Hierarchical Nonnegative Tensor Decompositions

by Jamie Haddock
(Harvey Mudd College, Department of Mathematics)
on September 30, 2023,
AWM Research Symposium 2023 “Tensor Methods for data modeling”

https://ieeexplore.ieee.org/document/9022678 (CAMSAP 2019)
joint with M. Gao•, D. Molitor, E. Sadovnik, T. Will•, R. Zhang•, D. Needell

https://ieeexplore.ieee.org/document/9723126 (ACSSC 2021)
joint with Joshua Vendrow•, Deanna Needell

https://ieeexplore.ieee.org/document/9747810 (ICASSP 2022)
joint with Joshua Vendrow•, Deanna Needell

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matH of Algorithms, Data & Decisions research group @ HARVEY MUDD COLLEGE

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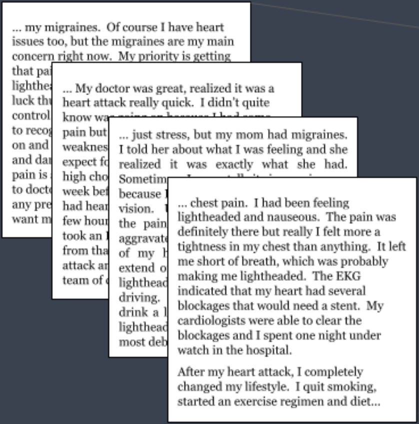
Motivation

» Learn trends in high-dimensional data

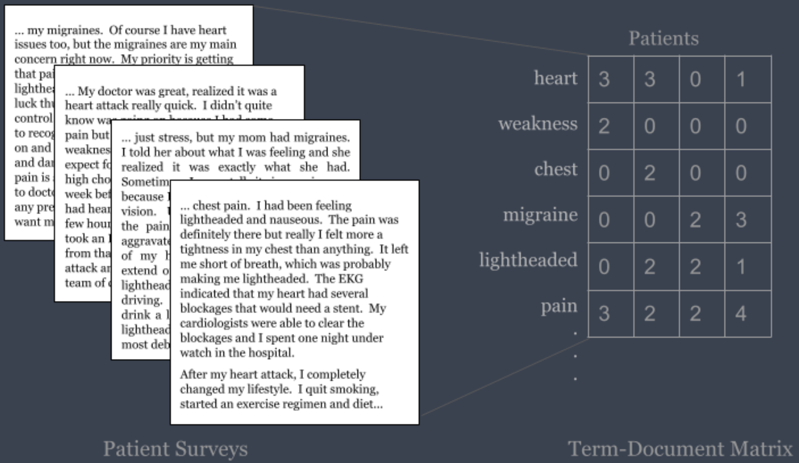


Patient Surveys

	Patients			
heart	3	3	0	1
weakness	2	0	0	0
chest	0	2	0	0
migraine	0	0	2	3
lightheaded	0	2	2	1
pain	3	2	2	4
⋮				

Term-Document Matrix

» Learn trends in high-dimensional data



Understand symptom trends and shared patient experiences automatically.

» Learn trends in high-dimensional data

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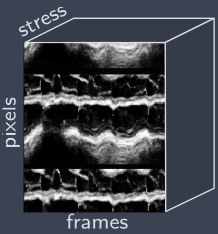
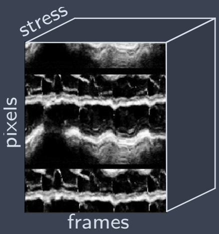


» Learn trends in high-dimensional data

Learn cohesive parts and separate noise in medical image studies.



Can we tell how the resulting parts/topics are related?

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How do we choose the number of topics or parts to learn?

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How do we choose the number of topics or parts to learn?

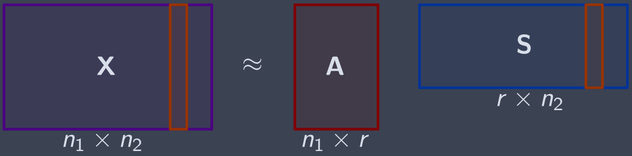
Hierarchical matrix factorization and tensor decomposition topic models!

Introduction

» Nonnegative Matrix Factorization (NMF)

Model: Given nonnegative data $\mathbf{X}$, compute nonnegative $\mathbf{A}$ and $\mathbf{S}$ of lower rank so that

$$\mathbf{X} \approx \mathbf{A}\mathbf{S}.$$



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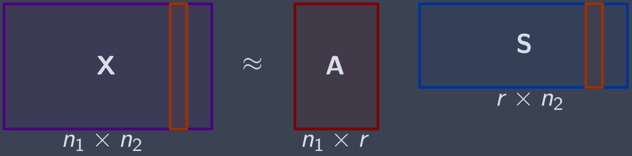

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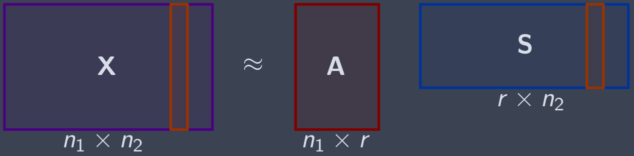

▷ Employed for dimensionality-reduction and topic modeling

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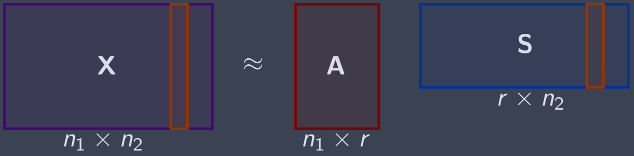

- ▷ Employed for dimensionality-reduction and topic modeling
- ▷ Often formulated as

$$\min_{\mathbf{A}\in\mathbb{R}_{\geq 0}^{n_1\times r},\mathbf{S}\in\mathbb{R}_{\geq 0}^{r\times n_2}} \|\mathbf{X}-\mathbf{AS}\|_F^2 \quad \text{or} \quad \min_{\mathbf{A}\in\mathbb{R}_{\geq 0}^{n_1\times r},\mathbf{S}\in\mathbb{R}_{\geq 0}^{r\times n_2}} D(\mathbf{X}\|\mathbf{AS}).$$ [1]

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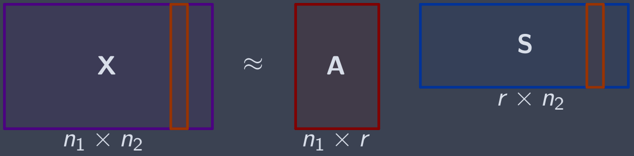

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- ▷ non-convex optimization problems

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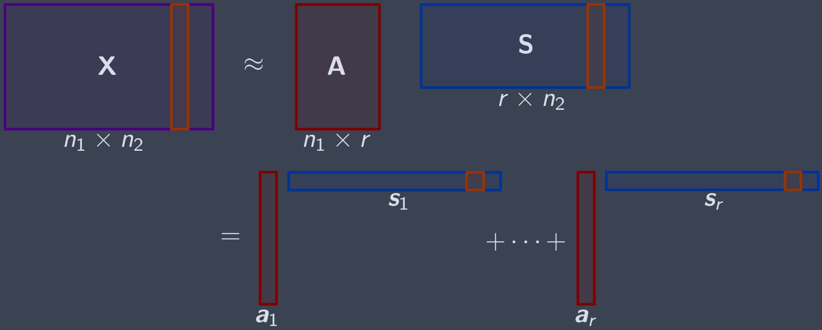

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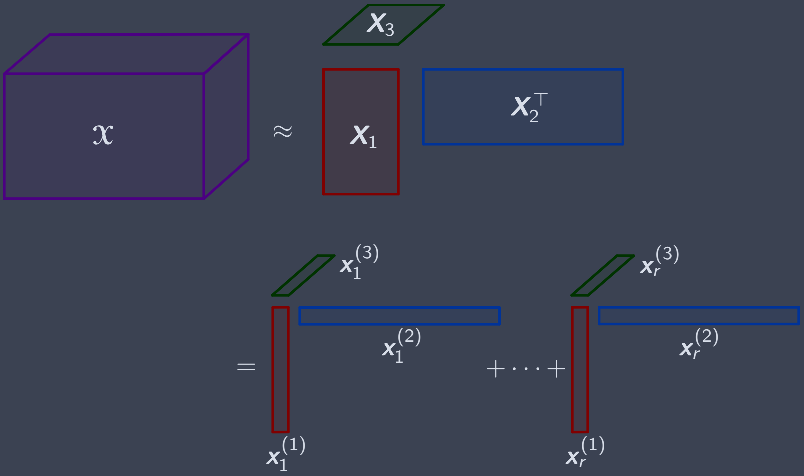
» Nonnegative CANDECOMP/PARAFAC (CP) decomposition (NCPD)



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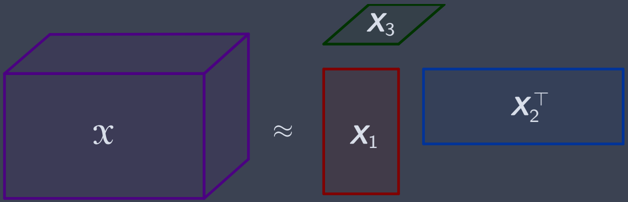

- formulated as $\min_{\boldsymbol{X}_i \geq 0} \|\mathcal{X} - [\![\boldsymbol{X}_1, \boldsymbol{X}_2, \cdots, \boldsymbol{X}_k]\!]\|_F^2$ where

$$[\![\boldsymbol{X}_1, \boldsymbol{X}_2, \cdots, \boldsymbol{X}_k]\!] \equiv \sum_{j=1}^{r} \boldsymbol{x}_j^{(1)} \otimes \boldsymbol{x}_j^{(2)} \otimes \cdots \otimes \boldsymbol{x}_j^{(k)}$$

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» Hierarchical NMF

Model: Sequentially factorize

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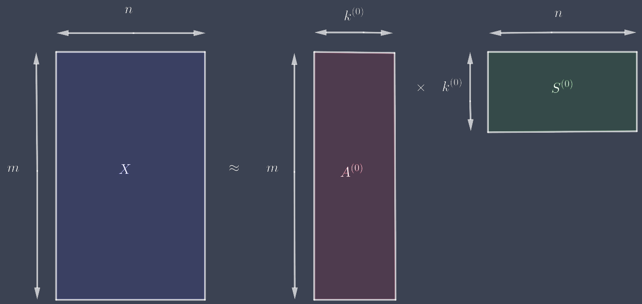

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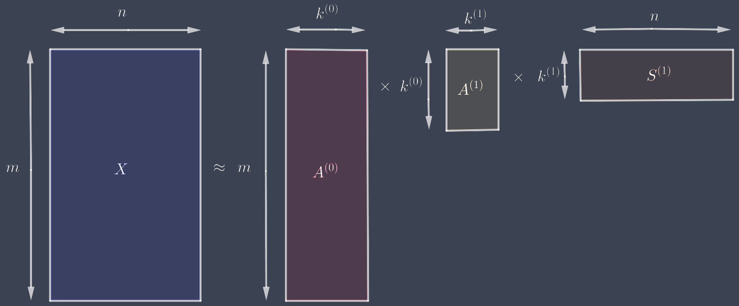
$$X \approx A^{(0)} S^{(0)}, S^{(0)} \approx A^{(1)} S^{(1)}$$



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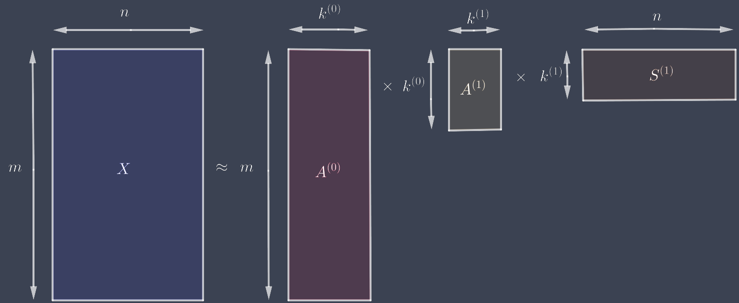
$$X \approx A^{(0)}S^{(0)}, S^{(0)} \approx A^{(1)}S^{(1)}, S^{(1)} \approx A^{(2)}S^{(2)}, ..., S^{(\mathcal{L}-1)} \approx A^{(\mathcal{L})}S^{(\mathcal{L})}.$$



- ▷ $k^{(\ell)}$: supertopics collecting $k^{(\ell-1)}$ subtopics

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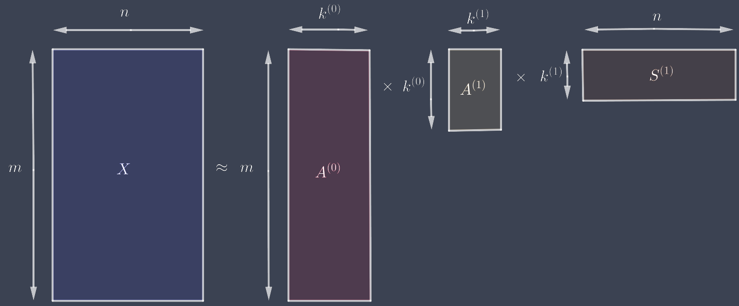

- ▷ $k^{(\ell)}$: supertopics collecting $k^{(\ell-1)}$ subtopics
- ▷ provides relationship between data matrix modes and $k^{(\ell)}$ topics

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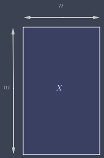

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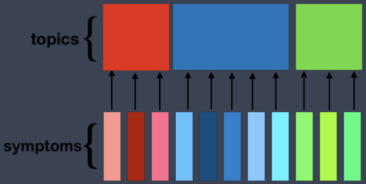

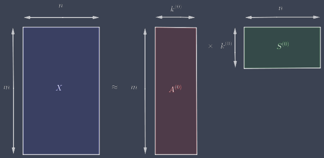

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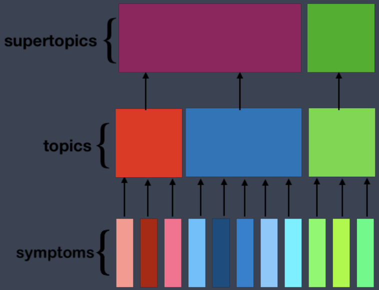

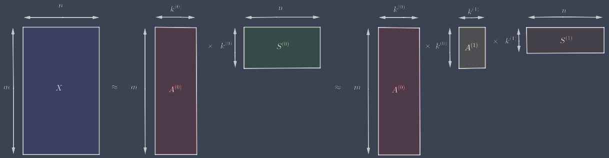

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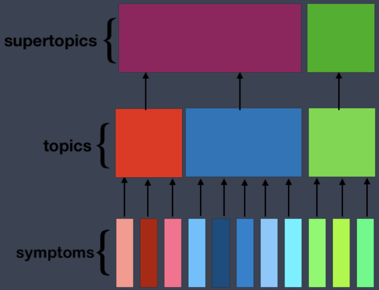
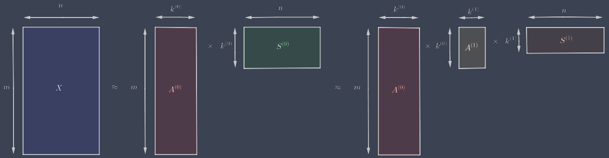


▷ elucidates the hierarchical relationships of learned topics



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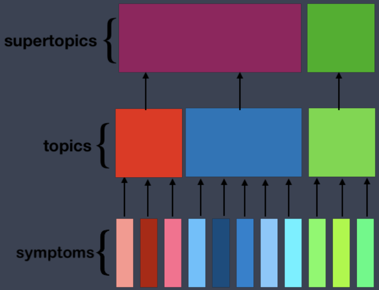
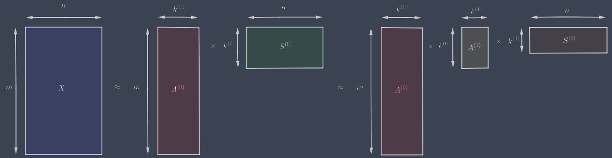


- ▷ elucidates the hierarchical relationships of learned topics
- ▷ no need to choose a fixed model rank (number of topics)



Hierarchical Models

» Hierarchical Tensor Decompositions

How do we generalize HNMF to a higher-order tensor model?

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Results depend upon hyperparameter choice (mode).

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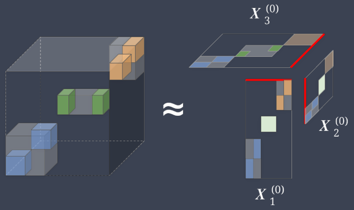
  ** Single hierarchical relationship, naive training method. **

» Multi-HNTF Model

This model learns

$$\mathcal{X} \approx [\![\boldsymbol{X}_1^{(0)}, \boldsymbol{X}_2^{(0)}, \cdots, \boldsymbol{X}_k^{(0)}]\!]$$



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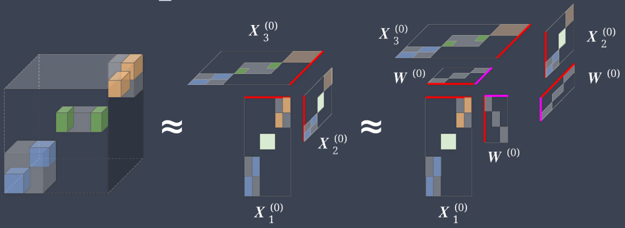
where

$$\boldsymbol{X}_j^{(\ell+1)} = \boldsymbol{X}_j^{(\ell)} \boldsymbol{W}^{(\ell)},$$

and $\boldsymbol{W}^{(\ell)} \in \mathbb{R}_{\geq 0}^{r^{(\ell-1)} \times r^{(\ell)}}$.



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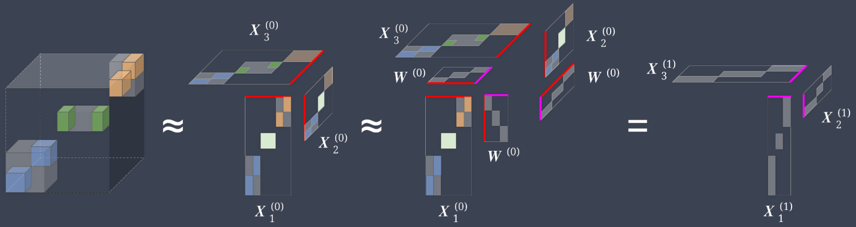

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$$\mathcal{X} \approx [\![X_1^{(0)}, X_2^{(0)}, \dots, X_k^{(0)}]\!] \approx [\![X_1^{(1)}, X_2^{(1)}, \dots, X_k^{(1)}]\!] \approx \cdots$$
$$\approx [\![X_1^{(\mathcal{L}-1)}, X_2^{(\mathcal{L}-1)}, \dots, X_k^{(\mathcal{L}-1)}]\!]$$

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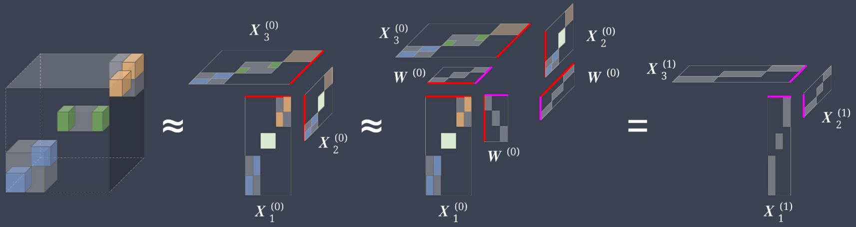

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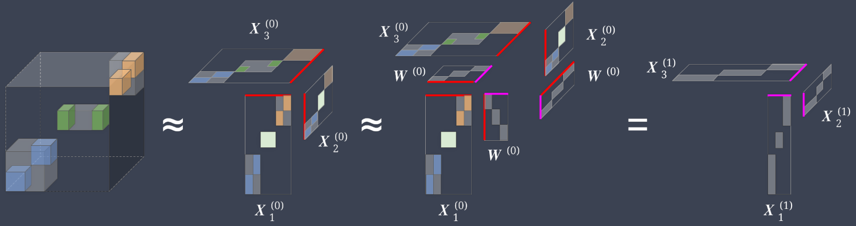
$$X_j^{(\ell+1)} = X_j^{(\ell)} W^{(\ell)},$$

and $W^{(\ell)} \in \mathbb{R}_{\geq 0}^{r^{(\ell-1)} \times r^{(\ell)}}$.



A single hierarchical relationship for all modes!

Vendrow, H., Needell. "A Generalized Hierarchical Nonnegative Tensor Decomposition." IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP). IEEE, 2022.

» Training Process

procedure $\textsc{Multi-HNTF}(\mathcal{X})$

$\quad \{\boldsymbol{X}_i^{(0)}\}_{i=1}^{k} \leftarrow \mathrm{NCPD}(\mathcal{X}, r_0)$

$\quad$ **for** $\ell = 0 \ldots \mathcal{L}$ **do**

$\quad\quad \boldsymbol{W}^{(\ell)} \leftarrow \mathrm{argmin}_{\boldsymbol{W} \in \mathbb{R}_+^{r_\ell \times r_{\ell+1}}} \|\mathcal{X} - [\![\boldsymbol{X}_1^{(\ell)}\boldsymbol{W}, \ldots, \boldsymbol{X}_k^{(\ell)}\boldsymbol{W}]\!]\|$

$\quad\quad$ **for** $i = 0 \ldots k$ **do**

$\quad\quad\quad \boldsymbol{X}_i^{(\ell+1)} = \boldsymbol{X}_i^{(\ell)}\boldsymbol{W}^{(\ell)}$

» Training Process

procedure MULTI-HNTF($\mathcal{X}$)
  $\{\boldsymbol{X}_i^{(0)}\}_{i=1}^{k} \leftarrow \mathrm{NCPD}(\mathcal{X}, r_0)$
  for $\ell = 0 \ldots \mathcal{L}$ **do**
    $\boldsymbol{W}^{(\ell)} \leftarrow \mathrm{argmin}_{\boldsymbol{W} \in \mathbb{R}_+^{r_\ell \times r_{\ell+1}}} \|\mathcal{X} - [\![\boldsymbol{X}_1^{(\ell)}\boldsymbol{W}, \ldots, \boldsymbol{X}_k^{(\ell)}\boldsymbol{W}]\!]\|$
    for $i = 0 \ldots k$ **do**
      $\boldsymbol{X}_i^{(\ell+1)} = \boldsymbol{X}_i^{(\ell)}\boldsymbol{W}^{(\ell)}$

▷ Can be approximated via NMF method on each mode with averaging of learned $\boldsymbol{W}$ matrix across modes.

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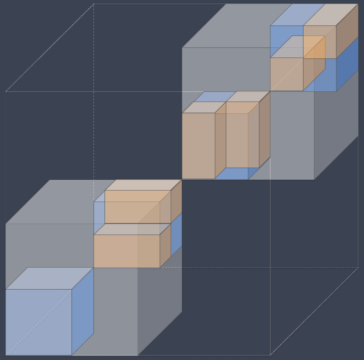
- Can be approximated via NMF method on each mode with averaging of learned $\boldsymbol{W}$ matrix across modes.
- Could/should also be trained in a neural network framework.

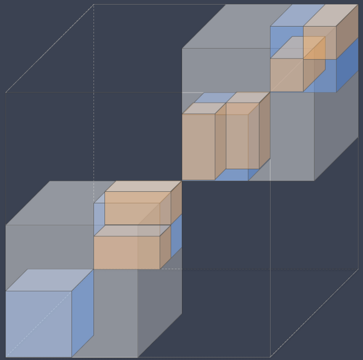
Experiments

» Synthetic Tensor



The table lists relative reconstruction errors on the tensor on the left for models learned with 7-4-2 topic structure. Below, we visualize the Multi-HNTF learned approximations for a synthetic tensor with 7-3 topic structure.

» Synthetic Tensor



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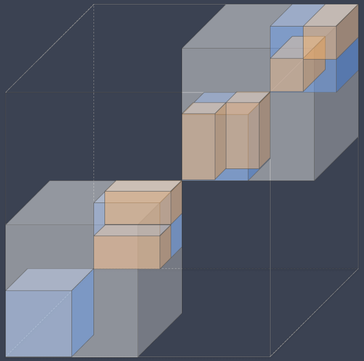
Relative reconstruction error.

Method	$r_0 = 7$	$r_1 = 4$	$r_2 = 2$
Multi-HNTF	0.454	0.548	0.721
Standard HNCPD [Vendrow, et. al.]	0.454	0.612	0.892
HNTF-1 [Cichocki, et. al.]	0.454	0.576	0.781
HNTF-2 [Cichocki, et. al.]	0.454	0.587	0.765
HNTF-3 [Cichocki, et. al.]	0.454	0.560	0.747

» Synthetic Tensor



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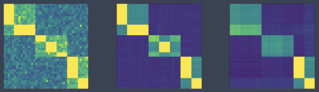

Projections of tensor approximation at each layer of Multi-HNTF.

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Neural HNCPD [Vendrow, et. al.]	0.454	**0.508**	**0.714**

Conclusions

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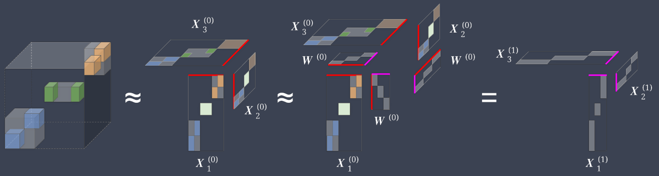
- Multi-HNTF is a hierarchical tensor decomposition model that generalizes hierarchical NMF.



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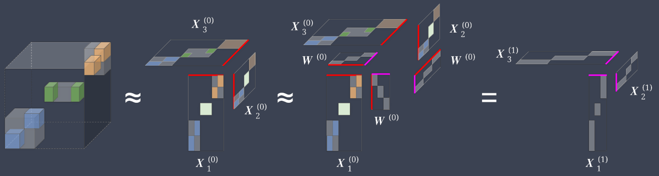

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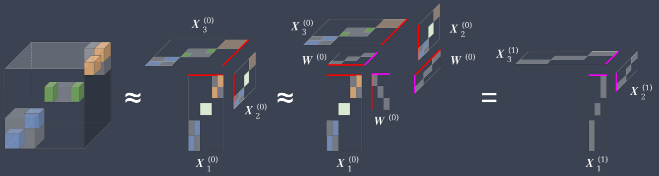

- Model can be trained by your `favorite NMF method` with an additional projection step.

- Develop backpropagation framework for Multi-HNTF and first layer NCPD.

» Thanks for listening! Questions?

[1] M. Gao, J. Haddock, D. Molitor, D. Needell, E. Sadovnik, T. Will, and R. Zhang. Neural nonnegative matrix factorization for hierarchical multilayer topic modeling. In Proc. Interational Workshop on Computational Advances in Multi-Sensor Adaptive Processing, 2019.

[2] J. Vendrow, J. Haddock, and D. Needell. Neural nonnegative CP decomposition for hierarchical tensor analysis. In Asilomar Conf. on Signals, Systems, Computers (ACSSC), 2021.

[3] J. Vendrow, J. Haddock, and D. Needell. A generalized hierarchical nonnegative tensor decomposition. In Proc. Int. Conf. on Acoustics, Speech, and Signal Processing (ICASSP), 2022.

[4] Daniel D Lee and H Sebastian Seung. Learning the parts of objects by non-negative matrix factorization. Nature, 401(6755):788–791, 1999.

[5] J Douglas Carroll and Jih-Jie Chang. Analysis of individual differences in multidimensional scaling via an N-way generalization of "Eckart-Young" decomposition. Psychometrika, 35(3):283–319, 1970.

[6] Richard A Harshman et al. Foundations of the PARAFAC procedure: Models and conditions for an" explanatory" multimodal factor analysis. 1970.

[7] Andrzej Cichocki and Rafal Zdunek. Multilayer nonnegative matrix factorisation. Electronics Letters, 42(16):947–948, 2006.

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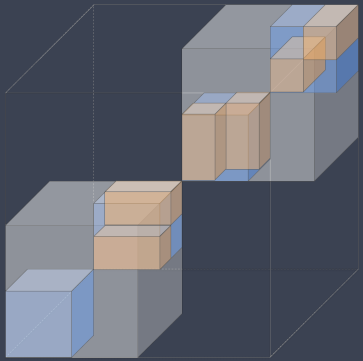

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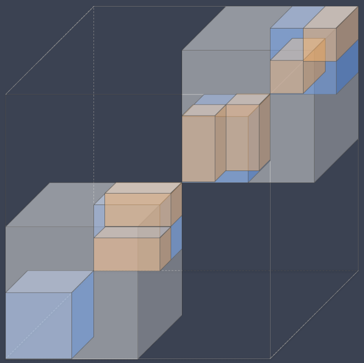

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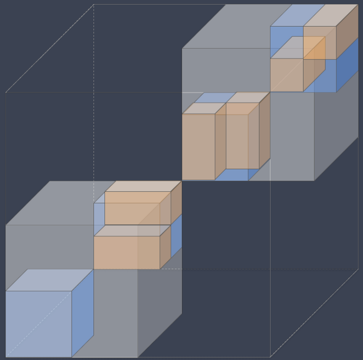

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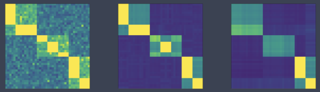

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