

Data Mining using Matrix/Tensor Factorizations & Applications

Evrim Acar

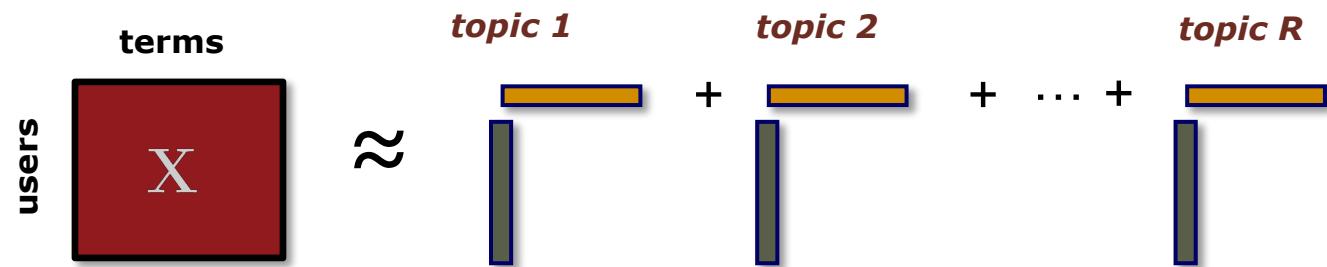
Simula Metropolitan Center for Digital Engineering

Oslo, Norway

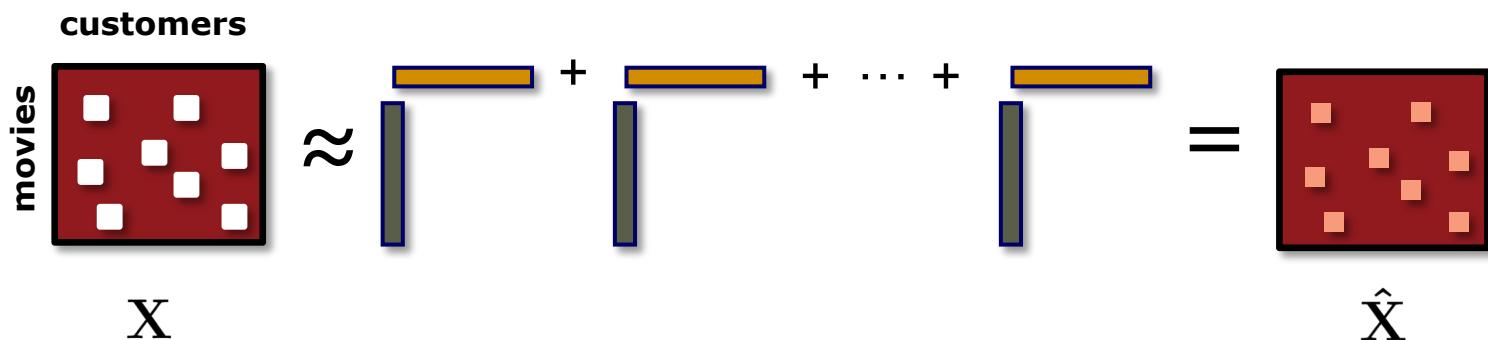
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Matrix Factorizations in Data Mining

Capturing underlying hidden factors/patterns



**Incomplete Matrix Factorization/
Matrix Completion**



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Data is often squeezed to be two-way!

2-way

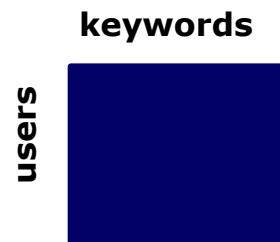
Social networks : **<users, keywords>**
<employee, employee>
<users, users>

Text mining: **< documents, terms>**

Recommender
Systems: **<customers, items>**

Computer vision: **<people, pixels>**

Neuroscience: **<electrodes, time>**



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Multi-way

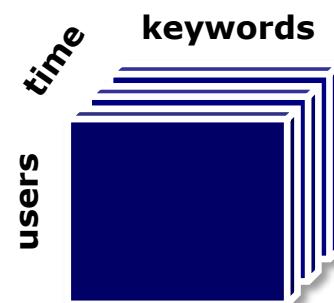
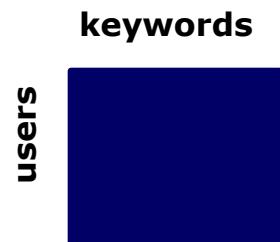
< users, keywords, time>
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< users, users, communication type>

< documents, terms, terms>

<customers, items, tags>

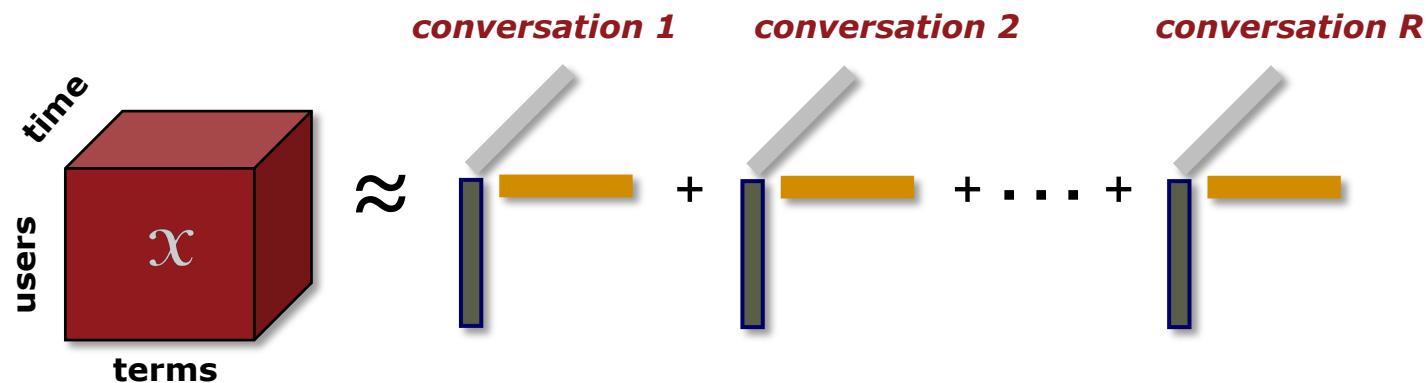
<people, pixels, viewpoints>

<electrodes, time, frequency>
<electrodes, time, subjects>

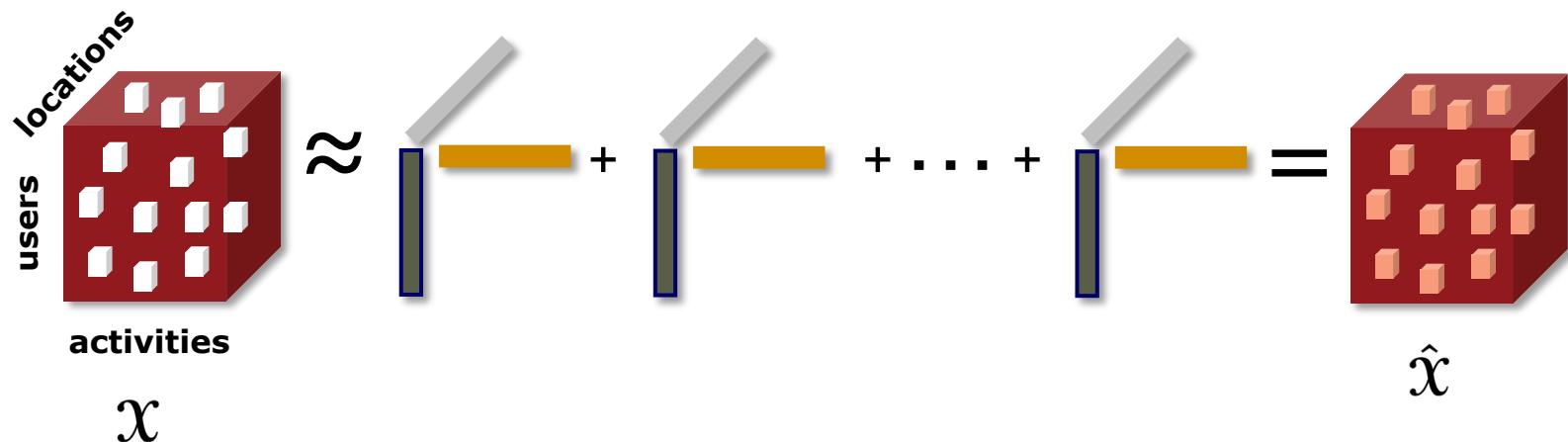


Data is often multi-way!

Capturing underlying hidden factors/patterns



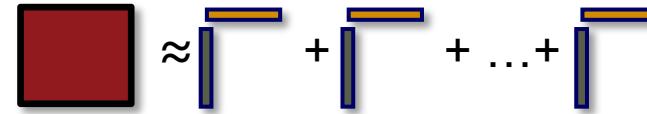
Incomplete Tensor Factorization/
Tensor Completion



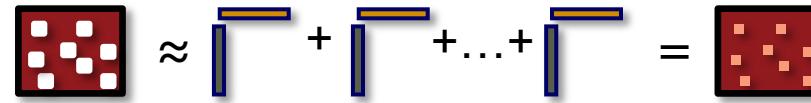
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Matrix Factorizations in Data Mining

Matrix Factorizations

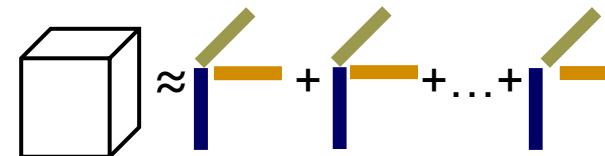


Matrix Completion

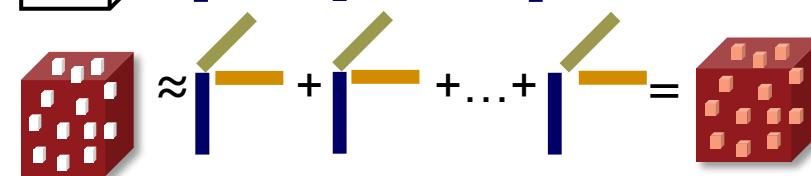


Data sets are often multi-way: Tensor Factorizations

Tensor Factorizations

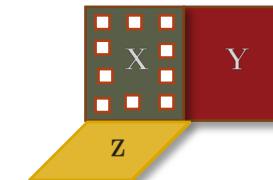


Tensor Completion

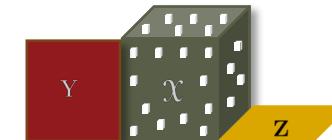
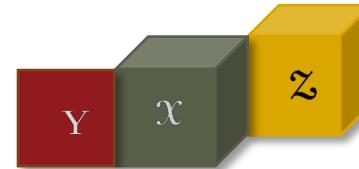


Data sets often come from multiple sources: Data Fusion

Coupled Matrix Factorizations

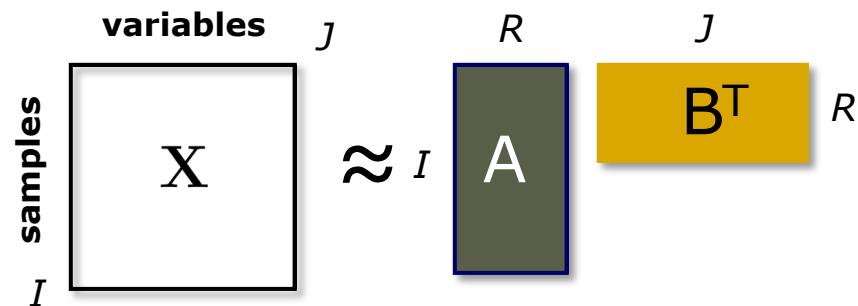


Coupled Tensor Factorizations



Matrix Factorizations

Matrix Factorizations, e.g., SVD (Singular Value Decomposition), NMF (Nonnegative Matrix Factorization), are commonly used in data mining.



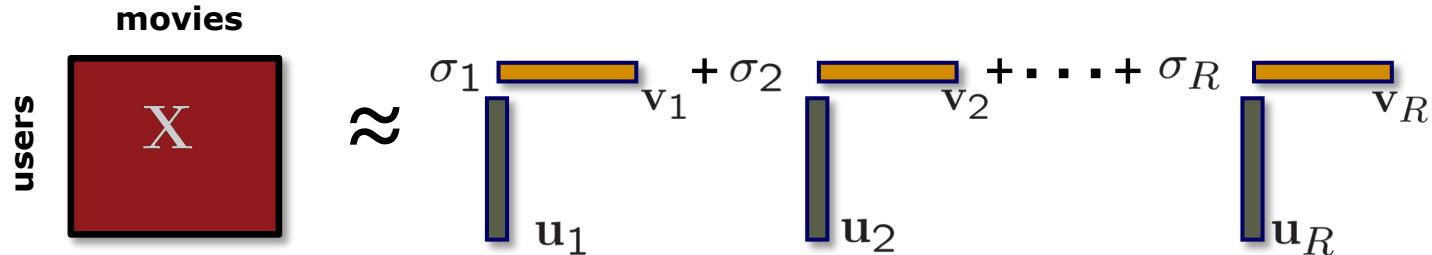
$$\begin{aligned} X &\approx \sum_{r=1}^R \mathbf{a}_r \mathbf{b}_r^\top \\ &\approx \mathbf{A} \mathbf{B}^\top \end{aligned}$$

$$\mathbf{A} \in \mathbb{R}^{I \times R} = [\mathbf{a}_1 \ \cdots \ \mathbf{a}_R]$$

$$\mathbf{B} \in \mathbb{R}^{J \times R} = [\mathbf{b}_1 \ \cdots \ \mathbf{b}_R]$$

Matrix Factorizations: Finding Underlying Structures

We can use SVD to find the underlying structures in a data set. For instance, using SVD of a *users* by *movies* matrix, we can capture the movie types and user groups.



$$\begin{aligned} X &\approx \sum_{r=1}^R \sigma_r \mathbf{u}_r \mathbf{v}_r^\top \\ &\approx \mathbf{U} \Sigma \mathbf{V}^\top \end{aligned}$$

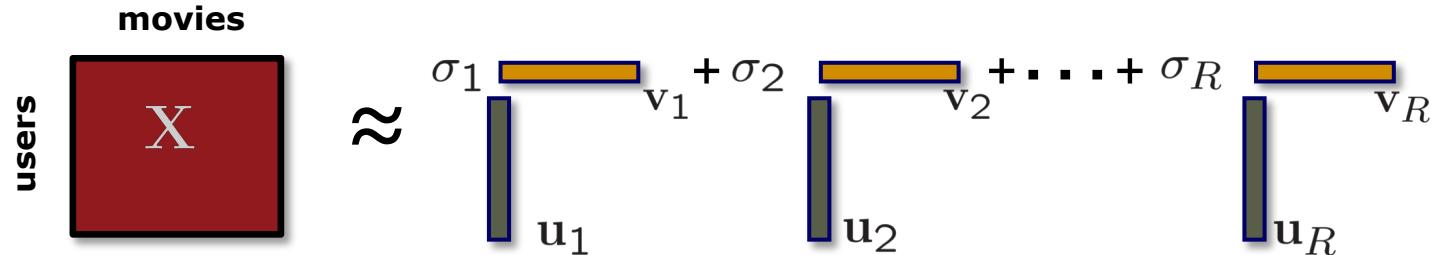
$$\min_{\mathbf{U}, \mathbf{V}, \sigma} \| \mathbf{X} - \mathbf{U} \Sigma \mathbf{V}^\top \|^2$$

$$\text{s.t. } \mathbf{U}^\top \mathbf{U} = \mathbf{I}, \mathbf{V}^\top \mathbf{V} = \mathbf{I}$$

$$\sigma_r \geq 0 \text{ for } r \in \{1 : R\}.$$

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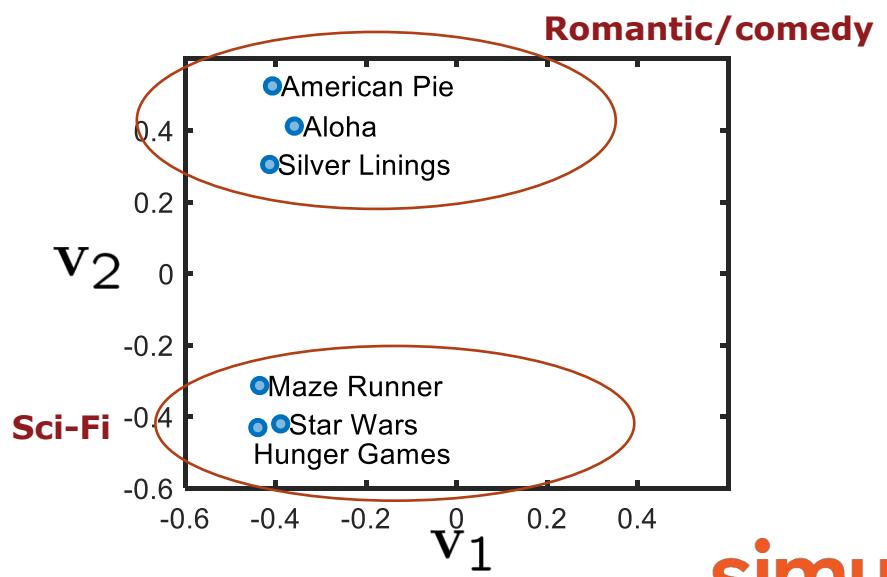
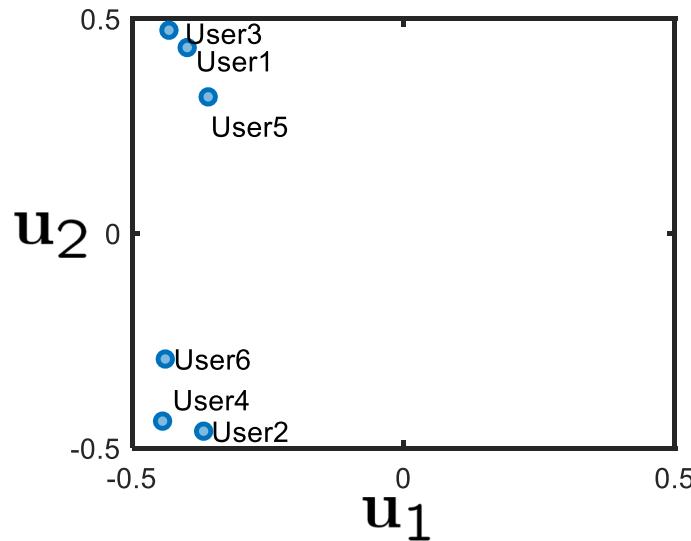
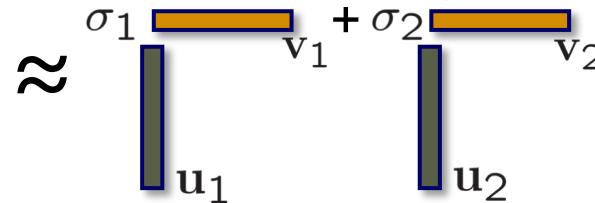
	Aloha	Star Wars	American Pie	Hunger Games	Silver Linings	Maze Runner
User 1	5	2	4	1	3	2
User 2	1	4	1	4	1	4
User 3	3	1	5	2	5	2
User 4	1	4	1	5	3	4
User 5	3	1	4	2	3	2
User 6	2	4	2	4	2	4

Who likes what type of movies?

Matrix Factorizations: Finding Underlying Structures

Tool: Singular Value Decomposition

	Aloha	Star Wars	American Pie	Hunger Games	Silver Linings	Maze Runner
User 1	5	2	4	1	3	2
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Principal Component Analysis (PCA)

PCA is a dimension reduction method often used for exploratory analysis to find the main axes of variation in the data.

Let \mathbf{X} be a *sample* by *variable* matrix and centered across the samples mode, e.g., each column has mean zero. PCA reveals scores and loadings, where columns of \mathbf{P} show the principal component directions and \mathbf{T} will have the corresponding principal component scores.

$$\mathbf{X} \approx \mathbf{T}\mathbf{P}^T$$

↑
scores ↓
 loadings

The diagram illustrates the decomposition of matrix \mathbf{X} into scores \mathbf{T} and loadings \mathbf{P}^T . On the left, the equation $\mathbf{X} \approx \mathbf{T}\mathbf{P}^T$ is shown with arrows indicating the flow from \mathbf{X} to \mathbf{T} and \mathbf{P}^T , labeled "scores" and "loadings" respectively. To the right, a large square matrix \mathbf{X} is shown with "samples" on the vertical axis and "variables" on the horizontal axis. This matrix is approximately equal (\approx) to the product of matrix \mathbf{T} (dimensions $I \times R$) and matrix \mathbf{P}^T (dimensions $R \times J$). Matrix \mathbf{T} is represented by a dark green rectangle, and matrix \mathbf{P}^T is represented by a yellow rectangle.

How do we find the scores and loadings?

Direction of the first principal component p_1 can be found by solving the following:

$$\max_{\|p_1\|=1} \text{var}(t_1), \text{ where } t_1 = Xp_1$$

The second direction p_2 is then found in the same way with the constraint that p_1 is orthogonal to p_2 .

Eigenvalue decomposition of the covariance matrix gives the principal component directions.

$$X^T X = P \Lambda P^T$$

How does this relate to SVD?

$$\begin{aligned} X &= U \Sigma V^T \\ X^T X &= V \Sigma U^T U \Sigma V^T \\ &= V \Sigma^2 V^T \end{aligned}$$

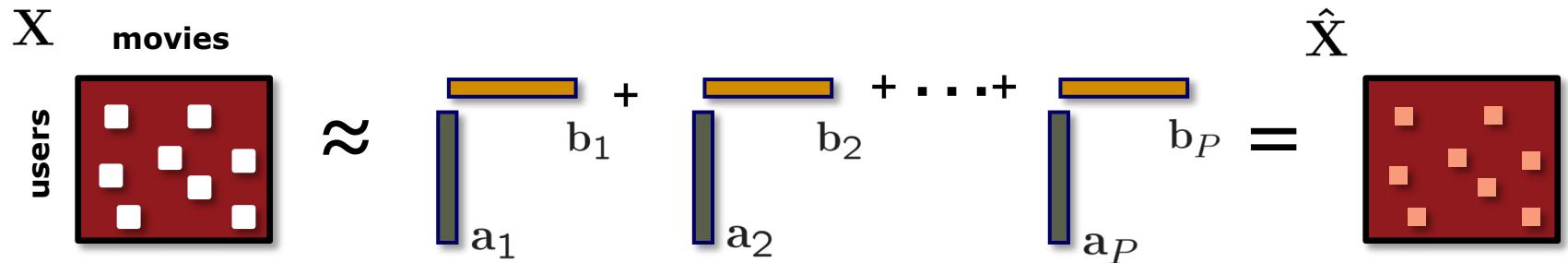


Right singular vectors
are the principal
component directions

The variance captured by
each component is the
square of the singular values

Matrix Factorizations: Missing Data Estimation (a.k.a. matrix completion)

In the case of incomplete data, matrix factorizations can be used to fill in the missing entries:



Finding low-rank approximation:

$$\min_{A,B} \| W * (X - AB^\top) \|^2$$

$$w_{ij} = \begin{cases} 1 & \text{if } x_{ij} \text{ is known,} \\ 0 & \text{if } x_{ij} \text{ is missing.} \end{cases}$$

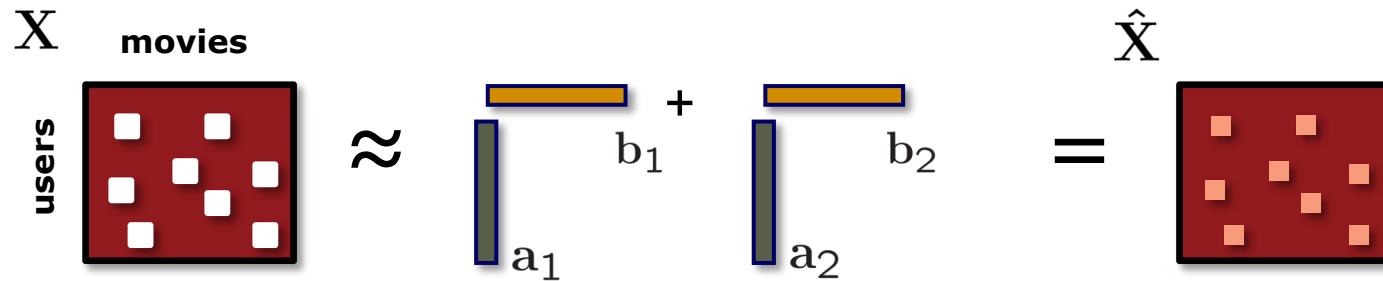
Data reconstruction:

$$\hat{X} = AB^\top$$

It is possible to recover an unknown low-rank matrix from a nearly minimal set of entries. For more on matrix completion [Candes and Plan, 2010]

Matrix Factorizations: Missing Data Estimation

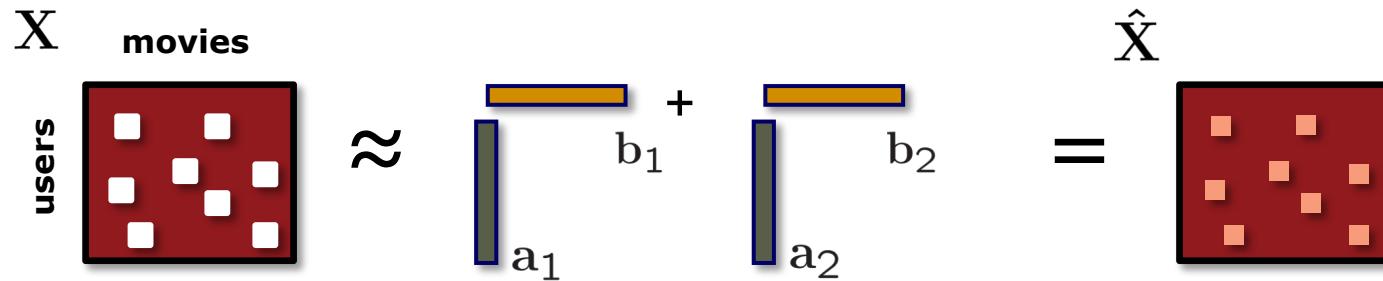
For instance, we can still factorize the incomplete \mathbf{X} and then use those factors to reconstruct the matrix and estimate the missing entries.



X	Aloha	Star Wars	American Pie	Hunger Games	Silver Linings	Maze Runner	$\hat{\mathbf{X}} = \mathbf{AB}^T$
User 1	5	2	4	1	3	?	3.72 1.27 4.41 1.60 3.78 1.91
User 2	1	4	1	4	1	4	0.82 3.91 0.74 4.05 1.53 3.91
User 3	3	1	5	2	5	2	4.06 1.37 4.82 1.72 4.12 2.07
User 4	1	4	1	?	3	4	1.37 4.06 1.39 4.24 2.08 4.15
User 5	3	1	4	2	3	2	3.15 1.38 3.71 1.65 3.25 1.90
User 6	2	?	2	4	2	4	1.77 3.76 1.89 3.97 2.40 3.94

Matrix Factorizations: Missing Data Estimation

For instance, we can still factorize the incomplete \mathbf{X} and then use those factors to reconstruct the matrix and estimate the missing entries.



X	Aloha	Star Wars	American Pie	Hunger Games	Silver Linings	Maze Runner	$\hat{X} = AB^T$
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User 3	3	1	5	2	5	2	4.06 1.37 4.82 1.72 4.12 2.07
User 4	1	4	1	5	3	4	1.37 4.06 1.39 4.24 2.08 4.15
User 5	3	1	4	2	3	2	3.15 1.38 3.71 1.65 3.25 1.90
User 6	2	4	2	4	2	4	1.77 3.76 1.89 3.97 2.40 3.94

Text Mining

Suppose we have the documents with the following titles and we want to group them into topics:

Document 1: Tiger stopped playing golf

Document 2: News about Tiger and his golf career

Document 3: Golf career of Tiger in jeopardy

Document 4: Tiger and his wife in the news

Document 5: The new zoo featuring the big cat family: tigers and lions

Document 6: Tigers – the big cats – in the new zoo

Document 7: Tigers and lions, which are the biggest cats?

	tiger	stop	play	golf	news	career	jeopardy	wife	zoo	featuring	new	big	cat	family	lions	which
Doc1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0
Doc2	1	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0
Doc3	1	0	0	1	0	1	1	0	0	0	0	0	0	0	0	0
Doc4	1	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0
Doc5	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1	0
Doc6	1	0	0	0	0	0	0	0	1	0	1	1	1	0	0	0
Doc7	1	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1

Text Mining (cont.)

Document 1: Tiger stopped playing golf

Document 2: News about Tiger and his golf career

Document 3: Golf career of Tiger in jeopardy

Document 4: Tiger and his wife in the news

Document 5: The new zoo featuring the big cat family: tigers and lions

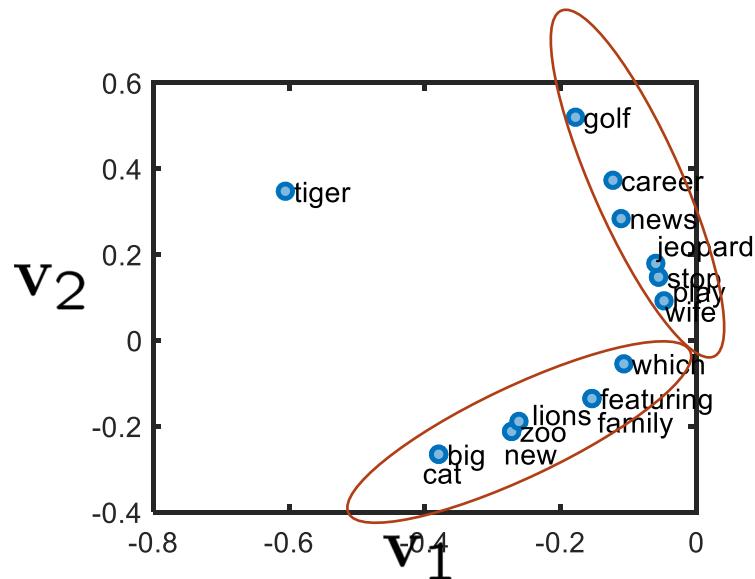
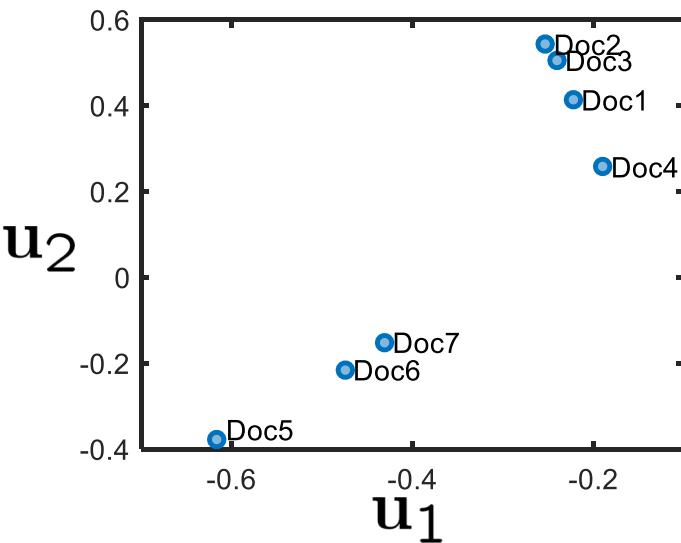
Document 6: Tigers – the big cats – in the new zoo

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	X																	
	tiger	stop	play	golf	news	career	jeopardy	wife	zoo	featuring	new	big	cat	family	lions	which		
Doc1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0		
Doc2	1	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0		
Doc3	1	0	0	1	0	1	1	0	0	0	0	0	0	0	0	0		
Doc4	1	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0		
Doc5	1	0	0	0	0	0	0	1	1	1	1	1	1	1	0	0		
Doc6	1	0	0	0	0	0	0	1	0	1	1	1	0	0	0	0		
Doc7	1	0	0	0	0	0	0	0	0	0	1	1	0	1	1	1		

$$X = U\Sigma V^T$$

$$\approx \sigma_1 \begin{matrix} \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ u_1 \end{matrix} v_1 + \sigma_2 \begin{matrix} \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ u_2 \end{matrix} v_2$$



You may be interested in:

- Clustering
- Document classification

Text Mining (cont.)

Document 1: Tiger stopped playing golf

Document 2: News about Tiger and his golf career

Document 3: Golf career of Tiger in jeopardy

Document 4: Tiger and his wife in the news

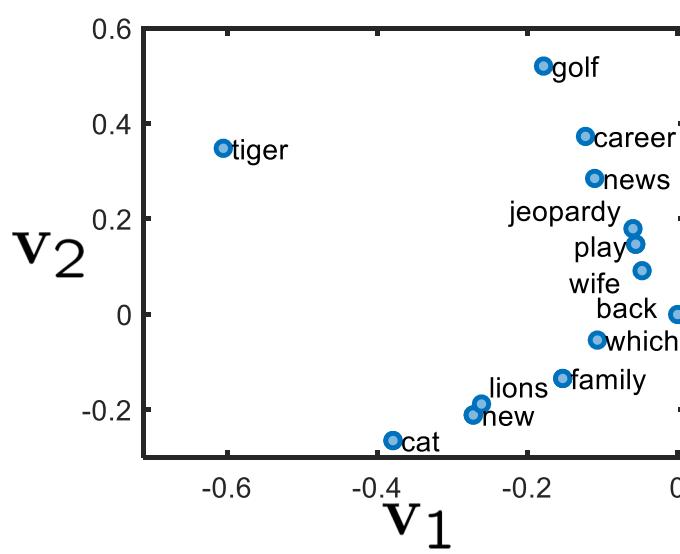
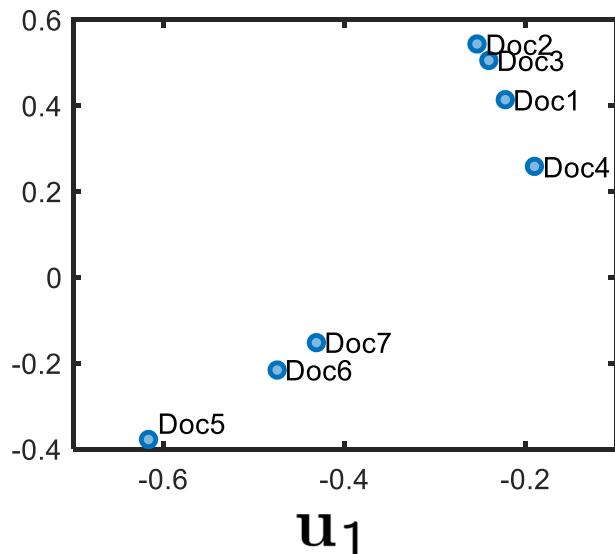
Document 5: The new zoo featuring the big cat family: tigers and lions

Document 6: Tigers – the big cats – in the new zoo

Document 7: Tigers and lions, which are the biggest cats?

Document 8: Tiger back to golf

$$q^T = [\begin{array}{ccccccccc} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{array}]$$



X

	tiger	stop	play	golf	news	career	jeopardy	wife	zoo	featuring	new	big	cat	family	lions	which
Doc1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0
Doc2	1	0	0	1	1	1	0	0	0	0	0	0	0	0	0	0
Doc3	1	0	0	1	0	1	1	0	0	0	0	0	0	0	0	0
Doc4	1	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0
Doc5	1	0	0	0	0	0	0	1	1	1	1	1	1	1	0	0
Doc6	1	0	0	0	0	0	0	1	0	1	1	1	0	0	0	0
Doc7	1	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1

$$\approx \sigma_1 \begin{matrix} \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \end{matrix} v_1 + \sigma_2 \begin{matrix} \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \end{matrix} v_2$$

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Text Mining (cont.)

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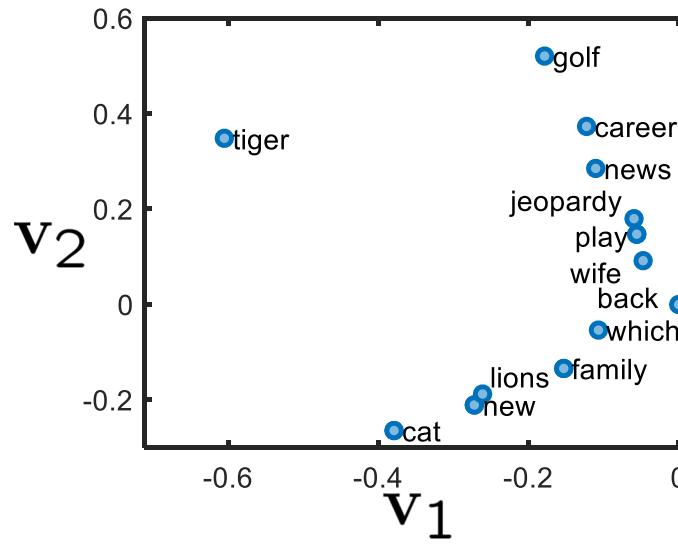
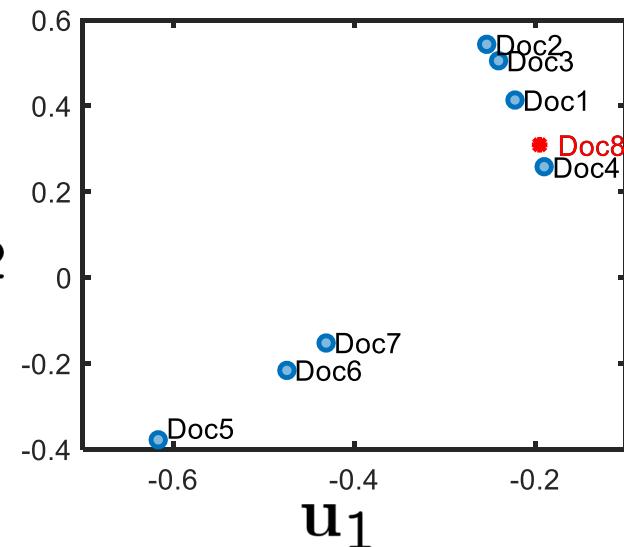
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$$q^T = [\begin{array}{ccccccccc} 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{array}]$$



Tool: Singular Value Decomposition

X

	tiger	stop	play	golf	news	career	jeopardy	wife	zoo	featuring	new	big	cat	family	lions	which
Doc1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0
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Doc5	1	0	0	0	0	0	0	0	1	1	1	1	1	1	0	0
Doc6	1	0	0	0	0	0	0	1	0	1	1	1	0	0	0	0
Doc7	1	0	0	0	0	0	0	0	0	0	0	1	1	0	1	1

$$\approx \sigma_1 \begin{matrix} \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \end{matrix} v_1 + \sigma_2 \begin{matrix} \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \\ \textcolor{blue}{\square} \end{matrix} v_2$$

$$\begin{matrix} \textcolor{darkblue}{\square} \\ \textcolor{darkblue}{\square} \\ \textcolor{darkblue}{\square} \end{matrix} u_1 \quad \begin{matrix} \textcolor{darkblue}{\square} \\ \textcolor{darkblue}{\square} \\ \textcolor{darkblue}{\square} \end{matrix} u_2$$

You may be interested in:

- Clustering
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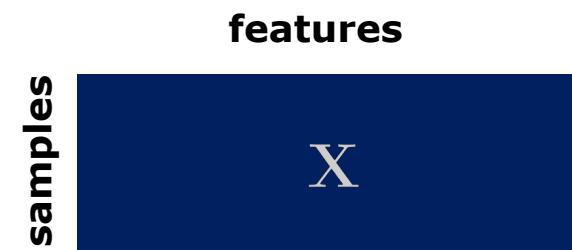
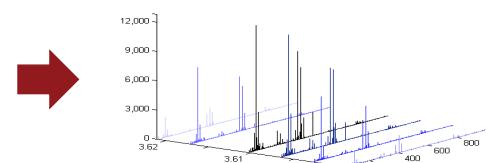
Metabolomics

The goal is to **detect** a wide range of **metabolites** in biological samples, e.g., blood or urine, and to **discover** the significant metabolic **biomarkers** related to certain conditions such as food intake or various diseases.

Some are fed with 10g apple while
some are controls (no apple)



Liquid Chromatography-
Mass Spectrometry (LC-MS)



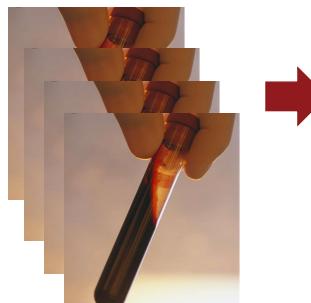
$$\approx \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_R u_R v_R^T$$

Metabolomics

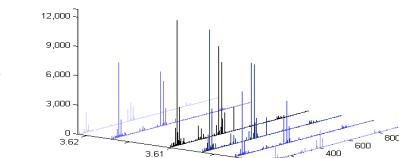
Tool: Singular Value Decomposition

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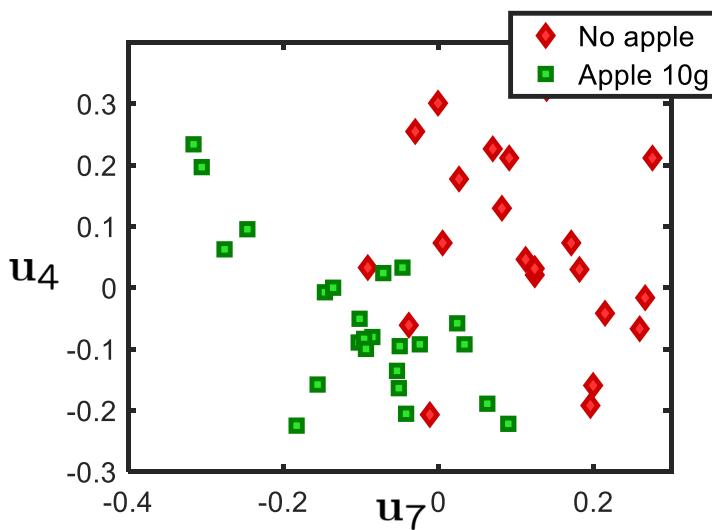
Liquid Chromatography-
Mass Spectrometry (LC-MS)



features

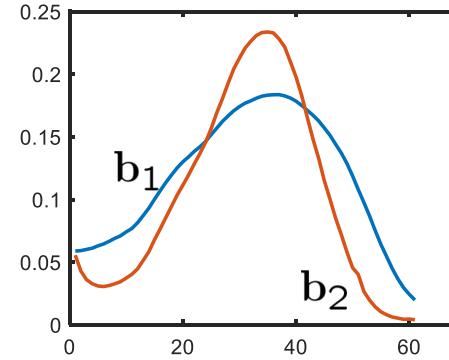
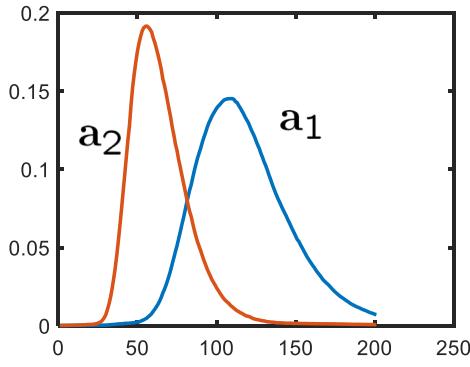


$$X = U\Sigma V^T$$



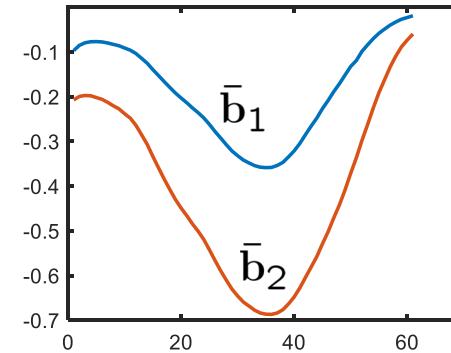
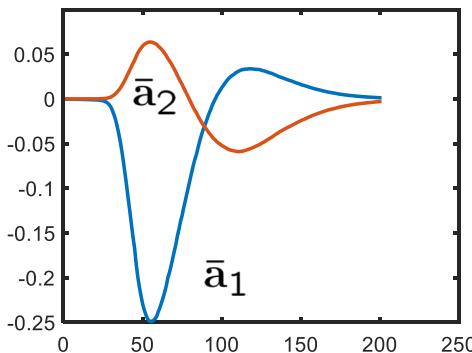
You may then check the corresponding columns in V to discover the metabolites

Matrix factorizations are not unique!



$$A \in \mathbb{R}^{201 \times 2} = [a_1 \ a_2] \quad B \in \mathbb{R}^{61 \times 2} = [b_1 \ b_2]$$

$$\begin{aligned} X &= AB^T \\ &= A M M^{-1} B^T \\ &= \bar{A} \bar{B}^T \end{aligned}$$



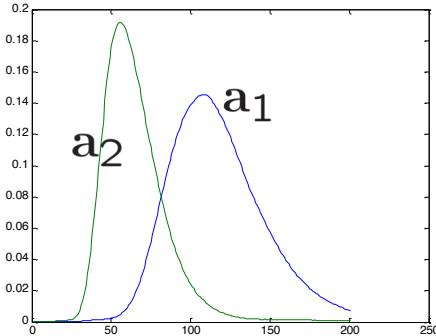
Uniqueness is an issue

$$\mathbf{X} = \mathbf{AB}^T = \mathbf{AMM}^{-1}\mathbf{B}^T = \bar{\mathbf{A}}\bar{\mathbf{B}}^T$$

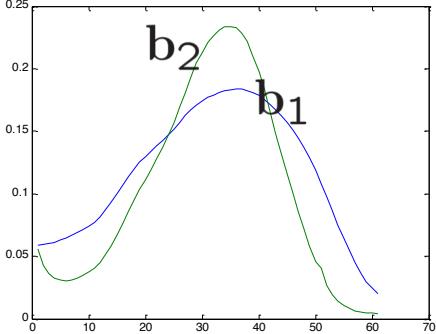
Constraints are used to deal with the uniqueness problem, e.g., SVD. However, factorizations with constraints may not be meaningful in terms of the application.

True factors

$$\mathbf{A} \in \mathbb{R}^{201 \times 2} = [\mathbf{a}_1 \quad \mathbf{a}_2]$$

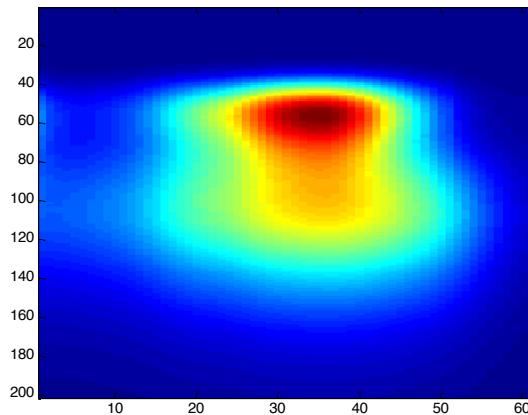


$$\mathbf{B} \in \mathbb{R}^{61 \times 2} = [\mathbf{b}_1 \quad \mathbf{b}_2]$$



Data matrix

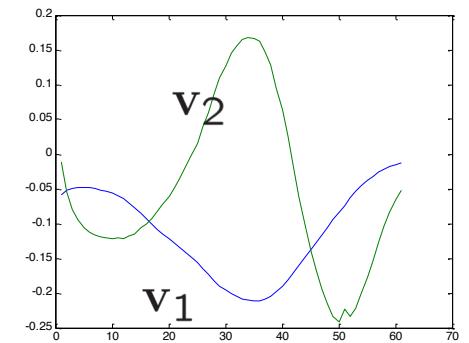
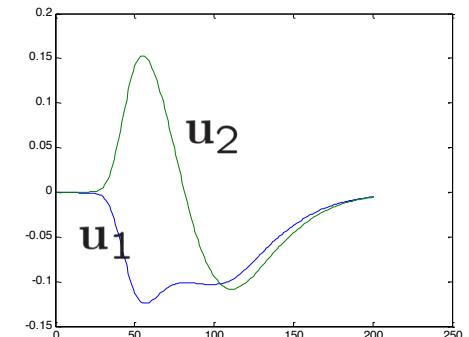
$$\mathbf{X} = \mathbf{AB}^T$$



Given \mathbf{X} , can we recover
the true factors?

SVD captures...

$$\mathbf{X} \approx \hat{\mathbf{X}} = \mathbf{U}\Sigma\mathbf{V}^T$$



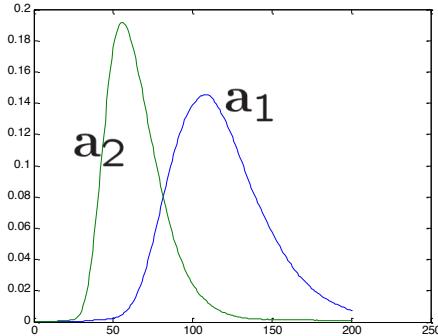
Uniqueness is an issue

$$\mathbf{X} = \mathbf{AB}^T = \mathbf{AMM}^{-1}\mathbf{B}^T = \bar{\mathbf{A}}\bar{\mathbf{B}}^T$$

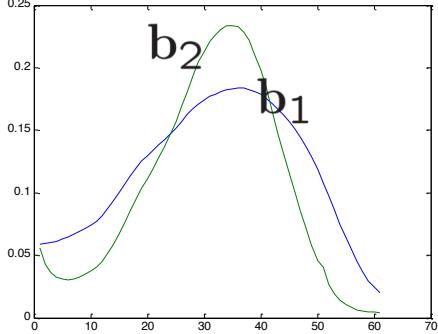
Constraints are used to deal with the uniqueness problem, e.g., SVD. However, factorizations with constraints may not be meaningful in terms of the application.

True factors

$$\mathbf{A} \in \mathbb{R}^{201 \times 2} = [\mathbf{a}_1 \quad \mathbf{a}_2]$$

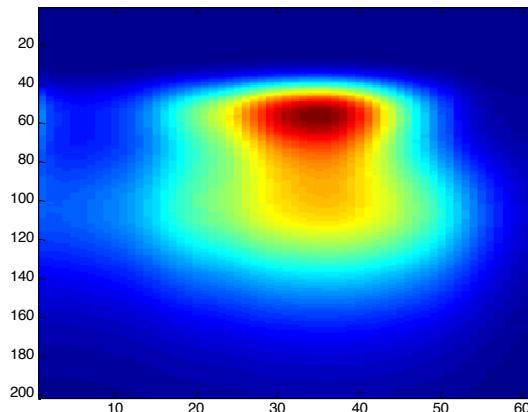


$$\mathbf{B} \in \mathbb{R}^{61 \times 2} = [\mathbf{b}_1 \quad \mathbf{b}_2]$$



Data matrix

$$\mathbf{X} = \mathbf{AB}^T$$

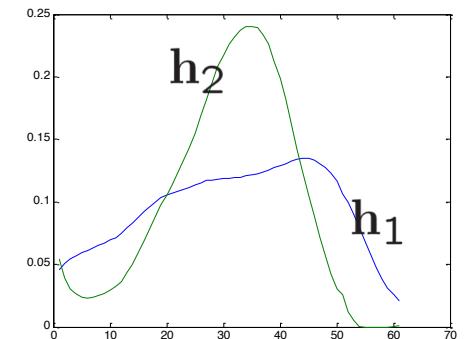
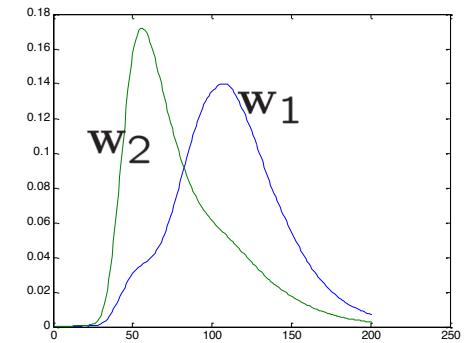


Given \mathbf{X} , can we recover the true factors?

NMF captures...

$$\mathbf{X} \approx \hat{\mathbf{X}} = \mathbf{WH}^T$$

$$w_{ir}, h_{jr} \geq 0$$



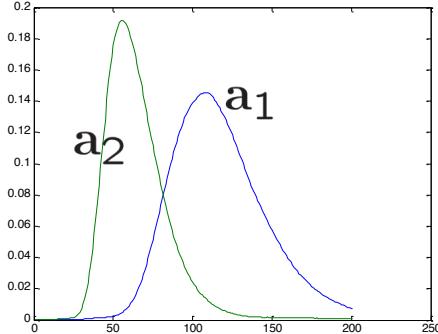
Uniqueness is an issue

$$\mathbf{X} = \mathbf{AB}^T = \mathbf{AMM}^{-1}\mathbf{B}^T = \bar{\mathbf{A}}\bar{\mathbf{B}}^T$$

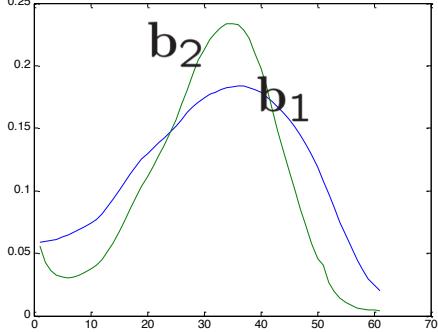
Constraints are used to deal with the uniqueness problem, e.g., SVD. However, factorizations with constraints may not be meaningful in terms of the application.

True factors

$$\mathbf{A} \in \mathbb{R}^{201 \times 2} = [\mathbf{a}_1 \quad \mathbf{a}_2]$$

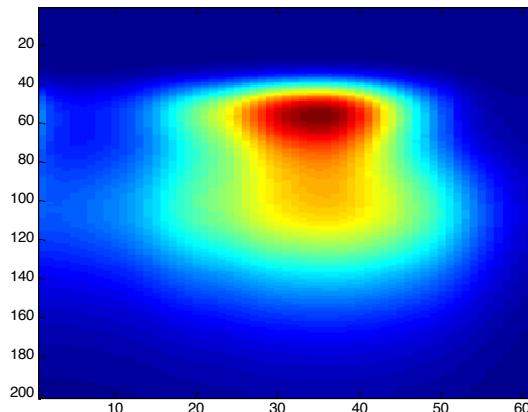


$$\mathbf{B} \in \mathbb{R}^{61 \times 2} = [\mathbf{b}_1 \quad \mathbf{b}_2]$$



Data matrix

$$\mathbf{X} = \mathbf{AB}^T$$

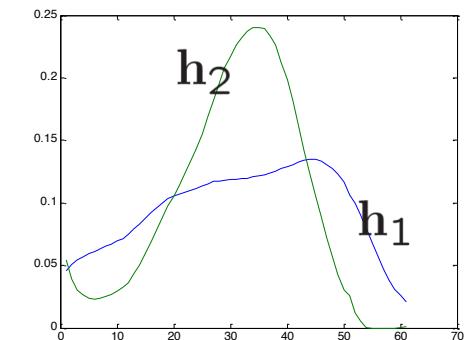
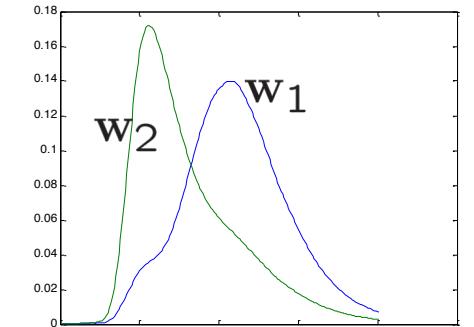


Given \mathbf{X} , can we recover the true factors?

NMF captures...

$$\mathbf{X} \approx \hat{\mathbf{X}} = \underbrace{\mathbf{W}}_{\bar{\mathbf{W}}} \underbrace{\mathbf{M}}_{\mathbf{M}} \underbrace{\mathbf{M}^{-1}}_{\bar{\mathbf{H}}^T} \underbrace{\mathbf{H}^T}_{\bar{\mathbf{H}}^T}$$

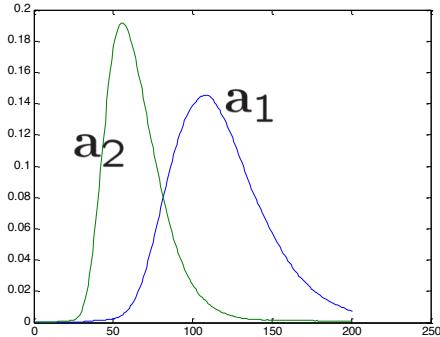
$$\bar{w}_{ir}, \bar{h}_{jr} \geq 0$$



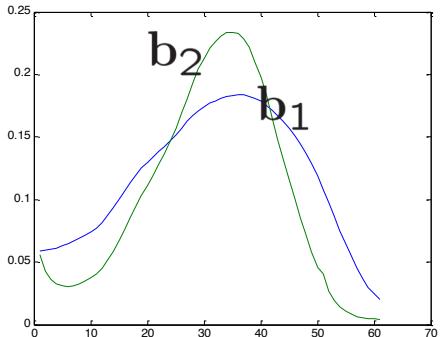
What if we have multiple matrices with the same underlying factors but in different proportions...

True factors

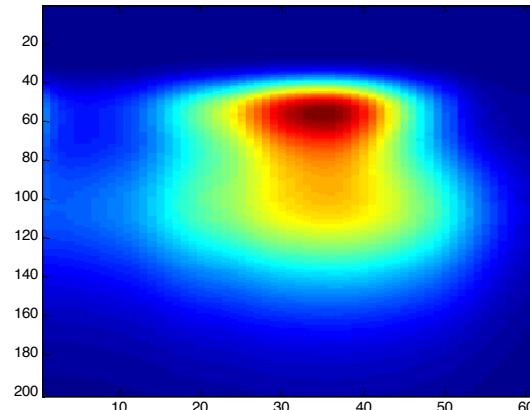
$$A \in \mathbb{R}^{201 \times 2} = [a_1 \ a_2]$$



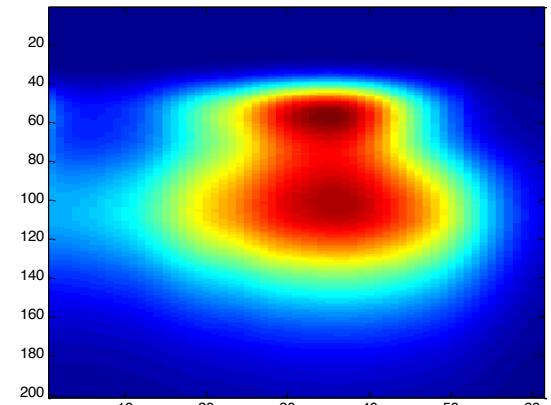
$$B \in \mathbb{R}^{61 \times 2} = [b_1 \ b_2]$$



$$X_1 = A \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} B^T$$



$$X_2 = A \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix} B^T$$



We can recover the true factors uniquely up to trivial indeterminacies, i.e., scaling and permutation.

Canonical Polyadic (CP) CANDECOMP/PARAFAC (CP)

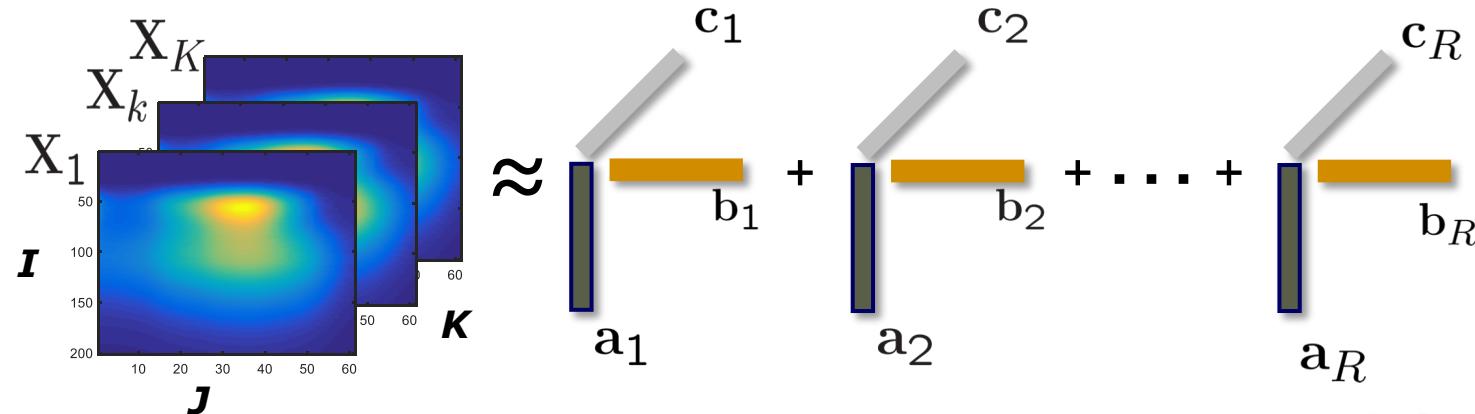
Hitchcock, 1927: Polyadic form of a tensor

Harshman, 1970: Parallel Factor Analysis (PARAFAC)

Carroll & Chang, 1970: Canonical Decomposition (CANDECOMP)

A popular tensor factorization model: CP

As an extension of matrix factorizations to higher-order tensors (multi-way arrays), tensor factorizations are used to extract the underlying factors in higher-order data sets. The CP model represents a tensor as a sum of rank-one tensors:



$$X_k \approx A \begin{bmatrix} c_{k1} & \dots & c_{kR} \end{bmatrix} B^T$$

$$\begin{aligned} \mathcal{X} &\approx \sum_{r=1}^R a_r \circ b_r \circ c_r \\ &\approx [\![A, B, C]\!] \end{aligned}$$

$$A \in \mathbb{R}^{I \times R} = [a_1 \ \dots \ a_R]$$

$$B \in \mathbb{R}^{J \times R} = [b_1 \ \dots \ b_R]$$

$$C \in \mathbb{R}^{K \times R} = [c_1 \ \dots \ c_R]$$

CP is unique up to scaling and permutation under the condition that

$$\text{krank}(A) + \text{krank}(B) + \text{krank}(C) \geq 2R + 2$$

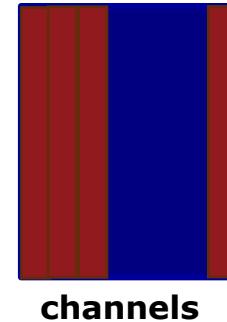
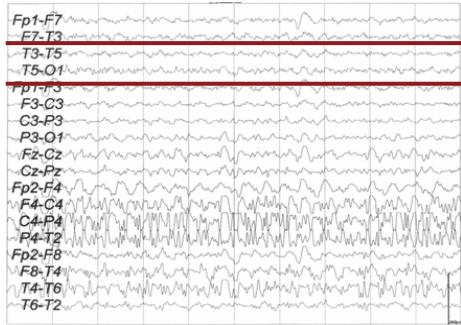
[Kruskal, 1977;
Sidiropoulos and Bro, 2000]

where $\text{krank}(A) = \max.$ value of k such that any k columns of A is linearly independent.

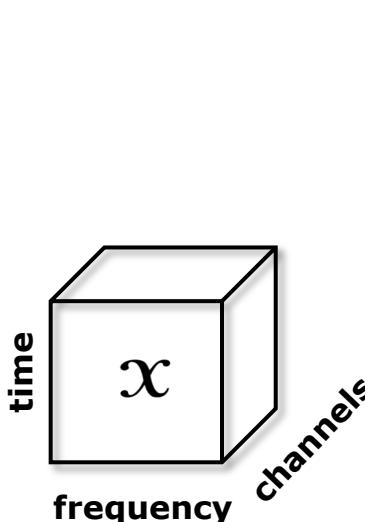
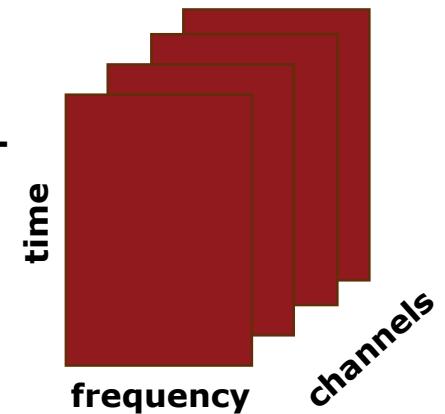
Neuroscience: CP has proved useful in epileptic seizure localization

[Acar et al., 2007; De Vos et al., 2007]

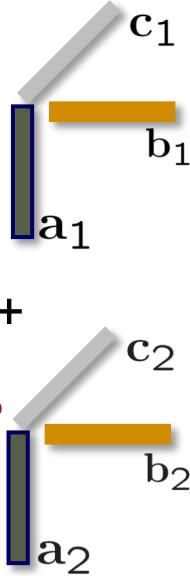
Tool: Tensor Factorizations



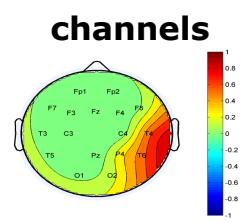
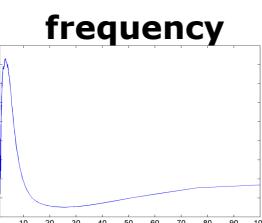
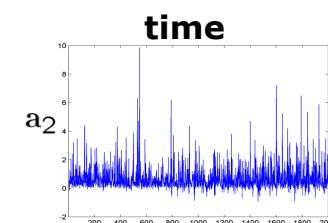
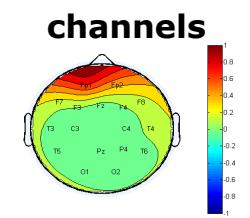
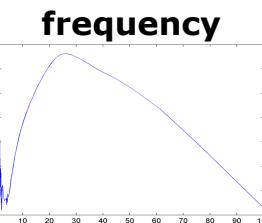
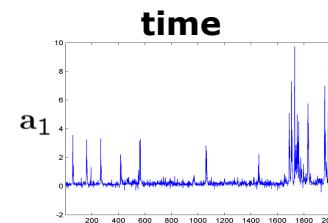
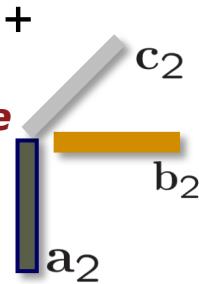
CWT
→



*Eye
artifact*



Seizure



Recommender Systems: CP can capture temporal patterns useful for link prediction

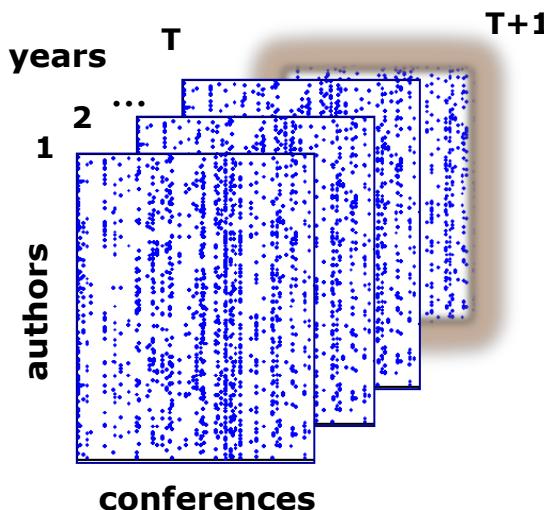
Tool: Tensor Factorizations

[Dunlavy, Kolda, Acar, 2011]

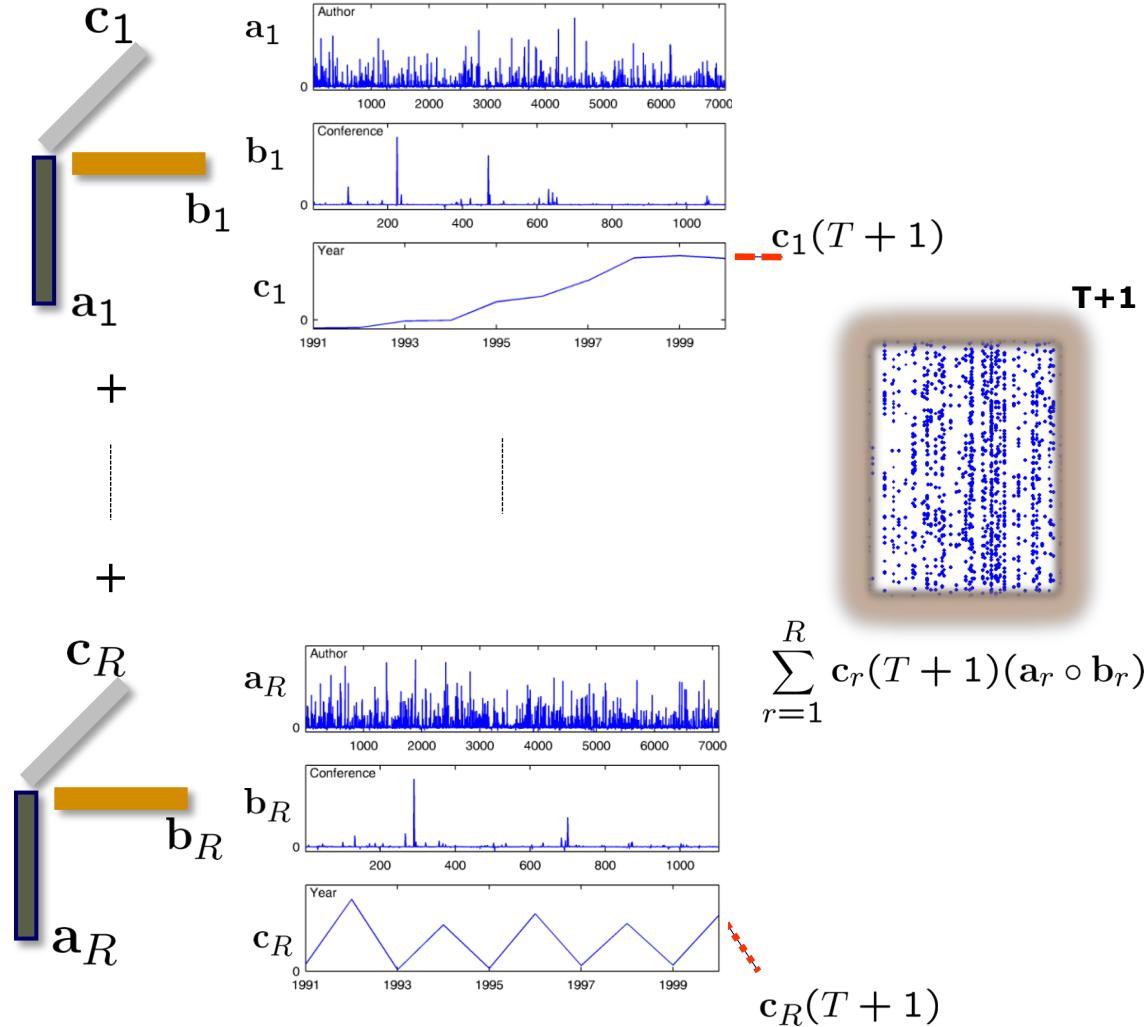
Temporal Link Prediction

Which customers will buy which products?

Which webpages will users visit?



\approx

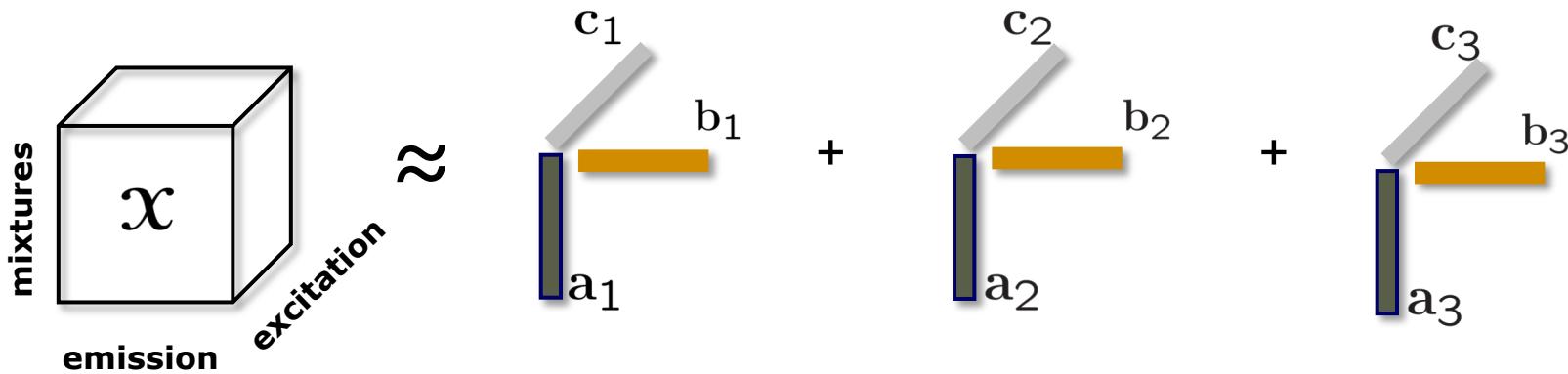


simula

Chemometrics: CP can separate the chemicals in mixtures

[Andersen and Bro, 2003]

A popular application of the CP model is the separation of individual chemicals from mixtures of chemicals measured using fluorescence spectroscopy.



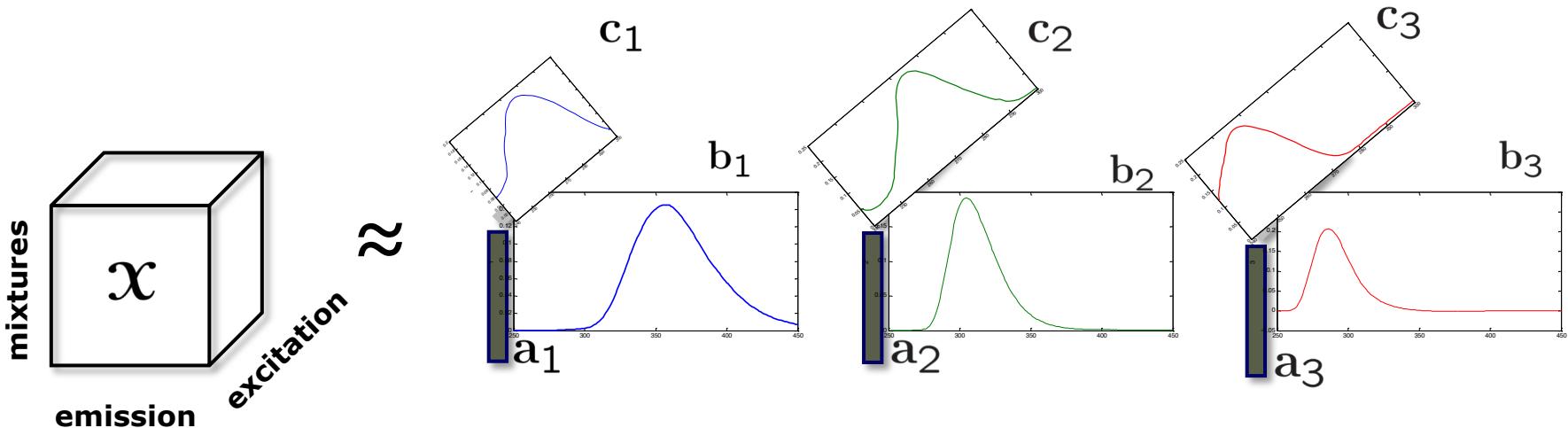
Amino Acid Data
<http://www.models.life.ku.dk/>

Chemometrics: CP can separate the chemicals in mixtures

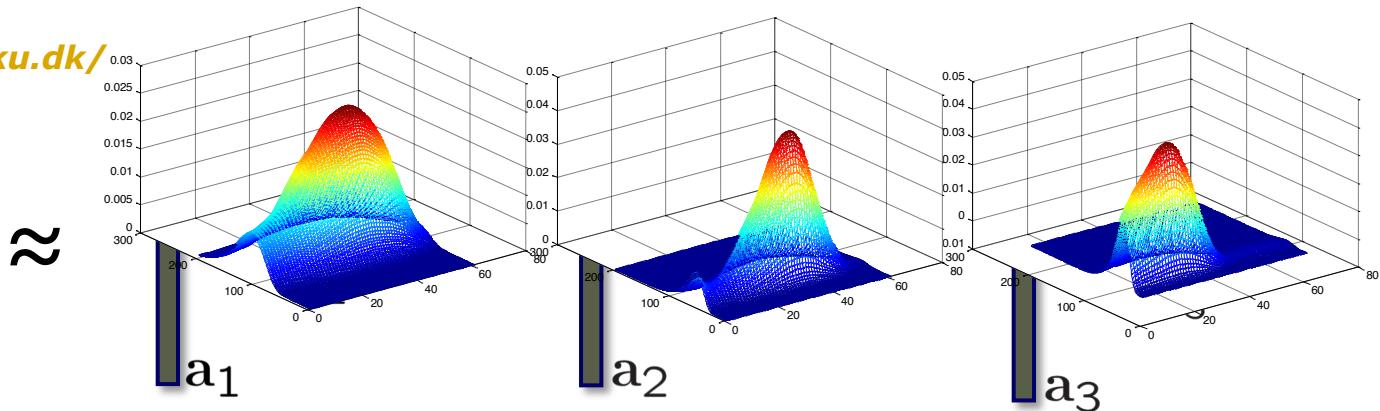
Tool: Tensor Factorizations

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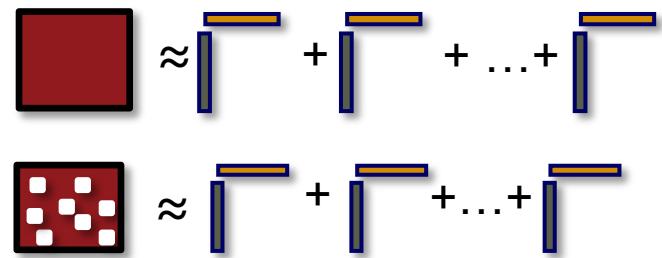
Amino Acid Data
<http://www.models.life.ku.dk/>



Summary

Matrix Factorizations: How to use matrix factorizations to

- (i) find the underlying factors,
- (ii) predict missing entries



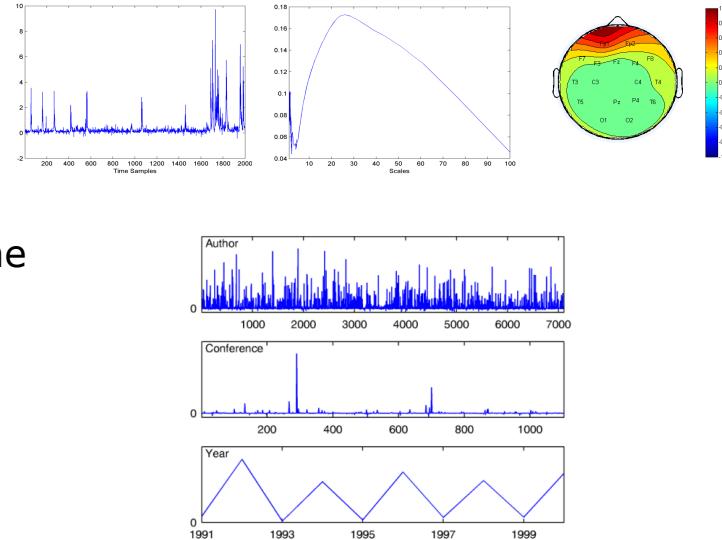
Matrix factorizations without constraints are not unique.

Constraints need to make sense in terms of the application; otherwise, the model will not reveal what we are looking for.

Tensor Factorizations

Tensor factorization methods such as CP have better uniqueness properties compared to matrix factorizations.

How to use tensor factorizations, in particular, CP, to find the underlying factors, e.g., chemometrics, neuroscience, temporal link prediction



Details, algorithms and more applications tomorrow!