# https://moodle.epfl.ch/course/view.php?id=16819 

## TENSOR FACTORIZATION

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| Thu. 21.09.2023 | (C) 1. ML introduction |
| :---: | :---: |
| Thu. 28.09.2023 | (C) 2. Bayesian 1 (C) 3. Bayesian 2 |
| Thu. 12.10.2023 | (C) 4. Hidden Markov Models |
| Thu. 19.10.2023 | (C) 5. Dimensionality reduction |
| Thu. 26.10.2023 | (C) 6. Decision trees |
| Thu. 02.11.2023 | (C) 7. Linear regression |
| Thu. 09.11.2023 | (C) 8. Nonlinear regression |
| Thu. 16.11.2023 | (C) 9. Kernel Methods - SVM |
| Thu. 23.11.2023 | (C) 10. Tensor factorization |
| Thu. 30.11.2023 | (C) 11. Deep learning 1 |
| Thu. 07.12.2023 | (C) 12. Deep learning 2 |
| Thu. 14.12.2023 | (C) 13. Deep learning 3 |
| Thu. 21.12.2023 | (C) 14. Deep learning 4 |

## Outline

## Linear algebra:

- Products (Hadamard, Kronecker, Khatri-Rao)
- Separation of variables
- Singular value decomposition (SVD)


## 3 tensor decomposition models:

- Canonical polyadic (CP)
- Tucker
- Tensor train

Products (Hadamard, Kronecker, Khatri-Rao)
Hadamard
(elementwise)

$$
\boldsymbol{A} * \boldsymbol{B}=\left[\begin{array}{cccc}
a_{1,1} b_{1,1} & a_{1,2} b_{1,2} & \cdots & a_{1, J} b_{1, J} \\
a_{2,1} b_{2,1} & a_{2,2} b_{2,2} & \cdots & a_{2, J} b_{2, J} \\
\vdots & \vdots & \ddots & \vdots \\
a_{I, 1} b_{I, 1} & a_{I, 2} b_{I, 2} & \cdots & a_{I, J} b_{I, J}
\end{array}\right]
$$

$$
\begin{aligned}
\boldsymbol{A} & \in \mathbb{R}^{I \times J} \\
\boldsymbol{B} & \in \mathbb{R}^{I \times J} \\
\boldsymbol{A} * \boldsymbol{B} & \in \mathbb{R}^{I \times J}
\end{aligned}
$$

Kronecker

$$
\boldsymbol{A} \otimes \boldsymbol{B}=\left[\begin{array}{cccc}
a_{1,1} \boldsymbol{B} & a_{1,2} \boldsymbol{B} & \cdots & a_{1, J} \boldsymbol{B} \\
a_{2,1} \boldsymbol{B} & a_{2,2} \boldsymbol{B} & \cdots & a_{2, J} \boldsymbol{B} \\
\vdots & \vdots & \ddots & \vdots \\
a_{I, 1} \boldsymbol{B} & a_{I, 2} \boldsymbol{B} & \cdots & a_{I, J} \boldsymbol{B}
\end{array}\right]
$$

$$
\boldsymbol{A} \in \mathbb{R}^{I \times J}
$$

$$
\boldsymbol{B} \in \mathbb{R}^{K \times L}
$$

$$
\boldsymbol{A} \otimes \boldsymbol{B} \in \mathbb{R}^{I K \times J L}
$$

Khatri-Rao

$$
\boldsymbol{A} \odot \boldsymbol{B}=\left[\begin{array}{cccc}
a_{1,1} \boldsymbol{b}_{1} & a_{1,2} \boldsymbol{b}_{2} & \cdots & a_{1, K} \boldsymbol{b}_{K} \\
a_{2,1} \boldsymbol{b}_{1} & a_{2,2} \boldsymbol{b}_{2} & \cdots & a_{2, K} \boldsymbol{b}_{K} \\
\vdots & \vdots & \ddots & \vdots \\
a_{I, 1} \boldsymbol{b}_{1} & a_{I, 2} \boldsymbol{b}_{2} & \cdots & a_{I, K} \boldsymbol{b}_{K}
\end{array}\right]
$$

$$
\boldsymbol{A} \in \mathbb{R}^{I \times K}
$$

$$
\boldsymbol{B} \in \mathbb{R}^{J \times K}
$$

$$
\boldsymbol{A} \odot \boldsymbol{B} \in \mathbb{R}^{I J \times K}
$$

Hadamard (elementwise) product - Example

$$
\begin{aligned}
\boldsymbol{A} & \in \mathbb{R}^{3 \times 2} \\
\boldsymbol{B} & \in \mathbb{R}^{3 \times 2} \\
\boldsymbol{A} * \boldsymbol{B} & \in \mathbb{R}^{3 \times 2}
\end{aligned}
$$



Kronecker product - Example

$\boldsymbol{A} \in \mathbb{R}^{3 \times 2}$

| $\boldsymbol{A}$ | $\in \mathbb{R}^{3 \times 2}$ |
| ---: | :--- |
| $\boldsymbol{B}$ | $\in \mathbb{R}^{5 \times 4}$ |
| $\boldsymbol{A} \otimes \boldsymbol{B}$ | $\in \mathbb{R}^{15 \times 8}$ |

## Khatri-Rao product - Example



$$
\begin{aligned}
\boldsymbol{A} & \in \mathbb{R}^{3 \times 2} \\
\boldsymbol{B} & \in \mathbb{R}^{5 \times 2} \\
\boldsymbol{A} \odot \boldsymbol{B} & \in \mathbb{R}^{15 \times 2}
\end{aligned}
$$

## Tensors



3rd-order tensors

Images: 3D tensors
(width, height, color channels)

Videos: 4D tensors
(frame, width, height, color channels)

## r

Tensors appear in various forms:

- Raw data (arrays of sensors, multidimensional channels)
- Data evolution over time window
(sets of short sequences)
- Data in multiple coordinate systems
- Basis functions expansion


## Tensor methods - Motivation



Tensor factorization
$\rightarrow$ Multiway analysis of the data


Couldn't we simply vectorize/flatten our data before further processing?


Tensor data in robotics: Available processing tools


Figures from: Andrzej CICHOCKI (2014), Era of Big Data Processing: A New Approach via Tensor Networks and Tensor Decompositions

## Separation of variables: a factorization problem

Matrix factorization with standard linear algebra:

(singular value decomposition)

Rank-1 decomposition:

$$
\boldsymbol{X}_{i, j}=\boldsymbol{U}_{i} \boldsymbol{V}_{j} \rightarrow \text { Representation in a separable form }
$$

Rank-R decomposition:

$$
\boldsymbol{X}_{i, j}=\sum_{r=1}^{R} \boldsymbol{U}_{i, r} \boldsymbol{V}_{j, r} \quad \underset{\text { (in matrix form) }}{\boldsymbol{X}=\boldsymbol{U} \boldsymbol{V}^{\top}}
$$

Extension to data with more indices (tensors):

$$
\boldsymbol{X}_{i, j, k, \ldots}=\sum_{r=1}^{R} \boldsymbol{U}_{i, r} \boldsymbol{V}_{j, r} \boldsymbol{W}_{k, r} \cdots
$$

(CP decomposition)

## Data structured as tensors



Tensor indexing - Slices and fibers


## Tensor matricization / unfolding

A matrix $\boldsymbol{X}_{(n)} \in \mathbb{R}^{I_{n} \times\left(I_{1} \cdots I_{n-1} I_{n+1} \cdots I_{N}\right)}$ results from the mode- $n$ matricization (unfolding) of a tensor $\mathcal{X} \in \mathbb{R}^{I_{1} \times I_{2} \times \cdots \times I_{N}}$, which consists of turning the mode- $n$ fibers of $\boldsymbol{\mathcal { X }}$ into the columns of a matrix $\boldsymbol{X}_{(n)}$.


$$
\boldsymbol{\mathcal { X }} \in \mathbb{R}^{8 \times 6 \times 4}
$$



$$
\boldsymbol{X}_{(1)} \in \mathbb{R}^{8 \times 24}
$$

(mode-1 unfolding)

## Mode-n product



Intuitively, the operation corresponds to multiplying each mode- $n$ fiber of $\boldsymbol{\mathcal { X }}$ by the matrix $\boldsymbol{M}$.

Modern product - Example

$$
\begin{aligned}
\mathcal{X} & \in \mathbb{R}^{8 \times 6 \times 4} \\
\boldsymbol{M} & \in \mathbb{R}^{6 \times 3} \\
\mathcal{Y} & \in \mathbb{R}^{8 \times 3 \times 4}
\end{aligned}
$$



## Outer product and inner product

## Singular value decomposition (SVD)



$$
\begin{aligned}
\tilde{\boldsymbol{u}}_{i}=\sigma_{i} \boldsymbol{u}_{i} & =\sigma_{1}^{2} \boldsymbol{u}_{1} \boldsymbol{v}_{1}^{\top}+\sigma_{2}^{2} \boldsymbol{u}_{2} \boldsymbol{v}_{2}^{\top} \\
\tilde{\boldsymbol{v}}_{i}=\sigma_{i} \boldsymbol{v}_{i} & =\tilde{\boldsymbol{u}}_{1} \tilde{\boldsymbol{v}}_{1}^{\top}+\tilde{\boldsymbol{u}}_{2} \tilde{\boldsymbol{v}}_{2}^{\top} \\
& =\tilde{\boldsymbol{u}}_{1} \circ \tilde{\boldsymbol{v}}_{1}+\tilde{\boldsymbol{u}}_{2} \circ \tilde{\boldsymbol{v}}_{2} \\
& = \\
&
\end{aligned}
$$

## Data structured as tensors



## $C P$ decomposition



## $C P$ decomposition



The tensor rank $r$ corresponds to the smallest number of components required in the CP decomposition.

## CP parameters estimation: Alternating least squares (ALS)

The CP decomposition can be solved by alternating least squares (ALS),
$\boldsymbol{\mathcal { X }} \in \mathbb{R}^{n_{1} \times n_{2} \times n_{3}}$ by repeating

$$
\begin{aligned}
& \boldsymbol{A} \leftarrow \arg \min _{\boldsymbol{A}}\left\|\boldsymbol{X}_{(1)}-\boldsymbol{A}(\boldsymbol{C} \odot \boldsymbol{B})^{\top}\right\|_{\mathrm{F}}^{2} \\
& \boldsymbol{B} \leftarrow \arg \min _{\boldsymbol{B}}\left\|\boldsymbol{X}_{(2)}-\boldsymbol{B}(\boldsymbol{C} \odot \boldsymbol{A})^{\top}\right\|_{\mathrm{F}}^{2} \\
& \boldsymbol{C} \leftarrow \arg \min _{\boldsymbol{C}}\left\|\boldsymbol{X}_{(3)}-\boldsymbol{C}(\boldsymbol{B} \odot \boldsymbol{A})^{\top}\right\|_{\mathrm{F}}^{2}
\end{aligned}
$$


until convergence, yielding the update rules

$$
\begin{aligned}
& \boldsymbol{A} \leftarrow \boldsymbol{X}_{(1)}\left((\boldsymbol{C} \odot \boldsymbol{B})^{\top}\right)^{\dagger} \\
& \boldsymbol{B} \leftarrow \boldsymbol{X}_{(2)}\left((\boldsymbol{C} \odot \boldsymbol{A})^{\top}\right)^{\dagger} \\
& \boldsymbol{C} \leftarrow \boldsymbol{X}_{(3)}\left((\boldsymbol{B} \odot \boldsymbol{A})^{\top}\right)^{\dagger}
\end{aligned}
$$

$$
\boldsymbol{A}=\left[\boldsymbol{a}_{1}, \boldsymbol{a}_{2}, \boldsymbol{a}_{3}\right]
$$

## Data structured as tensors



Matrix factorization with standard linear algebra:


## Tucker decomposition



Tucker parameters estimation: Higher-order SVD (HO-SVD)

The Tucker decomposition can be estimated by computing the truncated singular value decompositions (SVD)

$$
\begin{aligned}
& \boldsymbol{X}_{(1)}=\boldsymbol{A} \boldsymbol{S} \boldsymbol{V}^{\top} \\
& \boldsymbol{X}_{(2)}=\boldsymbol{B} \boldsymbol{S} \boldsymbol{V}^{\top} \\
& \boldsymbol{X}_{(3)}=\boldsymbol{C} \boldsymbol{S} \boldsymbol{V}^{\top}
\end{aligned}
$$

$$
\begin{array}{rlrl}
\boldsymbol{\mathcal { X }} & \in \mathbb{R}^{n_{1} \times n_{2} \times n_{3}} & & \\
\mathcal{G} \in \mathbb{R}^{r_{1} \times r_{2} \times r_{3}} & & \\
\boldsymbol{A} \in \mathbb{R}^{n_{1} \times r_{1}} & \boldsymbol{A}^{\top} \boldsymbol{A}=\boldsymbol{I}_{r_{1}} \\
\boldsymbol{B} \in \mathbb{R}^{n_{2} \times r_{2}} & \boldsymbol{B}^{\top} \boldsymbol{B}=\boldsymbol{I}_{r_{2}} \\
\boldsymbol{C} \in \mathbb{R}^{n_{3} \times r_{3}} & \boldsymbol{C}^{\top} \boldsymbol{C}=\boldsymbol{I}_{r_{3}}
\end{array}
$$

with $\mathcal{G}$ finally evaluated as

$$
\mathcal{G} \leftarrow \mathcal{X} \times_{1} \boldsymbol{A}^{\top} \times_{2} \boldsymbol{B}^{\top} \times_{3} \boldsymbol{C}^{\boldsymbol{\top}}
$$

In contrast to CP, the Tucker decomposition is generally not unique $\rightarrow A, B$ and $C$ constrained to be orthogonal matrices

## Data structured as tensors



Tensor train parameters estimation: TT-SVD

$$
\begin{aligned}
& \mathcal{X} \in \mathbb{R}^{n_{1} \times n_{2} \times n_{3} \times n_{4}} \\
& \boldsymbol{\mathcal { P }}^{k} \in \mathbb{R}^{r_{k-1} \times n_{k} \times r_{k}}
\end{aligned}
$$

- $\mathcal{X}$ is reshaped as a $n_{1} \times n_{2} n_{3} n_{4}$ matrix $\boldsymbol{X}_{1}$
- $\boldsymbol{X}_{1} \approx \boldsymbol{U}_{1} \boldsymbol{S}_{1} \boldsymbol{V}_{1}^{\top}$, where $\boldsymbol{U}_{1}$ is a $n_{1} \times r_{1}$ matrix, reshaped as $1^{\text {st }}$ core $\mathcal{P}^{1}$
- $\boldsymbol{S}_{1} \boldsymbol{V}_{1}^{\top}$ is a $r_{1} \times n_{2} n_{3} n_{4}$ matrix reshaped into a $r_{1} n_{2} \times n_{3} n_{4}$ matrix $\boldsymbol{X}_{2}$
- $\boldsymbol{X}_{2} \approx \boldsymbol{U}_{2} \boldsymbol{S}_{2} \boldsymbol{V}_{2}^{\top}$, where $\boldsymbol{U}_{2}$ is a $r_{1} n_{2} \times r_{2}$ matrix, reshaped as $2^{\text {nd }}$ core $\mathcal{P}^{2}$
- $\boldsymbol{S}_{2} \boldsymbol{V}_{2}^{\top}$ is a $r_{2} \times n_{3} n_{4}$ matrix reshaped into a $r_{2} n_{3} \times n_{4}$ matrix $\boldsymbol{X}_{3}$
- $\boldsymbol{X}_{3} \approx \boldsymbol{U}_{3} \boldsymbol{S}_{3} \boldsymbol{V}_{3}^{\top}$, where $\boldsymbol{U}_{3}$ is a $r_{2} n_{3} \times r_{3}$ matrix, reshaped as $3^{\text {rd }}$ core $\mathcal{P}^{3}$
- $\boldsymbol{S}_{3} \boldsymbol{V}_{3}^{\top}$ is a $r_{3} \times n_{4}$ matrix, reshaped as $4^{\text {th }}$ core $\mathcal{P}^{4}$


## Example: Tensor train for global optimization

For 2D decision variable:

decision variable

decision variable

For nD decision variable:


Tensor train (TT)

## Example: Tensor train for global optimization

Cross approximation (skeleton decomposition) of a probability distribution:


$\rightarrow$ Can be used to approximate an unknown matrix by querying rows and columns of the matrix in an iterative manner, while estimating the rank of the matrix

## Example: Tensor train for global optimization

Cross approximation (skeleton decomposition) of a probability distribution:

$\rightarrow$ Can be used to approximate an unknown matrix by querying rows and columns of the matrix in an iterative manner, while estimating the rank of the matrix

## Example: Tensor train for global optimization

Optimization benchmarks with Himmelblau functions

task param. $(3,3)$ task param. $(3,14)$ task param. $(7,11)$ task param. $(13,5)$

| Inverse kinematics <br> (success rate) | Number of samples |  |  |  |
| :--- | :---: | :---: | :---: | :---: |
|  | 1 | 10 | 100 | 1000 |
| TTGO | $94.00 \%$ | $98.00 \%$ | $98.00 \%$ | $99.00 \%$ |
| Uniform | $37.75 \%$ | $45.50 \%$ | $59.25 \%$ | $75.00 \%$ |


| Target reaching <br> (success rate) | Number of samples |  |  |  |
| :--- | :---: | :---: | :---: | :---: |
|  | 1 | 10 | 100 | 1000 |
| TTGO | $62.00 \%$ | $86.00 \%$ | $86.00 \%$ | $88.00 \%$ |
| Uniform | $19.25 \%$ | $28.75 \%$ | $41.00 \%$ | $53.50 \%$ |


| Pick-and-place <br> (success rate) | Number of samples |  |  |  |
| :--- | :---: | :---: | :---: | :---: |
|  | 1 | 10 | 100 | 1000 |
| TTGO | $70.00 \%$ | $81.00 \%$ | $79.00 \%$ | $89.00 \%$ |
| Uniform | $23.75 \%$ | $30.25 \%$ | $39.5 \%$ | $44.25 \%$ |



## Ergodic control: Spectral multiscale coverage problem



Aim: Matching Fourier series coefficients


## Ergodic control for insertion tasks



Insertion task (Siemens gears benchmark)


Demonstration of insertion pose variations to provide a spatial reference distribution

The Fourier basis functions expansion does not scale well for more than 3 dimensions:
$\rightarrow$ low-rank tensor factorization is required

We evaluate the proposed approach using two different peg grasps:


Grasp \#1


Grasp \#2

## References

## Tensor methods

Kolda T, Bader B (2009) Tensor decompositions and applications. SIAM Review 51(3):455-500
Rabanser S, Shchur O, Günnemann S (2017) Introduction to tensor decompositions and their applications in machine learning. arXiv:171110781 pp 1-13

Shetty, S., Lembono, T., Löw, T. and Calinon, S. (2023). Tensor Train for Global Optimization Problems in Robotics. International Journal of Robotics Research (IJRR).

Shetty, S., Silvério, J. and Calinon, S. (2022). Ergodic Exploration using Tensor Train: Applications in Insertion Tasks. IEEE Trans. on Robotics (T-RO), 38:2, 906-921.

## Tensor methods - Softwares

https://tensornetwork.org http://tensorly.org (Python) https://www.tensorlab.net (Matlab)

A MATLAB package for tensor computations


