Hierarchical and Neural Nonnegative Tensor Decompositions

by Jamie Haddock
(Harvey Mudd College, Department of Mathematics)
on December 2, 2022,
IPAM "Multi-Modal Imaging with Deep Learning and 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

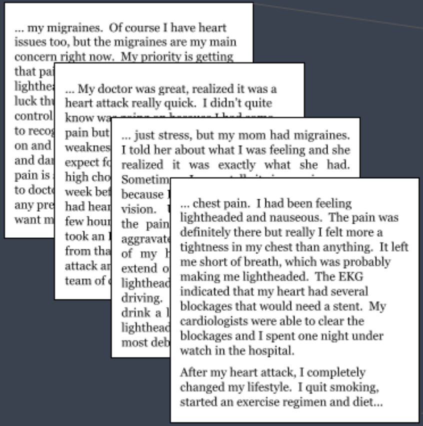
https://ieeexplore.ieee.org/document/9747810 (ICASSP 2022)
joint with Joshua Vendrow•, Deanna Needell

NSF DMS #2211318

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

Motivation

» Learn trends in high-dimensional data



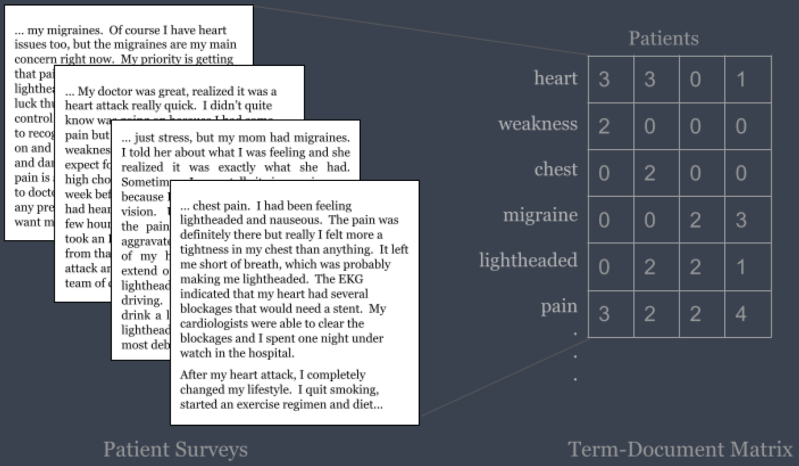
Patient Surveys

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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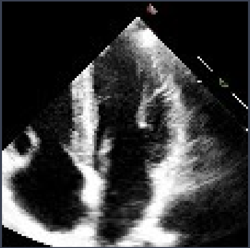
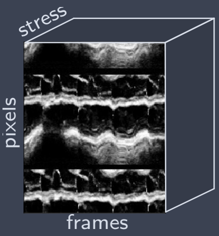
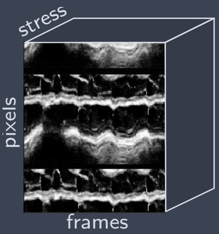




» Learn trends in high-dimensional data

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?

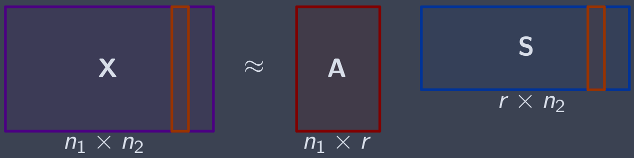
Hierarchical matrix factorization and tensor decomposition topic models!

Introduction

» Nonnegative Matrix Factorization (NMF)

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

$$\mathbf{X} \approx \mathbf{AS}.$$



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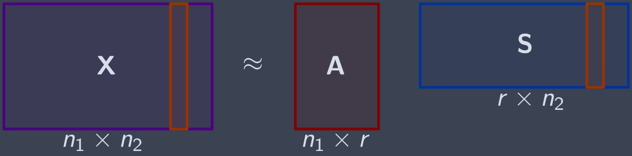

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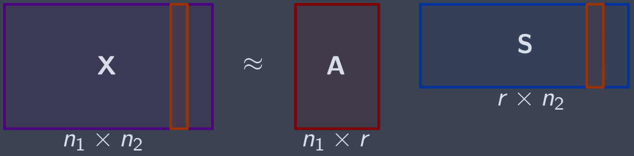

▷ Employed for dimensionality-reduction and topic modeling

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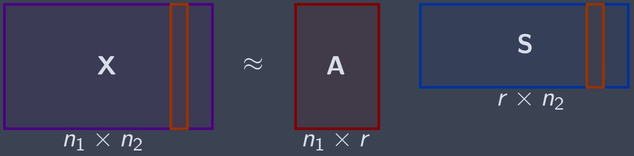

- ▷ Employed for dimensionality-reduction and topic modeling
- ▷ Often formulated as

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

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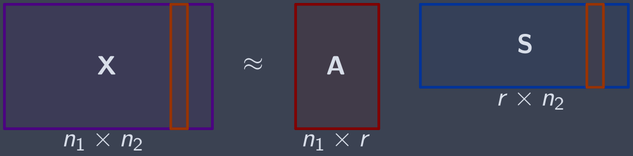

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- non-convex optimization problems

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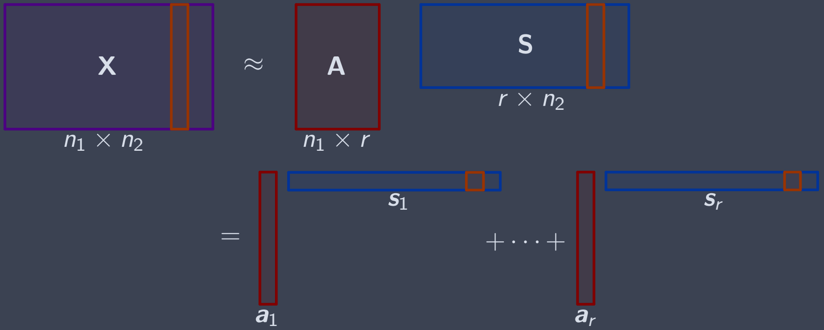

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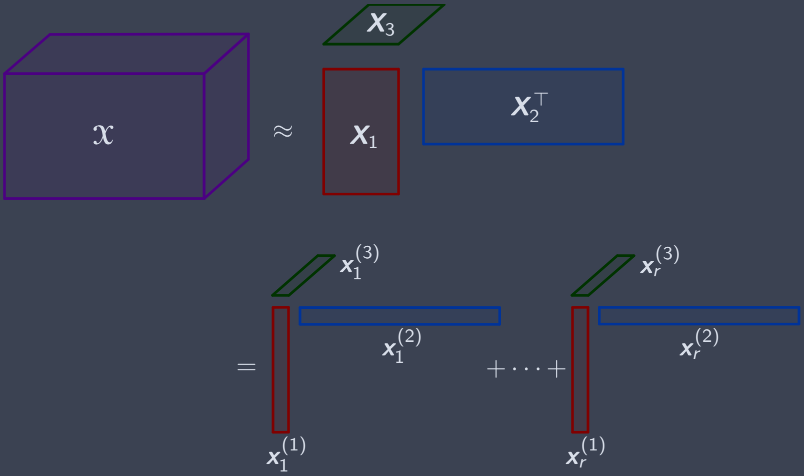

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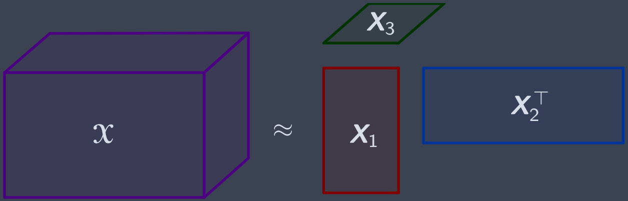

- ▷ formulated as $\min_{X_i \geq 0} \|\mathcal{X} - [\![X_1, X_2, \cdots, X_k]\!]\|_F^2$ where

$$[\![X_1, X_2, \cdots, X_k]\!] \equiv \sum_{j=1}^{r} x_j^{(1)} \otimes x_j^{(2)} \otimes \cdots \otimes x_j^{(k)}$$

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» Hierarchical NMF

Model: Sequentially factorize

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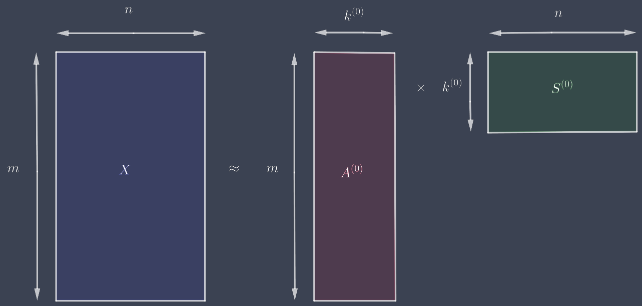
$$X \approx A^{(0)} S^{(0)}$$



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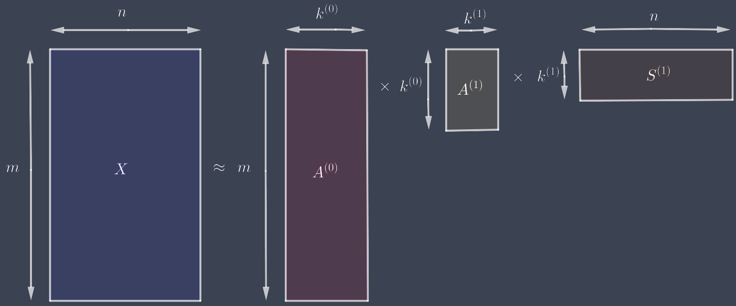
$$X \approx A^{(0)} S^{(0)}, S^{(0)} \approx A^{(1)} S^{(1)}$$



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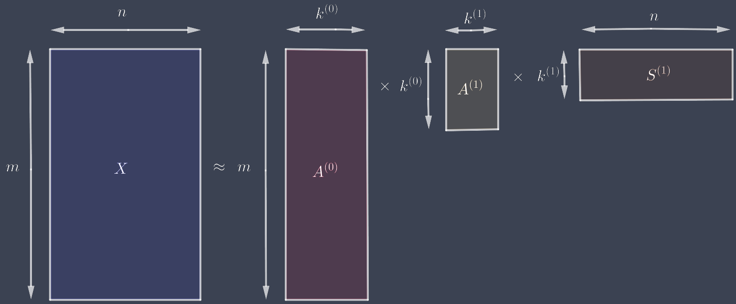
$$X \approx A^{(0)}S^{(0)}, S^{(0)} \approx A^{(1)}S^{(1)}, S^{(1)} \approx A^{(2)}S^{(2)}, ..., S^{(\mathcal{L}-1)} \approx A^{(\mathcal{L})}S^{(\mathcal{L})}.$$



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

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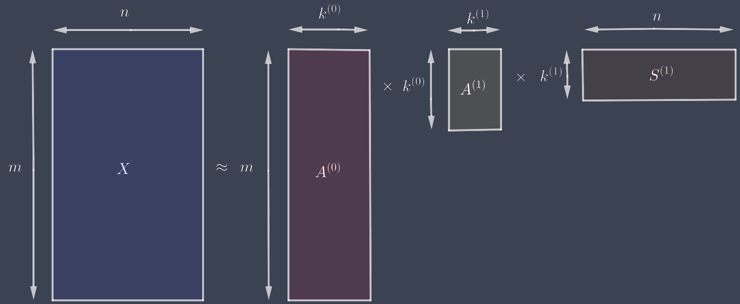

- $k^{(\ell)}$: supertopics collecting $k^{(\ell-1)}$ subtopics
- provides relationship between data matrix modes and $k^{(\ell)}$ topics

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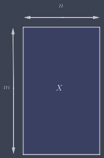

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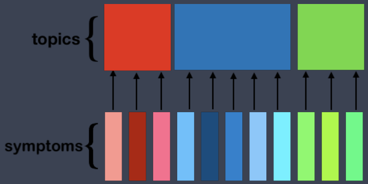

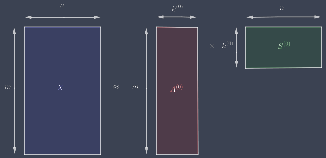

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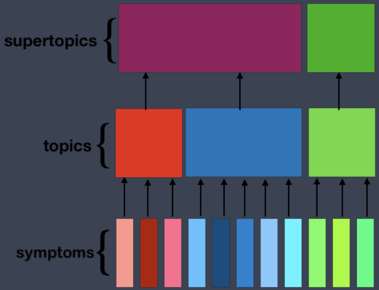

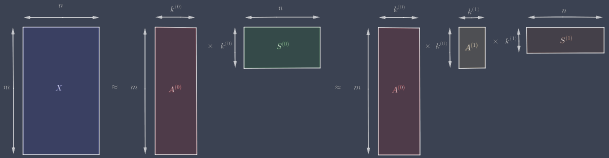

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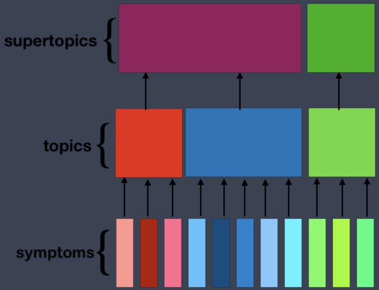
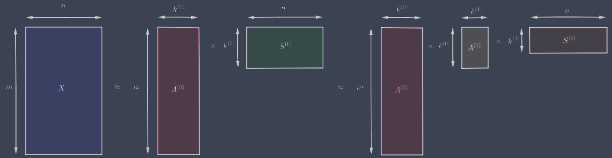


- ▷ elucidates the hierarchical relationships of learned topics



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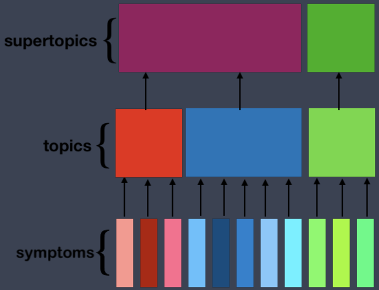
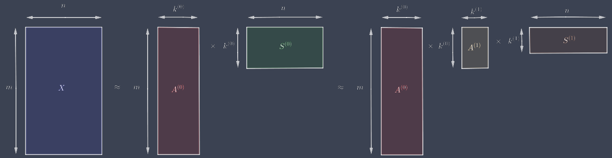


- ▷ elucidates the hierarchical relationships of learned topics
- ▷ no need to choose a fixed model rank (number of topics)



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.

» Hierarchical NCPD Model (Take 1)

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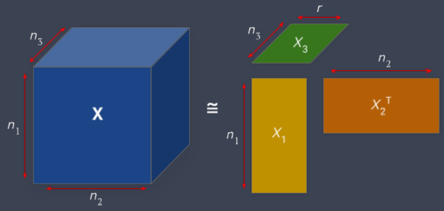
» Hierarchical NCPD Model (Take 1)

Learn an initial rank-r NCPD model,

$$\mathcal{X} \approx [\![\mathbf{X}_1, \mathbf{X}_2, \cdots, \mathbf{X}_k]\!]$$



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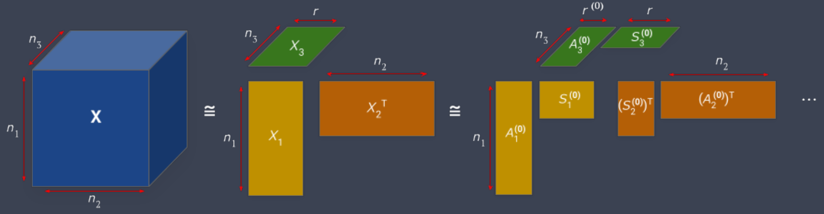
Learn an initial rank-r NCPD model,

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

and apply a hierarchical NMF model independently to each factor matrix,

$$\boldsymbol{X}_i \approx \boldsymbol{A}_i^{(0)} \boldsymbol{A}_i^{(1)} \cdots \boldsymbol{A}_i^{(l)} \boldsymbol{S}_i^{(l)}.$$



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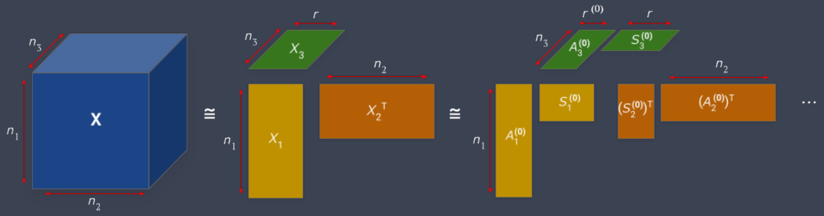

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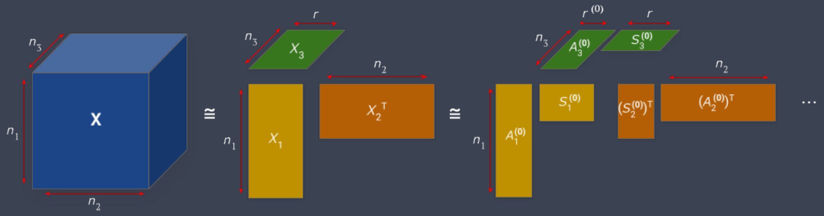

- ▷ can extend good training method for HNMF (Neural NMF) → Neural NCPD (later in this talk!)

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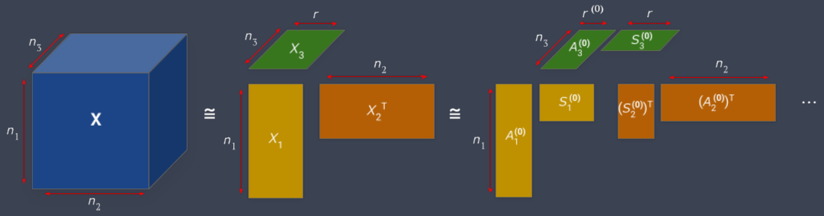

- ▷ can extend good training method for HNMF (Neural NMF) $\rightarrow$ Neural NCPD (later in this talk!)
- ▷ `Different hierarchy across tensor modes.  :(`

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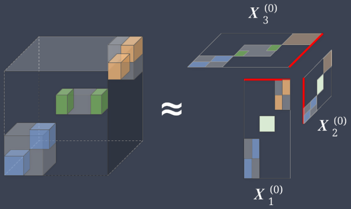
» Multi-HNTF Model (Take 2)

This model learns

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



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» Multi-HNTF Model (Take 2)

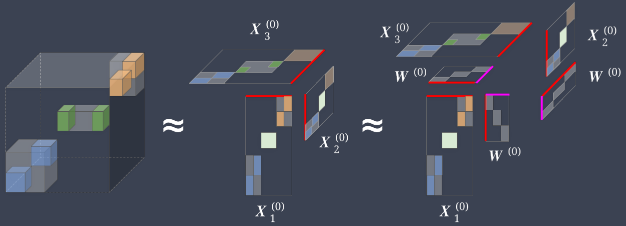
This model learns

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

where

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

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



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

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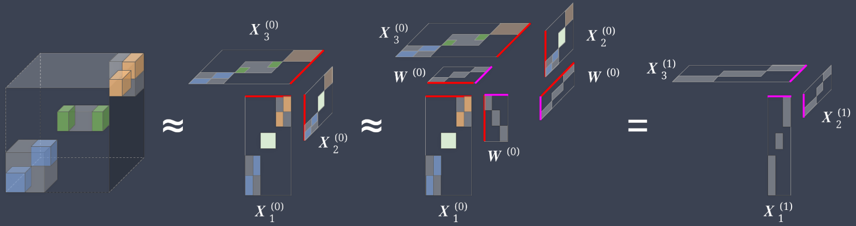

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$$\approx [\![X_1^{(\mathcal{L}-1)}, X_2^{(\mathcal{L}-1)}, \dots, X_k^{(\mathcal{L}-1)}]\!]$$

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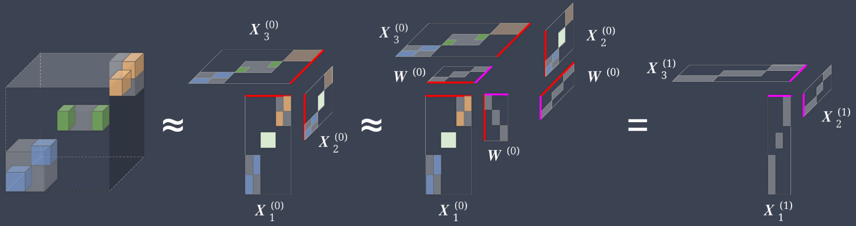

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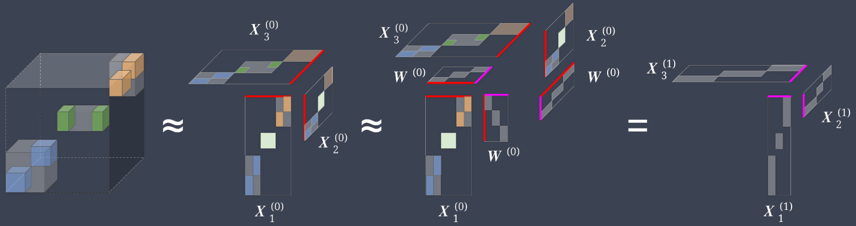


A single hierarchical relationship for all modes!

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

» Training Process

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

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

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

$\quad\quad W^{(\ell)} \leftarrow \operatorname{argmin}_{W \in \mathbb{R}_+^{r_\ell \times r_{\ell+1}}} \|\mathcal{X} - [\![X_1^{(\ell)} W, \dots, X_k^{(\ell)} W]\!]\|$

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

$\quad\quad\quad X_i^{(\ell+1)} = X_i^{(\ell)} W^{(\ell)}$

» Training Process

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

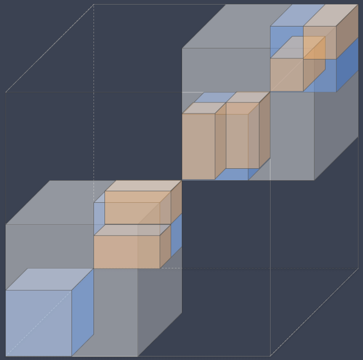
» Training Process

1: **procedure** MULTI-HNTF($\mathcal{X}$)
2: $\{X_i^{(0)}\}_{i=1}^k \leftarrow \text{NCPD}(\mathcal{X}, r_0)$
3: **for** $\ell = 0 \dots \mathcal{L}$ **do**
4: $W^{(\ell)} \leftarrow \text{argmin}_{W \in \mathbb{R}_+^{r_\ell \times r_{\ell+1}}} \|\mathcal{X} - [\![X_1^{(\ell)} W, \dots, X_k^{(\ell)} W]\!]\|$
5: **for** $i = 0 \dots k$ **do**
6: $X_i^{(\ell+1)} = X_i^{(\ell)} W^{(\ell)}$

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

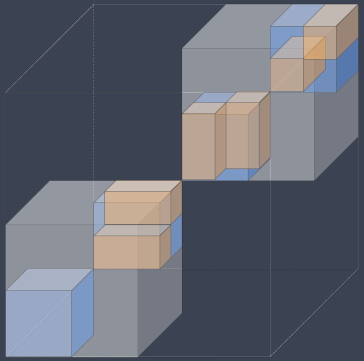
Experiments

» 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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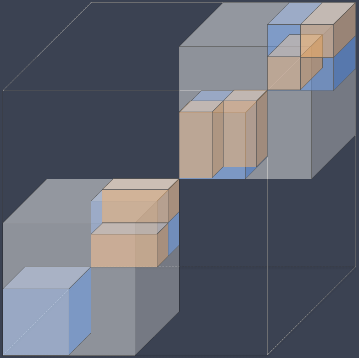
Relative reconstruction error.

Method	$r_0 = 7$	$r_1 = 4$	$r_2 = 2$
Multi-HNTF	0.454	0.548	0.721
~~Neural HNCPD [Vendrow, et. al.]~~	~~0.454~~	~~**0.508**~~	~~**0.714**~~
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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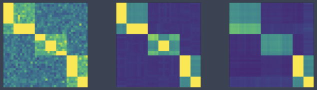

Projections of tensor approximation at each layer of Multi-HNTF.

Relative reconstruction error.

Method	$r_0 = 7$	$r_1 = 4$	$r_2 = 2$
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» Political Twitter Data

- A data set of tweets sent by political candidates during the 2016 election season
- We subset the tweets from eight politicians, four Republicans and four Democrats:

  Hillary Clinton, Tim Kaine, Martin O'Malley, Bernie Sanders, Ted Cruz, John Kasich, Marco Rubio, and Donald Trump.

» Political Twitter Data

Rank 8 Topics

Topic 1	Topic 2	Topic 3	Topic 4
trump	senate	martinomalley	berniesanders
hillary	florida	hillaryclinton	people
donald	zika	realdonaldtrump	bernie
president	venezuela	campaigning	must
timkaine	nicolasmaduro	maryland	change
Topic 5	**Topic 6**	**Topic 7**	**Topic 8**
tedcruz	johnkasich	marcorubio	crooked
cruz	kasich	teammarco	hillary
ted	ohio	vote	thank
internet	john	flsen	great
choosecruz	gov	click	clinton

Rank 4 Topics

Topic 1	Topic 2
trump	tedcruz
hillary	cruz
vote	ted
people	internet
berniesanders	choosecruz
Topic 3	**Topic 4**
johnkasich	crooked
kasich	hillary
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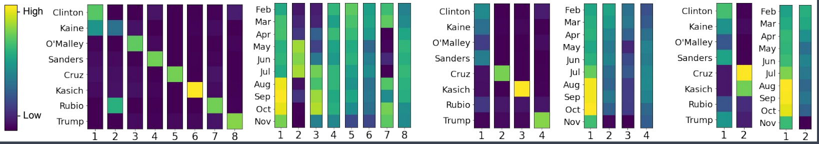
gov	realdonaldtrump

Rank 2 Topics

Topic 1
trump
hillary
people
vote
realdonaldtrump
Topic 2
tedcruz
cruz
ted
johnkasich
kasich



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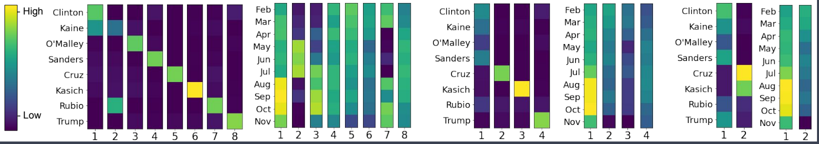
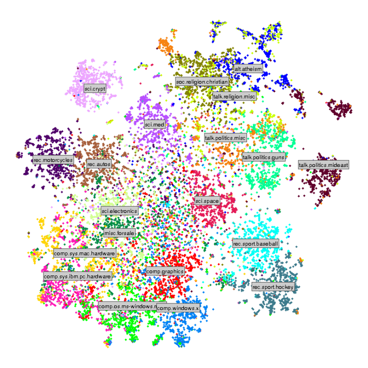


Method	$r_0 = 8$	$r_1 = 4$	$r_2 = 2$
Multi-HNTF	0.834	0.887	0.920
~~Neural HNCPD [Vendrow, et. al.]~~	~~0.834~~	~~**0.883**~~	~~**0.918**~~
Standard HNCPD [Vendrow, et. al.]	0.834	0.889	0.919
Standard NCPD	0.834	0.931	0.950
HNTF-1 [Cichocki, et. al.]	0.834	0.890	0.927
HNTF-2 [Cichocki, et. al.]	0.834	0.909	0.956
HNTF-3 [Cichocki, et. al.]	0.834	0.895	0.942

» 20 Newsgroups Data



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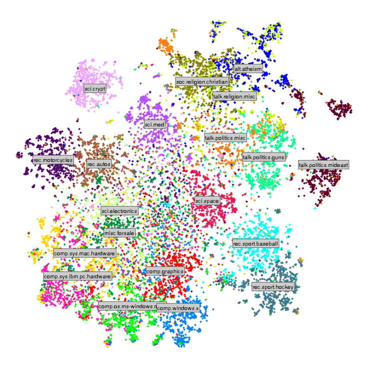


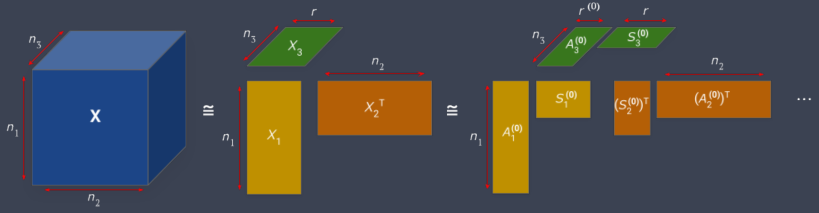
Reconstruction loss and classification accuracy at the second layer of two layer Multi-HNTF and HNMF on the 20 newsgroup data set.

Method	Recon Loss		Accuracy	
	Unsup.	Sup.	Unsup.	Sup.
Multi-HNTF	**30.81**	**30.91**	**0.516**	**0.737**
HNMF	30.82	31.45	0.507	0.636

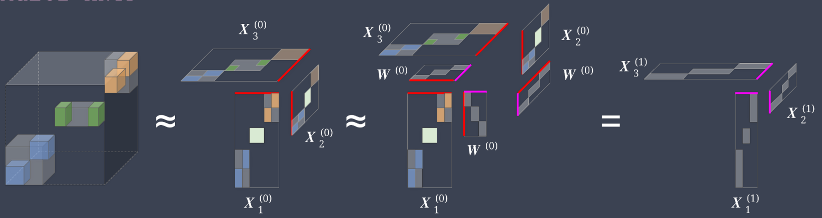
Backpropagation

» Hierarchical Tensor Decompositions

Hierarchical NCPD

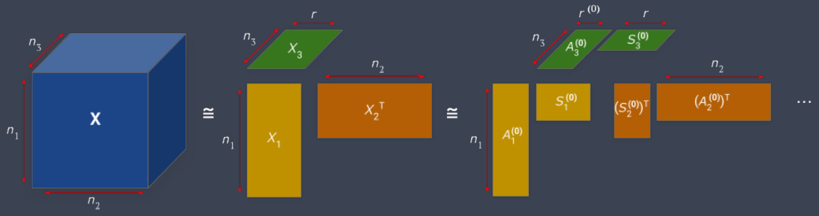


Multi-HNTF

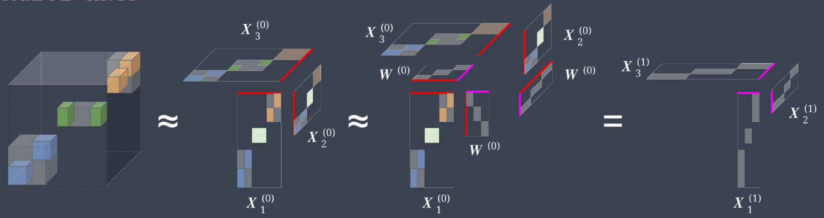


» Hierarchical Tensor Decompositions

Hierarchical NCPD



Multi-HNTF

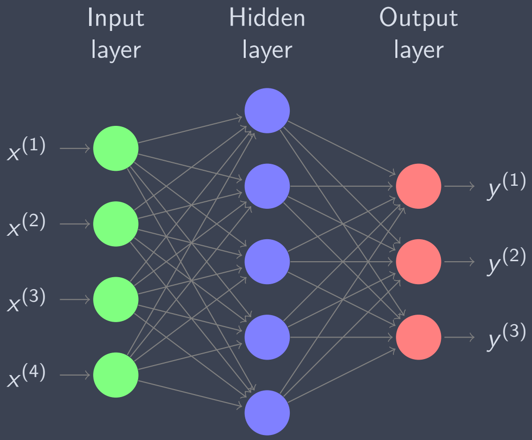


Devastating error propagation through layers!

» Reminder

Neural Network: Learn weights $W^{(1)}, W^{(2)}, ..., W^{(L)}$ to minimize model error

$$E(\{W^{(i)}\}) = \sum_{n=1}^{N} f(\mathbf{y}(\mathbf{x}_n, \{W^{(i)}\}), \mathbf{x}_n, \mathbf{t}_n).$$



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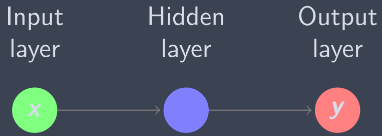

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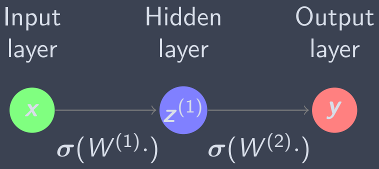


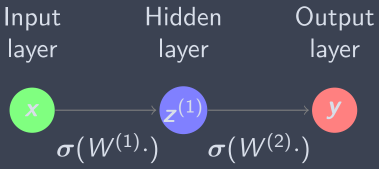
Training:

- forward propagation:
  $\boldsymbol{z}^{(1)} = \sigma(W^{(1)}\boldsymbol{x})$,
  $\boldsymbol{z}^{(2)} = \sigma(W^{(2)}\boldsymbol{z}_1)$,
  $\dots$,
  $\boldsymbol{y} = \sigma(W^{(L)}\boldsymbol{z}^{(L-1)})$

» Reminder

Neural Network: Learn weights $W^{(1)}, W^{(2)}, \dots, W^{(L)}$ to minimize model error

$$E(\{W^{(i)}\}) = \sum_{n=1}^{N} f(\boldsymbol{y}(\boldsymbol{x}_n, \{W^{(i)}\}), \boldsymbol{x}_n, \boldsymbol{t}_n).$$

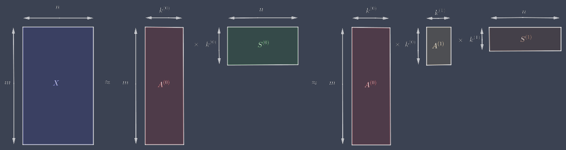


Training:

- ▷ forward propagation: $\boldsymbol{z}^{(1)} = \boldsymbol{\sigma}(W^{(1)}\boldsymbol{x})$, $\boldsymbol{z}^{(2)} = \boldsymbol{\sigma}(W^{(2)}\boldsymbol{z}_1)$, ..., $\boldsymbol{y} = \boldsymbol{\sigma}(W^{(L)}\boldsymbol{z}^{(L-1)})$
- ▷ back propagation: update $\{W^{(i)}\}$ with $\nabla E(\{W^{(i)}\})$

» Training via backpropagation

Neural NMF: Forward and back propagation algorithms for hNMF.



Gao, Mengdi, et al. "Neural nonnegative matrix factorization for hierarchical multilayer topic modeling." 2019 IEEE 8th International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP). IEEE, 2019.

Related work: [Flenner, Hunter 2018], [Trigeorgis, Bousmalis, Zafeiriou, Schuller 2016], [Le Roux, Hershey, Weninger 2015], [Sun, Nasrabadi, Tran 2017]

» Training via backpropagation

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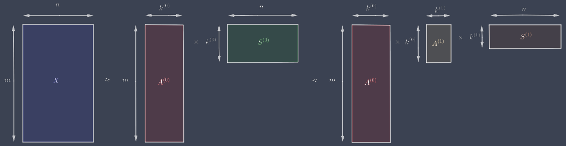

- ▷ Regard the A matrices as independent variables, determine the S matrices from the A matrices.

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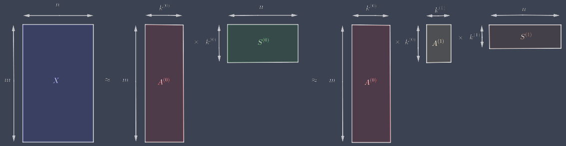

- ▷ Regard the A matrices as independent variables, determine the S matrices from the A matrices.
- ▷ Define $q(X, A) := \text{argmin}_{S \geq 0} \|X - AS\|_F^2$ (least-squares).

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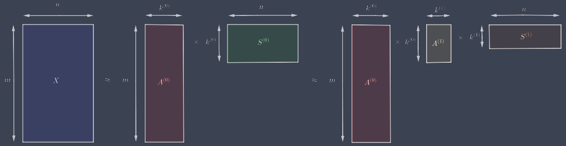

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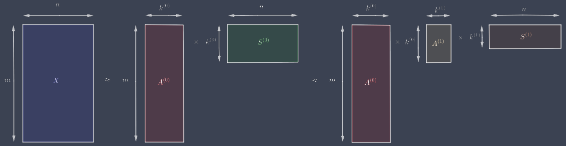

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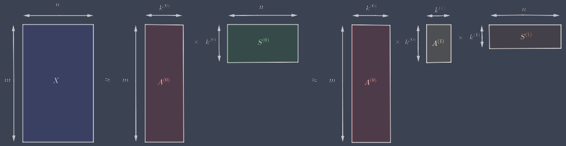

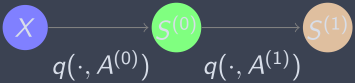

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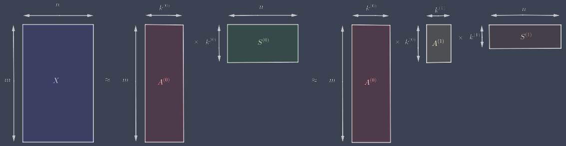

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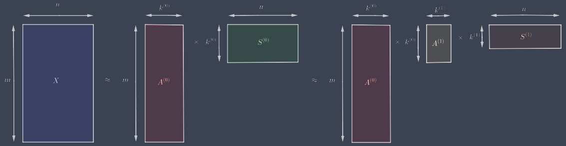

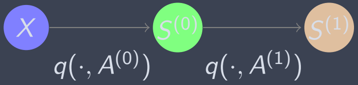

Training:

- forward propagation:
  $S^{(0)} = q(X, A^{(0)})$,
  $S^{(1)} = q(S^{(0)}, A^{(1)})$, ...,
  $S^{(L)} = q(S^{(L-1)}, A^{(L)})$
- back propagation: update $\{A^{(i)}\}$ with $\nabla E(\{A^{(i)}\})$

Gao, Mengdi, et al. "Neural nonnegative matrix factorization for hierarchical multilayer topic modeling." 2019 IEEE 8th International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP). IEEE, 2019.

Related work: [Flenner, Hunter 2018], [Trigeorgis, Bousmalis, Zafeiriou, Schuller 2016], [Le Roux, Hershey, Weninger 2015], [Sun, Nasrabadi, Tran 2017]

» Training via backpropagation

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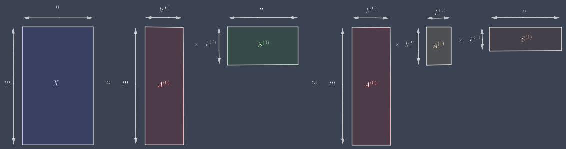

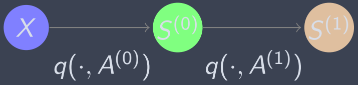

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Apply this approach to each mode of HNCPD!

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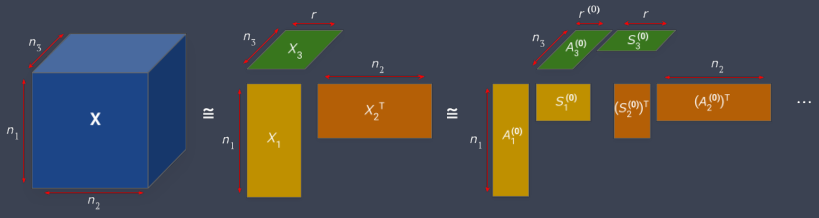
» Neural NCPD

Train independent neural NMF models for each mode of tensor from fixed NCPD factor matrices.



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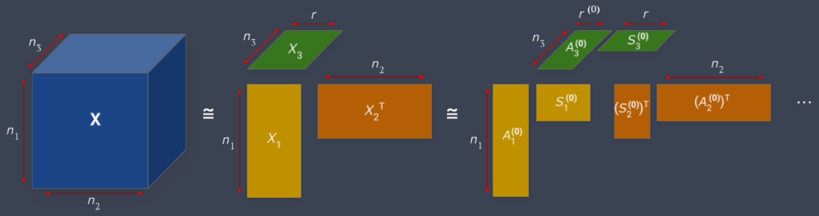

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» Gradient Calculation

Theorem-ish [Will, Zhang, Sadovnik, Gao, Vendrow, H., Molitor, Needell, 22+]

Given knowledge of the support of $q(\boldsymbol{A}, \boldsymbol{X})$, the gradient $\nabla_{\boldsymbol{A}} q(\boldsymbol{A}, \boldsymbol{X})$ has a closed-form expression almost everywhere in the space of real-valued matrix pairs. This gradient expression is inherited from unconstrained least-squares.

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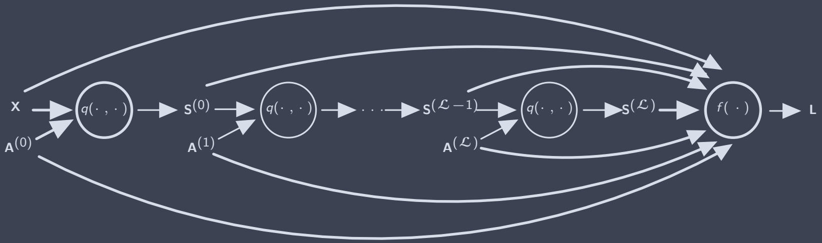
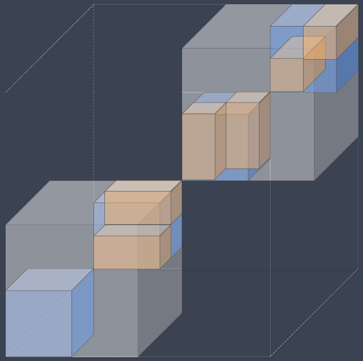


» Synthetic Tensor



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.

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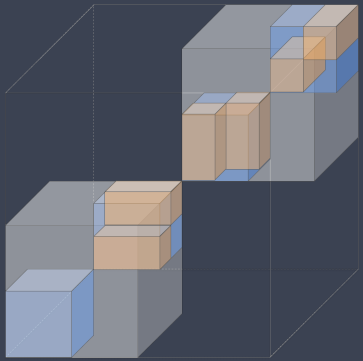

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Relative reconstruction error.

Method	$r_0 = 7$	$r_1 = 4$	$r_2 = 2$
Multi-HNTF	0.454	0.548	0.721
Neural HNCPD [Vendrow, et. al.]	0.454	**0.508**	**0.714**
Standard HNCPD [Vendrow, et. al.]	0.454	0.612	0.892
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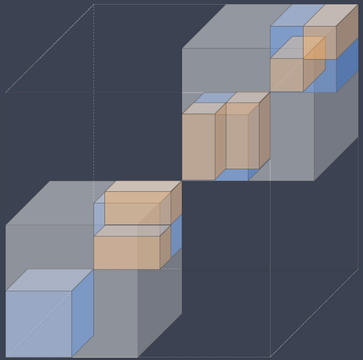

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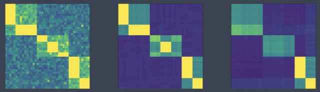

Projections of tensor approximation at each layer of Multi-HNTF.

Relative reconstruction error.

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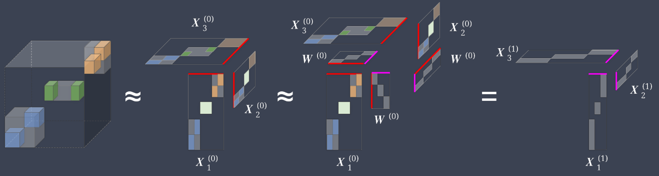

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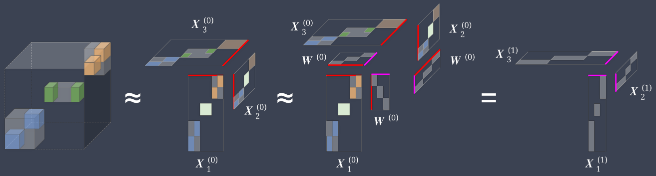
- Multi-HNTF is a hierarchical tensor decomposition model that `generalizes` hierarchical NMF.



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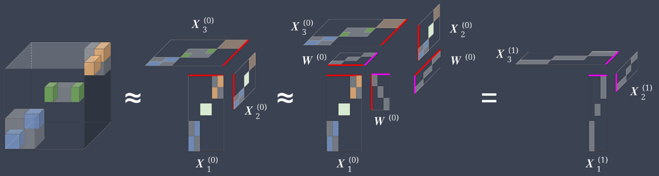

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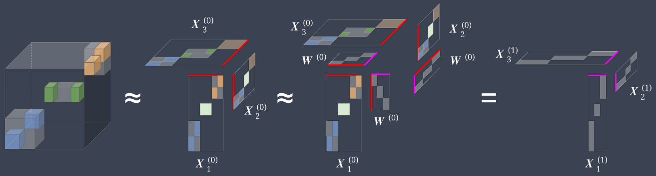

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- Develop backpropagation framework for Multi-HNTF and first layer NCPD.

» 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.

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