Aproksimacija antisimetričnih tenzora tenzorima nižeg ranga

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SADRŽAJ

- Tenzori - Uvod
- Osnovne dekompozicije tenzora
- Tenzorski rang i multilinearni rang

- Aproksimacija tenzorima nižeg multilinearnog ranga
- Jacobijeva metoda
- Numerički primjeri

- Aproksimacija tenzorima multilinearnog ranga d
- Numerički primjeri

E. Begović Kovač, D. Kressner: Structure-preserving low multilinear rank approximation of antisymmetric tensors. submitted.

TENZORI - Oznake i osnovni pojmovi

- **Tenzor** je višedimenzionalni (konačni) niz
- Matrica $\mathbf{M}(i,j) \dashrightarrow$ Tenzor $\mathcal{T}(i_1, i_2, \ldots, i_d)$
- **Red** tenzora (order) - dimenzija d

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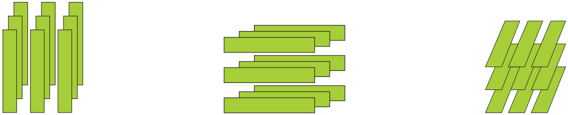
- **Red** tenzora (order) - dimenzija d
- **Fiber** - vektor koji se dobije fiksiranjem svih osim jednog indeksa, npr. $\mathcal{T}(:, i_2, \ldots, i_d)$, **mode**-$k$



- **Slice** - matrica koja se dobije fiksiranjem svih osim dva indeksa, npr. $\mathcal{T}(:, :, i_3, \ldots, i_d)$

SIMETRIČNI I ANTISIMETRIČNI TENZORI

- Simetrični tenzor

$$\mathcal{X}(i_1, i_2, \ldots, i_d) = \mathcal{X}(i_{\sigma(1)}, i_{\sigma(2)}, \ldots, i_{\sigma(d)})$$

- Antisimetrični tenzor

$$\mathcal{A}(i_1, i_2, \ldots, i_d) = (-1)^{|\sigma|}\mathcal{A}(i_{\sigma(1)}, i_{\sigma(2)}, \ldots, i_{\sigma(d)})$$

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Löwdin rules - Pravila za antisimetrične tenzore:

$$\begin{aligned}
(i)\ \mathcal{A}(i,j,k) &= 0, \quad \text{ako je } i=j \text{ ili } i=k \text{ ili } j=k,\\
(ii)\ \mathcal{A}(i,j,k) &= \mathcal{A}(j,k,i) = \mathcal{A}(k,i,j)\\
&= -\mathcal{A}(j,i,k) = -\mathcal{A}(k,j,i) = -\mathcal{A}(i,k,j), \quad \text{inače.}
\end{aligned}$$

Antisimetrizator anti($\mathcal{X}$) - projekcija na prostor antisimetričnih tenzora

PRIMJENE

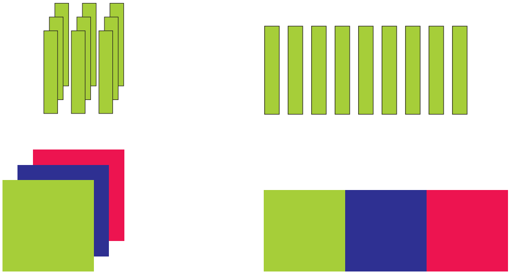
- Fizika (kvantna fizika, elektromagnetizam)
- Kemija (kvantna kemija, računarska kemija, kemometrija)
- Inženjerstvo (obrada signala, obrada slike i videa)
- Društvene znanosti (sociologija, psihometrika)

- Antisimetrični tenzori:
  Valna funkcija koja opisuje **kvantno stanje fermiona** je antisimetrična.

MATRICIZACIJA

- **Unfolding** (matricization/flattening) - matrična reprezentacija tenzora

$$\mathcal{T} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d} \quad \dashrightarrow \quad \mathbf{T}_{(k)} \in \mathbb{R}^{n_k \times (n_1 \cdots n_{k-1} n_{k+1} \cdots n_d)}$$



MATRICIZACIJA - Primjer 1

$d = 3, n_1 = 3, n_2 = 4, n_3 = 2$

$$\mathcal{X}(:,:,1) = \left[\begin{array}{cccc} 9 & 4 & 5 & 4 \\ 2 & 8 & 0 & 6 \\ 6 & 7 & 8 & 1 \end{array}\right], \quad \mathcal{X}(:,:,2) = \left[\begin{array}{cccc} 2 & 0 & 1 & 5 \\ 3 & 3 & 9 & 1 \\ 7 & 6 & 5 & 0 \end{array}\right]$$

$$\mathbf{X}_{(1)} = \left[\begin{array}{cccc|cccc} 9 & 4 & 5 & 4 & 2 & 0 & 1 & 5 \\ 2 & 8 & 0 & 6 & 3 & 3 & 9 & 1 \\ 6 & 7 & 8 & 1 & 7 & 6 & 5 & 0 \end{array}\right]$$

$$\mathbf{X}_{(2)} = \left[\begin{array}{ccc|ccc} 9 & 2 & 6 & 2 & 3 & 7 \\ 4 & 8 & 7 & 0 & 3 & 6 \\ 5 & 0 & 8 & 1 & 9 & 5 \\ 4 & 6 & 1 & 5 & 1 & 0 \end{array}\right]$$

$$\mathbf{X}_{(3)} = \left[\begin{array}{ccc|ccc|ccc|ccc} 9 & 2 & 6 & 4 & 8 & 7 & 5 & 0 & 8 & 4 & 6 & 1 \\ 2 & 3 & 7 & 0 & 3 & 6 & 1 & 9 & 5 & 5 & 1 & 0 \end{array}\right]$$

MATRICIZACIJA - Primjer 2

- Neka je $\mathcal{A} \in \mathbb{R}^{n \times n \times \cdots \times n}$ antisimetrični tenzor reda d. Vrijedi

$$\mathbf{A}_{(k)} = (-1)^{|k-l|} \mathbf{A}_{(l)}, \quad \text{za sve } 1 \leq k, l \leq d.$$

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- $d = 3, n = 4$:

$$\mathcal{A}(:,:,1) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 \\ 0 & -1 & 0 & 3 \\ 0 & -2 & -3 & 0 \end{bmatrix}, \quad \mathcal{A}(:,:,2) = \begin{bmatrix} 0 & 0 & -1 & -2 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 4 \\ 2 & 0 & -4 & 0 \end{bmatrix}$$

$$\mathcal{A}(:,:,3) = \begin{bmatrix} 0 & 1 & 0 & -3 \\ -1 & 0 & 0 & -4 \\ 0 & 0 & 0 & 0 \\ 3 & 4 & 0 & 0 \end{bmatrix}, \quad \mathcal{A}(:,:,4) = \begin{bmatrix} 0 & 2 & 3 & 0 \\ -2 & 0 & 4 & 0 \\ -3 & -4 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{A}_{(1)} = \mathbf{A}_{(3)} = \left[\begin{array}{cccc|cccc|cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & -1 & -2 & 0 & 1 & 0 & -3 & 0 & 2 & 3 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -4 & -2 & 0 & 4 & 0 \\ 0 & -1 & 0 & 3 & 1 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & -3 & -4 & 0 & 0 \\ 0 & -2 & -3 & 0 & 2 & 0 & -4 & 0 & 3 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right]$$

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KVADRATNA MATRICIZACIJA

- **Square unfolding** - $\mathcal{T} \in \mathbb{R}^{n_1 \times n_2 \times n_3 \times n_4} \dashrightarrow \mathbf{T} \in \mathbb{R}^{n_1 n_3 \times n_2 n_4}$

$d = 4, n_1 = 3, n_2 = 2, n_3 = 2, n_4 = 2$

$$\mathcal{X}(:,:,1,1) = \begin{bmatrix} 2 & 3 \\ 6 & 5 \\ 9 & 1 \end{bmatrix}, \quad \mathcal{X}(:,:,1,2) = \begin{bmatrix} 8 & 3 \\ 6 & 9 \\ 2 & 2 \end{bmatrix},$$
$$\mathcal{X}(:,:,2,1) = \begin{bmatrix} 6 & 8 \\ 7 & 5 \\ 5 & 3 \end{bmatrix}, \quad \mathcal{X}(:,:,2,2) = \begin{bmatrix} 3 & 3 \\ 5 & 8 \\ 3 & 0 \end{bmatrix},$$

$$\mathbf{A}_{(12)} = \left[\begin{array}{cc|cc} 2 & 3 & 8 & 3 \\ 6 & 5 & 6 & 9 \\ 9 & 1 & 2 & 2 \\ \hline 6 & 8 & 3 & 3 \\ 7 & 5 & 5 & 8 \\ 5 & 3 & 3 & 0 \end{array}\right]$$

MNOŽENJE I NORMA

- **Mode-k product**

$$\mathcal{X} \times_k \mathbf{M}$$

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- $\mathcal{T} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$, Frobeniusova norma

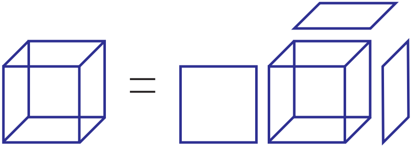
$$\|\mathcal{T}\|^2 = \sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} \cdots \sum_{i_d=1}^{n_d} \mathcal{T}(i_1, i_2, \ldots, i_d)^2$$

Osnovne dekompozicije tenzora

TUCKEROVA DEKOMPOZICIJA I HOSVD

$\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$

- Tucker (1966.) $\qquad \mathcal{X} = \mathcal{T} \times_1 \mathbf{M}_1 \times_2 \mathbf{M}_2 \cdots \times_d \mathbf{M}_d$



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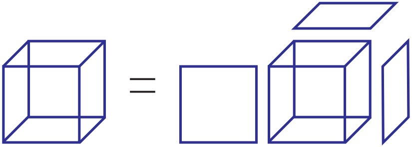

- **Higher order SVD** (multilinearni SVD)
  De Lathauwer et al. (2000.)

$$\mathcal{X} = \mathcal{S} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \cdots \times_d \mathbf{U}_d,$$

gdje je $\mathcal{S} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ core tenzor, a $U_k \in \mathbb{R}^{n_k \times n_k}$ su unitarne matrice, $1 \leq k \leq d$.

HOSVD

$\mathcal{S}$ **nije** dijagonalni tenzor!

Svaki "podtenzor" od $\mathcal{S}$ je okomit na svaki drugi "podtenzor" i njihove norme padaju kako se udaljavamo od "gornjeg lijevog" vrha.

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$$\mathcal{S} = \mathcal{X} \times_1 \mathbf{U}_1^T \times_2 \mathbf{U}_2^T \cdots \times_d \mathbf{U}_d^T$$

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HOSVD algoritam, $\mathcal{X}$

FOR $k = 1, \ldots, d$
  Compute SVD of $\mathbf{X}_{(k)}$, $\mathbf{X}_{(k)} = \mathbf{U}_k \mathbf{S}_k \mathbf{V}_k^T$.
ENDFOR
$\mathcal{S} = \mathcal{X} \times_1 \mathbf{U}_1^T \times_2 \mathbf{U}_2^T \times_3 \cdots \times_d \mathbf{U}_d^T$

HOSVD ANTISIMETRIČNOG TENZORA

U slučaju antisimetričnog tenzora $\mathcal{A}$ vrijedi

$$\mathbf{A}_{(1)} = -\mathbf{A}_{(2)} = \mathbf{A}_{(3)} = -\mathbf{A}_{(4)} = \cdots ,$$

pa HOSVD ima oblik

$$\mathcal{A} = \mathcal{S} \times_1 \mathbf{U} \times_2 \mathbf{U} \cdots \times_d \mathbf{U},$$

$$\text{tj.} \qquad \mathbf{U}_1 = \mathbf{U}_2 = \cdots = \mathbf{U}_d = \mathbf{U}.$$

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HOSVD algoritam, $\mathcal{A}$

Compute SVD of $\mathbf{A}_{(1)}$, $\mathbf{A}_{(1)} = \mathbf{USV}^T$.
$\mathcal{S} = \mathcal{A} \times_1 \mathbf{U}^T \times_2 \mathbf{U}^T \times_3 \cdots \times_d \mathbf{U}^T$

HOSVD $\dashrightarrow$ SVD

$$\mathbf{M}_{(1)} = \mathbf{U}_1 \Sigma_1 \mathbf{V}_1^T, \qquad \mathbf{M}_{(1)} = \mathbf{M} = \mathbf{U}\Sigma\mathbf{V}^T$$
$$\mathbf{M}_{(2)} = \mathbf{U}_2 \Sigma_2 \mathbf{V}_2^T, \qquad \mathbf{M}_{(2)} = \mathbf{M}^T = \mathbf{V}\Sigma\mathbf{U}^T$$

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$$\Rightarrow \mathbf{U} = \mathbf{U}_1 = \mathbf{V}_2, \quad \mathbf{V} = \mathbf{V}_1 = \mathbf{U}_2, \quad \Sigma = \Sigma_1 = \Sigma_2$$

HOSVD ⇢ SVD

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CP DEKOMPOZICIJA

- Hitchcock (1927.)
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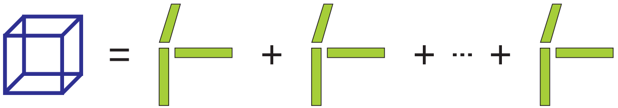
- **CP dekompozicija**, $\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$

$$\mathcal{X} \approx \sum_{j=1}^{R} x_1^{(j)} \circ x_2^{(j)} \circ \ldots \circ x_d^{(j)},$$

gdje je $R \in \mathbb{N}$, $x_k^{(j)} \in \mathbb{R}^{n_k}$, za $1 \leq k \leq d$, $1 \leq j \leq R$.
$\circ$ označava tenzorski produkt,

$$\mathcal{T} = x \circ y \circ z \quad \Leftrightarrow \quad \mathcal{T}(i,j,k) = x(i)y(j)z(k).$$



RANG TENZORA

- Najmanji R u egzaktnoj CP dekompoziciji je **tenzorski rang** (CP rang).
- Ova je definicija analogna definiciji ranga matrice, ali rang tenzora ima bitno drukčija svojstva.

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- Ova je definicija analogna definiciji ranga matrice, ali rang tenzora ima bitno drukčija svojstva.

- Rang tenzora $\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ je često veći od $\min\{n_1, n_2, \ldots, n_d\}$.
  Primjer:

$$\mathbf{X}_{(1)} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{X}_{(2)} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \quad \text{je ranga 3.}$$

- Za $\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$, $\text{rank}(\mathcal{X}) \leq \min\{n_1 n_2, n_1 n_3, n_2 n_3\}$.

- Problem određivanja tenzorskog ranga je NP-težak.

MULTILINEARNI RANG

- **Multilinearni rang** (k-rang) tenzora $\mathcal{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ je uređena d-torka

$$(r_1, r_2, \ldots, r_d), \quad \text{gdje je } r_k = \operatorname{rank}(\mathbf{X}_{(k)}),\ 1 \leq k \leq d.$$

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- U slučaju antisimetričnog tenzora $\mathcal{A}$ vrijedi

$$r_1 = r_2 = \cdots = r_d = r.$$

- Kažemo da $\mathcal{A}$ ima multilinearni rang r i pišemo $\mathcal{A} \in \mathcal{M}_r$.

MULTILINEARNI RANG ANTISIMETRIČNOG TENZORA

Teorem (B., Kressner)

Neka je $\mathcal{A} \in \mathbb{R}^{n \times n \times \cdots \times n}$ antisimetrični tenzor reda $d \geq 3$. Onda za multilinearni rang r od $\mathcal{A}$ vrijedi

(i) $r = 0$, za $n < d$;

(ii) $r \leq d$, za $n = d$ or $n = d + 1$;

(iii) $r \leq n$, za $n \geq d + 2$.

Postoje tenzori $\mathcal{A}$ takvi da u (ii) i (iii) vrijedi jednakost.

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$$\{0, d, d + 2, \ldots, n\}.$$

Aproksimacija tenzorima nižeg multilinearnog ranga

FORMULACIJA PROBLEMA

- Za dani antisimetrični tenzor $\mathcal{A}$ tražimo antisimetrični tenzor $\hat{\mathcal{A}} \in \mathcal{M}_r$ koji dobro aproksimira $\mathcal{A}$.
- **Minimizacijski problem**:

$$\|\mathcal{A} - \hat{\mathcal{A}}\|^2 \to \min, \quad \text{uz uvjet } \hat{\mathcal{A}} \in \mathcal{M}_r.$$

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$$\|\mathcal{A} - \hat{\mathcal{A}}\|^2 \to \min, \quad \text{uz uvjet } \hat{\mathcal{A}} \in \mathcal{M}_r.$$

Taj problem možemo zapisati kao

$$\|\mathcal{A} - \mathcal{B} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \cdots \times_d \mathbf{U}_d\|^2 \to \min,$$

gdje je $\hat{\mathcal{A}} = \mathcal{B} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \cdots \times_d \mathbf{U}_d$ HOSVD od $\hat{\mathcal{A}}$.

FORMULACIJA PROBLEMA

- Za dani antisimetrični tenzor $\mathcal{A}$ tražimo antisimetrični tenzor $\hat{\mathcal{A}} \in \mathcal{M}_r$ koji dobro aproksimira $\mathcal{A}$.
- **Minimizacijski problem**:

$$\|\mathcal{A} - \hat{\mathcal{A}}\|^2 \to \min, \quad \text{uz uvjet } \hat{\mathcal{A}} \in \mathcal{M}_r.$$

  Taj problem možemo zapisati kao

$$\|\mathcal{A} - \mathcal{B} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \cdots \times_d \mathbf{U}_d\|^2 \to \min,$$

  gdje je $\hat{\mathcal{A}} = \mathcal{B} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \cdots \times_d \mathbf{U}_d$ HOSVD od $\hat{\mathcal{A}}$.
- Dualni **maksimizacijski problem** (De Lathauwer, 2000.):

$$\|\mathcal{A} \times_1 \mathbf{U}_1^T \times_2 \mathbf{U}_2^T \times_3 \cdots \times_d \mathbf{U}_d^T\|^2 \to \max.$$

T-HOSVD

- **Truncated HOSVD** ($\sim$ 2000.)

  FOR $k = 1, \ldots, d$
  Compute SVD of $\mathbf{A}_{(k)}$, $\mathbf{A}_{(k)} = \mathbf{U}_k \mathbf{S}_k \mathbf{V}_k^T$.
  $\mathbf{W}_k = \mathbf{U}_k(:, 1 : r_k)$
  ENDFOR
  $\mathcal{S} = \mathcal{A} \times_1 \mathbf{W}_1^T \times_2 \mathbf{W}_2^T \times_3 \cdots \times_d \mathbf{W}_d^T$

- Ne vrijedi Eckart-Young teorem, ali T-HOSVD **daje dobru početnu aproksimaciju za iterativne metode**.

HOOI

- **Higher order orthogonal iterations** ($\sim$ 2006.)
- ALS algoritam. Tražimo $\hat{\mathcal{A}} = \mathcal{B} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \cdots \times_d \mathbf{U}_d$ tako da u svakoj mikroiteraciji optimiziramo samo po jednoj matrici U_k, $1 \leq k \leq d$, dok su ostale fiksne.

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- **U praksi konvergira prema stacionarnoj točki**.

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- **U praksi konvergira prema stacionarnoj točki**.

HOOI algoritam, $d = 3$

Take initial U_1, U_2, U_3.
REPEAT
  $\mathcal{X} = \mathcal{A} \times_2 U_2^T \times_3 U_3^T$
  Compute SVD of $\mathbf{X}_{(1)}$, $\mathbf{X}_{(1)} = \mathbf{USV}^T$, $U_1 = U(:, 1:r_1)$.
  $\mathcal{X} = \mathcal{A} \times_1 U_1^T \times_3 U_3^T$
  Compute SVD of $\mathbf{X}_{(2)}$, $\mathbf{X}_{(2)} = \mathbf{USV}^T$, $U_2 = U(:, 1:r_2)$.
  $\mathcal{X} = \mathcal{A} \times_1 U_1^T \times_2 U_2^T$
  Compute SVD of $\mathbf{X}_{(3)}$, $\mathbf{X}_{(3)} = \mathbf{USV}^T$, $U_3 = U(:, 1:r_3)$.
UNTIL convergence
$\mathcal{B} = \mathcal{A} \times_3 U_3^T$
$\hat{\mathcal{A}} = \mathcal{B} \times_1 U_1 \times_2 U_2 \times_3 U_3$

Jacobijeva metoda

JACOBIJEVA METODA

Zbog jednostavnosti uzmimo $d = 3$, $\mathcal{A} \in \mathbb{R}^{n\times n\times n}$.

Definiramo funkcije

$$g : \mathbf{U} \mapsto \|\mathcal{A} \times_1 \mathbf{U}^T \times_2 \mathbf{U}^T \times_3 \mathbf{U}^T\|^2,$$
$$f : \mathbf{Q} \mapsto g(\mathbf{U}), \quad \text{gdje je } \mathbf{Q} = [\mathbf{U}\mathbf{U}_\perp].$$

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$$f : \mathbf{Q} \mapsto g(\mathbf{U}), \quad \text{gdje je } \mathbf{Q} = [\mathbf{U}\mathbf{U}_\perp].$$

Za $M = \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}$, funkciju f možemo zapisati kao

$$f(\mathbf{Q}) = \|\mathcal{A} \times_1 \mathbf{M}\mathbf{Q}^T \times_2 \mathbf{M}\mathbf{Q}^T \times_3 \mathbf{M}\mathbf{Q}^T\|^2.$$

Tražimo maksimum funkcije f.

JACOBIJEVA METODA

Ideja: primjenjujemo Jacobijeve rotacije s ciljem da povećamo normu (r, r, r)-podtenzora s najmanjim indeksima.
(Ishteva et al., 2013.)

Jacobijeve rotacije su $n \times n$ matrice oblika

$$R(i,j,\phi) = \begin{bmatrix} 1 & & & & & & & & & & \\ & \ddots & & & & & & & & & \\ & & 1 & & & & & & & & \\ & & & \cos\phi & & & & -\sin\phi & & & \\ & & & & 1 & & & & & & \\ & & & & & \ddots & & & & & \\ & & & & & & 1 & & & & \\ & & & \sin\phi & & & & \cos\phi & & & \\ & & & & & & & & 1 & & \\ & & & & & & & & & \ddots & \\ & & & & & & & & & & 1 \end{bmatrix} \begin{matrix} \\ \\ \\ i \\ \\ \\ \\ j \\ \\ \\ \\ \end{matrix},$$

gdje je $(i,j) = (i(k), j(k))$ pivotni par u k-tom koraku.

JACOBIJEVA METODA - Algoritam

Take initial Q. (Koristeći HOSVD $Q = U$ ili $Q = I_n$.)
$\mathcal{A}_1 = \mathcal{A} \times_1 Q^T \times_2 Q^T \times_3 Q^T$
REPEAT
Choose $(i(k), j(k))$.
Find ϕ.
$R_k = R(i(k), j(k), \phi(k))$
$Q_{k+1} = Q_k R_k$
$\mathcal{A}_{k+1} = \mathcal{A}_k \times_1 R_k^T \times_2 R_k^T \times_3 R_k^T$
UNTIL convergence
$U = Q(1:n, 1:r)$
$\hat{\mathcal{A}} = (\mathcal{A} \times_1 U^T \times_2 U^T \times_3 U^T) \times_1 U \times_2 U \times_3 U$

PIVOTNA STRATEGIJA

- Pivotne parove biramo iz skupa

$$(1, r+1), (1, r+2), \ldots, (1, n), (2, r+1), \ldots, (r, n).$$

- Uzimamo pivotne parove (i, j) za koje vrijedi

$$|(\mathrm{grad} f(\mathbf{Q}), d_{ij}(\mathbf{Q}))| \geq \epsilon \|\mathrm{grad} f(\mathbf{Q})\|,$$

za $\epsilon \ll 1$ i

$$d_{ij}(\mathbf{Q}) = Q \cdot \frac{d}{d\phi} R_{i,j,\phi}\Big|_{\phi=0} = Q \begin{bmatrix} 0 & & & & & \\ & \ddots & & & & \\ & & 0 & & -1 & \\ & & & \ddots & & \\ & & 1 & & 0 & \\ & & & & & \ddots & \\ & & & & & & 0 \end{bmatrix} \begin{matrix} \\ \\ i \\ \\ j \\ \\ \\ \end{matrix} .$$

- To će osigurati **konvergenciju prema stacionarnoj točki**. (Ishteva et al. 2013. za slučaj simetričnih tenzora.)

IZBOR KUTA ROTACIJE

Rotacija $R(i, j, \phi)$ mijenja elemente na pozicijama

$$(i, :, :), (j, :, :), (:, i, :), (:, j, :), (:, :, i), (:, :, j).$$

Bitni su nam elementi u (r, r, r)-podtenzoru. Zbog $1 \leq i \leq r < j \leq n$, ograničimo se na $(i, :, :)$, $(:, i, :)$, $(:, :, i)$, a kako je tenzor antisimetričan dovoljno je gledati pozicije $(i, :, :)$.

IZBOR KUTA ROTACIJE

Rotacija $R(i,j,\phi)$ mijenja elemente na pozicijama

$$(i,:,:),(j,:,:),(:,i,:),(:,j,:),(:,:,i),(:,:,j).$$

Bitni su nam elementi u (r,r,r)-podtenzoru. Zbog $1 \leq i \leq r < j \leq n$, ograničimo se na $(i,:,:)$, $(:,i,:)$, $(:,:,i)$, a kako je tenzor antisimetričan dovoljno je gledati pozicije $(i,:,:)$.

Za fiksni k i $(i,j) = (i(k),j(k))$, označimo $c = \cos\phi$, $s = \sin\phi$.

$$\|\mathcal{A}(i,:,:)\|^2 = \sum_{p,q=1}^{r} \mathcal{A}(i,p,q)^2 = \sum_{\substack{p,q=1\\ p,q\neq i}}^{r} \mathcal{A}(i,p,q)^2$$

$$\|\mathcal{A}'(i,:,:)\|^2 = (c\mathcal{A}(i,p,q) + s\mathcal{A}(j,p,q))^2 = \psi(c,s).$$

IZBOR KUTA ROTACIJE

Potrebno je maksimizirati funkciju
$\psi(c, s) = (c\mathcal{A}(i, p, q) + s\mathcal{A}(j, p, q))^2$ s obzirom na ϕ.

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Označimo

$$S_1 = \sum_{\substack{p,q=1 \\ p,q\neq i}}^{r} \mathcal{A}(i,p,q)^2,\ S_2 = \sum_{\substack{p,q=1 \\ p,q\neq i}}^{r} \mathcal{A}(i,p,q)\mathcal{A}(j,p,q),\ S_3 = \sum_{\substack{p,q=1 \\ p,q\neq i}}^{r} \mathcal{A}(j,p,q)^2.$$

Trebamo

$$\psi_\phi(c,s) = -6csS_1 + 6(c^2 - s^2)S_2 + 6csS_3 = 0.$$

IZBOR KUTA ROTACIJE

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$\psi(c,s) = (c\mathcal{A}(i,p,q) + s\mathcal{A}(j,p,q))^2$ s obzirom na ϕ.

Označimo

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Trebamo

$$\psi_\phi(c,s) = -6csS_1 + 6(c^2 - s^2)S_2 + 6csS_3 = 0. \Big/ \ : c^2$$

$$\Rightarrow t^2 S_2 + t(S_1 - S_3) - S_2 = 0, \quad \text{gdje je } t = \frac{s}{c}.$$

Za kut ϕ uzimamo rješenje gornje jednadžbe koje maksimizira ψ.

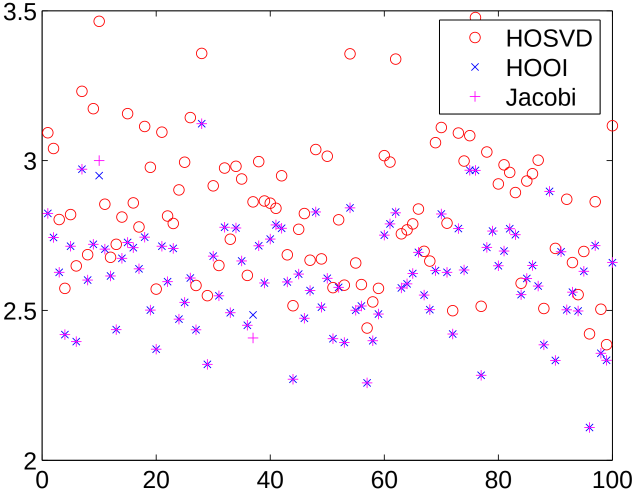
JACOBIJEVA METODA - Konvergencija

Teorem (B., Kressner)

Neka je $(Q_k)_k$ niz ortogonalnih matrica generiranih Jacobijevim algoritmom primijenjenim na antisimetrični tenzor $\mathcal{A} \in \mathbb{R}^{n \times n \times \cdots \times n}$. Svako gomilište niza $(Q_k)_k$ je stacionarna točka funkcije $f(\mathbf{Q}) = \|\mathcal{A} \times_1 \mathbf{MQ}^T \times_2 \mathbf{MQ}^T \times_3 \mathbf{MQ}^T\|^2$.

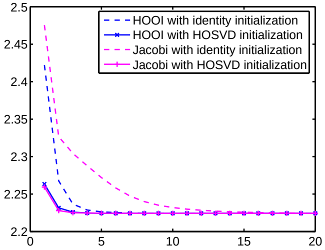
Numerički primjeri

Greška aproksimacije

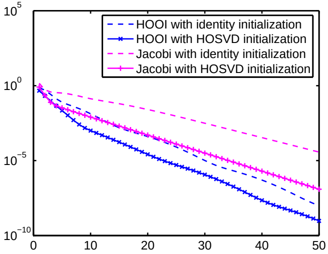


Slika: 100 slučajnih antisimetričnih $10 \times 10 \times 10$ tenzora aproksimiramo tenzorima multilinearnog ranga 3.

Konvergencija



(a) Greška aproksimacije



(b) Norma gradijenta

Slika: Aproksimacija slučajnog $10 \times 10 \times 10$ tenzora tenzorom multilinearnog ranga 6.

Aproksimacija tenzorima multilinearnog ranga d

FORMULACIJA PROBLEMA

- Za dani antisimetrični tenzor $\mathcal{A}$ odredimo aproksimaciju tenzorom $\mathcal{B}$ ranga 1,

$$\mathcal{B} = x_1 \circ x_2 \circ \cdots \circ x_d.$$

- $\mathcal{B}$ ranga 1 $\dashrightarrow$ $\hat{\mathcal{A}}$ multilinearnog ranga d

VEZA DVA PROBLEMA

Teorem (B., Kressner)

Neka je $\mathcal{A} \in \mathbb{R}^{n\times\cdots\times n}$ antisimetrični tenzor reda d. Vrijedi

$$\begin{aligned}
&\max\left\{\|\mathcal{A} \times_1 U^T \cdots \times_d U^T\| : \ U \in \mathbb{R}^{n\times d}, U^T U = I_d\right\} \\
=&d! \max\left\{|\mathcal{A} \times_1 u_1^T \cdots \times_d u_d^T| : \ [u_1, \ldots, u_d]^T [u_1, \ldots, u_d] = I_d\right\} \\
=&d! \max\left\{|\mathcal{A} \times_1 v_1^T \cdots \times_d v_d^T| : \ \|v_1\|_2 = \cdots = \|v_d\|_2 = 1\right\}.
\end{aligned}$$

VEZA DVA PROBLEMA

Teorem (B., Kressner)

Neka je $\mathcal{A} \in \mathbb{R}^{n\times\cdots\times n}$ antisimetrični tenzor reda d. Vrijedi

$$\begin{aligned} &\max\left\{\|\mathcal{A} \times_1 U^T \cdots \times_d U^T\| : \; U \in \mathbb{R}^{n\times d}, U^T U = I_d\right\} \\ =&d!\max\left\{|\mathcal{A} \times_1 u_1^T \cdots \times_d u_d^T| : \; [u_1,\ldots,u_d]^T[u_1,\ldots,u_d] = I_d\right\} \\ =&d!\max\left\{|\mathcal{A} \times_1 v_1^T \cdots \times_d v_d^T| : \; \|v_1\|_2 = \cdots = \|v_d\|_2 = 1\right\}. \end{aligned}$$

Ako je

$$\mathcal{B} = \alpha u_1 \circ u_2 \circ \cdots \circ u_d$$

najbolja aproksimacija rangom 1, u_k ortonormirani, $1 \leq k \leq d$, onda je

$$\hat{\mathcal{A}} = d! \text{ anti}(\mathcal{B})$$

najbolja aproksimacija multilinearnim rangom d.

APROKSIMACIJA TENZOROM RANGA-1

- **Minimizacijski problem**:

$$\|\mathcal{A} - x_1 \circ x_2 \circ \ldots \circ x_d\|^2 \to \min,$$

- Dualni **maksimizacijski problem** (Zhang, Golub, 2001.):

$$\sum_{i_1,\ldots,i_d} (\mathcal{A}(i_1, \ldots, i_d) x_1(i_1) \cdots x_d(i_d)) \to \max,$$

uz uvjet $\|x_1\|_2 = \cdots = \|x_d\|_2 = 1.$

HOPM

- **Higher order power method** ($\sim$ 2002.)
- ALS algoritam. Tražimo vektore $x_1, x_2, \ldots, x_d$ tako da u svakoj mikroiteraciji optimiziramo samo po jednom od njih dok su ostali fiksni.

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- **Konvergira prema lokalnom minimumu/maksimumu**.

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- **Konvergira prema lokalnom minimumu/maksimumu**.

HOPM algoritam

Take initial $u_1, u_2, \ldots, u_d$.
REPEAT
$u_1 = \mathcal{A} \times_2 u_2^T \times_3 u_3^T \cdots \times_d u_d^T$, $u_1 = u_1/\|u_1\|$.
$\ldots$
$u_d = \mathcal{A} \times_1 u_1^T \times_2 u_2^T \cdots \times_{d-1} u_{d-1}^T$, $u_d = u_d/\|u_d\|$.
UNTIL convergence
$\alpha = \mathcal{A} \times_1 u_1^T \times_2 u_2^T \cdots \times_d u_d^T$
Return approximation $\alpha u_1 \circ u_2 \circ \cdots \circ u_d$

DVIJE LEME

Lema (B., Kressner)

Neka je $\mathcal{A} \in \mathbb{R}^{n\times\cdots\times n}$ antisimetrični tenzor reda $d \leq n$. Vektori $u_1, u_2, \ldots, u_d$ generirani HOPM algoritmom čine ortonormiranu bazu, ukoliko niti jedan od vektora iz HOPM nije nul-vektor.

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Lema (B., Kressner)

Neka je $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ antisimetričan. Vrijedi:

(i) Kvadratna matricizacija $\mathbf{A}_{(1,2)}$ je simetrična matrica.

(ii) Ako je (λ, v) svojstveni par matrice $\mathbf{A}_{(1,2)}$, $\lambda \neq 0$, onda je matricizacija vektora v, $\bar{\mathbf{V}} \in \mathbb{R}^{n\times n}$, antisimetrična.

INICIJALIZACIJA HOPM ALGORITMA

- Standardna inicijalizacija HOSVD-om:

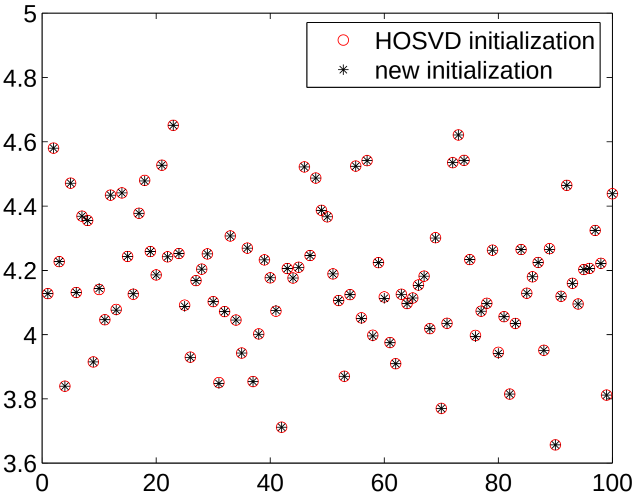
$$u_k = \mathbf{U}_k(:,1), \quad 1 \leq k \leq d.$$

- **Nova inicijalizacija** za $d = 4$

Form $\mathbf{A}_{(1,2)}$.
Compute eigenvector $v \in \mathbb{R}^{n^2}$ belonging to largest eigenvalue of $\mathbf{A}_{(1,2)}$.
Form $\bar{\mathbf{V}} \in \mathbb{R}^{n \times n}$.
Compute $\bar{\mathbf{V}} = \mathbf{U}\Sigma\mathbf{V}^T$.
$u_i = \mathbf{U}(:,i),\ 1 \leq i \leq 4$.

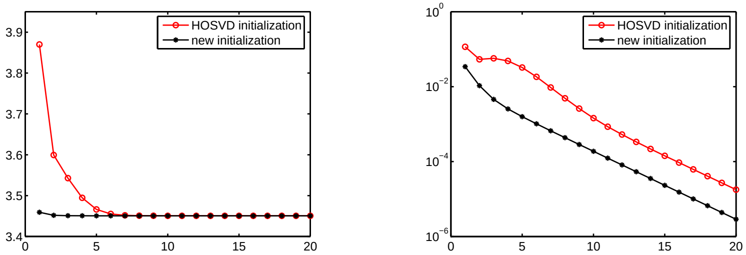
Numerički primjeri

Greška aproksimacije



Slika: HOPM aproksimacija 100 slučajnih antisimetričnih $10 \times 10 \times 10 \times 10$ tenzora multilinearnim rangom 4.

Konvergencija



(a) Greška aproksimacije (b) Norma gradijenta

Slika: Aproksimacija slučajnog $10 \times 10 \times 10 \times 10$ tenzora tenzorom multilinearnog ranga 4.

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