

# Unsupervised data decompositions

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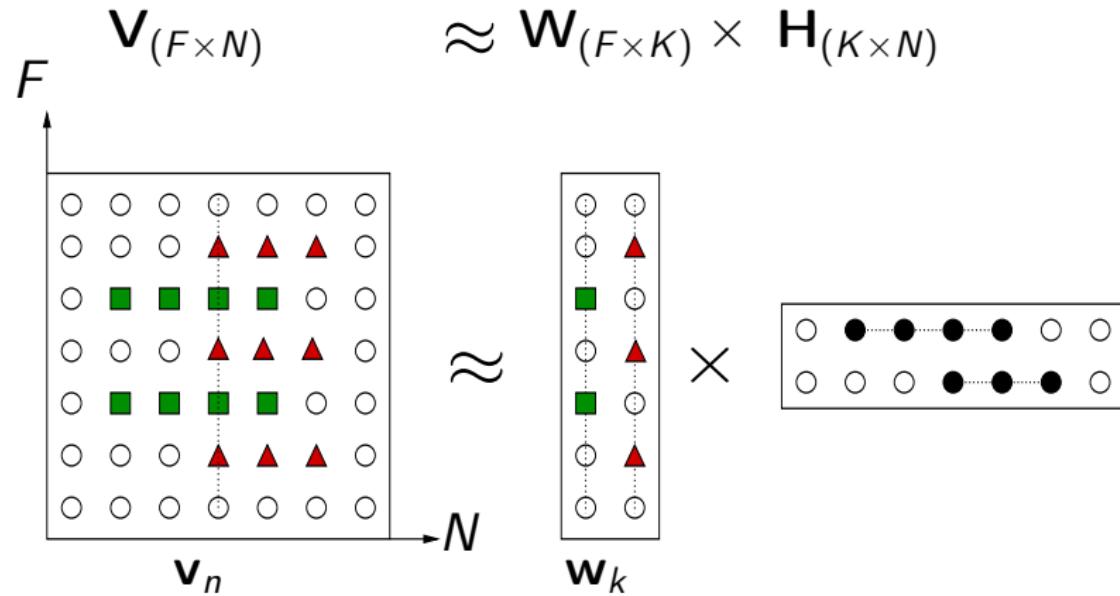
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- ▶ Introduction
- ▶ Principal Component Analysis (PCA)
- ▶ NMF models
- ▶ Algorithms for solving NMF
- ▶ Constrained NMF schemes
- ▶ Multi-stream and cross-modal NMF schemes
- ▶ Applications
- ▶ Conclusion

# Explaining data by factorisation

## General formulation

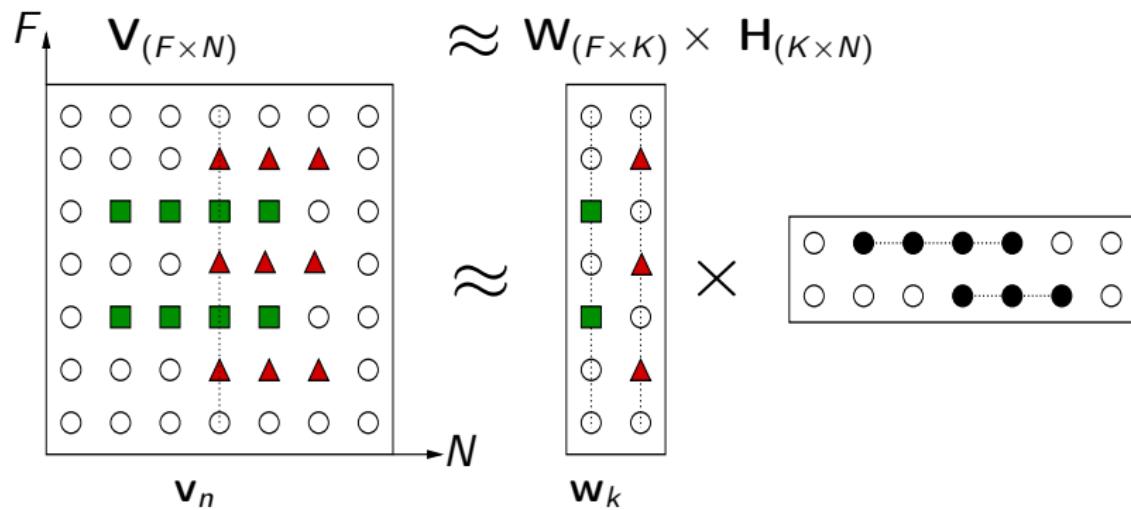


$$\mathbf{v}_n \approx \sum_{k=1}^K h_{kn} \mathbf{w}_k$$

*Illustration by C. Févotte*

# Explaining data by factorisation

## General formulation



data matrix

“explanatory variables”  
“basis”, “dictionary”,  
“patterns”, “topics”

“regressors”,  
“activation coefficients”,  
“expansion coefficients”

Illustration by C. Févotte

# PCA

- The data is assumed real-valued ( $\mathbf{v}_n \in \mathbb{R}^F$ ) and centered ( $E\{\mathbf{v}_n\} = 0$ )
- PCA returns the best linear approximation to the data in **least squares** sense:

$$\mathbf{v}_n \approx \hat{\mathbf{v}}_n = \mathbf{W}\mathbf{W}^T\mathbf{v}_n = \sum_{k=1}^K \langle \mathbf{v}_n, \mathbf{w}_k \rangle \mathbf{w}_k$$

where  $\mathbf{W} \in \mathbb{R}^{F \times K}$  is such that the least squares error is minimized:

$$\mathbf{W}_{PCA} = \min_{\mathbf{W}} \frac{1}{N} \sum_{n=1}^N \|\mathbf{v}_n - \hat{\mathbf{v}}_n\|_2^2 = \frac{1}{N} \|\mathbf{V} - \mathbf{W}\mathbf{W}^T\mathbf{V}\|_F^2$$

# PCA

- The solution can be shown to be of the form

$$\mathbf{W}_{PCA} = \mathbf{E}_{1:K} \mathbf{U}$$

where  $\mathbf{E}_{1:K}$  denotes the  $K$  dominant eigenvectors of  $\mathbf{C}_v$ :

$$\mathbf{C}_v = \mathbb{E}\{\mathbf{v}\mathbf{v}^T\} \approx \frac{1}{N} \sum_n \mathbf{v}_n \mathbf{v}_n^T$$

and where  $\mathbf{U}$  is any unitary matrix of size  $K \times K$ .

# Compression

The residual least square error of the decomposition can be shown to be

$$\frac{1}{N} \sum_n \|\mathbf{v}_n - \hat{\mathbf{v}}_n\|_2^2 = \sum_{i=K+1}^F d_i$$

where  $\{d_i\}_i$  are the eigenvalues of  $\mathbf{C}_v$ , sorted in order of decreasing value.  
PCA can be used for **compression** and **dimensionality reduction**:

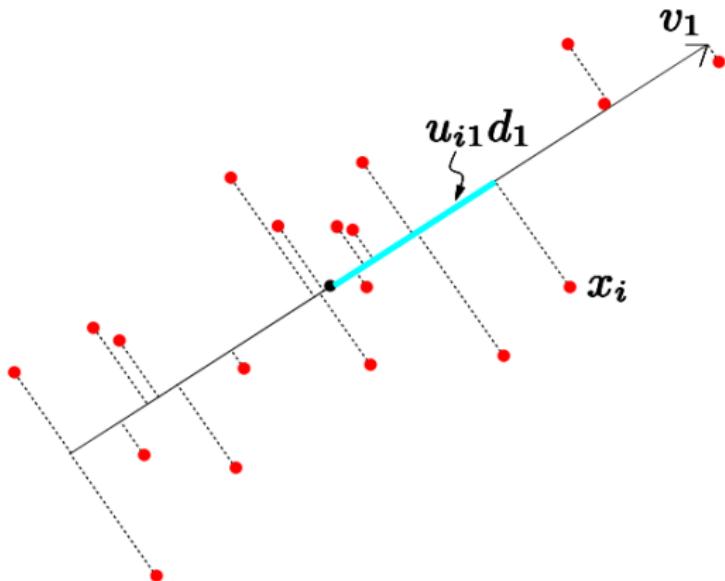
the original  $F \times N$  data matrix  $\mathbf{V}$  can be approximated by  $FK + KN$  coefficients of the matrices  $\mathbf{W}_{PCA}$  and  $\mathbf{H}_{PCA} = \mathbf{W}_{PCA}^T \mathbf{V}$ .

## Uncorrelatedness

When  $\mathbf{U} = \mathbf{I}$ , the expansion coefficients in the PCA model are uncorrelated; indeed, we have

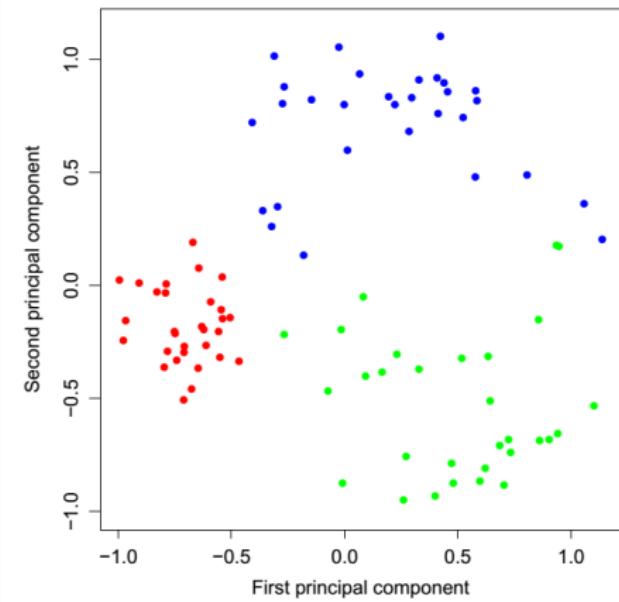
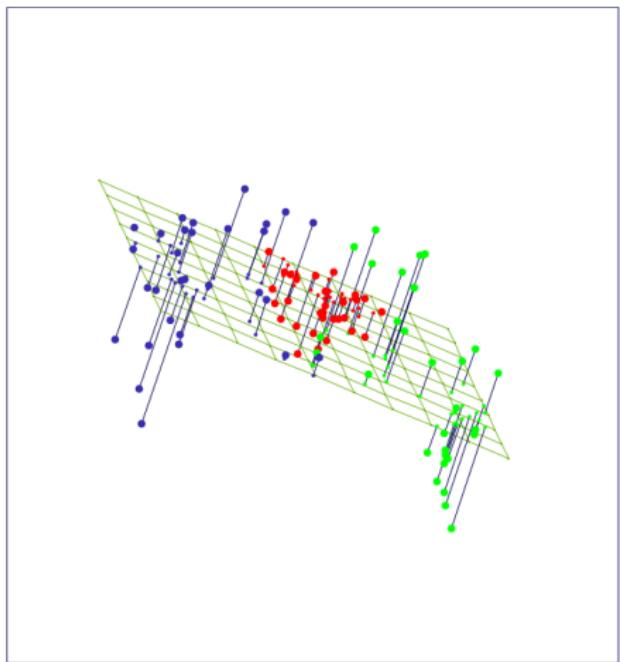
$$\begin{aligned}\mathbf{C}_h &= E\{(\mathbf{W}^T \mathbf{v})(\mathbf{W}^T \mathbf{v})^T\} \\ &= \mathbf{W}^T \mathbf{C}_v \mathbf{W} \\ &= \text{diag}([d_1, \dots, d_K]) \\ &\stackrel{\text{def}}{=} \mathbf{D}_K\end{aligned}$$

## 2D data example



After (Hastie *et al.*, 2008)

# 3D data example



After (Hastie *et al.*, 2008)

# Explaining face images by PCA<sup>1</sup>

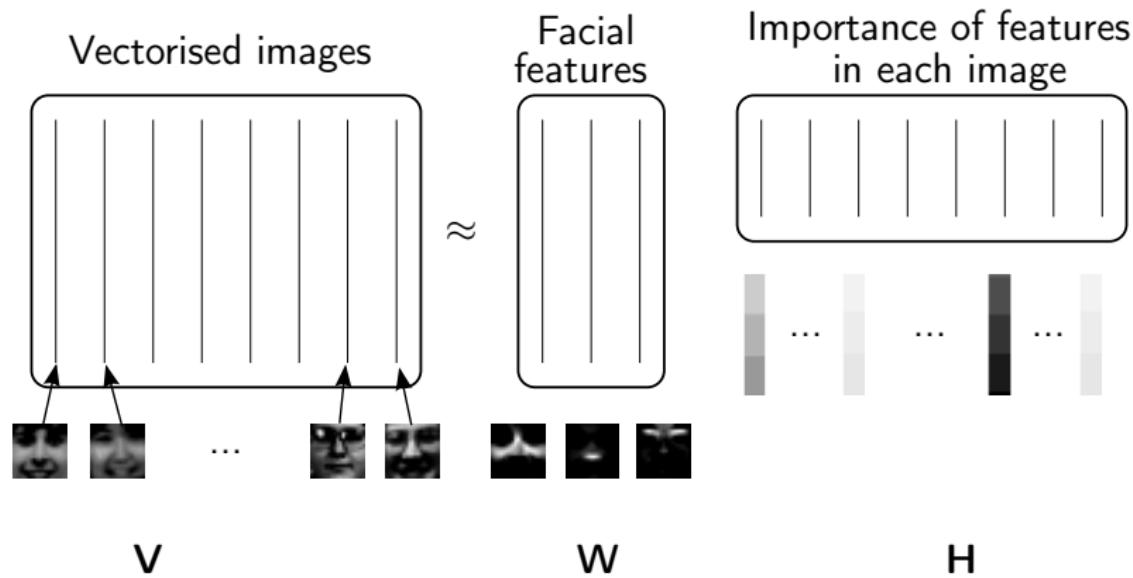
Image example: 49 images among 2429 from MIT's CBCL face dataset



<sup>1</sup>slide adapted from (Févotte, 2012).

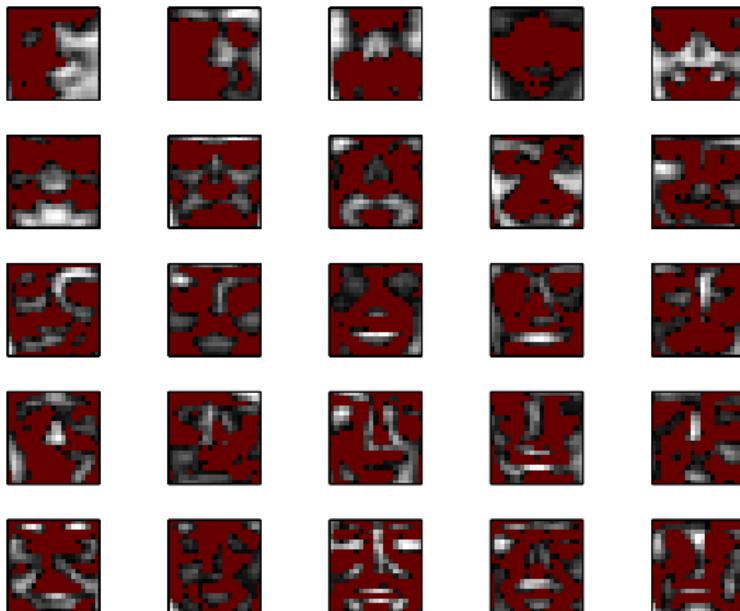
# Explaining face images by PCA

## Method



# Explaining face images by PCA<sup>2</sup>

## Eigenfaces



*Red pixels indicate negative values! How to interpret this?*

<sup>2</sup>slide adapted from (Févotte, 2012).

# Data is often nonnegative by nature<sup>3</sup>

- pixel intensities;
- amplitude spectra;
- occurrence counts;
- food or energy consumption;
- user scores;
- stock market values;
- ...

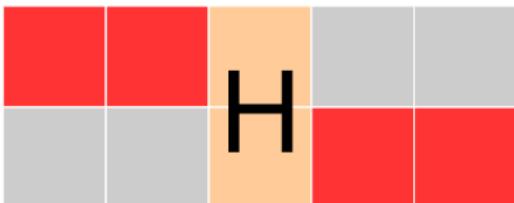
For the sake of **interpretability** of the results, optimal processing of **nonnegative data** may call for processing under **nonnegativity constraints**.

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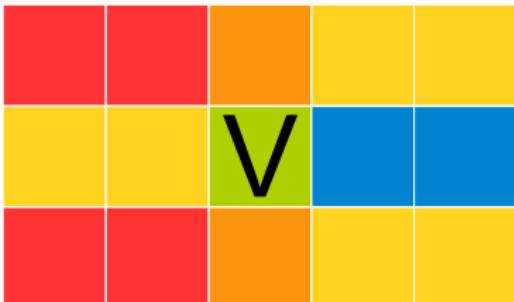
<sup>3</sup>slide adapted from (Févotte, 2012).

# The Nonnegative Matrix Factorisation model

NMF provides an unsupervised linear representation of the data:



$$\mathbf{V} \approx \mathbf{W}\mathbf{H};$$



- $\mathbf{W} = [w_{fk}]$  s.t.  $w_{fk} \geq 0$   
and
- $\mathbf{H} = [h_{kn}]$  s.t.  $h_{kn} \geq 0$ .

Illustration by N. Seichepine

# Why nonnegative factors?

- Nonnegativity induces **sparsity**.
- Nonnegativity leads to **part-based decompositions**.

"Atoms energy cancellation" is not allowed: once an atom is selected with some energy, it cannot be further concealed by other atoms.

# NMF outputs

Image example



*Illustration by C. Févotte*

# NMF outputs

## Audio example

NMF produces **part-based** representations of the data:

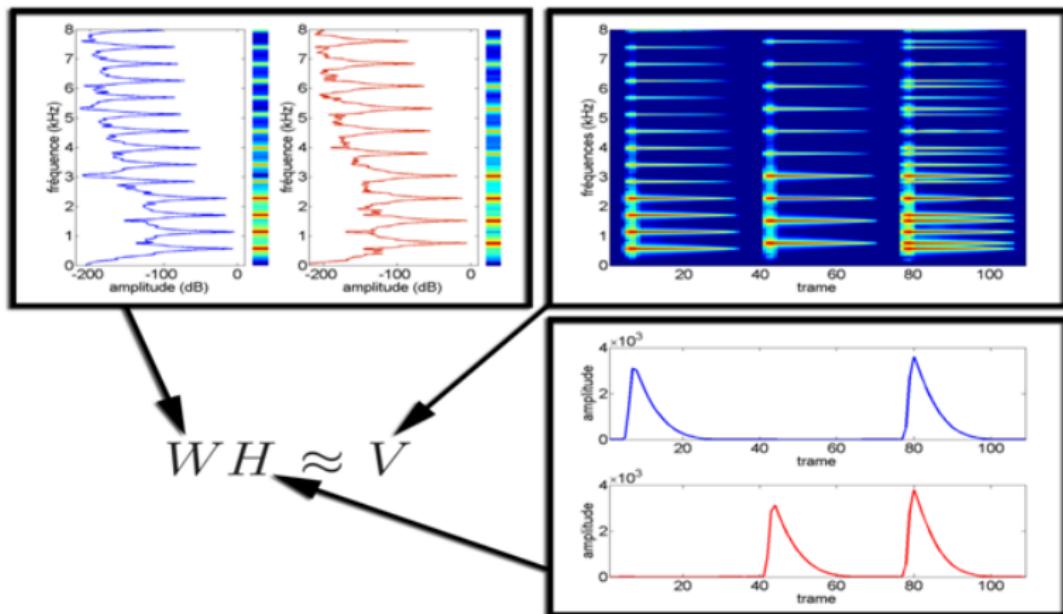


Illustration by R. Hennequin.

# History

NMF is more than **30-year old!**

- previous variants referred to as:
  - **nonnegative rank factorisation** (Jeter and Pye, 1981; Chen, 1984);
  - **positive matrix factorisation** (Paatero and Tapper, 1994);
- popularized by Lee and Seung (1999) for “**learning the parts of objects**”.

Since then, widely used in various research areas for diverse applications.

# Notations I

- $\mathbf{V}$  : the  $F \times N$  **data matrix**:
  - $F$  features (rows),
  - $N$  observations/examples/feature vectors (columns);
- $\mathbf{v}_n = (v_{1n}, \dots, v_{Fn})^T$ : the  $n$ -th **feature vector** observation among a collection of  $N$  observations  $\mathbf{v}_1, \dots, \mathbf{v}_N$ ;
- $\mathbf{v}_n$  is a column vector in  $\mathbb{R}_+^F$ ;  $\mathbf{v}_f$  is a row vector;
- $\mathbf{W}$  : the  $F \times K$  **dictionary matrix**:
  - $w_{fk}$  is one of its coefficients,
  - $\mathbf{w}_k$  a dictionary/basis vector among  $K$  elements;

## Notations II

- $\mathbf{H}$  : the  $K \times N$  activation/expansion matrix:
  - $\mathbf{h}_n$  : the **column vector** of activation coefficients for observation  $\mathbf{v}_n$  :
  - $\mathbf{h}_{k:}$  : the **row vector** of activation coefficients relating to basis vector  $\mathbf{w}_k$ .

$$\mathbf{v}_n \approx \sum_{k=1}^K h_{kn} \mathbf{w}_k ;$$

# General usages of NMF I

## What for?

NMF is a non-supervised data decomposition technique, akin to **latent variable analysis**, that can be used for:

- **feature learning**: like Principal Component Analysis (PCA);
- learn NMF on training dataset  $\mathbf{V}_{train} \rightarrow$  dictionary  $\mathbf{W}$
- exploit  $\mathbf{W}$  to decompose new test examples  $\mathbf{v}_n$  :  
$$\mathbf{v}_n \approx \sum_{k=1}^K h_{kn} \mathbf{w}_k ; h_{kn} \geq 0$$
- use  $\mathbf{h}_n$  as **feature vector** for example  $n$ .

### Evaluation for face recognition:

- **Dataset**: Olivetti faces, 40 classes
- **Classifiers**: LDA (Linear Discriminant Analysis)
- **Cross-validated results**:

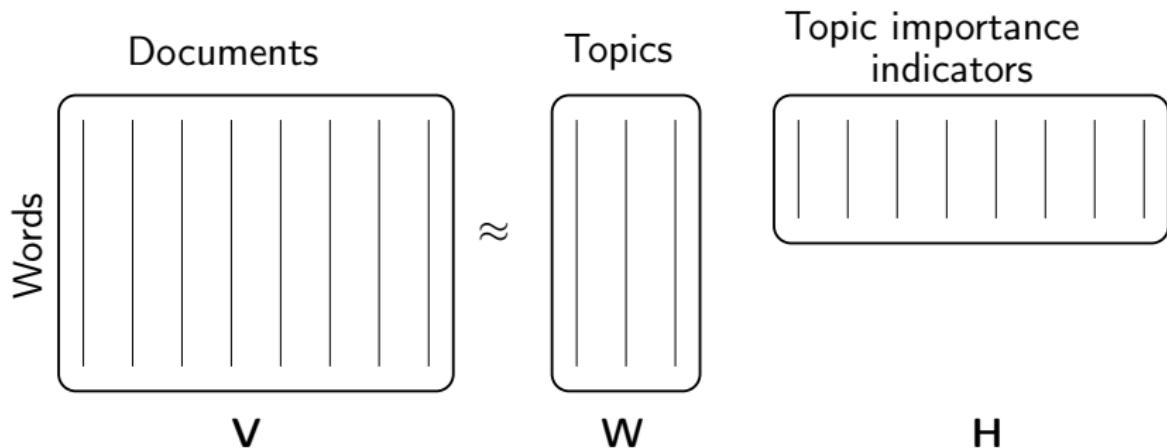
	Accuracy
PCA	93%
ICA	93%
NMF	96%

# General usages of NMF II

What for?

- **topics recovery:**

assume  $\mathbf{V} = [v_{fn}]$  is a (scaled) **term-document** co-occurrence matrix:  
 $v_{fn}$  is the frequency of occurrences of word  $m_f$  in document  $d_n$ ;



# Text document analysis example

After sklearn topics extraction demo (Pedregosa et al., 2011)

Analysing the 20 newsgroups dataset with NMF, the following topics are automatically determined:

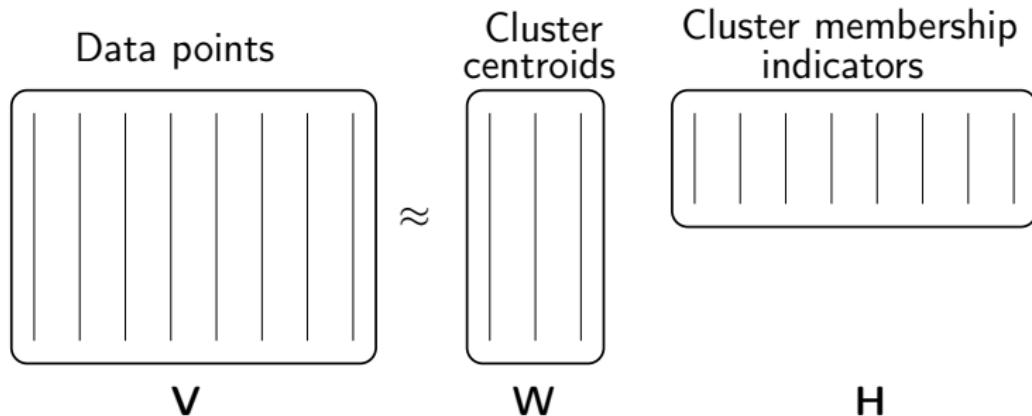
- **Topic #0:** god people bible israel jesus christian true moral think christians believe don say human israeli church life children jewish
- **Topic #1:** drive windows card drivers video scsi software pc thanks vga graphics help disk uni dos file ide controller work
- **Topic #2:** game team nhl games ca hockey players buffalo edu cc year play university teams baseball columbia league player toronto
- **Topic #3:** window manager application mit motif size display widget program xlib windows user color event information use events values
- **Topic #4:** pitt gordon banks cs science pittsburgh univ computer soon disease edu reply pain health david article medical medicine

Topics described by most frequent words in each dictionary element  $W_k$ .

# General usages of NMF III

What for?

- **clustering:** like K-means (Ding et al., 2005, 2010; Xu et al., 2003):

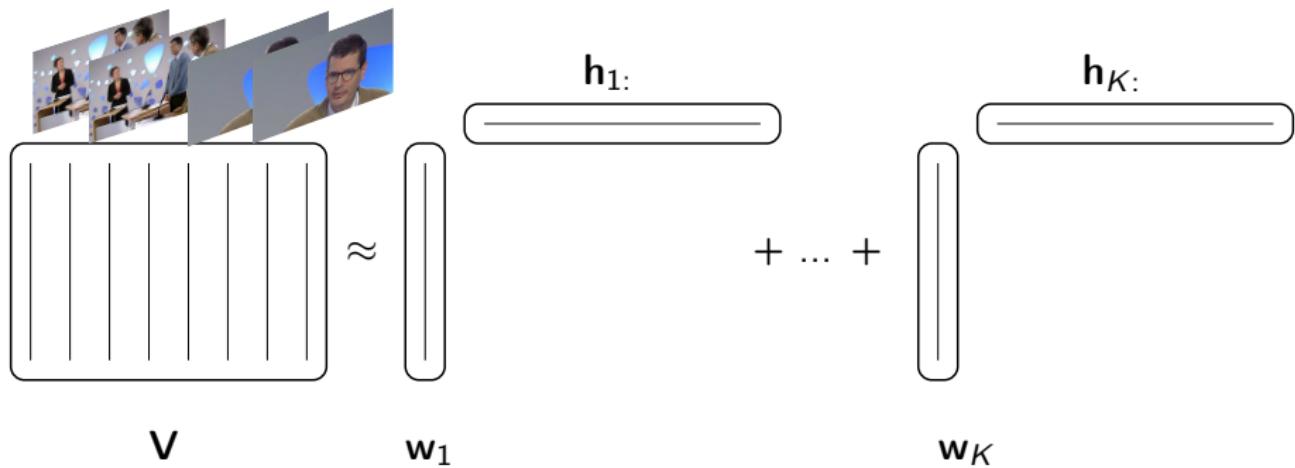


- ▶ NMF can handle overlapping clusters and provides *soft* cluster membership indications.

# General usages of NMF IV

What for?

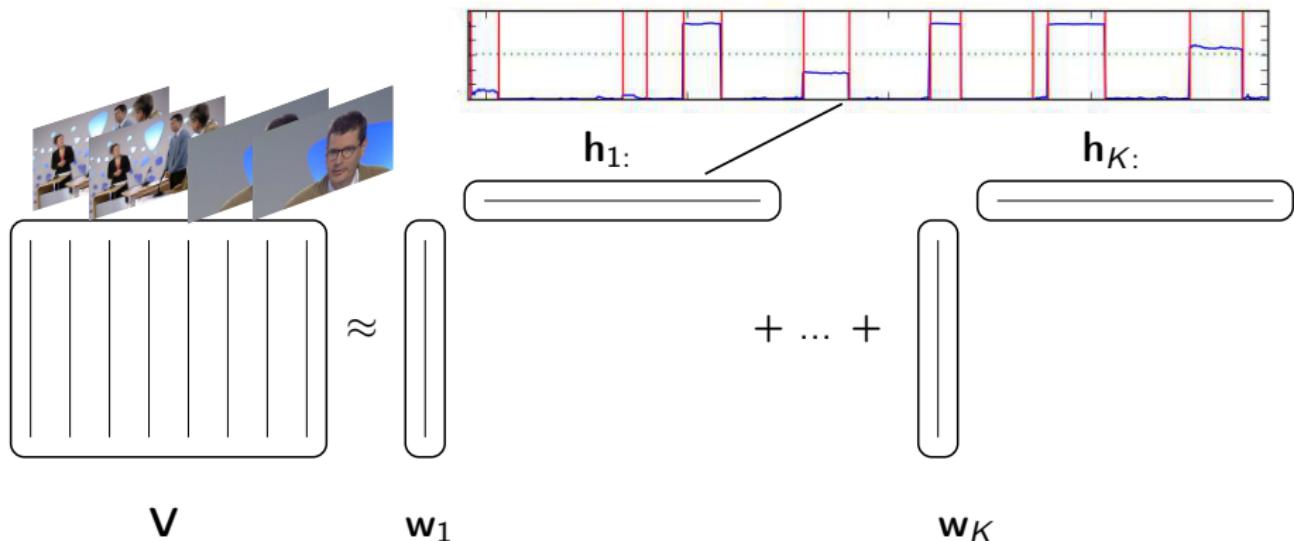
- **temporal segmentation:** like Hidden Markov Models (HMM); analysing temporal data sequences, e.g., videos:



# General usages of NMF IV

What for?

- **temporal segmentation:** like Hidden Markov Models (HMM); analysing temporal data sequences, e.g., videos:

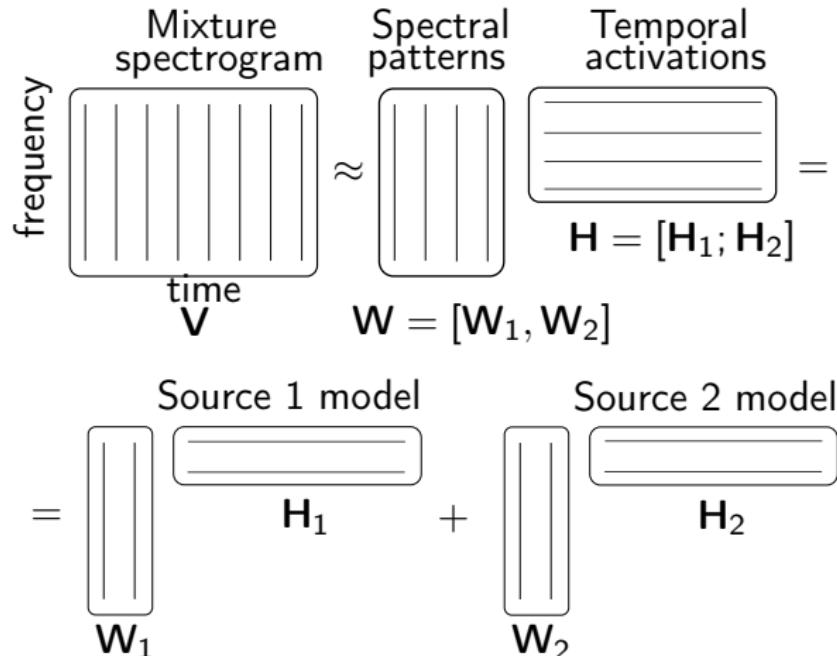


Temporal segmentation can be achieved by thresholding the temporal activations relating to components of interest.

# General usages of NMF V

What for?

- **filtering and source separation:** as with Independent Component Analysis (ICA):



# In summary...

## What for?

NMF is a non-supervised data decomposition technique, akin to **latent variable analysis**, that can be used for:

- **topics recovery**: like Probabilistic Latent Semantic Analysis (PLSA);
- **feature learning**: like Principal Component Analysis (PCA);
- **clustering**: like K-means;
- **temporal segmentation**: like Hidden Markov Models (HMM);
- **filtering and source separation**: as with Independent Component Analysis (ICA);
- **coding** as with vector quantization.

# Overview of NMF application domains I

A variety of successful applications:

- **Text mining:** (Xu et al., 2003; Berry and Browne, 2006; Kim and Park, 2008)
- **Images:**
  - unsupervised object discovery (Sivic et al., 2005)
  - object and face recognition (Soukup and Bajla, 2008)
  - tagging (Kalayeh et al., 2014)
  - denoising and inpainting (Mairal et al., 2010)
  - texture classification (Sandler and Lindenbaum, 2011)
  - spectral data (Berry et al.)
  - hashing (Monga and Mihcak, 2007)
  - watermarking (Lu et al., 2009)
- **Electroencephalography (EEG) data:**
  - feature extraction (Cichocki and Rutkowski, 2006; Lee et al., 2009)
  - artifact rejection (Damon et al., 2013a,b)

# Overview of NMF application domains II

- **Bioinformatics:**

- gene expression analysis (Brunet et al., 2004; Gao and Church, 2005)
  - protein interaction clustering (Greene et al., 2008)

- **Other:**

- collaborative filtering (Melville and Sindhvai, 2010)
  - community discovery (Wang et al., 2010)
  - portfolio diversification (Drakakis et al., 2007)
  - food consumption analysis (Zetlaoui et al., 2010)
  - industrial source apportionment (Limen et al., 2013)

- **Audio and music**

- **Videos**

# Audio and music processing

- **Source separation** (NMF is state-of-the art):
  - **speech**: separating voices in speech mixtures or voice from background (Virtanen, 2007; Virtanen and Cemgil, 2009; Mohammadiha et al., 2013)
  - **music**: separating singing voice/melody from accompaniment or musical instruments in polyphonic mixtures (Durrieu et al., 2009; Ozerov and Fevotte, 2010; Hennequin et al., 2011; Ozerov et al., 2013; Rafii et al., 2013)
- **Signal enhancement/denoising**:  
(Wilson et al., 2008; Schmidt et al., 2007; Sun and Mazumder, 2013)
- **Audio inpainting**  
(Roux et al., 2011; Yilmaz et al., 2011)

# Audio and music processing

- **Compression**

(Ozerov et al., 2011b; Nikunen et al., 2011)

- **Music transcription:** recognizing musical notes played by Piano, Drums or multiple instruments

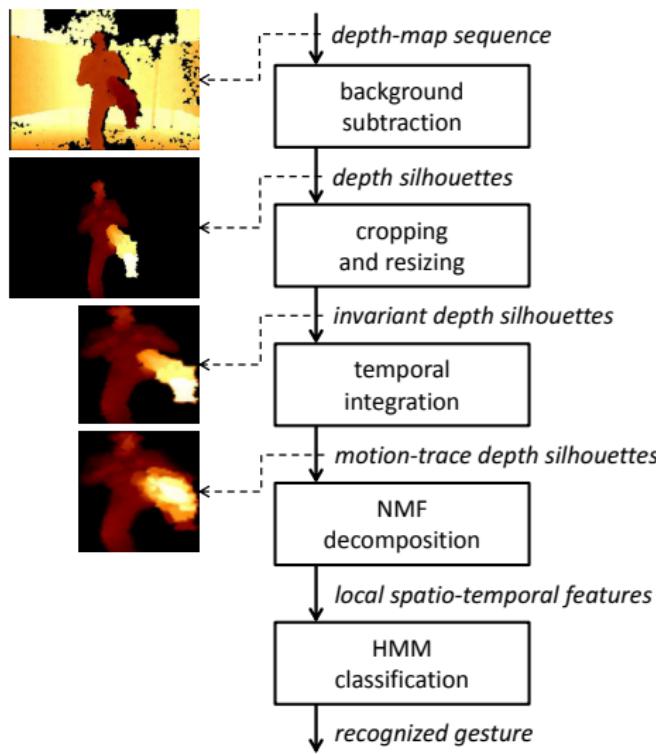
(Smaragdis and Brown, 2003; Abdallah and Plumbley, 2004; Vincent et al., 2007; E. Vincent et al., 2008; Févotte et al., 2009; Bertin et al., 2010; Vincent et al., 2010)

# Video processing

- NMF use for video processing remains quite limited, despite its potential.
- Known works:
  - Video summarization (Cooper and Foote, 2002)
  - Dynamic video content representation and scene change detection (Bucak and Gunsel, 2007)
  - Onscreen person spotting and shot-type classification (Essid and Fevotte, 2012, 2013)
  - Fingerprinting (Cirakman et al., 2010)
  - Action recognition (Krausz and Bauckhage, 2010; Masurelle et al., 2014)
  - Compression (Türkan and Guillemot, 2011)

# Action recognition using depth silhouettes

Using NMF for feature learning (Masurelle et al., 2014)



Skeleton features	PCA	NMF
78%	89%	91%

## Recognition accuracies

- considering Kinect recordings of 8 actions;
- using Huawei/3DLife grand challenge dataset for action recognition.

# Video Structuring

Using NMF for temporal segmentation and soft-clustering (Essid and Fevotte, 2013)

Discovering the video editing structure (Essid and Fevotte, 2012)



Performing speaker diarization  
(Seichepine et al., 2013)

"Who spoke when?"



illustration by N. Seichepine

Using the **Canal9** political debates database (Vinciarelli et al., 2009).

► Introduction

► Principal Component Analysis (PCA)

- First look at the model
- General usages and applications
- Difficulties in NMF

► NMF models

► Algorithms for solving NMF

► Constrained NMF schemes

► Multi-stream and cross-modal NMF schemes

► Applications

# Model order choice

A suitable choice of  $K$  is very important

Model order  $K$  corresponds to the number of rank-1 matrices within the approximation

The choice of  $K$  results in a compromise between

## Data fitting

A greater  $K$  leads to a better data approximation

## Model complexity

A smaller  $K$  leads to a less complex model (easier to estimate, less parameters to transmit, etc ...)

A right **model order choice is important** and it depends on the data  $\mathbf{V}$  and on the application.

# NMF is ill-posed

The solution is not unique

Given  $\mathbf{V} = \mathbf{WH}$ ;  $\mathbf{W} \geq 0$ ,  $\mathbf{H} \geq 0$ ; any matrix  $\mathbf{Q}$  such that:

- $\mathbf{WQ} \geq 0$
- $\mathbf{Q}^{-1}\mathbf{H} \geq 0$

provides an alternative factorisation  $\mathbf{V} = \tilde{\mathbf{W}}\tilde{\mathbf{H}} = (\mathbf{WQ})(\mathbf{Q}^{-1}\mathbf{H})$ .

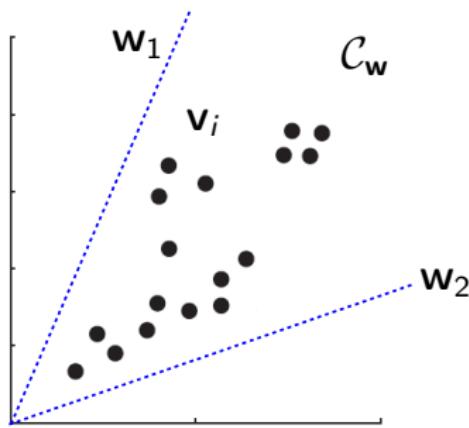
In particular,  $\mathbf{Q}$  can be any **nonnegative generalised permutation matrix**; e.g., in  $\mathbb{R}^3$ :

$$\mathbf{Q} = \begin{bmatrix} 0 & 0 & 2 \\ 0 & 3 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

This case is not so problematic: merely accounts for **scaling** and **permutation** of basis vectors  $\mathbf{w}_k$ .

## Geometric interpretation and ill-posedness

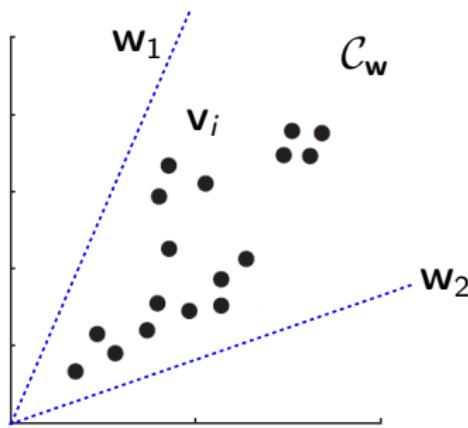
NMF assumes the data is well described by a **simplicial convex cone**  $\mathcal{C}_w$  generated by the columns of  $W$ :



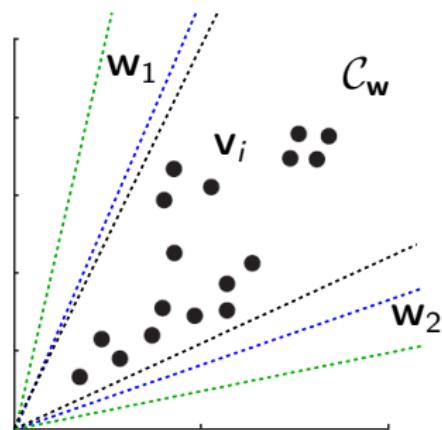
$$\mathcal{C}_w = \left\{ \sum_{k=1}^K \lambda_k w_k; \lambda_k \geq 0 \right\}$$

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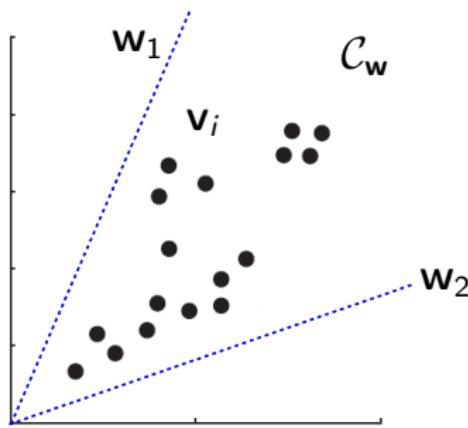
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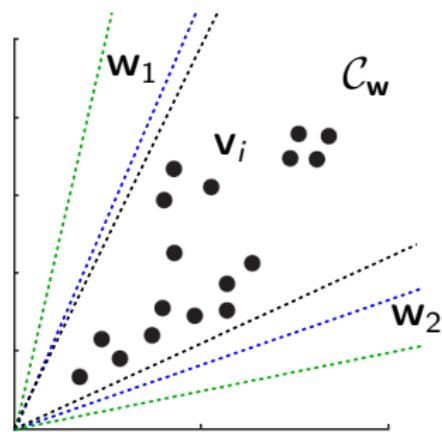
**Problem:** which  $\mathcal{C}_w$ ?

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$$\mathcal{C}_w = \left\{ \sum_{k=1}^K \lambda_k w_k; \lambda_k \geq 0 \right\}$$



**Problem:** which  $\mathcal{C}_w$ ?

- Need to impose **constraints** on the set of possible solutions to select the most “useful” ones.

# Constrained NMF methods

Different types of constraints have been considered in previous works:

- **Sparsity** constraints: either on  $\mathbf{W}$  or  $\mathbf{H}$  (e.g., Hoyer, 2004; Eggert and Korner, 2004);
- **Shape** constraints on  $\mathbf{w}_k$ , e.g.:
  - ▶ **convex NMF**:  $\mathbf{w}_k$  are convex combinations of inputs (Ding et al., 2010);
  - ▶ **harmonic NMF**:  $\mathbf{w}_k$  are mixtures of harmonic spectra (Vincent et al., 2008).
- **Spatial coherence** or **temporal** constraints on  $\mathbf{h}_k$ : activations are **smooth** (Virtanen, 2007; Jia and Qian, 2009; Essid and Fevotte, 2013);
- **Cross-modal correspondence** constraints: factorisations of related modalities are related, e.g., temporal activations are correlated (Seichepine et al., 2013; Liu et al., 2013; Yilmaz et al., 2011);
- **Geometric** constraints: e.g., select particular cones  $\mathcal{C}_{\mathbf{w}}$  (Klingenberg et al., 2009; Essid, 2012).

- ▶ Introduction
- ▶ Principal Component Analysis (PCA)
- ▶ NMF models
  - Cost functions
  - Weighted NMF schemes
- ▶ Algorithms for solving NMF
- ▶ Constrained NMF schemes
- ▶ Multi-stream and cross-modal NMF schemes
- ▶ Applications

## NMF optimization criteria

NMF approximation  $\mathbf{V} \approx \mathbf{WH}$  is usually obtained through:

$$\min_{\mathbf{W}, \mathbf{H} \geq 0} D(\mathbf{V} | \mathbf{WH}),$$

where  $D(\mathbf{V} | \hat{\mathbf{V}})$  is a *separable matrix divergence*:

$$D(\mathbf{V} | \hat{\mathbf{V}}) = \sum_{f=1}^F \sum_{n=1}^N d(v_{fn} | \hat{v}_{fn}),$$

and  $d(x|y)$  defined for all  $x, y \geq 0$  is a *scalar divergence* such that:

- $d(x|y)$  is continuous over  $x$  and  $y$ ;
- $d(x|y) \geq 0$  for all  $x, y \geq 0$ ;
- $d(x|y) = 0$  if and only if  $x = y$ .

## Popular (scalar) divergences

Euclidean (EUC) distance (Lee and Seung, 1999)

$$d_{EUC}(x, y) = (x - y)^2$$

Kullback-Leibler (KL) divergence (Lee and Seung, 1999)

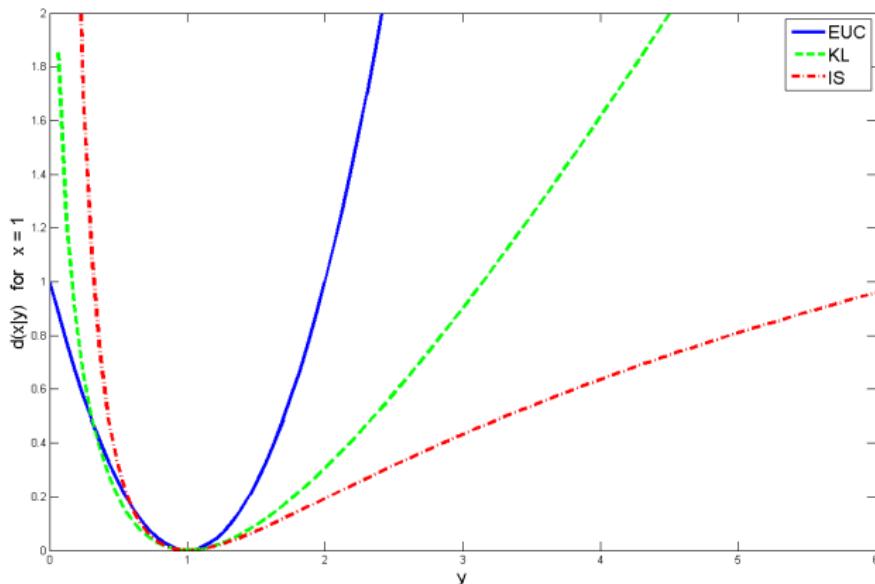
$$d_{KL}(x, y) = x \log \frac{x}{y} - x + y$$

Itakura-Saito (IS) divergence (Févotte et al., 2009)

$$d_{IS}(x, y) = \frac{x}{y} - \log \frac{x}{y} - 1$$

# Convexity properties

Divergence $d(x y)$	EUC	KL	IS
Convex on $x$	yes	yes	yes
Convex on $y$	yes	yes	<b>no</b>



## Scale invariance properties<sup>4</sup>

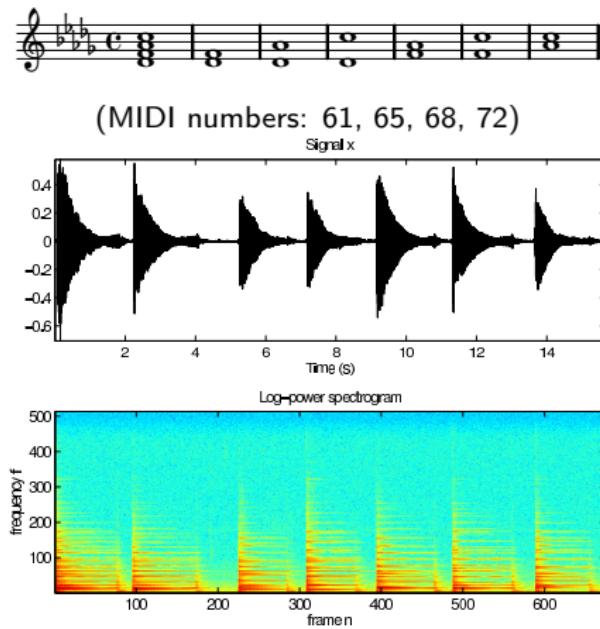
$$\begin{aligned} d_{EUC}(\lambda x | \lambda y) &= \lambda^2 d_{EUC}(x|y) \\ d_{KL}(\lambda x | \lambda y) &= \lambda d_{KL}(x|y) \\ d_{IS}(\lambda x | \lambda y) &= d_{IS}(x|y) \end{aligned}$$

The IS divergence is **scale-invariant** → it provides higher accuracy in the representation of data with large dynamic range, such as audio spectra.

<sup>4</sup>slide adapted from (Févotte, 2012).

# Music transcription demo

Demo slide courtesy of C. Févotte (Fevotte et al., 2009)

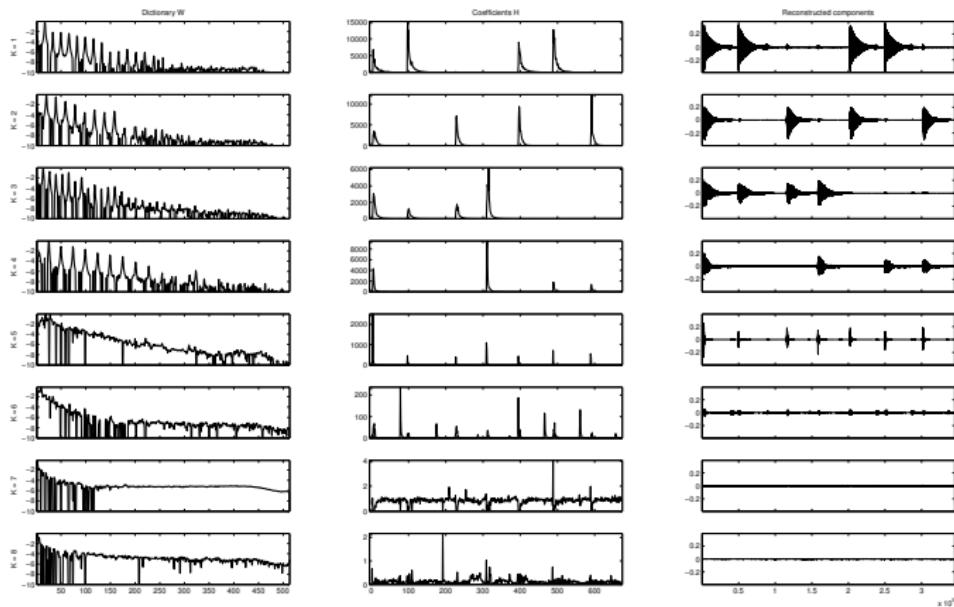


Three representations of the data.

# Music transcription demo

Demo slide courtesy of C. Févotte (Fevotte et al., 2009)

NMF decomposition with  $K = 8$



Pitch estimates:    65.0    68.0    61.0    72.0    0    0    0  
(True values: 61, 65, 68, 72)

# General parametric families of divergences

$\beta$ -divergence (Eguchi and Kano., 2001)

$$d_\beta(x|y) = \begin{cases} \frac{1}{\beta(\beta-1)} (x^\beta + (\beta-1)y^\beta - \beta x y^{\beta-1}) & \beta \in \mathbb{R} \setminus \{0, 1\} \\ x \log \frac{x}{y} - x + y & \beta = 1 \\ \frac{x}{y} - \log \frac{x}{y} - 1 & \beta = 0 \end{cases}$$

Generalizes IS ( $\beta = 0$ ), KL ( $\beta = 1$ ) divergences and EUC ( $\beta = 2$ ) distance.

# Which divergence to choose?

NMF divergence choice depends on the **data** and on the **application**.

One can choose the divergence as follows:

- by **intuition** or from some **prior knowledge of the application goal** (e.g., NMF is used for predicting the unseen data while minimizing the mean squared error  $\Rightarrow$  EUC distance) or **invariances** (e.g., scale invariance for music analysis with IS divergence) ;
- from some **probabilistic considerations** (presented in the upcoming section);
- **optimize the divergence** (e.g. from some parametric family) on some development data within a particular application.

# Statistical viewpoint

For many divergences a probabilistic formulation is possible: the **divergence minimization** becomes equivalent to a **maximum likelihood** criterion (Févotte et al., 2009; Cemgil, 2009b):

$$D(\mathbf{V}|\hat{\mathbf{V}}) = -\log p(\mathbf{V}|\hat{\mathbf{V}}) + \text{const}$$

Examples:

Divergence $D(\mathbf{V} \hat{\mathbf{V}})$	Probability distribution	p.d.f. $p(\mathbf{V} \hat{\mathbf{V}})$
EUC	$\sum_{f,n} (v_{fn} - \hat{v}_{fn})^2$	$v_{fn} \sim \text{Gaussian}(\hat{v}_{fn}, \sigma^2)$
KL	$\sum_{f,n} \left( v_{fn} \log \frac{v_{fn}}{\hat{v}_{fn}} - v_{fn} + \hat{v}_{fn} \right)$	$v_{fn} \sim \text{Poisson}(\hat{v}_{fn})$
IS	$\sum_{f,n} \left( \frac{v_{fn}}{\hat{v}_{fn}} - \log \frac{v_{fn}}{\hat{v}_{fn}} - 1 \right)$	$v_{fn} \sim \text{Exponential}\left(\frac{1}{\hat{v}_{fn}}\right)$

## Statistical viewpoint

Numerous advantages of a probabilistic NMF formulation:

- possibility of using efficient **probabilistic inference algorithms** such as the Expectation-Maximization (EM) algorithm (Févotte et al., 2009) and the Monte Carlo methods (Cemgil, 2009b; Schmidt et al., 2009);
- possibility of **introducing various constraints** into NMF modeling via prior distributions (Arngren et al., 2011);
- possibility of learning the NMF from **partially missing** (Roux et al., 2011) or **noisy** (Arberet et al., 2012) data;
- possibility of combining the NMF with **different probabilistic models** (Ozerov et al., 2012), e.g., the hidden Markov models (HMMs) (Ozerov et al., 2009).

- ▶ Introduction
- ▶ Principal Component Analysis (PCA)
- ▶ NMF models
- ▶ Algorithms for solving NMF
  - Preliminaries
  - Multiplicative update rules
  - Model order selection, initialization and stopping criteria
- ▶ Constrained NMF schemes
- ▶ Multi-stream and cross-modal NMF schemes
- ▶ Applications

# Optimization difficulties

An efficient solution of the NMF optimization problem

$$\min_{\mathbf{W}, \mathbf{H} \geq 0} D(\mathbf{V}|\mathbf{WH}) \Leftrightarrow \min_{\theta} C(\theta); \quad C(\theta) \stackrel{\text{def}}{=} D(\mathbf{V}|\mathbf{WH})$$

(where  $\theta \stackrel{\text{def}}{=} \{\mathbf{W}, \mathbf{H}\}$  denotes the NMF parameters) must cope with the following difficulties:

- the **nonnegativity constraints** must be taken into account;
- **no uniqueness** of the solution is guaranteed in general;
- the optimization problem has usually a **multitude of local and global minima**.

## Alternating optimization strategy

The problem is usually easier to optimize over one matrix (say  $\mathbf{H}$ ) given the other matrix (say  $\mathbf{W}$ ) is known and fixed.

Indeed, for several divergences  $D(\mathbf{V}|\mathbf{WH})$  is even convex separately w.r.t.  $\mathbf{H}$  and w.r.t.  $\mathbf{W}$ , but not w.r.t.  $\{\mathbf{W}, \mathbf{H}\}$ .

For this reason many state-of-the-art NMF optimization algorithms rely on the following iterative alternating optimization strategy.

Alternating optimization a.k.a block-coordinate descent (one iteration):

- update  $\mathbf{W}$ , given  $\mathbf{H}$  fixed,
- update  $\mathbf{H}$ , given  $\mathbf{W}$  fixed.

## Multiplicative update rules

A heuristic approach introduced by (Lee and Seung, 2001) to solve  $\min_{\theta} C(\theta)$

Multiplicative update (MU) rule for  $\mathbf{H}$  (similarly for  $\mathbf{W}$ ) is defined as:

$$h_{kn} \leftarrow h_{kn} [\nabla_{h_{kn}} C(\theta)]_- / [\nabla_{h_{kn}} C(\theta)]_+,$$

where

$$\nabla_{h_{kn}} C(\theta) = [\nabla_{h_{kn}} C(\theta)]_+ - [\nabla_{h_{kn}} C(\theta)]_-,$$

and the summands are both nonnegative.

**NOTE:** The nonnegativity of  $\mathbf{W}$  and  $\mathbf{H}$  is guaranteed by construction.

## MU rules for the $\beta$ -divergence

For example, in the case of the  $\beta$ -divergence (generalizing the three popular divergences) the following decomposition:

$$\nabla_y d_\beta(x|y) = \underbrace{y^{\beta-1}}_{[\nabla_y d_\beta(x|y)]_+} - \underbrace{xy^{\beta-2}}_{[\nabla_y d_\beta(x|y)]_-}$$

leads to the following MU rules (in matrix form) (Févotte et al., 2009):

MU rules for NMF with the  $\beta$ -divergence (one iteration):

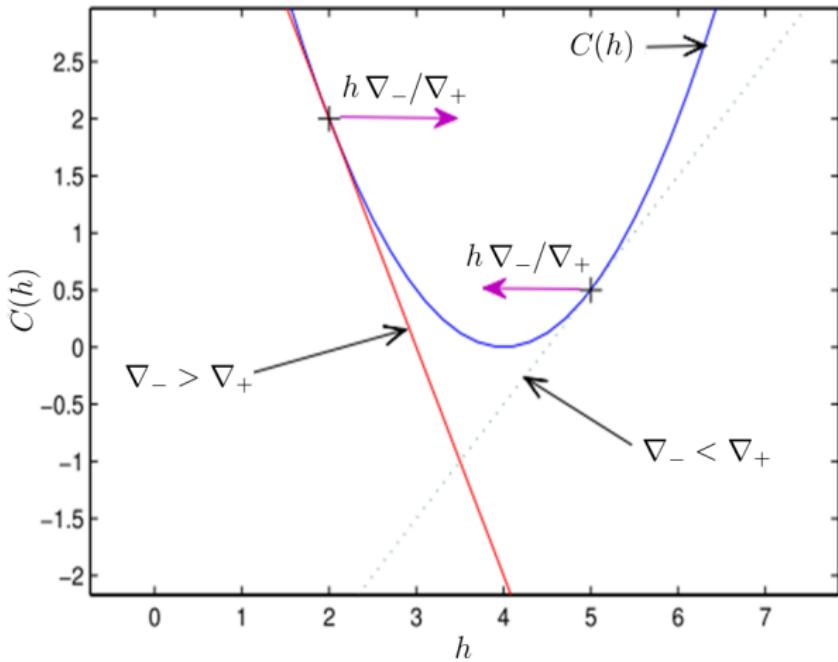
$$\mathbf{H} \leftarrow \mathbf{H} \odot \frac{\mathbf{W}^T \left( (\mathbf{W}\mathbf{H})^{[\beta-2]} \odot \mathbf{V} \right)}{\mathbf{W}^T (\mathbf{W}\mathbf{H})^{[\beta-1]}},$$

$$\mathbf{W} \leftarrow \mathbf{W} \odot \frac{\left( (\mathbf{W}\mathbf{H})^{[\beta-2]} \odot \mathbf{V} \right) \mathbf{H}^T}{(\mathbf{W}\mathbf{H})^{[\beta-1]} \mathbf{H}^T},$$

Re-normalize  $\mathbf{W}$  columns and  $\mathbf{H}$  rows to address scale-invariance (see Févotte et al. 2009).

## Intuitive explanation

We consider for simplicity  $\nabla_h C(h) = \nabla_+ - \nabla_-$



## Discussion

The only two things guaranteed by this approach:

- the newly updated value lies in the **direction of partial derivative decrease**;
- the newly updated value is **always nonnegative**.

Nothing more can be guaranteed in general, and all the other algorithm properties depend on the “**positive-negative**” decomposition chosen:

$$\nabla_{h_{kn}} C(\theta) = [\nabla_{h_{kn}} C(\theta)]_+ - [\nabla_{h_{kn}} C(\theta)]_- .$$

## Gradient descent viewpoint

Each MU rule can be interpreted as a **rescaled gradient descent** (Lee and Seung, 2001):

$$h_{kn} \leftarrow h_{kn} - \mu_{kn} \nabla_{h_{kn}} C(\theta),$$

where the step-size  $\mu_{kn}$  is defined as  $\mu_{kn} \stackrel{\Delta}{=} h_{kn} / [\nabla_{h_{kn}} C(\theta)]_+$ .

Though this re-formulation does not bring any new properties for the algorithm (e.g., the convergence).

## Majorisation-minimisation viewpoint

For many divergences and certain “positive-negative” decompositions each MU rule can be interpreted as a **Majorisation-Minimisation (MM)** procedure (Hunter and Lange, 2004):

To minimise  $C(s)$ , e.g.,  $s = w_{fk}$  or  $s = h_{kn}$ :

- build  $G(s|\tilde{s})$  such that  $G(s|\tilde{s}) \geq C(s)$  and  $G(\tilde{s}|\tilde{s}) = C(\tilde{s})$ ;
- optimize iteratively  $G(s|\tilde{s})$  instead of  $C(s)$ .

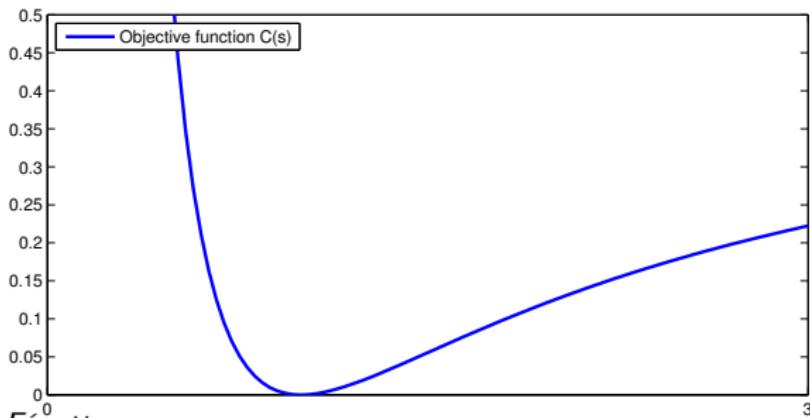


Illustration by C. Févotte

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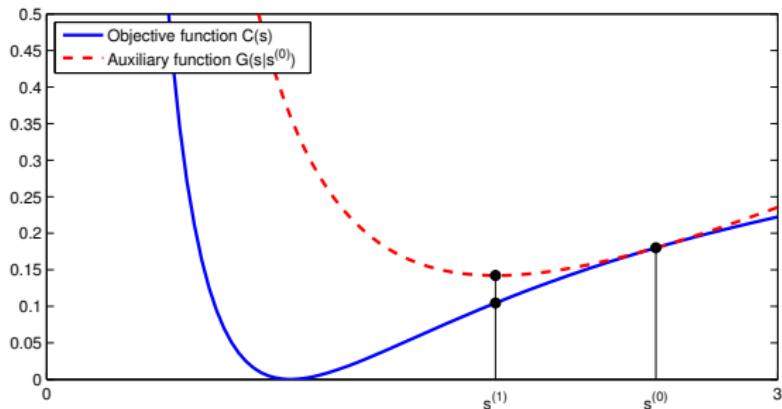


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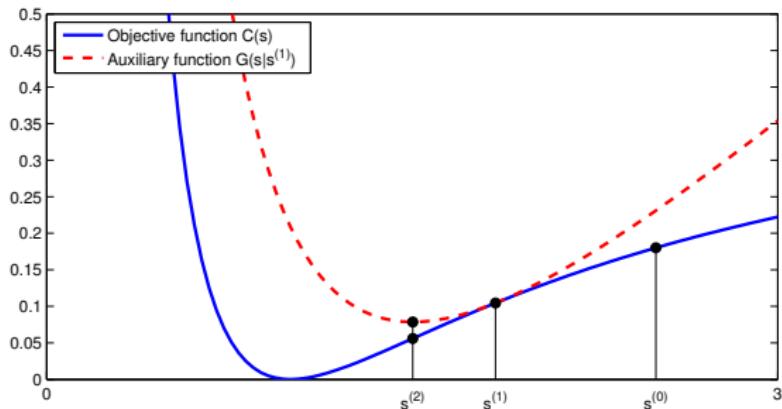


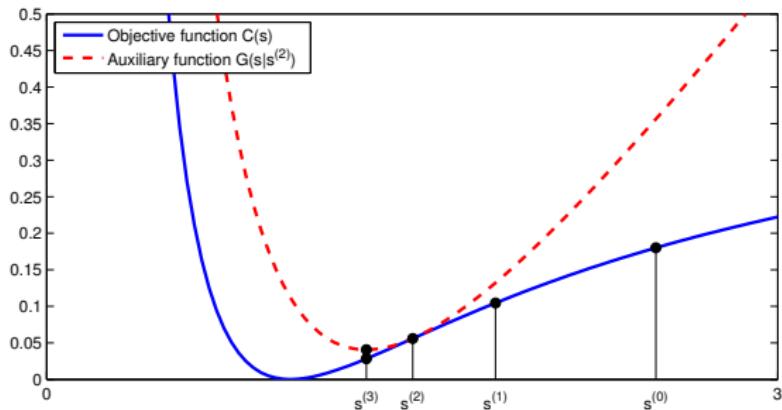
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*Illustration by C. Févotte*

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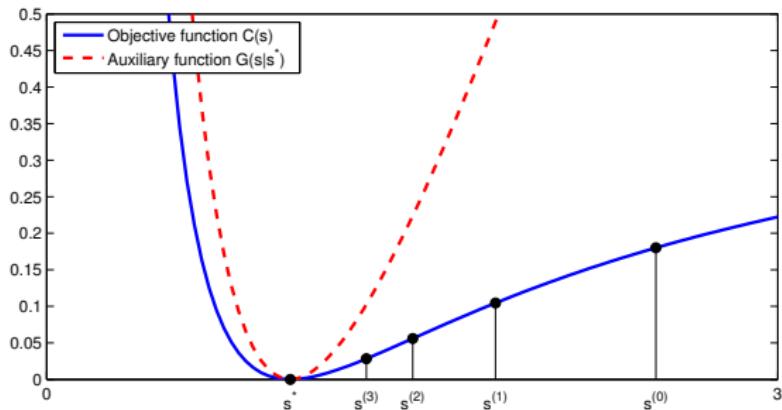


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- optimize iteratively  $G(s|\tilde{s})$  instead of  $C(s)$ .

► **NOTE:** The MM procedure guarantees the cost is non-increasing at each iteration:

$$C(s^{(t+1)}) \leq G(s^{(t+1)}|s^{(t)}) \leq G(s^{(t)}|s^{(t)}) = C(s^{(t)}).$$

# Convergence analysis

**Monotonicity** (“convergence” in terms of **non-increase** of the cost):

- is not guaranteed in general for MU rules;
- is proven (via the majorisation-minimisation formulation) for some divergences (e.g.,  $\beta$ -divergences) with particular “positive-negative” decompositions (see, e.g., Févotte and Idier 2010; Yang and Oja 2011).

**Local convergence in parameters** (whether the solution converges to a stationary point?)

- very few positive results for MU rules (see, e.g., Lin 2007a; Badeau et al. 2010);
- the main difficulty is due to non-uniqueness of the NMF.

# Summary

## Advantages:

- easy to implement;
- non-negativity of  $\mathbf{W}$  and  $\mathbf{H}$  is guaranteed.

## Drawbacks:

- monotonicity is not always guaranteed;
- among other algorithms the convergence rate is not the highest one.

## Other alternating optimization algorithms

**Gradient-like** algorithms (Lin, 2007b)

- **Advantages:** may “converge” faster than MU rules
- **Drawbacks:** nonnegativity constraints must be explicitly handled.

**Newton-like** algorithms (Zdunek and Cichocki, 2006)

- **Advantages:** “converge” faster than Gradient-like algos and MU rules
- **Drawbacks:** nonnegativity constraints must be explicitly handled; limited to convex divergences

**Expectation-maximization (EM)** algorithms (Févotte et al., 2009; Cemgil, 2009a)

- **Advantages:** nonnegativity constraints are implicitly handled; possibility of introducing other constraints via probabilistic priors
- **Drawbacks:** may “converge” slower than MU rules; limited to NMF with probabilistic formulation

# Online algorithms

Online algorithms to handle **continuous data streams** (Bucak and Gunsel, 2009; Simon and Vincent, 2012)

Online algorithms to handle **big data** (stochastic gradient-like) (Mairal et al., 2010)

# How to choose model order?

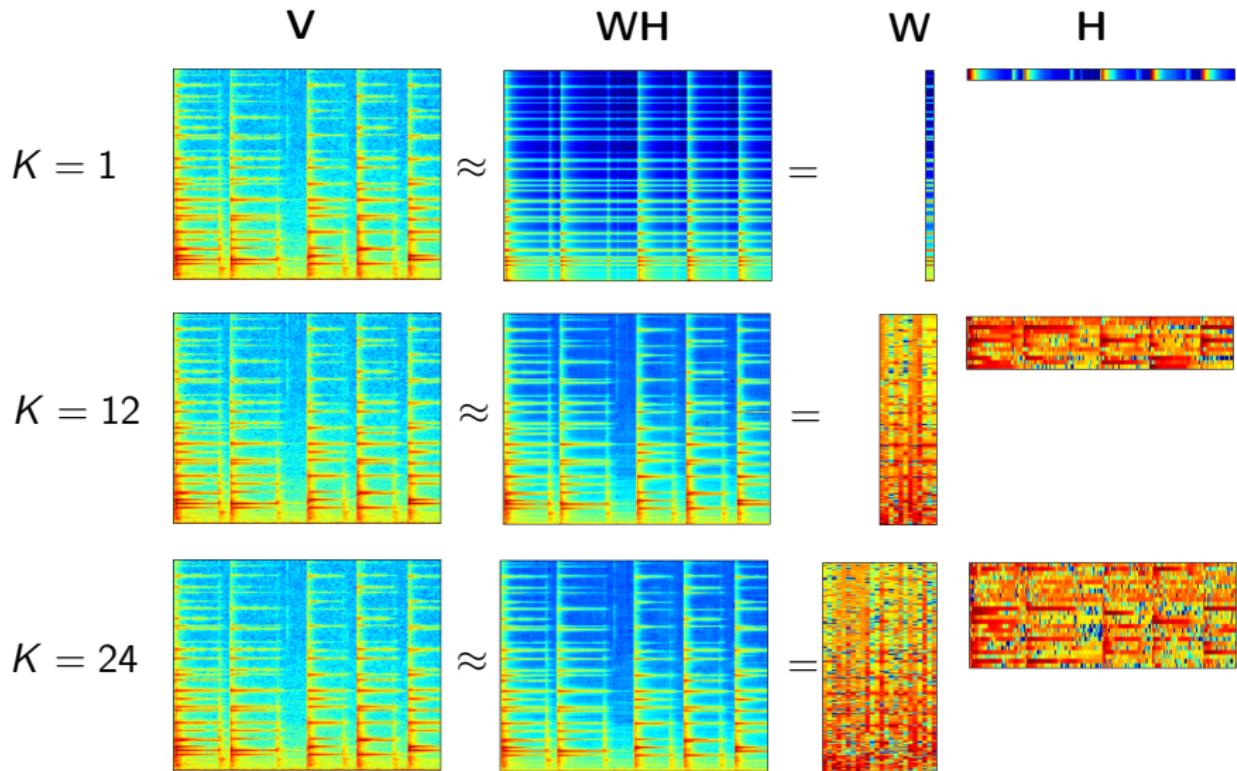
A right **model order choice is important** and it depends on the data  $\mathbf{V}$  and on the application.

The following strategies are usually used to set up an appropriate model order:

- **Model order  $K$  is fixed** during the NMF decomposition, and it was
  - either chosen by intuition,
  - either chosen based on some prior knowledge (e.g., known number of clusters for clustering),
  - or trained on some development data within a particular application.
- **Model order  $K$  is estimated automatically** within the NMF decomposition (Tan and Févotte, 2013; Schmidt and Morup, 2010).

# Model order choice

Illustration on audio data



# Initialization

A good **initialization** of parameters ( $\mathbf{W}$  and  $\mathbf{H}$ ) is **important for any local optimization** approach (including MU rules) due to the existence of many local minima.

## Random initializations:

- initialize (nonnegative) parameters **randomly several times**;
- keep the solution with the lowest final cost.

## Structural data-driven initializations:

- initialize  $\mathbf{W}$  by **clustering** of data points  $\mathbf{V}$  (Kim and Choi, 2007);
- initialize  $\mathbf{W}$  by **singular value decomposition (SVD)** of data points  $\mathbf{V}$  (Boutsidis and Galloopoulos, 2008);
- etc ...

# Stopping criteria

How many iterations?

For any iterative optimization strategy (including MU rules) **the total number of iterations is important** and results in a tradeoff between:

- the computational load from one side, and
- the data fitting (approximation error) and model quality from the other side.

**Stopping criteria** (Albright et al., 2006):

- after a **fixed number of iterations**;
- once the **approximation error** (the cost) is below a pre-defined **threshold**;
- once the **approximation error relative decrease** is below a pre-defined **threshold**;
- etc ...

# Take-home messages I

- NMF is a **versatile** data decomposition technique that has proven effective for **diverse applications** across **numerous disciplines**,
  - it tends to provide “meaningful” and “natural” **part-based** data representations,
  - it can be used both for feature learning, topic extraction, clustering, segmentation, source separation, coding...
- For NMF to be successful, it has to be estimated using **appropriate cost-functions** reflecting prior knowledge about the data.
- Being non-unique, NMF should **incorporate constraints** relating to the data, either though:
  - **regularized cost-functions** accounting for sparsity, shape, smoothness, cross-modal dependency constraints..., or
  - alternative formulations, e.g, **geometric** approaches having the potential to estimate **exact NMF** models.

## Take-home messages II

- Many algorithms are available to estimate NMF, mostly alternating updates of  $\mathbf{W}$  and  $\mathbf{H}$ ; variants include:
  - **multiplicative updates**: heuristic, simple and easy to implement, but slow and unstable,
  - **majorisation-minimisation**: well-founded for a variety of cost functions, stable, still slow,
  - **gradient-descent** and **Newton**: fast but unstable.
- NMF is a state-of-the-art technique for a number of audio-processing tasks (transcription, source separation...),
- it has a great potential for video (and RGB+depth) analysis tasks, especially temporal structure analysis.

# Ongoing and future research

- How to properly estimate the **model-order  $K$ ?**
- How to achieve **better** and faster “convergence”?
- How to perform **non-linear** data decompositions?
- How to handle **big data**?

# A selection of NMF software

Software	Language	Main features
beta_ntf	Python	Weighted tensor decomposition, all $\beta$ -divergences, MM
sklearn.decomposition.NMF	Python	$\ell_2$ -norm, gradient-descent, sparsity
IMM DTU NMF toolbox	Matlab	$\ell_2$ -norm, MM, gradient-descent, ALS
Févotte's matlab scripts	Matlab	$\ell_2$ -norm, KL and IS-div, MM, probabilistic
Seichepine's matlab scripts	Matlab	Soft <b>co-factorisation</b> , $\ell_2$ -norm, KL and IS-div, $\ell_1/\ell_2$ -norm <b>temporal smoothing</b> , MM
svmnmf	Matlab	Geometric SVM-based NMF, <b>kernel</b> -based non-linear decompositions, fast
libNMF	C	$\ell_2$ -norm, MM, gradient-descent, ALS, multi-core, fast

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