Matrix and Tensor Functions in Conflict with Approximation

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Outline

Low Rank Matrices and Tensors

The Hierarchical Tucker Format

Determine Largest Element

Interesting Problems

Low Rank Matrices and Tensors

Our objects of interest are multivariate functions

$$f(x_1, \dots, x_d) \in \mathbb{R}, \qquad x \in I = I_1 \times \cdots \times I_d$$

with typically **finite** univariate index sets I_μ

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We want to represent or approximate the function in low rank form

$$f(x_1, \ldots, x_d) \approx \sum_j f_{j,1}(x_1) \cdots f_{j,d}(x_d)$$

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- Data-sparse representation of each $f_{j,\mu}$ easy
- Curse of dimensionality lifted **provided few summands**
- Need to find/determine the $f_{j,\mu}$

Low Rank Matrices and Tensors

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Hilbert-Schmidt (SVD) in $d = 2$

$$f(x_1, x_2) = \sum_{j=1}^{r} f_{j,1}(x_1) f_{j,2}(x_2)$$

s.t. $f_{\cdot,1}$ and $f_{\cdot,2}$ orthogonal / normalized

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Our goal is to extend this to high dimension $d \gg 1000$

Example: d-dimensional Laplacian

We solve [Computing 2004, G.]

$$-\Delta u(x) = 1, \qquad x \in \Omega = [0,1]^d, \qquad u|_{\partial\Omega} = 0$$

on a grid with 1024^d grid points and rel. pointwise accuracy $\approx 10^{-5}$

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ease of presentation, cf. [FOCM 16,2016, Dahmen,DeVore,G.,Süli]
Results based on exponential sums $\frac{1}{x} \approx \sum_{j=1}^{r} w_j \exp(t_j x)$

Example: d-dimensional Laplacian

$$-\Delta u(x) = 1, \qquad x \in \Omega = [0,1]^d, \qquad u|_{\partial\Omega} = 0$$

The operator discretized leads to a (sparse) matrix A and we solve

$$Ax = b$$

We apply the matrix function

$$F(A) = \sum_{j=1}^{r} w_j \exp(t_j A) \approx A^{-1}$$

and obtain — for structured b — a structured solution

$$x \approx \tilde{x} = \sum_{j=1}^{r} w_j \exp(t_j A) b$$

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Low Rank Matrices and Tensors

Remarks:

1. The operator (and thus A) is structured

Low Rank Matrices and Tensors

Remarks:

2. The right-hand side is assumed to be structured

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3. We require an explicit a priori exponential sum approximation

$$\frac{1}{x} \approx \sum_{j=1}^{r} w_j \exp(t_j x), \qquad x \in (1, \infty)$$

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$$\boxed{\text{We need to change the low rank format}}$$

The Hierarchical Tucker Format

Low rank matrix representation $M = UV^T$

$$M(i_1, i_2) = \sum_{j=1}^{k} U(i_1, j) V(i_2, j)$$

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Low rank tensor representation (CP) format

$$M(i_1, \ldots, i_d) = \sum_{j=1}^{k} M_{j,1}(i_1) \cdots M_{j,d}(i_d)$$

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Matrices of rank $\leq k$ closed

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Tensors of rank $\leq k$ not closed (and complicated)

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- Matrices of rank $\leq k$ closed
- Tensors of rank $\leq k$ not closed (and complicated)
- CP decomposition used e.g. in blind source separation

The Hierarchical Tucker Format

Idea (Hackbusch): Use a hierarchy of low rank matrices:

$$M(\boxed{i_1, i_2}, \boxed{i_3, i_4}) = \sum_{j=1}^{k} U^{(1,2)}(\boxed{i_1, i_2}, j)\, U^{(3,4)}(\boxed{i_3, i_4}, j)$$

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$$U^{(1,2)}(i_1, i_2, j) = \sum_{\ell=1}^{k} \sum_{m=1}^{k} B^{(1,2)}{}_{j,\ell,m} U^{(1)}(i_1, \ell) U^{(2)}(i_2, m)$$

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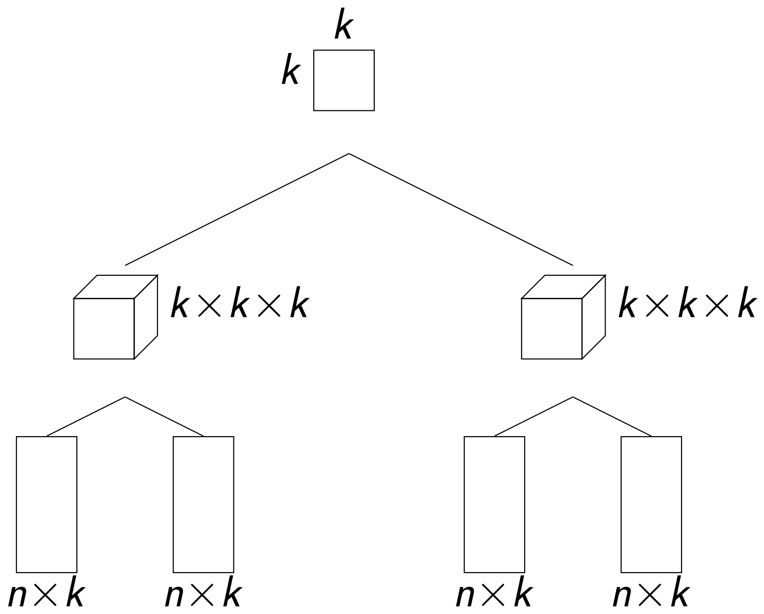
$\rightarrow$ (HT) format

HT Tensors of rank $\leq k$ closed (and simple)

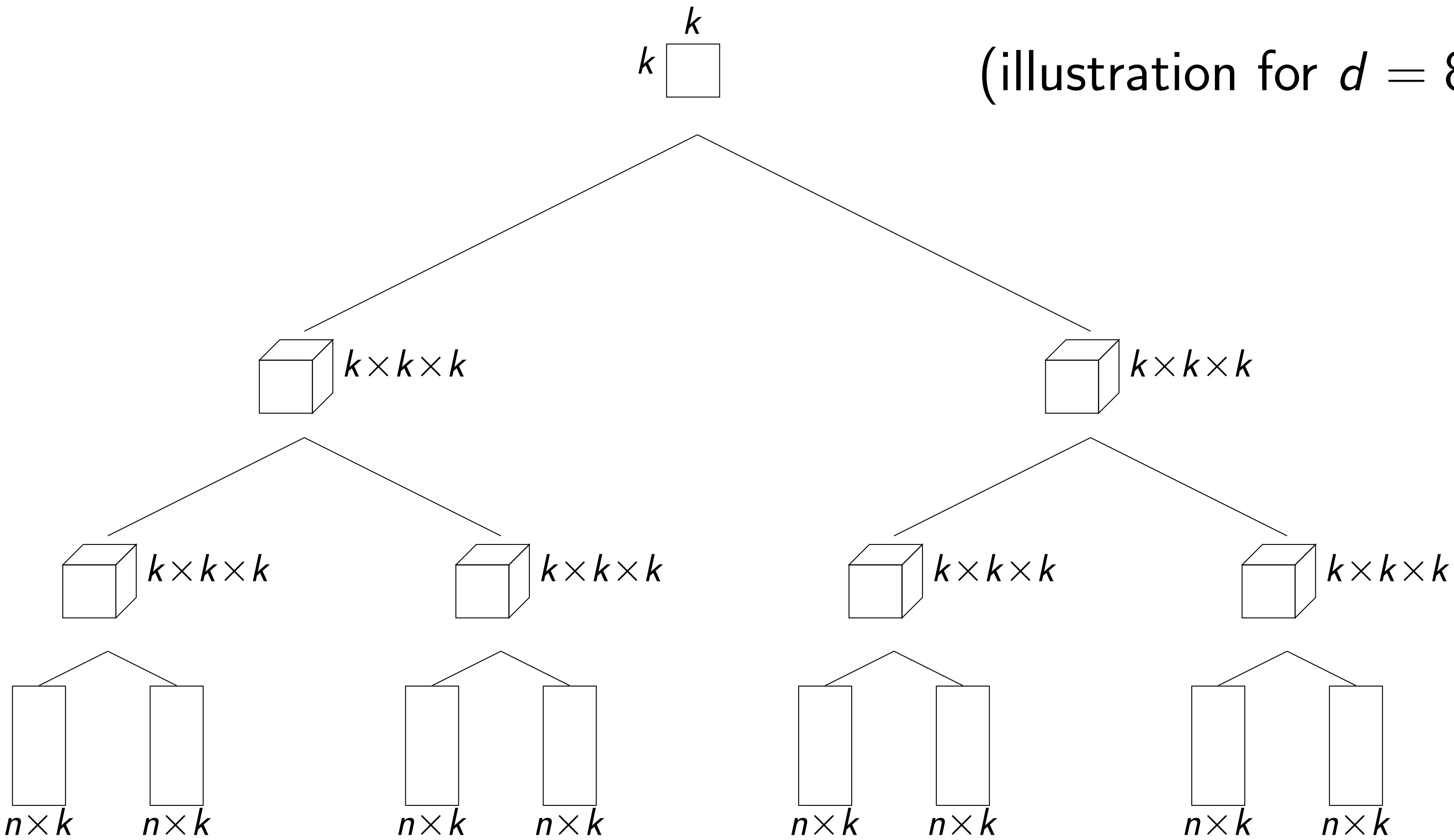
The Hierarchical Tucker Format



(illustration for $d = 4$)

The Hierarchical Tucker Format

(illustration for $d = 8$)



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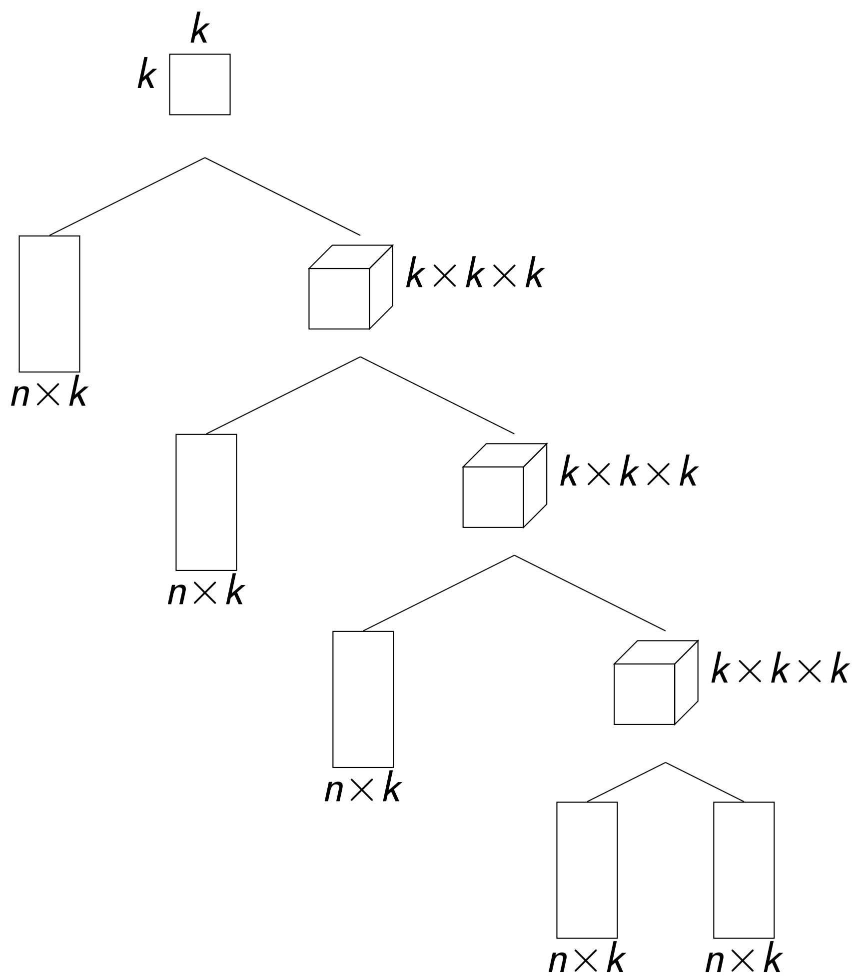

(illustration for $d = 5$)

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A d-dimensional tensor $M \in \mathbb{R}^{n \times \cdots \times n}$ (i.e. n^d entries) of **low rank** k allows for a representation in the Hierarchical Tucker Format with only

$$d \cdot n \cdot k + (d-2) \cdot k^3 + k^2 = \mathcal{O}(d) \text{ entries.}$$

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CP tensor:	$1,000$	parameters

The Hierarchical Tucker Format

Matricization and low rank representation for $t = \{2, 3, 5\}$:

$$M(\boxed{i_2, i_3, i_5}, \boxed{i_1, i_4, i_6, i_7}) = \sum_{j=1}^{k} U(\boxed{i_2, i_3, i_5}, j) V(\boxed{i_1, i_4, i_6, i_7}, j)$$

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Two main research directions:

1. Design algorithms to work with and exploit data-sparse tensor representations ($\gg$ 1000 articles)
2. Prove approximability / convergence (few articles)

Truncation of Hierarchical Tensors / Projection onto $HT(k)$

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(Truncation should be applied after a certain amount of summations or multiplications to keep the amount of data $dnk + (d-2)k^3 + k^2$ below some upper limit)

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Speed of truncation (single processor CPU, 9 years ago):

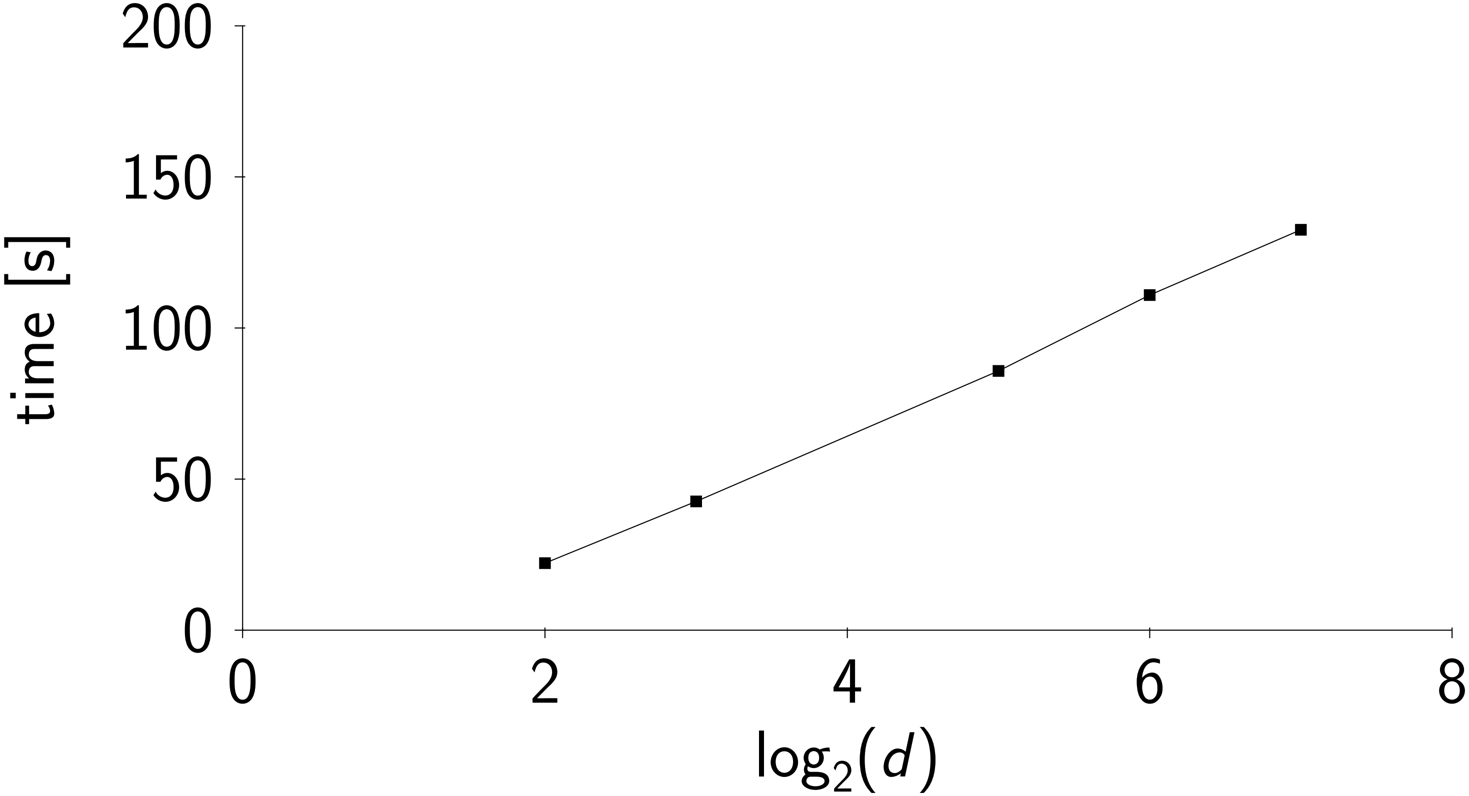
$n = 100$, $d = 1000$, input rank $k = 25$

Memory consumption: 138 MB

Time consumption: 19 seconds

Parallel Truncation [Num.Lin.Alg.Appl., G.,Löbbert, acc.]

time $\sim \log_2(d)$ (full tensor: 10^{512} entries)



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Postprocessing with low rank tensors can be easy:

$$QoI = \int f(x) d\pi(x)$$

with product measure π and

$$f(x_1, \ldots, x_d) = \sum_{j=1}^{k} f_{j,1}(x_1) \cdots f_{j,d}(x_d)$$

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...or complicated:

$$\max_{i_1,\dots,i_d} f(i_1, \dots, i_d) = ?$$

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Determine Largest Element

$$\max_{i_1,\ldots,i_d} f(i_1,\ldots,i_d) = ?$$

1. Conditioning of the problem
2. Numerical heuristics

Determine Largest Element

1. Conditioning

$$M := \max_{i_1,\dots,i_d} |f(i_1,\dots,i_d)| =?$$

Any elementwise perturbation E of size ε yields

$$\max_{i_1,\dots,i_d} |f(i_1,\dots,i_d) + E(i_1,\dots,i_d)| \in [M-\varepsilon, M+\varepsilon]$$

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What about

$$\max_{i_1,\dots,i_d} |f(i_1,\dots,i_d) + E(i_1,\dots,i_d)|$$

for $\|M\| \le \varepsilon \|f\|$?

Determine Largest Element

$$\max_{i_1,\ldots,i_d} |f(i_1,\ldots,i_d) + E(i_1,\ldots,i_d)| \in ?, \qquad \|M\| \leq \varepsilon \|f\|$$

Example: $\varepsilon \sim 1/\sqrt{n}$

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Example: $\varepsilon \sim 1/\sqrt{n}$

$$f = \left[\begin{array}{ccc|c} \varepsilon & \cdots & \varepsilon & 0 \\ \vdots & \ddots & \vdots & 0 \\ \varepsilon & \cdots & \varepsilon & 0 \\ \hline 0 & \cdots & 0 & 1 \end{array}\right] \in \mathbb{R}^{n+1 \times n+1}, \qquad \|f\|_F = \sqrt{n^2\varepsilon^2 + 1} \sim \sqrt{n}$$

$$M = \left[\begin{array}{ccc|c} 0 & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & 0 \\ 0 & \cdots & 0 & 0 \\ \hline 0 & \cdots & 0 & -1 \end{array}\right] \in \mathbb{R}^{n+1 \times n+1}, \qquad \|M\|_F = 1 \sim \varepsilon \|f\|_F$$

In higher dimension d ill-conditioned in $\|\cdot\|_F$

Determine Largest Element

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Example: $\varepsilon \sim n^{-d/4}$

$$f = \varepsilon v \otimes \cdots \otimes v \in \mathbb{R}^{(n+1)^d}, \qquad \|f\|_F = \sqrt{n^d \varepsilon^2 + 1} \sim n^{d/4}$$

$$M = -e_{n+1} \otimes \cdots \otimes e_{n+1} \in \mathbb{R}^{(n+1)^d}, \qquad \|M\|_F = 1 \sim \varepsilon \|f\|_F$$

In higher dimension d ill-conditioned in $\|\cdot\|_F$

2. Numerical Heuristics

First approach:

for any rank 1 tensor $v = v_1 \otimes \cdots \otimes v_d$ we have

$$\|v\|_\infty = \prod_{\mu=1}^{d} \|v_\mu\|_\infty$$

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$$\mathrm{argmax}_i |v(i)| = \left(\mathrm{argmax}_{i_\mu} |v_\mu(i_\mu)|\right)_{\mu=1}^{d}$$

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First approach:

for any rank 1 tensor $v = v_1 \otimes \cdots \otimes v_d$ we have

$$\|v\|_\infty = \prod_{\mu=1}^{d} \|v_\mu\|_\infty$$

$$\mathrm{argmax}_i |v(i)| = (\mathrm{argmax}_{i_\mu} |v_\mu(i_\mu)|)_{\mu=1}^{d}$$

truncate tensor M to rank 1 tensor $\tilde{M}$ and compute its max

2. Numerical Heuristics

First approach: truncate to rank 1
Example: $\varepsilon \sim n^{-d/2}$

$$M = \varepsilon v \otimes \cdots \otimes v + e_{n+1} \otimes \cdots \otimes e_{n+1}$$

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Rank 1 best approximation in $\|\cdot\|_F$ is

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Result: $\|M\|_\infty = 1$ estimated by $\|\tilde{M}\|_\infty = n^{-d/2}$,
gives completely wrong answer

2. Numerical Heuristics

Second approach: power iteration (Mike Espig)

compute Hadamard products

$$\hat{M} := M \odot M \odot M \cdots$$

2. Numerical Heuristics

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$$\hat{M} := M \odot M \odot M \cdots$$

truncate tensor $\hat{M}$ to rank 1 tensor $\tilde{M}$ and compute its argmax

2. Numerical Heuristics

Second approach: power iteration
Example: $\varepsilon \sim n^{-1}$

$$M = \varepsilon v \otimes \cdots \otimes v + e_{n+1} \otimes \cdots \otimes e_{n+1}$$

Determine Largest Element

2. Numerical Heuristics

Second approach: power iteration
Example: $\varepsilon \sim n^{-1}$

$$M = \varepsilon v \otimes \cdots \otimes v + e_{n+1} \otimes \cdots \otimes e_{n+1}$$

$$\hat{M} := M \odot M \odot M \cdots = \varepsilon^{\ell} v \otimes \cdots \otimes v$$

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Rank 1 best approximation in $\|\cdot\|_F$ is

$$\tilde{M} = \varepsilon^{\ell} v \otimes \cdots \otimes v$$

for all $\ell < d/2$

Determine Largest Element

2. Numerical Heuristics

Further approaches:

- subspace iterations (Lukas Juschka)
- local search
- many optimizations. . .

[cf. Higham and Relton 2015]

Determine Largest Element

2. Numerical Heuristics

Further approaches:

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- many optimizations...

[cf. Higham and Relton 2015]

Lower bound: largest known value
Good upper bound: ? some p-norm
$\rightarrow$ branach and bound

(work in progress)

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Interesting Problems

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1. Stability of Tensor Completion
   ($\rightarrow$ Krämer, G. arXiv:1701.08045) and other operations

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8. Relation between HT and deep convolutional neural networks

   ...

Thank You!

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