Topic Models, Methods, and Medicine

by Jamie Haddock
(Harvey Mudd College, Department of Mathematics)
on June 23, 2022,
Stauffer Lecture

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

`https://ieeexplore.ieee.org/document/9022678` (CAMSAP 2019)
joint with Mengdi Gao[•], Denali Molitor[*], Deanna Needell, Eli Sadovnik[*], Tyler Will[•], Runyu Zhang[•]
collaboration with LymeDisease.org

`https://arxiv.org/abs/2010.11365` (ICASSP 2021)
joint with Deanna Needell, Liza Rebrova, Joshua Vendrow[•]

`https://arxiv.org/abs/2010.07956` (ACSSC 2021)
joint with Miju Ahn, Rachel Grotheer, Lara Kassab[*], Alona Kryshchenko, Kathryn Leonard, Sixian Li[•], R. W. M. A. Madushani, Thomas Merkh[*], Deanna Needell, Elena Sizikova, Chuntian Wang

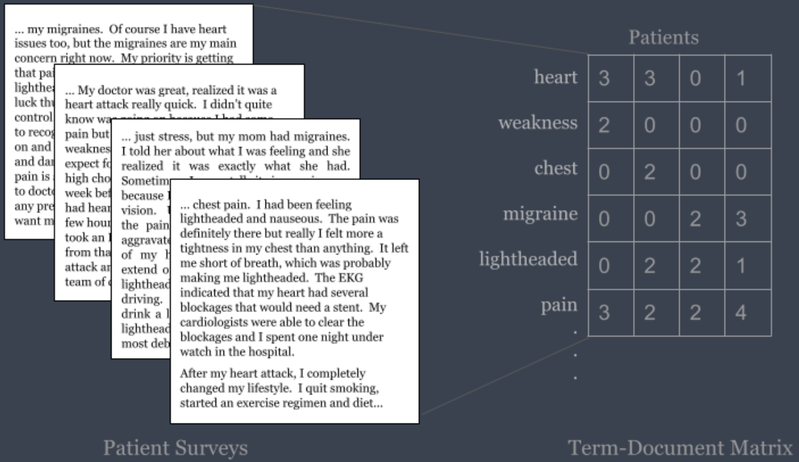
Soon to appear work (ACSSC 2021)
joint with Joshua Vendrow[•], Deanna Needell

`https://arxiv.org/pdf/2109.14820.pdf` (ICASSP 2022)
joint with Joshua Vendrow[•], Deanna Needell

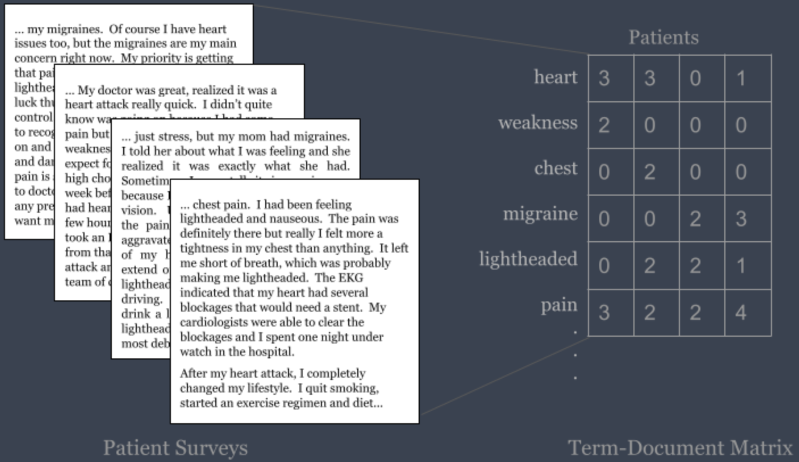
Forthcoming work
joint with Edwin Chau[•], Moisey Alaev[•], Joshua Vendrow[•], Rachel Grotheer, Alona Kryshchenko, Kathryn Leonard, Deanna Needell
collaboration with Harbor-UCLA Medical Center Department of Cardiology

Motivation

» Learn trends in high-dimensional data



» Learn trends in high-dimensional data



Can we understand symptom trends and shared patient experiences automatically?

» Learn trends in high-dimensional data

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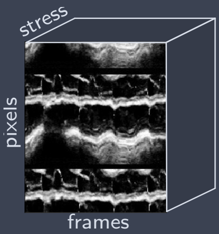
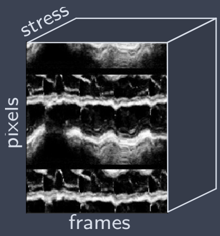


» Learn trends in high-dimensional data

Can we learn cohesive parts and separate noise in medical image studies?



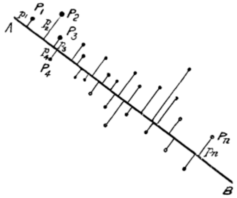
Introduction

» Topic Modeling

- ▷ principal component analysis (PCA)

  [Pearson 1901]

  [Hotelling 1933]



Pearson, K. (1901) *On lines and planes of closest fit to systems of points in space.*

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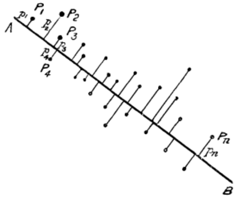

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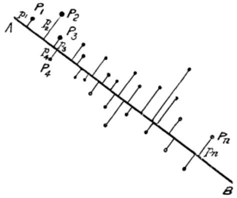

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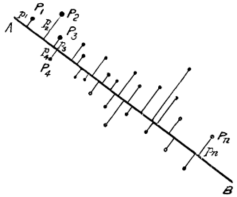

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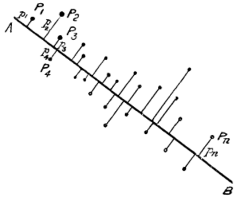

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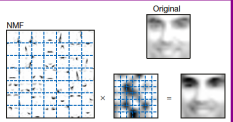

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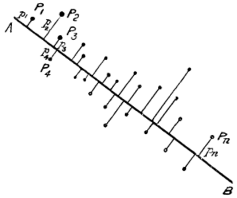

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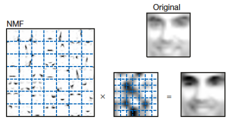

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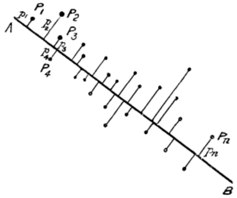

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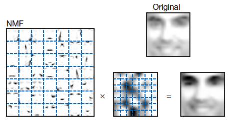

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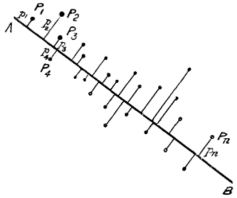

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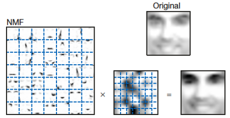

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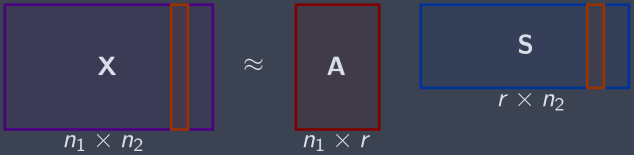
» Nonnegative Matrix Factorization (NMF)

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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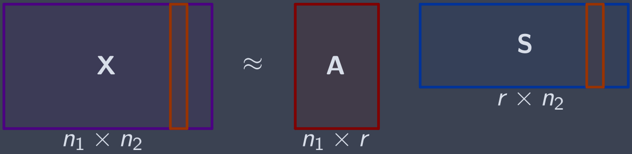

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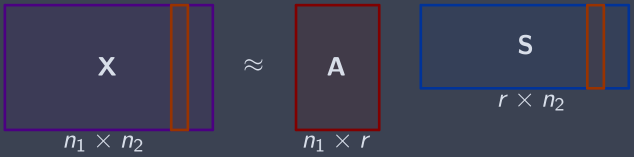

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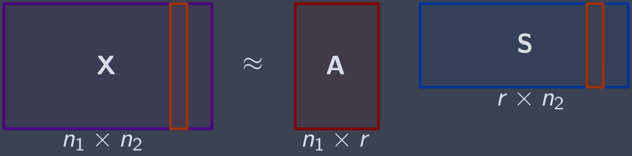

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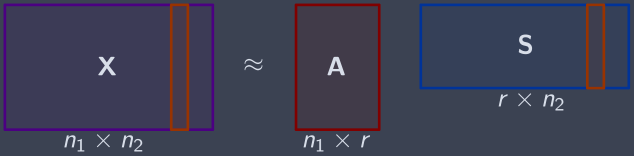

- ▷ Popularized by [Lee & Seung 1999]
- ▷ Employed for dimensionality-reduction and topic modeling
- ▷ Often formulated as

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

[1] information divergence $D(\mathbf{A}\|\mathbf{B}) = \sum_{i,j}\left(\mathbf{A}_{ij}\log\frac{\mathbf{A}_{ij}}{\mathbf{B}_{ij}} - \mathbf{A}_{ij} + \mathbf{B}_{ij}\right)$

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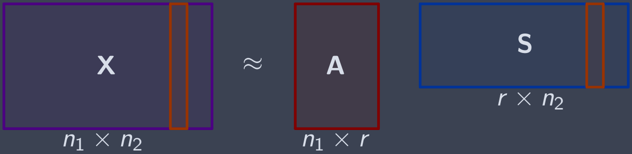

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- These formulations are MLE models

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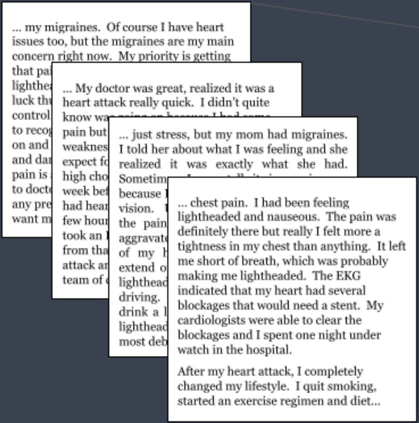
» NMF Example



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

» NMF Example

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	3	2	4
⋮				

NMF Example

$$
\begin{array}{r}
 \\ \text{heart} \\ \text{weakness} \\ \text{chest} \\ \text{migraine} \\ \text{lightheaded} \\ \text{pain} \\ \vdots
\end{array}
\begin{array}{c}
\text{Patients} \\
\begin{bmatrix} 3 & 3 & 0 & 1 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 3 \\ 0 & 2 & 2 & 1 \\ 3 & 3 & 2 & 4 \end{bmatrix} \\
\end{array}
\approx
\begin{bmatrix} 4.3 & 0.3 \\ 1.4 & 0 \\ 1.4 & 0 \\ 0 & 3.6 \\ 1.2 & 1.9 \\ 4.1 & 3.9 \end{bmatrix}
\begin{bmatrix} 0.7 & 0.7 & 0 & 0.1 \\ 0 & 0.1 & 0.6 & 0.8 \end{bmatrix}
$$

» NMF Example

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	3	2	4
⋮				

≈

Topics

4.3	0.3
1.4	0
1.4	0
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Lower-dimensional representation

» NMF Example

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⋮				

≈

Topics

Heart attack	Chronic migraine
4.3	0.3
1.4	0
1.4	0
0	3.6
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0.7	0.7	0	0.1
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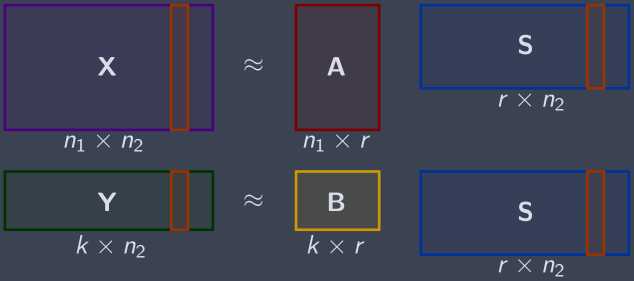
Lower-dimensional representation

Supervised Models

» Semi-supervised NMF (SSNMF)

Model: Jointly factorize nonnegative data $\mathbf{X}$ and supervision information $\mathbf{Y}$ so that

$$\mathbf{X} \approx \mathbf{AS} \text{ and } \mathbf{Y} \approx \mathbf{BS}.$$



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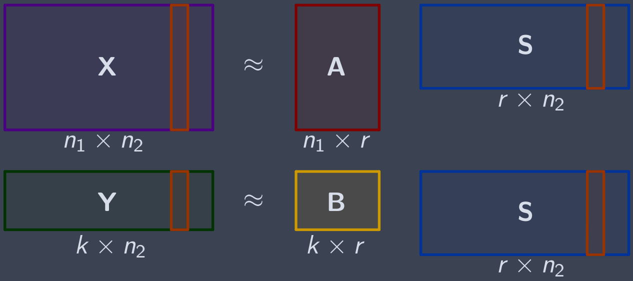

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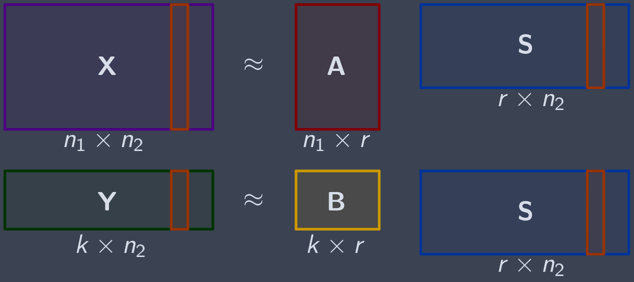

- ▷ Formulated in [Lee, Yoo & Choi 2009] as optimization problem

$$\min_{\mathbf{A}\in\mathbb{R}^{n_1\times r}_{\geq 0},\mathbf{B}\in\mathbb{R}^{k\times r}_{\geq 0},\mathbf{S}\in\mathbb{R}^{r\times n_2}_{\geq 0}} \|\mathbf{X}-\mathbf{AS}\|_F^2+\lambda\|\mathbf{Y}-\mathbf{BS}\|_F^2.$$

SSNMF example

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⋮				

Classes	1	1	0	1
	0	0	1	1

» SSNMF example

$$
\begin{array}{r}
\\
\text{heart}\\
\text{weakness}\\
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\overset{\text{Topics}}{\begin{bmatrix} 4.3 & 0.1\\ 1.4 & 0\\ 1.4 & 0\\ 0 & 3.6\\ 1.2 & 1.9\\ 4.2 & 3.8 \end{bmatrix}}
\begin{bmatrix} 0.7 & 0.7 & 0 & 0.2\\ 0 & 0.1 & 0.6 & 0.8 \end{bmatrix}
$$

Lower-dimensional representation

$$
\text{Classes}\ \begin{bmatrix} 1 & 1 & 0 & 1\\ 0 & 0 & 1 & 1 \end{bmatrix}
\approx
\begin{bmatrix} 1.5 & 0.6\\ 0 & 1.4 \end{bmatrix}
\begin{bmatrix} 0.7 & 0.7 & 0 & 0.2\\ 0 & 0.1 & 0.6 & 0.8 \end{bmatrix}
$$

» SSNMF example

Patients | Topics

$$
\begin{array}{r}
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\approx
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yields insight into relationship between symptom expression and diagnoses, insight into common co-occuring diagnoses, and a predictive model

» NMF and SSNMF Models

NMF formulations

» NMF and SSNMF Models

NMF formulations

- [Lee & Seung 1999] $\|\cdot\|_F$-NMF:
  $\operatorname{argmin}_{\mathbf{A},\mathbf{S}\geq 0}\|\mathbf{X}-\mathbf{AS}\|_F^2$

» NMF and SSNMF Models

NMF formulations

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- [Lee & Seung 2001] $D(\cdot\|\cdot)$-NMF: $\operatorname{argmin}_{\mathbf{A},\mathbf{S}\geq 0} D(\mathbf{X}\|\mathbf{AS})$

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* multiplicative updates [Lee & Seung 2001]

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SSNMF formulations

- [H. Lee, Yoo & Choi 2009] $(\|\cdot\|_F, \|\cdot\|_F)$-SSNMF: $\operatorname{argmin}_{\mathbf{A},\mathbf{B},\mathbf{S}\geq 0}\|\mathbf{X}-\mathbf{AS}\|_F^2+\lambda\|\mathbf{Y}-\mathbf{BS}\|_F^2$

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* multiplicative updates [Lee & Seung 2001]
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» NMF and SSNMF Models

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» Guided NMF

Idea: Instead of supervising factorization with class label matrix, supervise with model or seed topics.

[H., Needell, Rebrova, Vendrow 2021]
Related work: [Jagarlamudi, Jagadeesh, Daume, Udupa 2012]

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Idea: Instead of supervising factorization with class label matrix, supervise with model or seed topics.

Model: Jointly factorize nonnegative data $\mathbf{X} \in \mathbb{R}_{\geq 0}^{n_1 \times n_2}$ and seed matrix $\mathbf{Y} = [\boldsymbol{v}^{(1)}, \boldsymbol{v}^{(2)}, \ldots, \boldsymbol{v}^{(c)}] \in \mathbb{R}_{\geq 0}^{n_1 \times c}$ so that

$$\mathbf{X} \approx \mathbf{AS} \text{ and } \mathbf{Y} \approx \mathbf{AB}.$$

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- ▷ `allows for use of expert guidance`

[H., Needell, Rebrova, Vendrow 2021]
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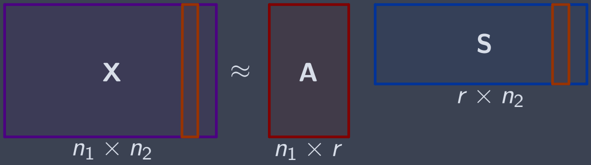
» What about tensor data?



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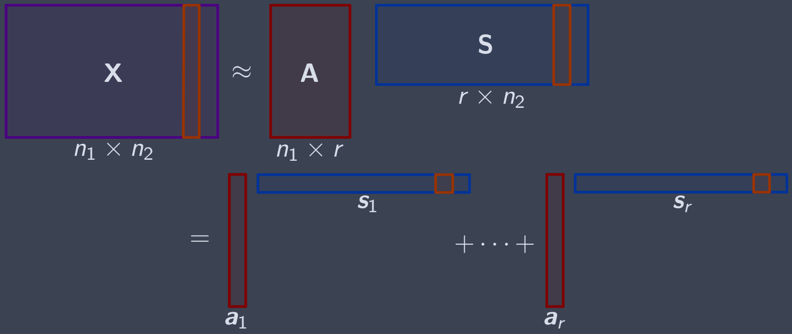

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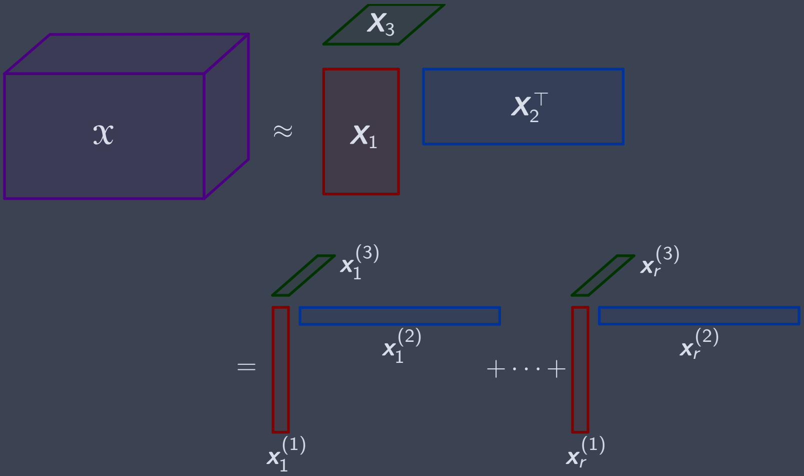

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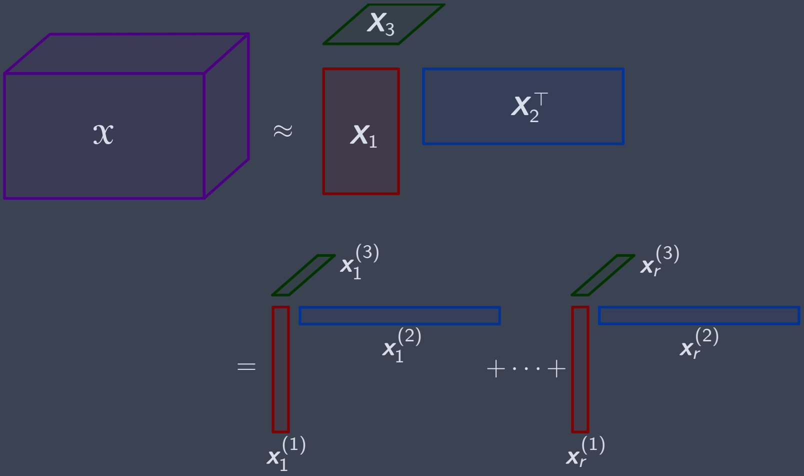
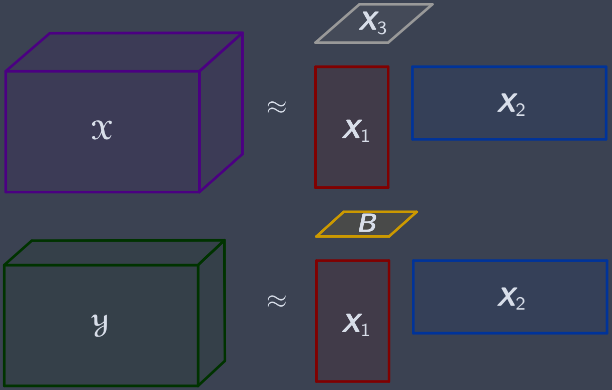


nonnegative CANDECOMP/PARAFAC (CP) decomposition (NCPD)

[Carroll, Chang 1970] [Harshman 1970]

» Semi-supervised NCPD



forthcoming work with Chau, Alaev, Vendrow, Grotheer, Kryshchenko, Leonard, Needell
Related work: [Verma, Liu, Wang, Zhu 2017], [Cao, Lu, Wei, Philip, Leow 2016], [Lock, Li 2018]

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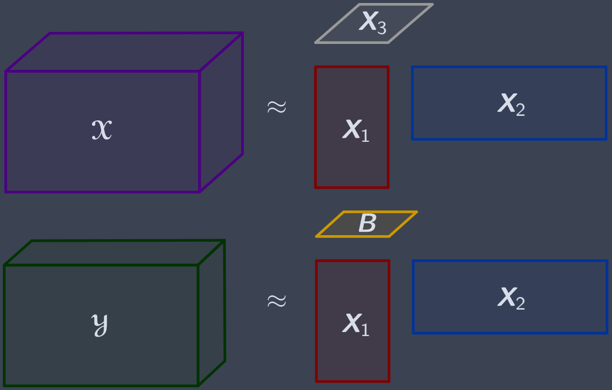

flexible to many forms of supervision

---

forthcoming work with Chau, Alaev, Vendrow, Grotheer, Kryshchenko, Leonard, Needell
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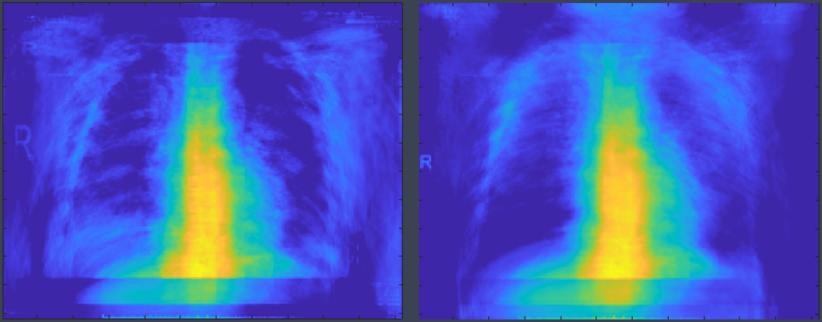

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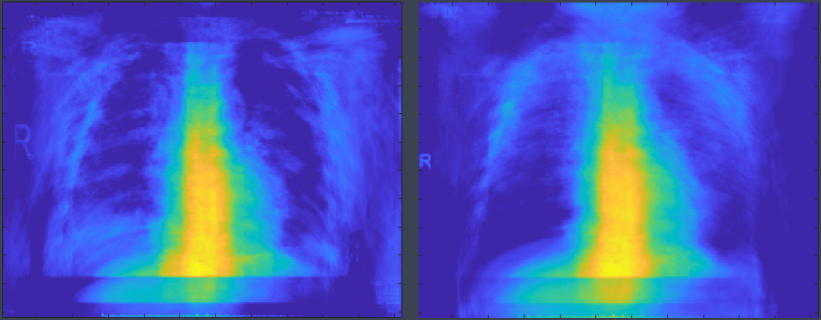

Left: ‘viral pneumonia’ topic; Right: ‘Normal’ topic.

Hierarchical Models

» Hierarchical NMF

Model: Sequentially factorize

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

[Cichocki, Zdunek 2006]

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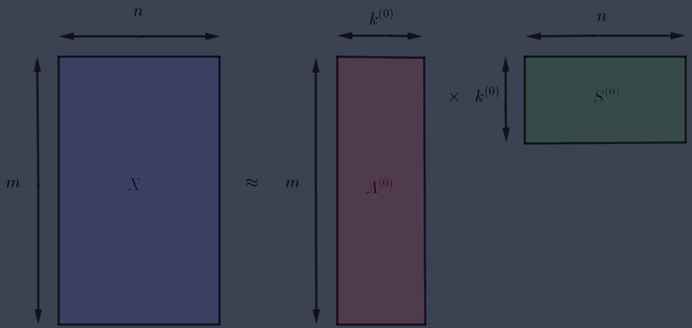

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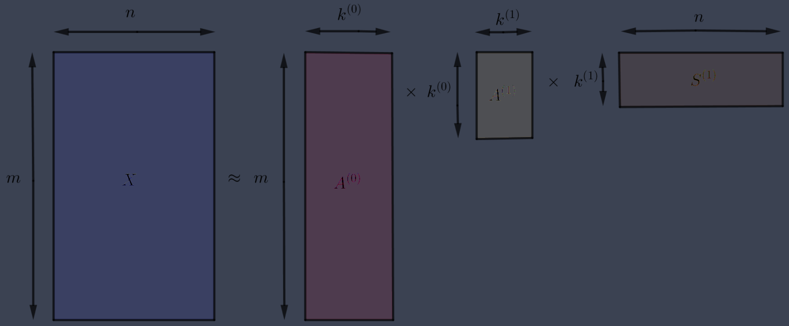

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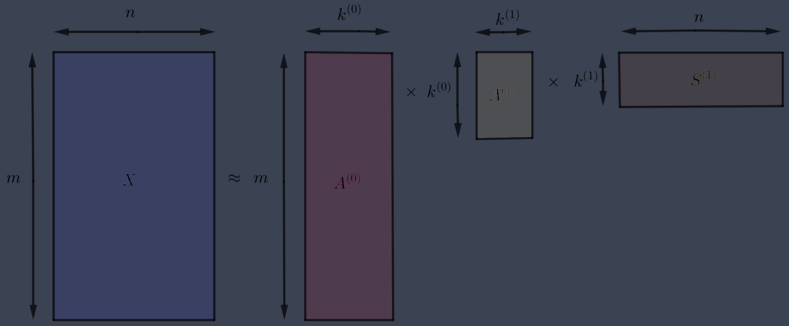

- ▷ $k^{(\ell)}$: supertopics collecting $k^{(\ell-1)}$ subtopics

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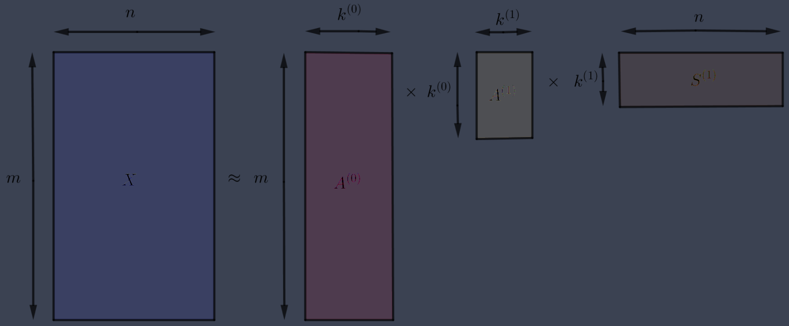

- ▷ $k^{(\ell)}$: supertopics collecting $k^{(\ell-1)}$ subtopics
- ▷ error propagates through layers

[Cichocki, Zdunek 2006]

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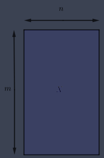

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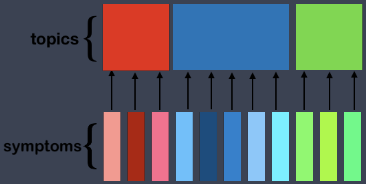

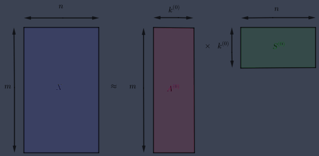

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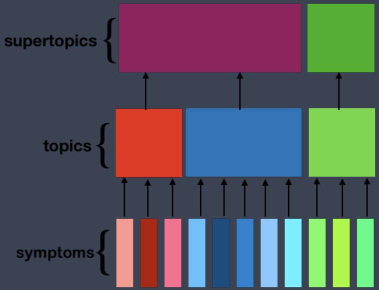

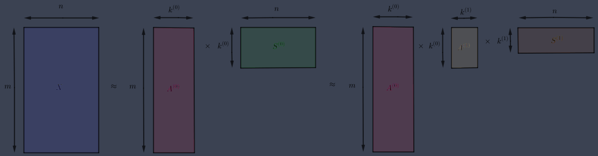

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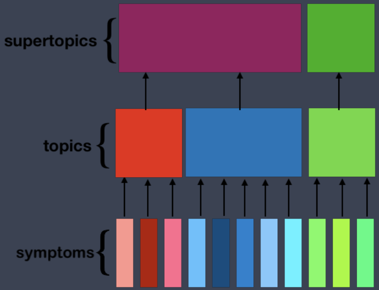
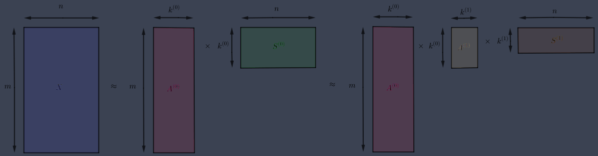


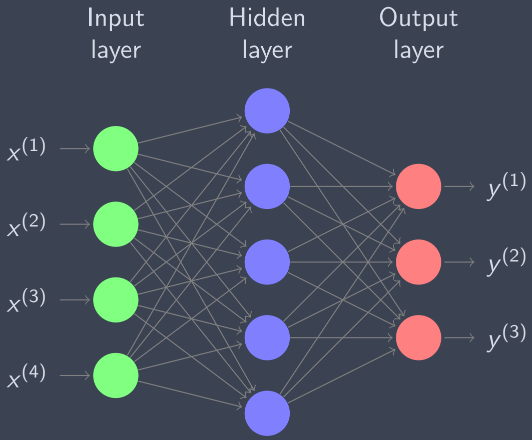
- ▷ hNMF can be implemented in a `feed-forward neural network` structure



» Feed-forward Neural Networks

Goal: Identify weights $W^{(1)}, W^{(2)}, \dots, W^{(L)}$ to minimize model error

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



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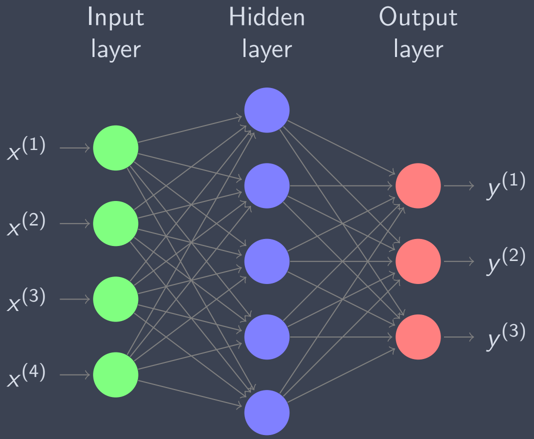

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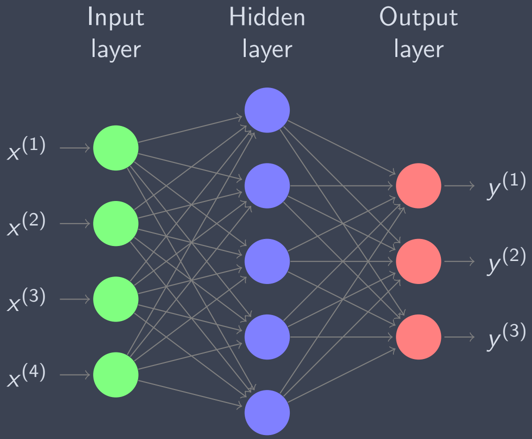

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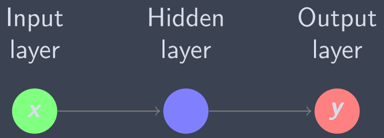

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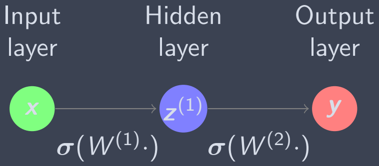

Training:

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

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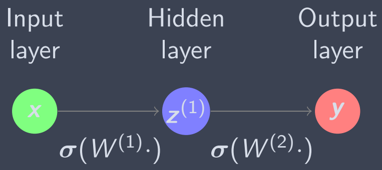

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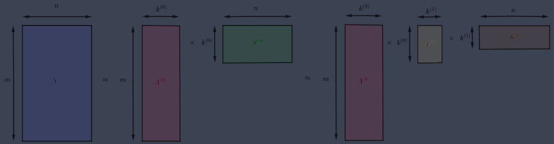
- ▷ back propagation: update $\{W^{(i)}\}$ with $\nabla E(\{W^{(i)}\})$

» Neural NMF

Goal: Develop forward and back propagation algorithms for hNMF.



[Gao, H., Molitor, Needell, Sadovnik, Will, Zhang 2019]
Related work: [Flenner, Hunter 2018], [Trigeorgis, Bousmalis, Zafeiriou, Schuller 2016], [Le Roux, Hershey, Weninger 2015], [Sun, Nasrabadi, Tran 2017]

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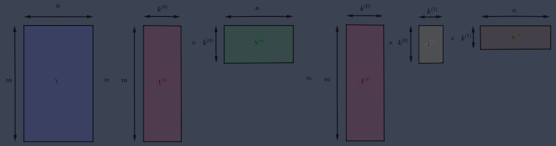

- ▷ Regard the A matrices as independent variables, determine the S matrices from the A matrices.

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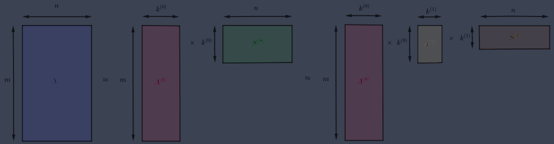

- ▷ Regard the A matrices as independent variables, determine the S matrices from the A matrices.
- ▷ Define $q(X, A) := \text{argmin}_{S \geq 0} \|X - AS\|_F^2$ (least-squares).

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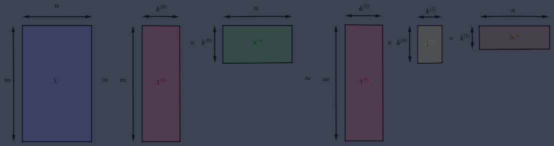

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- Pin the values of S to those of A by recursively setting $S^{(\ell)} := q(S^{(\ell-1)}, A^{(\ell)})$.

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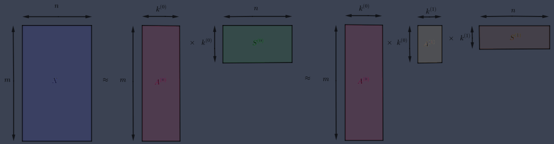

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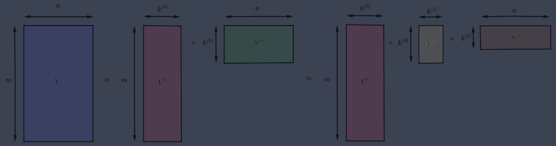
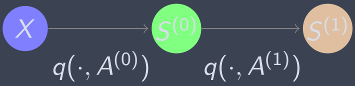
$$X \xrightarrow{q(\cdot, A^{(0)})} S^{(0)} \xrightarrow{q(\cdot, A^{(1)})} S^{(1)}$$

» Neural NMF

Goal: Develop forward and back propagation algorithms for hNMF.





[Gao, H., Molitor, Needell, Sadovnik, Will, Zhang 2019]
Related work: [Flenner, Hunter 2018], [Trigeorgis, Bousmalis, Zafeiriou, Schuller 2016], [Le Roux, Hershey, Weninger 2015], [Sun, Nasrabadi, Tran 2017]

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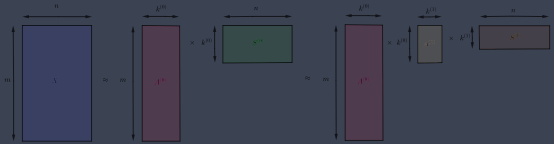
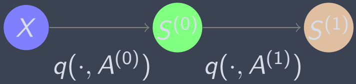


Training:



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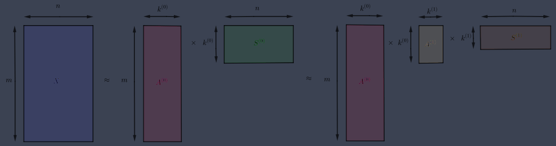
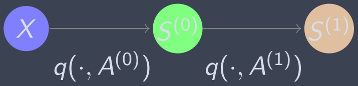


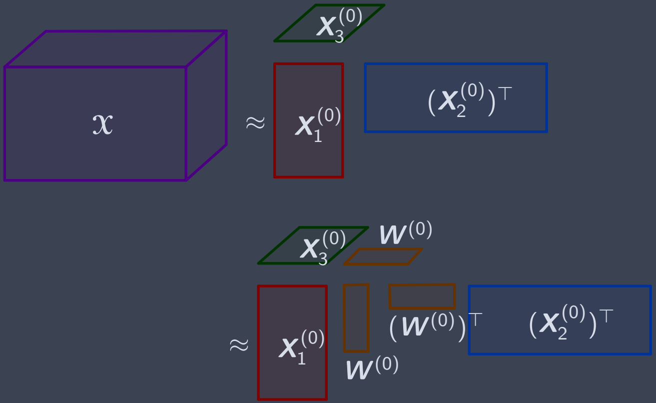


Training:

- 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, H., Molitor, Needell, Sadovnik, Will, Zhang 2019]
Related work: [Flenner, Hunter 2018], [Trigeorgis, Bousmalis, Zafeiriou, Schuller 2016], [Le Roux, Hershey, Weninger 2015], [Sun, Nasrabadi, Tran 2017]

» What about tensor data?



[Vendrow, H., Needell 2021]

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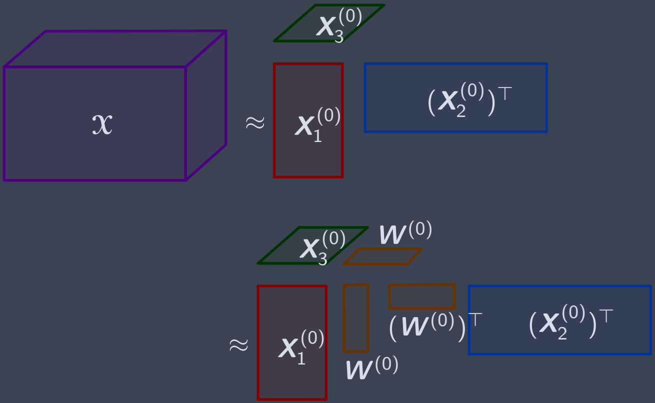
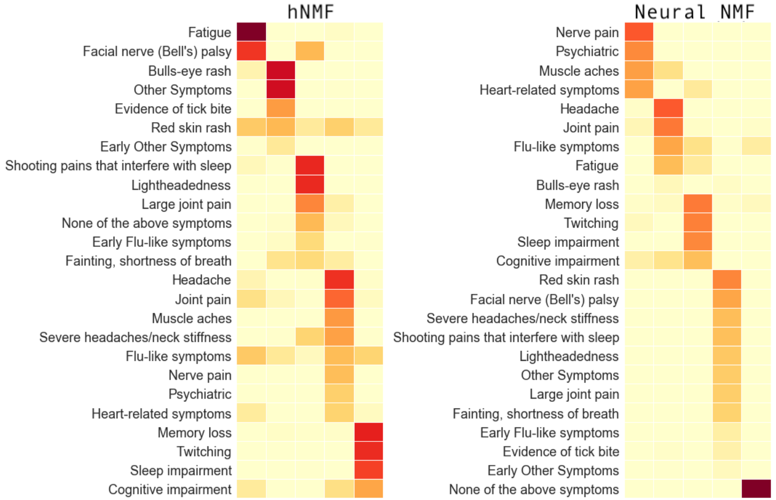


Neural NCPD model can again be formulated and trained in neural network framework

[Vendrow, H., Needell 2021]

» Application: MyLymeData



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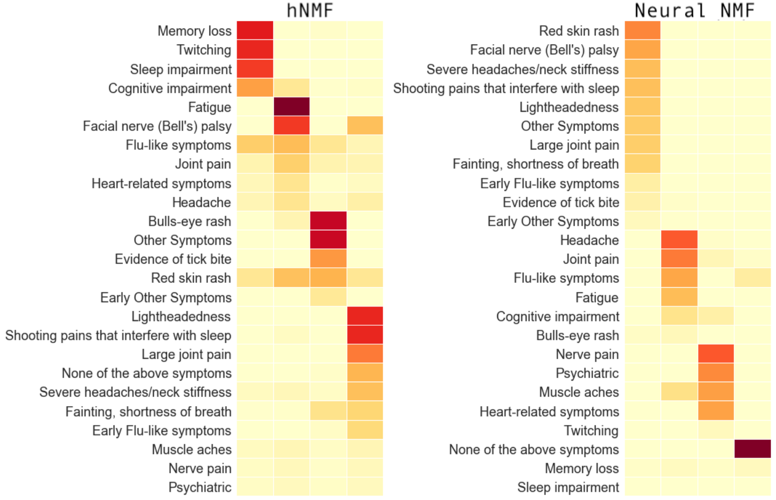

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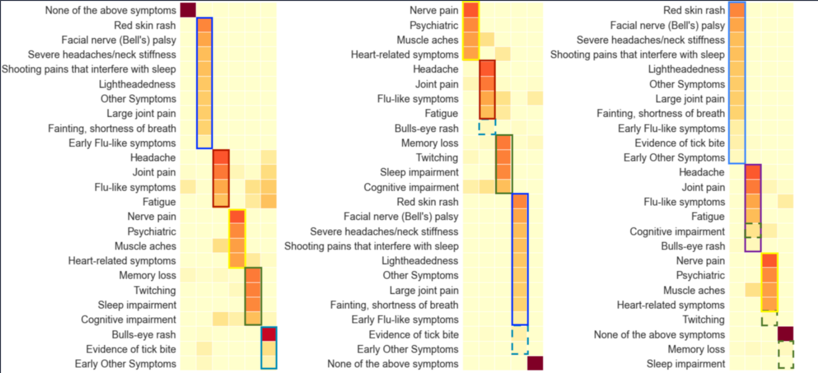

$k^{(0)} = 6$ $k^{(1)} = 5$ $k^{(2)} = 4$

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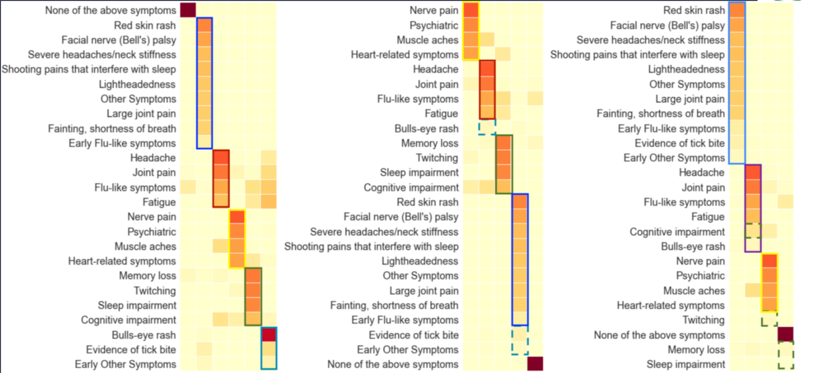

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bulls-eye rash (diagnosing symptoms) topic does not seem to persist for smaller number of topics

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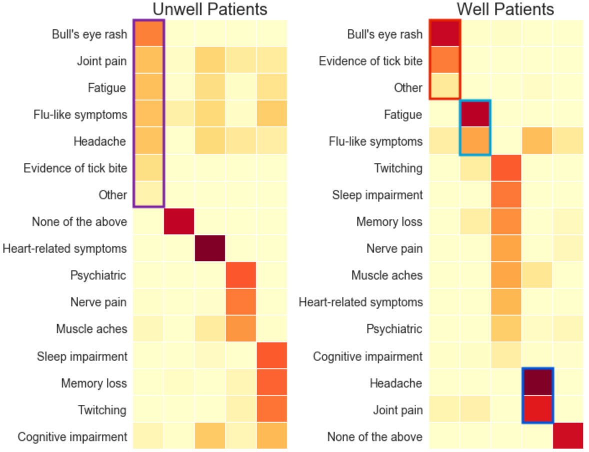

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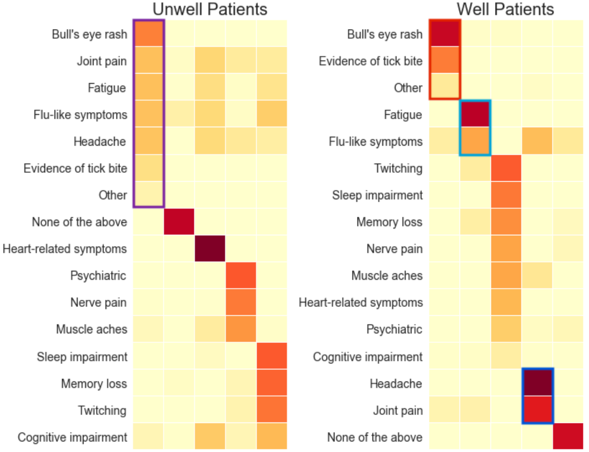

unwell and well patients have very different presentation of bulls-eye rash symptom in topics

Conclusions

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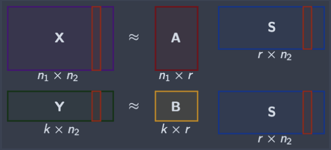
- SSNMF and SSNCPD models are maximum likelihood estimators



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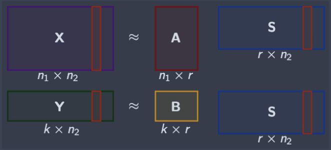

- ▷ they can be trained by `multiplicative updates`

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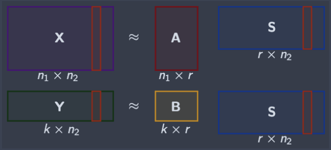

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» Conclusions

- ▷ SSNMF and SSNCPD models are maximum likelihood estimators

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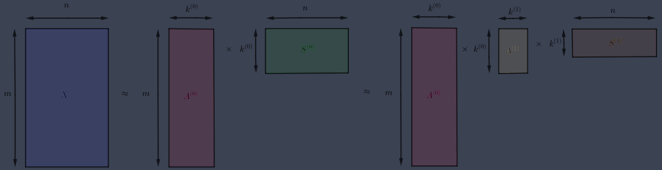
- ▷ hNMF model can be implemented as a feed-forward neural network



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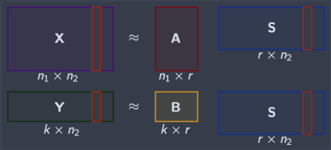

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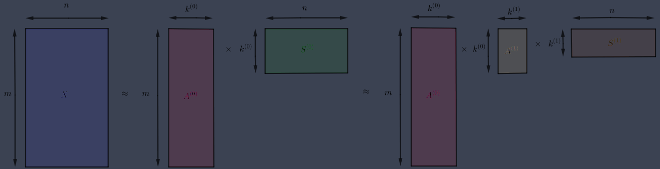

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Conclusions

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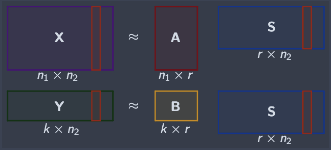

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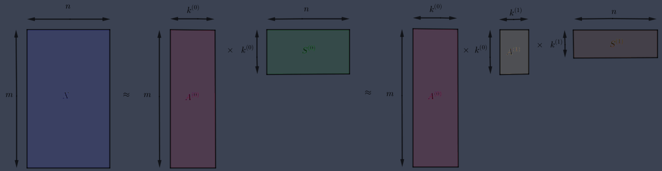

- `Neural NMF` and `Neural NCPD` can decrease error propagation
- elucidate hierarchical relationships between learned topics and decrease dependence upon hyperparameters

» Thanks for listening! Questions?

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