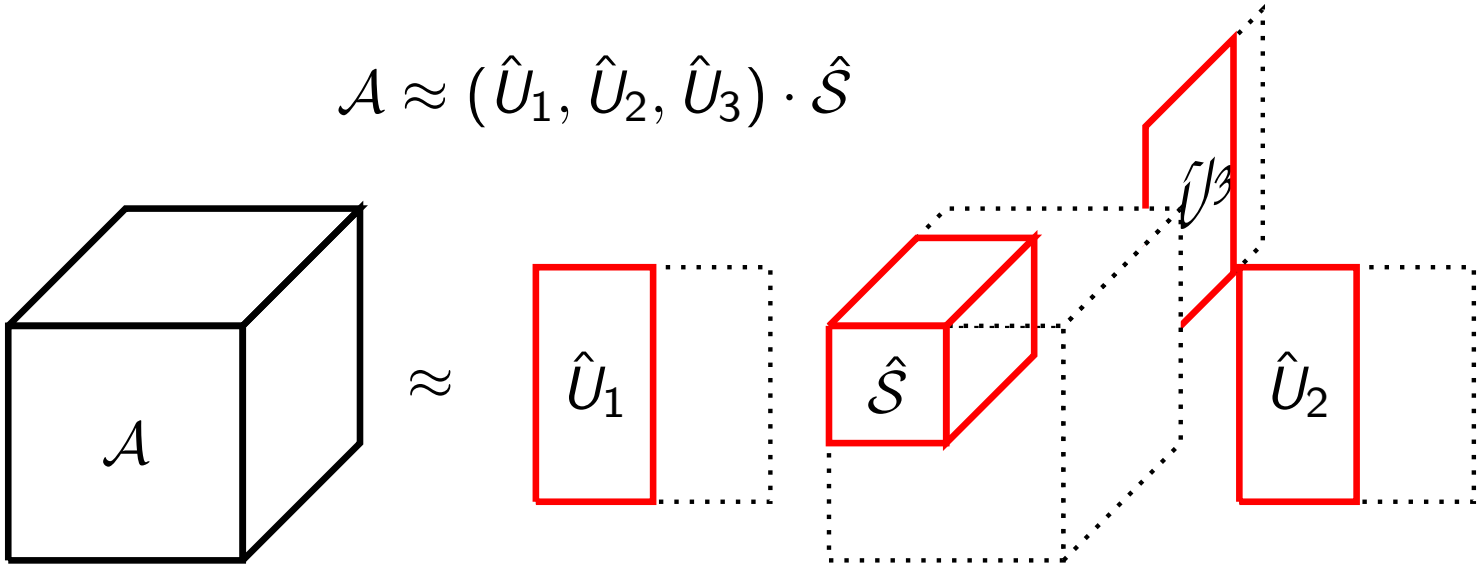
$$\min_{\text{rank}(\mathcal{B}) \leq (r_1, r_2, r_3)} \|\mathcal{A} - \mathcal{B}\|_F = \min_{U_i \in O(n_i, r_i)} \left\| \mathcal{A} - (U_1 U_1^T, U_2 U_2^T, \ldots, U_d U_d^T) \cdot \mathcal{A} \right\|_F .$$

with $O(n_i, r_i)$ the group of $n_i \times r_i$ matrices with orthonormal columns.

- Optimum is found by **orthogonal projection** onto a new, optimal tensor basis, but
- no closed solution known.

Orthogonal Tucker approximation I — Definition

$$\mathcal{A} \approx (\hat{U}_1, \hat{U}_2, \hat{U}_3) \cdot \hat{\mathcal{S}}$$



Rank (r_1, r_2, r_3) orthogonal Tucker approximation to $\mathcal{A}$

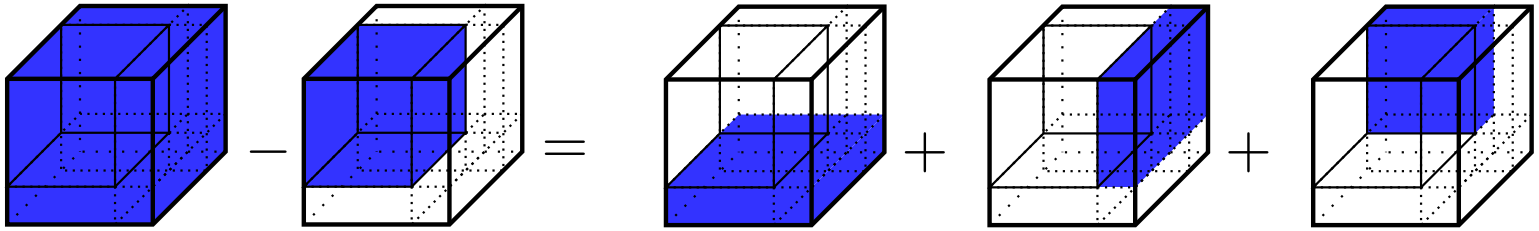
Columns of $\begin{cases} \hat{U}_1 \in \mathbb{R}^{n_1 \times r_1} \\ \hat{U}_2 \in \mathbb{R}^{n_2 \times r_2} \\ \hat{U}_3 \in \mathbb{R}^{n_3 \times r_3} \end{cases}$ can be extended to a basis of $\begin{cases} \mathbb{R}^{n_1} \\ \mathbb{R}^{n_2} \\ \mathbb{R}^{n_3} \end{cases}$

Orthogonal Tucker approximation II — Error [VVM2011]

If

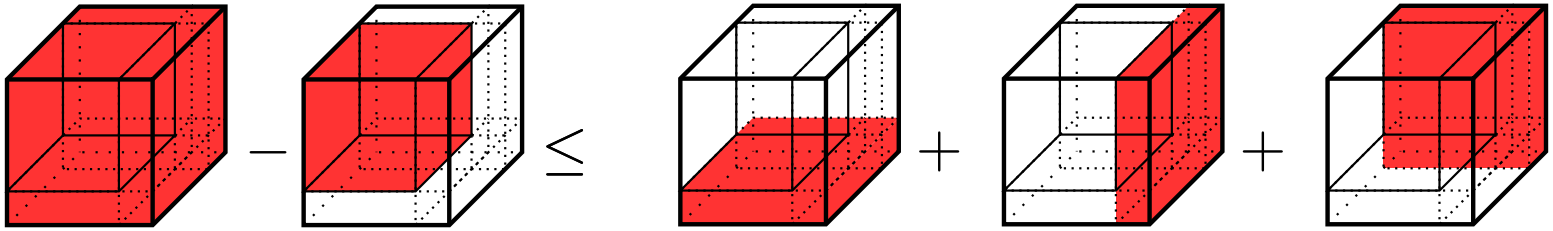
$$\mathcal{A} \approx \hat{\mathcal{A}} := \pi_1\pi_2\pi_3\mathcal{A} = (U_1U_1^T, U_2U_2^T, U_3U_3^T) \cdot \mathcal{A}.$$

Then an error expression is



$$\|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 = \|\pi_2^\perp\mathcal{A}\|^2 + \|\pi_1^\perp\pi_2\mathcal{A}\|^2 + \|\pi_3^\perp\pi_1\pi_2\mathcal{A}\|^2$$

with upper bound



$$\|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 \quad \|\pi_2^\perp\mathcal{A}\|^2 + \|\pi_1^\perp\mathcal{A}\|^2 + \|\pi_3^\perp\mathcal{A}\|^2$$

Orthogonal Tucker approximation II — Error [VVM2011]

If

$$\mathcal{A} \approx \hat{\mathcal{A}} := \pi_1\pi_2\pi_3\mathcal{A} = (U_1U_1^T, U_2U_2^T, U_3U_3^T) \cdot \mathcal{A}.$$

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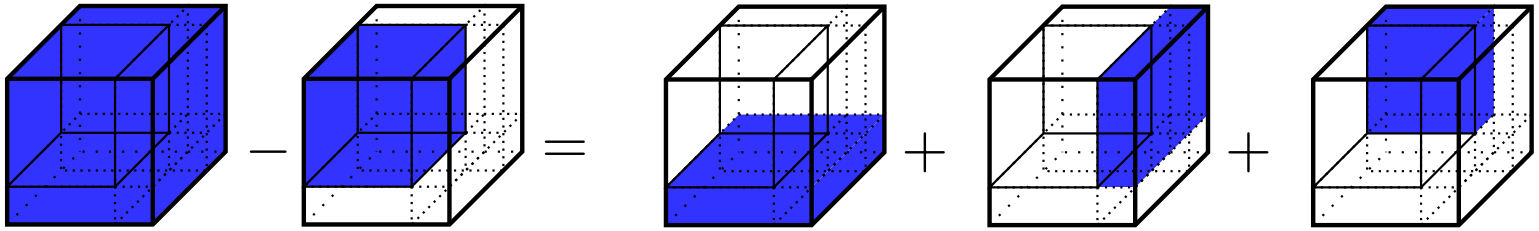
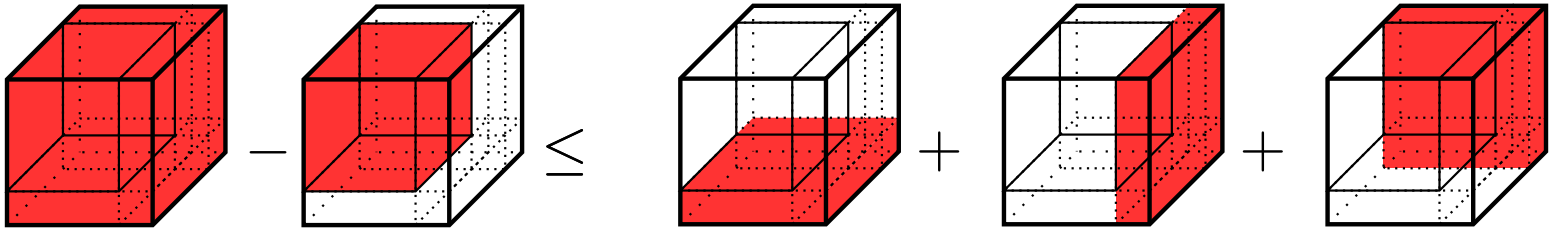


$$\|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 = \|\pi_2^\perp\mathcal{A}\|^2 + \|\pi_1^\perp\pi_2\mathcal{A}\|^2 + \|\pi_3^\perp\pi_1\pi_2\mathcal{A}\|^2$$

with upper bound



$$\|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 \quad \|\pi_2^\perp\mathcal{A}\|^2 + \|\pi_1^\perp\mathcal{A}\|^2 + \|\pi_3^\perp\mathcal{A}\|^2$$

Dependence on the **processing order** of the modes.

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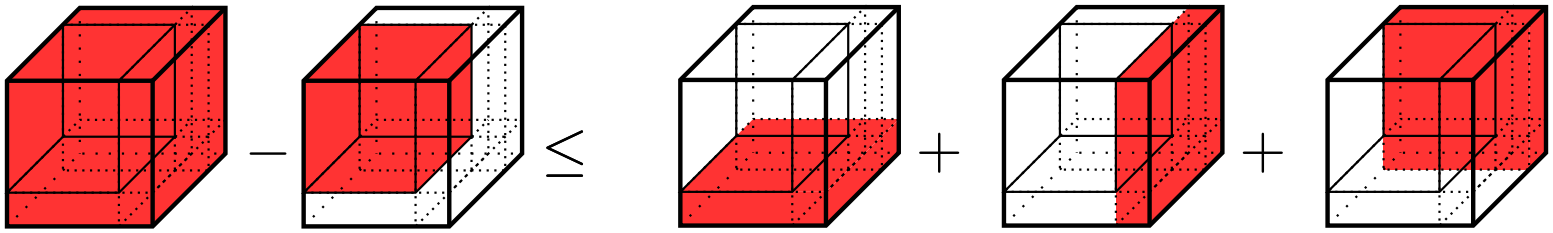
Truncated Higher-Order SVD (T-HOSVD) [DDV2000]

Recall upper bound?



$$\|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 \quad \|\pi_2^\perp\mathcal{A}\|^2 + \|\pi_1^\perp\mathcal{A}\|^2 + \|\pi_3^\perp\mathcal{A}\|^2$$

Minimize it!

$$\min_{\pi_1,\pi_2,\pi_3} \|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 \leq \min_{\pi_1,\pi_2,\pi_3} \sum_{k=1}^{3} \|\pi_k^\perp\mathcal{A}\|^2,$$

$$= \sum_{k=1}^{3} \min_{\pi_k} \|\pi_k^\perp\mathcal{A}\|^2.$$

Minimum given by r_k first singular vectors in every mode k!

Algorithm

Rank (r_1, r_2, r_3) T-HOSVD:

for every mode k **do**

Compute rank r_k truncated SVD:

$$\mathcal{A}_{(k)} = \begin{bmatrix} \bar{U}_k & \bar{U}_k^{\perp} \end{bmatrix} \begin{bmatrix} \bar{S}_k & \\ & \bar{S}_k^{\perp} \end{bmatrix} \begin{bmatrix} \bar{V}_k & \bar{V}_k^{\perp} \end{bmatrix}^T$$

end for

Project:

$$\bar{\mathcal{S}} = (\bar{U}_1^T, \bar{U}_2^T, \bar{U}_3^T) \cdot \mathcal{A}$$

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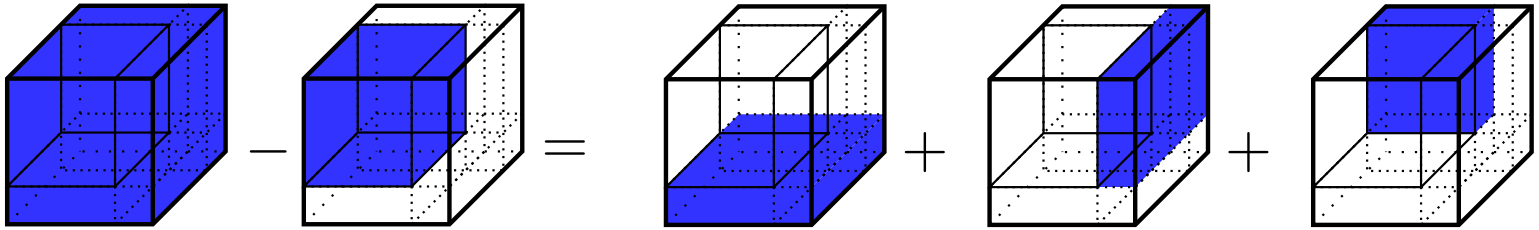
Sequentially truncated HOSVD (ST-HOSVD) [VVM2011]

Recall error expression?



$$\|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 = \|\pi_2^\perp\mathcal{A}\|^2 + \|\pi_1^\perp\pi_2\mathcal{A}\|^2 + \|\pi_3^\perp\pi_1\pi_2\mathcal{A}\|^2$$

(Try to) minimize it!

$$\min_{\pi_1,\pi_2,\pi_3} \|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2$$

$$= \min_{\pi_1,\pi_2,\pi_3} \left[\|\pi_1^\perp\mathcal{A}\|^2 + \|\pi_2^\perp\pi_1\mathcal{A}\|^2 + \|\pi_3^\perp\pi_1\pi_2\mathcal{A}\|^2\right]$$

$$= \min_{\pi_1} \left[\|\pi_1^\perp\mathcal{A}\|^2 + \min_{\pi_2} \left[\|\pi_2^\perp\pi_1\mathcal{A}\|^2 + \min_{\pi_3} \|\pi_3^\perp\pi_1\pi_2\mathcal{A}\|^2\right]\right]$$

Sequentially truncated HOSVD (ST-HOSVD) [VVM2011]

The sequentially truncated HOSVD computes solution to

$$\pi_1^* = \arg\min_{\pi_1} \|\pi_1^\perp \mathcal{A}\|^2$$
$$\pi_2^* = \arg\min_{\pi_2} \|\pi_2^\perp \pi_1^* \mathcal{A}\|^2$$
$$\pi_3^* = \arg\min_{\pi_3} \|\pi_3^\perp \pi_1^* \pi_2^* \mathcal{A}\|^2$$

π_k^* given by r_k first singular vectors of $[\pi_1^* \cdots \pi_{k-1}^* \mathcal{A}]_{(k)}$!

Algorithm

Rank (r_1, r_2, r_3) ST-HOSVD:

$\hat{\mathcal{S}} = \mathcal{A}$

for every mode k **do**

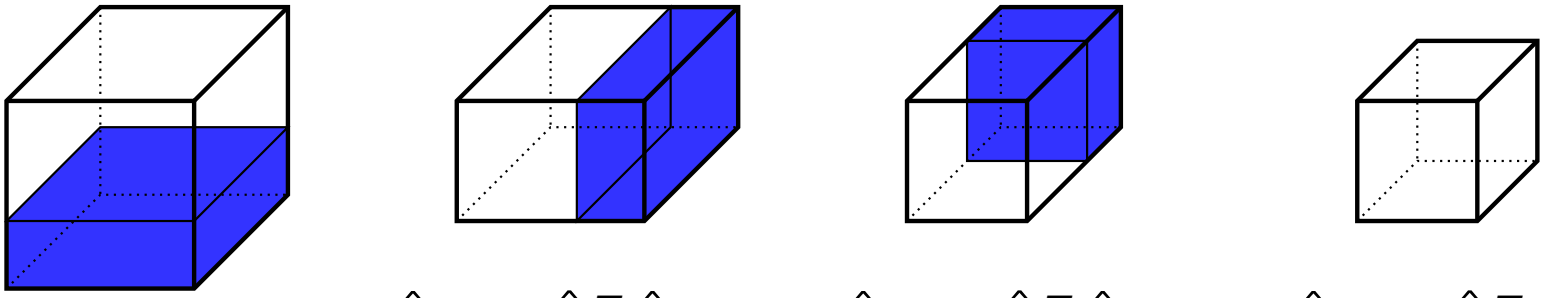
Compute rank r_k truncated SVD:

$$\hat{\mathcal{S}}_{(k)} = \begin{bmatrix} \hat{U}_k & \hat{U}_k^{\perp} \end{bmatrix} \begin{bmatrix} \hat{S}_k & \\ & \hat{S}_k^{\perp} \end{bmatrix} \begin{bmatrix} \hat{V}_k & \hat{V}_k^{\perp} \end{bmatrix}^T$$

Project:

$$\hat{\mathcal{S}}_{(k)} = \hat{U}_k^T \hat{\mathcal{S}}_{(k)}$$

end for



$\hat{\mathcal{S}} = \mathcal{A}$ $\quad$ $\hat{\mathcal{S}}_{(1)} = \hat{U}_1^T \hat{\mathcal{S}}_{(1)}$ $\quad$ $\hat{\mathcal{S}}_{(2)} = \hat{U}_2^T \hat{\mathcal{S}}_{(2)}$ $\quad$ $\hat{\mathcal{S}}_{(3)} = \hat{U}_3^T \hat{\mathcal{S}}_{(3)}$

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Operation count

Theorem

Let $\mathcal{A} \in \mathbb{R}^{n \times n \times \cdots \times n}$ be truncated to rank $(r, r, \ldots, r)$ by the ST-HOSVD and T-HOSVD. Assume an $O(m^2 n)$ algorithm to compute the SVD of an $m \times n$ matrix, $m \leq n$. Then, the ST-HOSVD requires

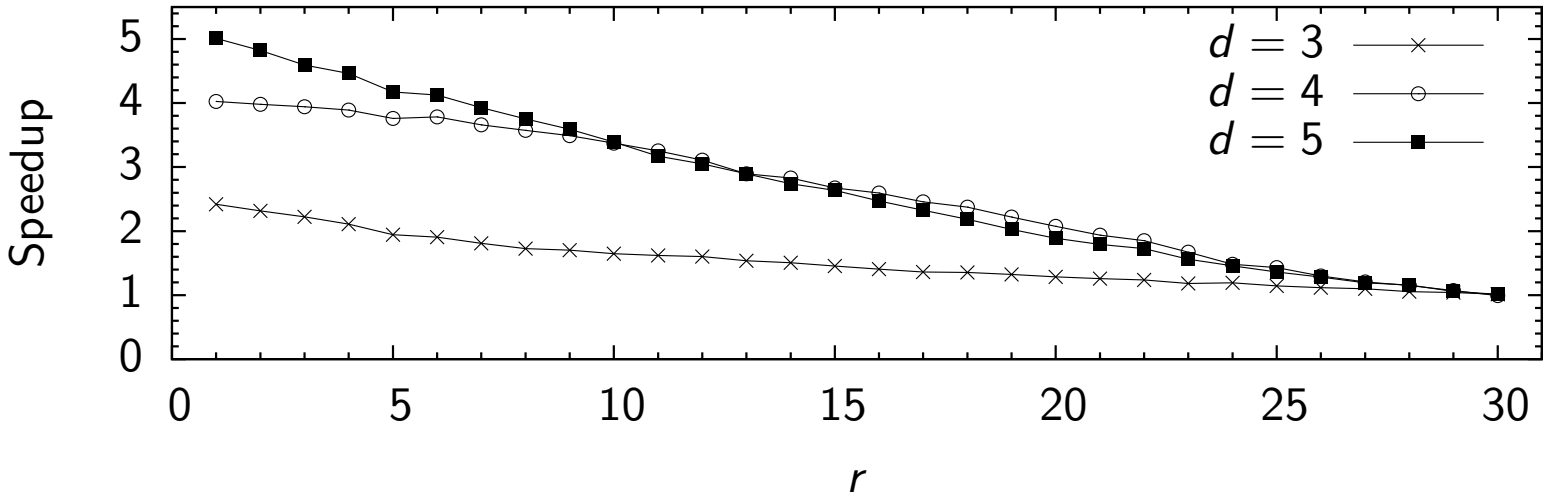
$$O\left(\sum_{k=1}^{d} r^{k-1} n^{d-k+2} + \sum_{k=1}^{d} r^k n^{d-k}\right)$$

operations, and T-HOSVD requires

$$O\left(dn^{d+1} + \sum_{k=1}^{d} r^k n^{d-k+1}\right)$$

operations to compute the approximation.

Operation count



Speedup of ST-HOSVD over T-HOSVD for an order-d tensor of size $30 \times 30 \times \cdots \times 30$ which is truncated to rank $(r, r, \ldots, r)$.

Speedups greater than d possible with non-cubic tensors.

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Approximation error I — Hypothesis

Hypothesis

Let $\mathcal{A}^*$ be an ST-HOSVD approximation, and $\mathcal{A}^*$ the T-HOSVD approximation of corresponding rank. Then,

$$\|\mathcal{A} - \mathcal{A}^*\|_F \overset{?}{\leq} \|\mathcal{A} - \mathcal{A}^*\|_F.$$

Not valid in general.

Approximation error II — Counterexample

Rank-$(1,1,1,1)$ approximation of

$$\mathcal{A}_{:,:,1,1} = \begin{bmatrix} 0.5 & -1.7 \\ -1.3 & -0.6 \end{bmatrix}, \qquad \mathcal{A}_{:,:,2,1} = \begin{bmatrix} -2.4 & -0.1 \\ -0.7 & 1.4 \end{bmatrix},$$

$$\mathcal{A}_{:,:,1,2} = \begin{bmatrix} 0.1 & 0.1 \\ 2.2 & -0.8 \end{bmatrix}, \qquad \mathcal{A}_{:,:,2,2} = \begin{bmatrix} -0.3 & -2.5 \\ 0.0 & 0.3 \end{bmatrix}.$$

T-HOSVD:

$$\mathcal{A}^* = \left(\begin{bmatrix} -0.97325 \\ -0.22975 \end{bmatrix}, \begin{bmatrix} -0.78940 \\ 0.61388 \end{bmatrix}, \begin{bmatrix} -0.31546 \\ 0.94894 \end{bmatrix}, \begin{bmatrix} -0.88167 \\ 0.47186 \end{bmatrix} \right) \cdot \begin{bmatrix} 2.57934 \end{bmatrix}.$$

ST-HOSVD:

$$\mathcal{A}^* = \left(\begin{bmatrix} -0.97325 \\ -0.22975 \end{bmatrix}, \begin{bmatrix} -0.97310 \\ 0.23037 \end{bmatrix}, \begin{bmatrix} -0.09956 \\ 0.99503 \end{bmatrix}, \begin{bmatrix} -0.99692 \\ 0.07841 \end{bmatrix} \right) \cdot \begin{bmatrix} 2.53595 \end{bmatrix}.$$

The approximation errors:

$$\|\mathcal{A} - \mathcal{A}^*\|_F^2 = 18.68700 \quad \text{and} \quad \|\mathcal{A} - \mathcal{A}^*\|_F^2 = 18.90896,$$

Approximation error III — Sufficient condition

Theorem

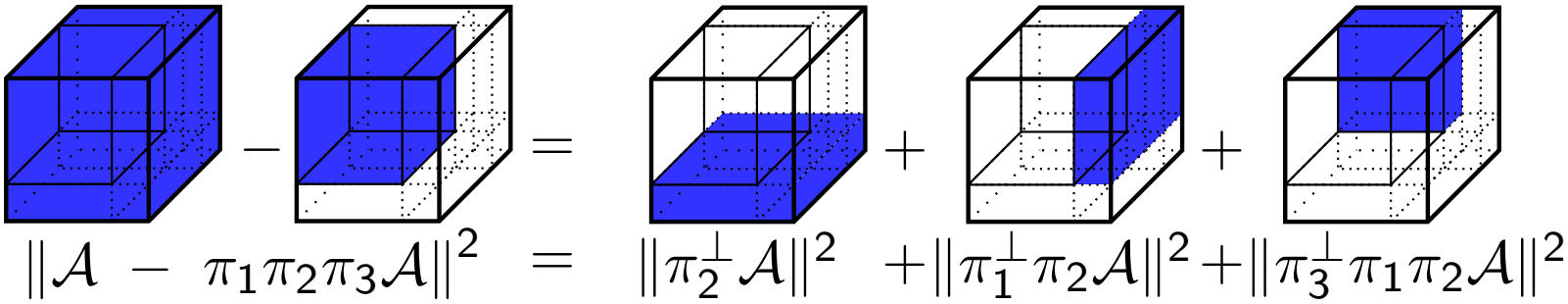
Let $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$. Let $\mathcal{A}^*$ be the rank-$(1, r, r)$ ST-HOSVD of $\mathcal{A}$ and let $\mathcal{A}^*$ be the T-HOSVD of $\mathcal{A}$ of the same rank. Then,

$$\|\mathcal{A} - \mathcal{A}^*\|_F \leq \|\mathcal{A} - \mathcal{A}^*\|_F.$$

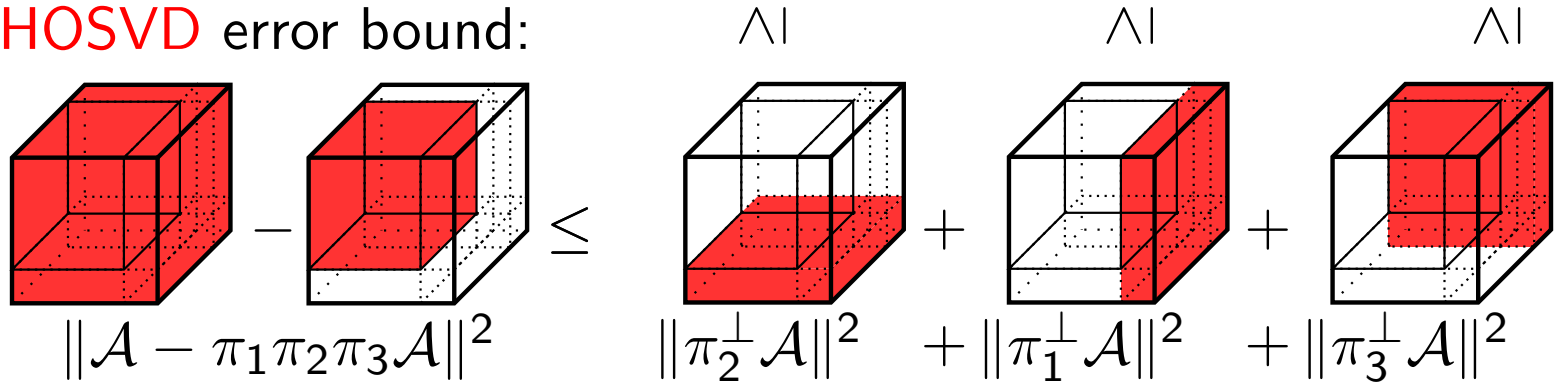
ST-HOSVD yields better rank-1 approximation for order-3 tensors.

Approximation error IV — Bounds

ST-HOSVD error bound:

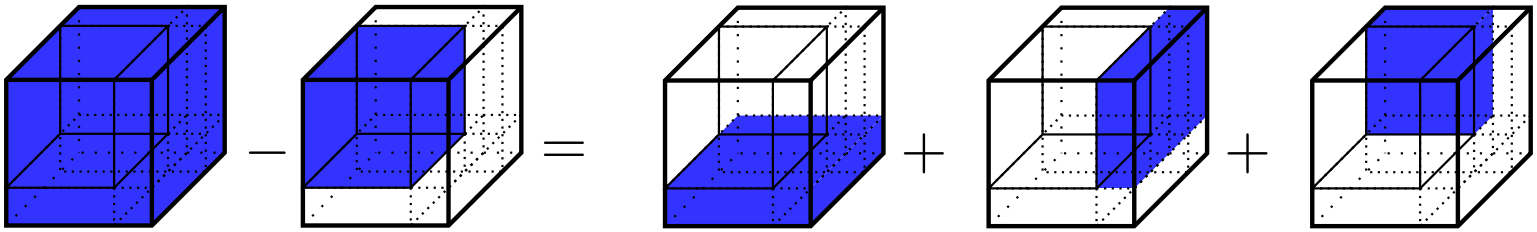


T-HOSVD error bound:



Approximation error IV — Bounds

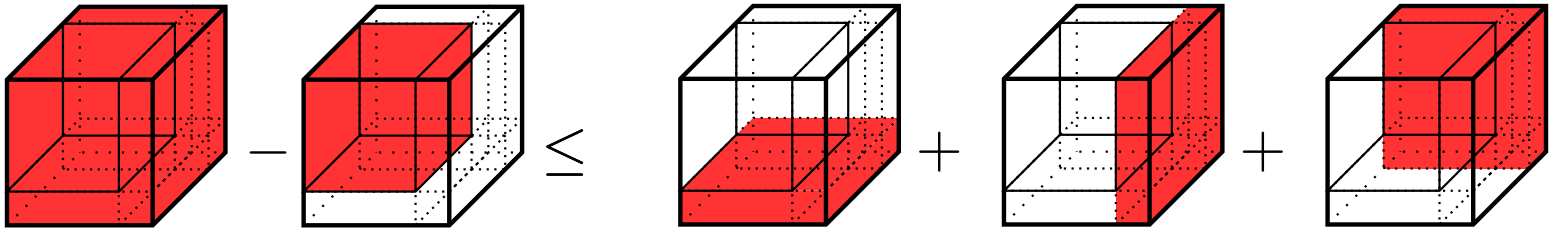
ST-HOSVD error bound:



$$\|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 = \|\pi_2^\perp\mathcal{A}\|^2 + \|\pi_1^\perp\pi_2\mathcal{A}\|^2 + \|\pi_3^\perp\pi_1\pi_2\mathcal{A}\|^2$$

T-HOSVD error bound:

$\wedge|$ $\wedge|$ $\wedge|$



$$\|\mathcal{A} - \pi_1\pi_2\pi_3\mathcal{A}\|^2 \leq \|\pi_2^\perp\mathcal{A}\|^2 + \|\pi_1^\perp\mathcal{A}\|^2 + \|\pi_3^\perp\mathcal{A}\|^2$$

Both bounded by:

$$\|\mathcal{A} - \mathcal{A}^*\|_F \leq \sqrt{d}\|\mathcal{A} - \mathcal{A}^{\text{opt}}\|_F.$$

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Compression of images I

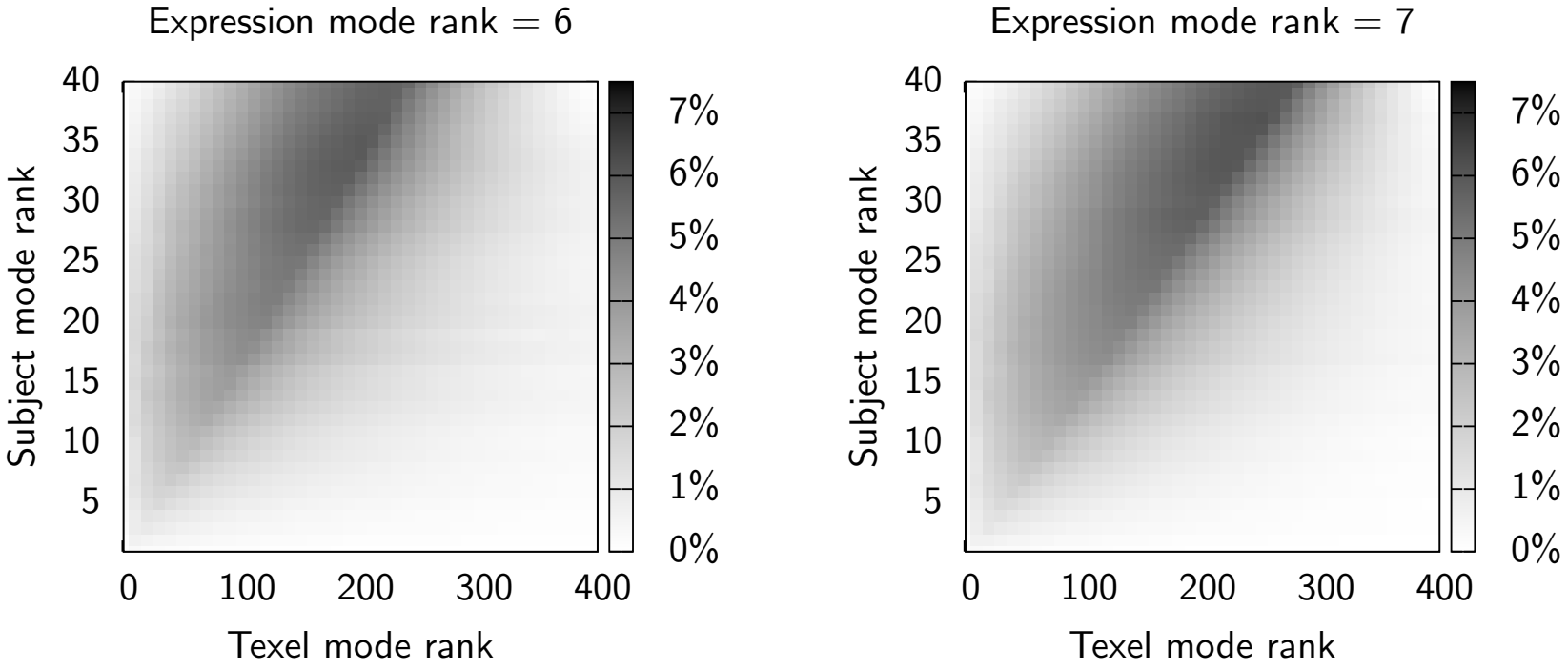
Compression of the Olivetti Research Laboratory faces database [SH1994, VT2003].

Tensor of size $10304 \times 40 \times 10$ (Texel $\times$ Subject $\times$ Expression).

- Unstructured, 4.1 million nonzeros.
- HOOI, T-HOSVD and ST-HOSVD approximations of 6560 different ranks.

Compression of images II

Relative difference between approximation error of T-HOSVD and HOOI: $(\mathrm{err}_{\mathrm{HOSVD}} - \mathrm{err}_{\mathrm{HOOI}})/\mathrm{err}_{\mathrm{HOOI}}$.

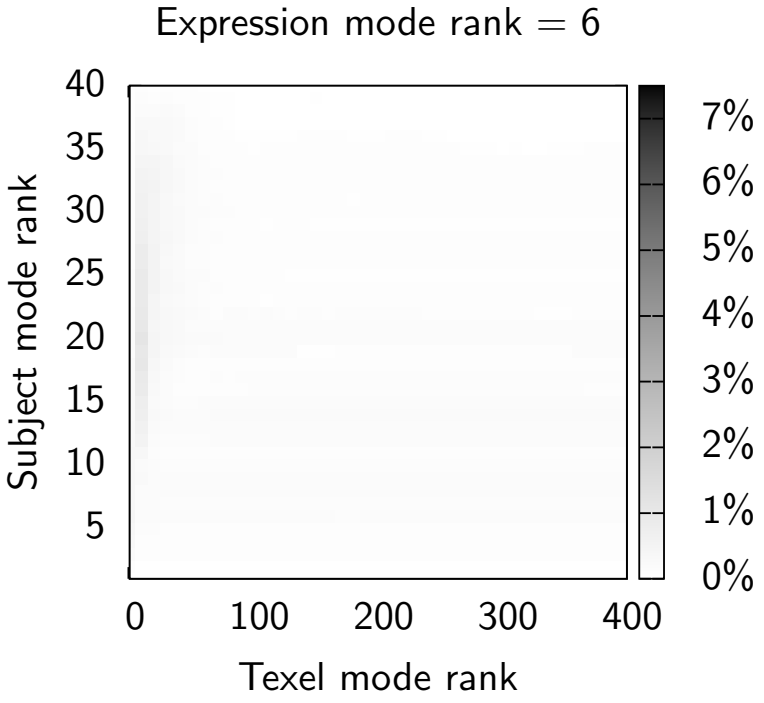


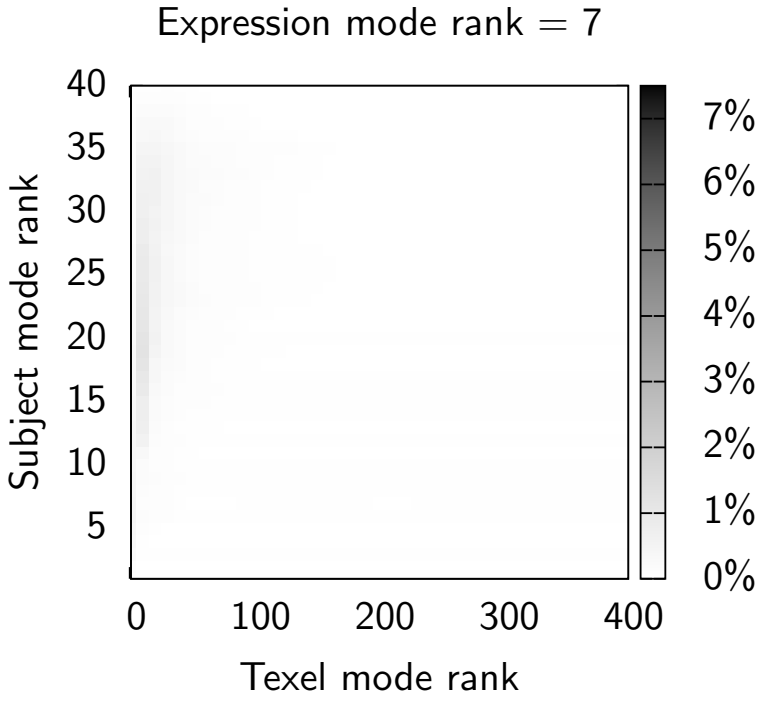
Average relative error: 2.115%

Maximum relative error: 6.340%

Compression of images II

Relative difference between approximation error of ST-HOSVD and HOOI: $(\mathrm{err}_{\mathrm{HOSVD}} - \mathrm{err}_{\mathrm{HOOI}})/\mathrm{err}_{\mathrm{HOOI}}$.





Average relative error: 0.099%

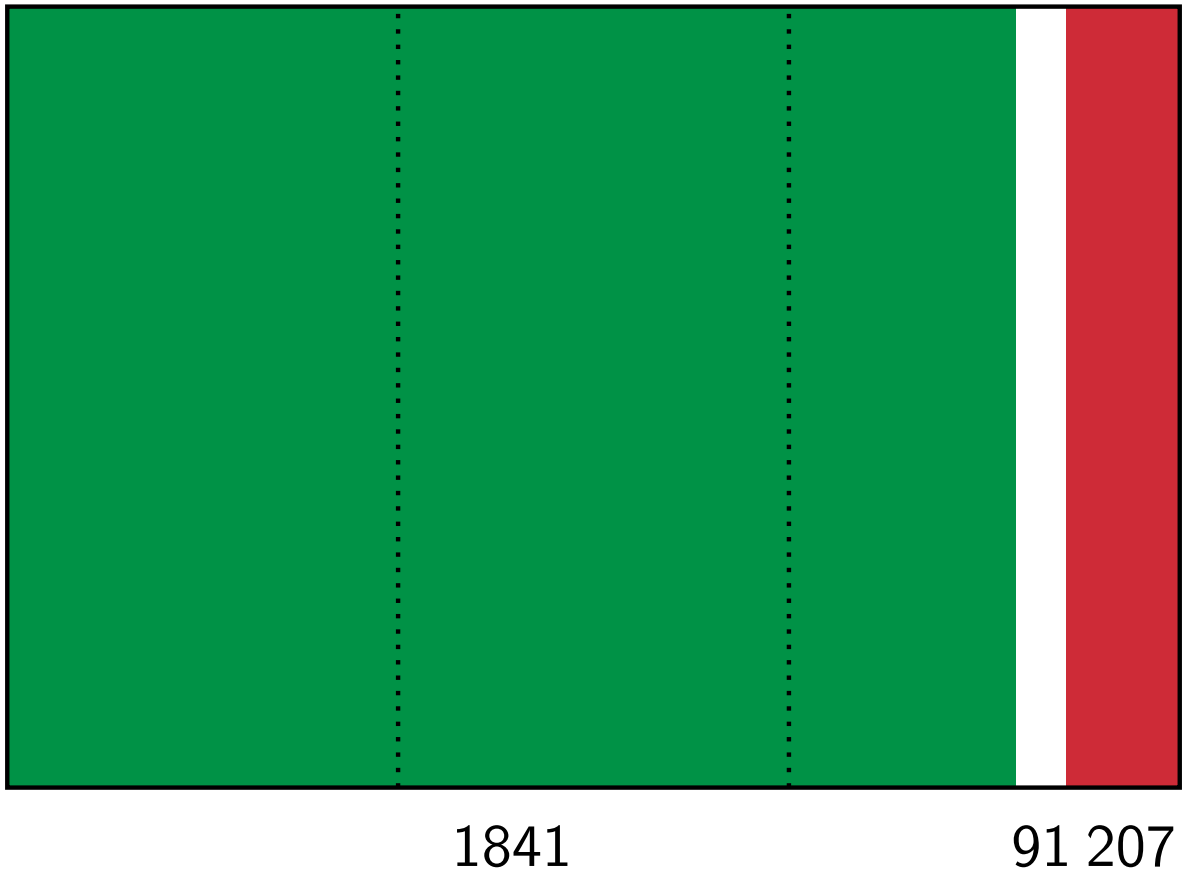
Maximum relative error: 1.012%

Dinner tonight

La Finestra at 19h30!

Compression of images III

Total compression time (min) of
HOOI, ST-HOSVD and T-HOSVD:



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Handwritten digit classification I

Classification of handwritten digits by T-HOSVD [SE2007].

Tensor of size $786 \times 5421 \times 10$ (Texel $\times$ Example $\times$ Digit).

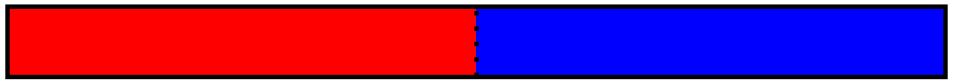
- Unstructured, 42.6 million non-zeros.
- T-HOSVD and ST-HOSVD truncated to relative error of 10%.

	T-HOSVD	ST-HOSVD
Rel. model error	9.90%	9.68%
Model rank	$(94, 511, 10)$	$(94, 511, 10)$

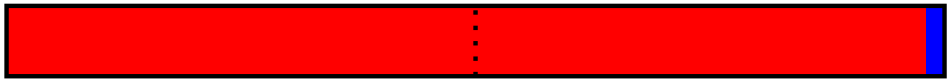
Handwritten digit classification II

T-HOSVD ST-HOSVD

Classification error

4.94%  4.94%

Factorization time

49m 26.0s  1m 8.7s

43x speedup!

Handwritten digit classification III — Why?

Recall truncation rank? $(94, 511, 10)$.

T-HOSVD requires:

- SVD of 786×54210 matrix,
- SVD of $\mathbf{5421} \times \mathbf{7860}$ matrix, and
- SVD of 10×4260906 matrix.

ST-HOSVD (only) requires:

1. SVD of 786×54210 matrix,
2. SVD of $\mathbf{5421} \times \mathbf{940}$ matrix, and
3. SVD of 10×48034 matrix.

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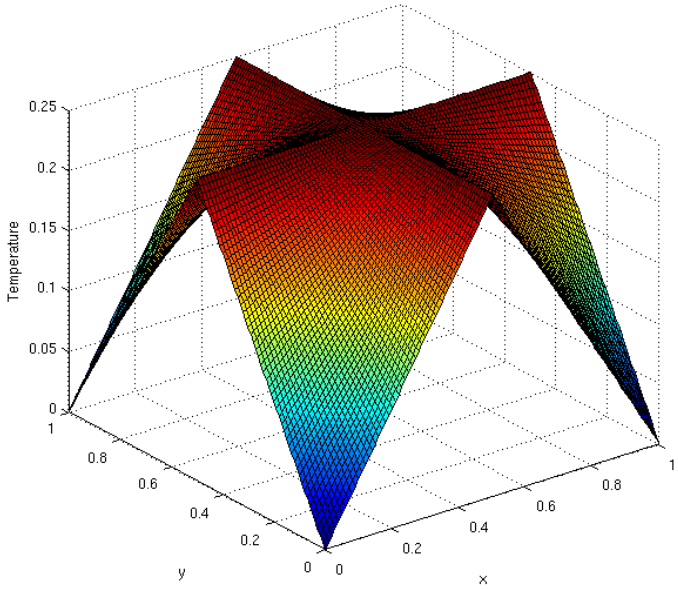
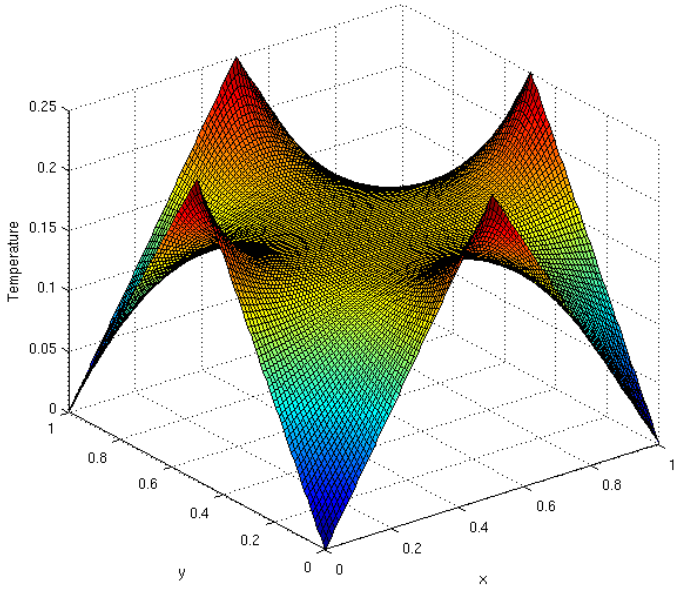
Compression of simulation results I

Compression of numerical solution of the heat equation on a square domain computed by explicit Euler. Inspired by [LVV2010].





Tensor of size $101 \times 101 \times 10001$ ($x \times y \times t$).

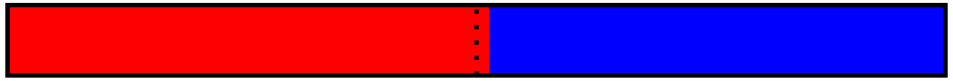
- Partially symmetric, 102.0 million non-zeros.
- T-HOSVD and ST-HOSVD truncated to absolute error of 10^{-4} (discretization accurary).

Compression of simulation results II

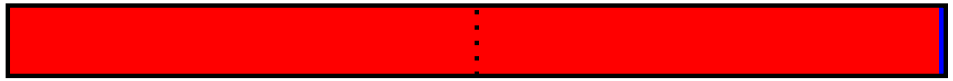
	T-HOSVD	ST-HOSVD
Abs. error	$8.512 \cdot 10^{-5}$	$9.587 \cdot 10^{-5}$
Rank	$(22, 22, 20)$	$(22, 21, 19)$

T-HOSVD ST-HOSVD

Storage (nb. of values)

214144  203140

Factorization time

2h 46m  1m 14.7s

133x speedup!

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Conclusions

Early projection, as in ST-HOSVD, can greatly improve the performance of T-HOSVD.

Thank you for your attention.

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SÉ2007 B. Savas and L. Eldén, *Handwritten digit classification using higher-order singular value decomposition*, Patt. Recog., 40 (2007)

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