Source Separation

for under-determined sound mixtures

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Material taken with permission from slides of Nicholas Bryan and Dennis Sun

Analysis of Sound Mixture

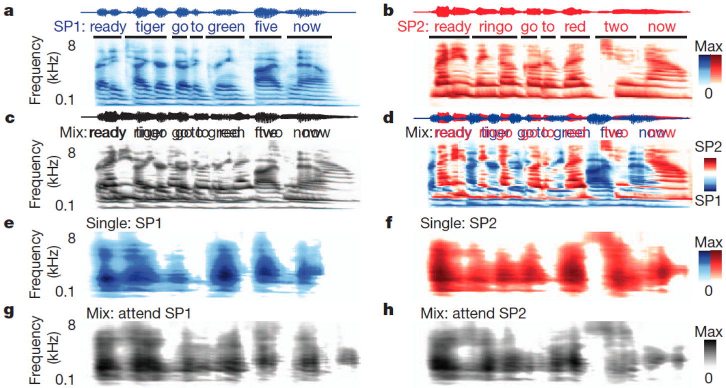
We aim at performing

- Computational Auditory Scene Analysis
- Humans focus on one source

Tasks:

- Source separation ?
- Source classification ?
- Something in-between ?

Human separate sounds, really ?

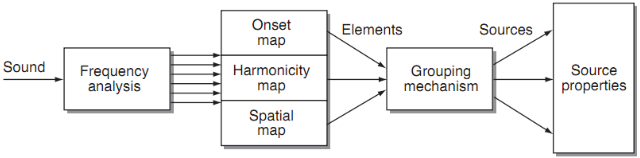


Mesgarani, N., & Chang, E. F. Selective cortical representation of attended speaker in multi-talker speech perception Nature

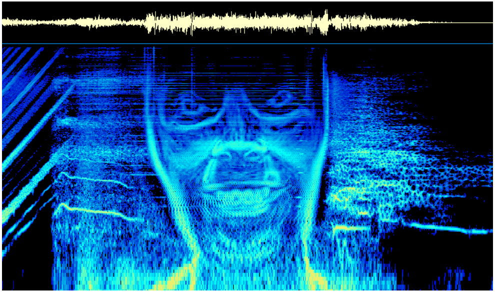
Computational Auditory Scene Analysis (CASA)

- How do people analyze sound mixtures ?
- break mixture into small elements (in time-freq)
- elements are grouped in to sources using cues
- sources have aggregate attributes

Computational Auditory Scene Analysis (CASA)



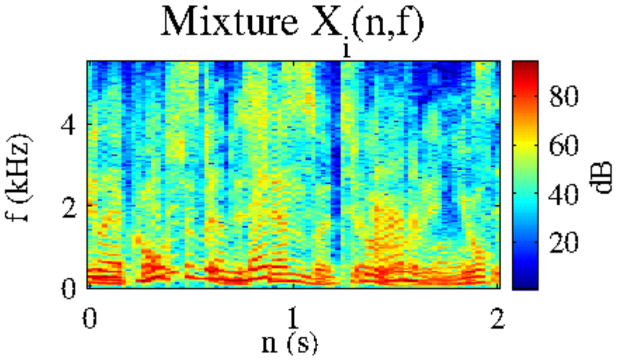
Frequency Analysis



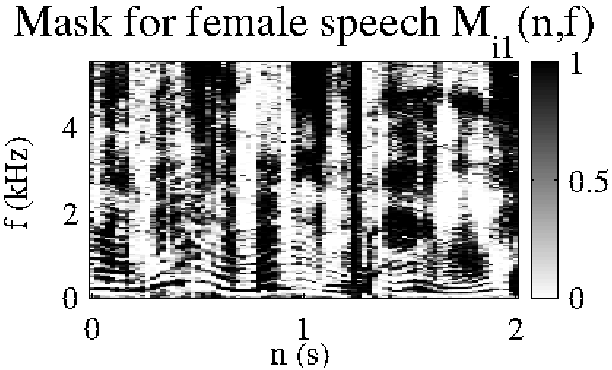
Grouping by masking

- Formulate the source separation problem as a masking one in the time / frequency domain
- Goal: find a mask M that retrieves one source when used to filter a given time-frequency representation.
- $$\hat{\mathbf{S}}_n(r,k) = \mathbf{M}_{mn}(r,k) \circ \mathbf{X}_m(r,k)$$
- Keep the phase of the mixture

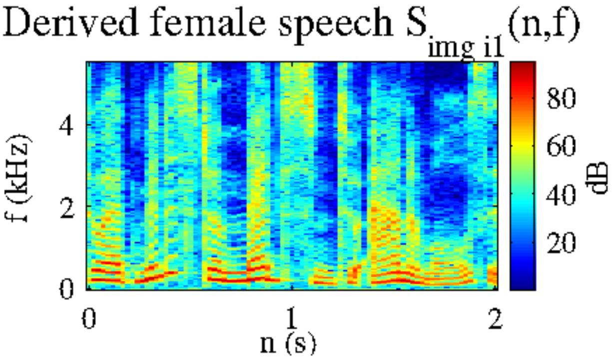
Grouping by masking



Grouping by masking



Grouping by masking



The Ideal Binary Mask (IBM)

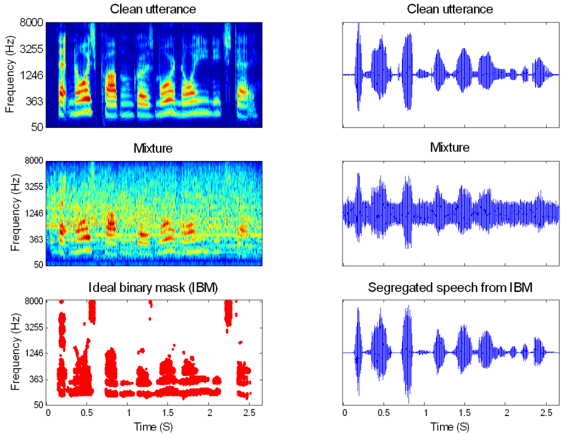
The IBM is an "oracle" separation method, that is we know something (everything ?) we need for separating the sources. It provides

- An upper bound for masking based approaches
- A way to understand issues with the front end
- like Time/frequency resolution tradeoff and phase issues

The Ideal Binary Mask (IBM)

- Utterance: "That noise problem grows more annoying each day"
- Interference: Crowd noise with music (0 SNR)

The Ideal Binary Mask (IBM)

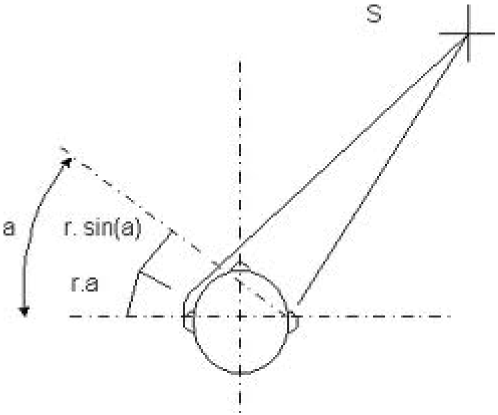


Binaural Cues

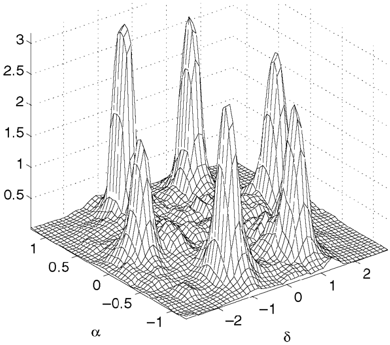
Stereo recording have spatial location cues

- Termed Interchannel or Interaural
- Encoded as Phase and Intensity Differences: IPD and IID
- Warning: professionally mastered audio does not preserve them.

Binaural Cues



DUET (Degenerate Unmixing Estimation Technique)



- Histogram of IPD and IID
- Binary Mask created by selecting bins around histogram peaks.

Yilmaz and Rickard Blind Separation of Speech Mixtures via Time-Frequency Masking IEEE Trans. on Signal Processing 2004

Human-assisted time-frequency masking

- Human-assisted selection of the time-frequency bins out of the DUET- like histogram for creating the unmixing mask
- Implementation as a VST plugin: the Audio Scanner

M.Vinyes, J. Bonada and A. Loscos. Demixing Commercial Music Productions via Human-Assisted Time-Frequency Masking. 120th AES convention, Paris, France, 2006.

Matrix Factorization

- Decompose a matrix as a product of two or more matrices

$$\mathbf{A} = \mathbf{B}\,\mathbf{C} \qquad\qquad \mathbf{A} \approx \mathbf{B}\,\mathbf{C}$$

$$\mathbf{D} = \mathbf{E}\,\mathbf{F}\,\mathbf{G} \qquad\qquad \mathbf{D} \approx \mathbf{E}\,\mathbf{F}\,\mathbf{G}$$

- Matrices have special properties depending on factorization
- Example factorizations:
  - Singular Value Decomposition (SVD)
  - Eigenvalue Decomposition
  - QR Decomposition (QR)
  - Lower Upper Decomposition (LU)
  - Non-Negative Matrix Factorization

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Non-Negative Matrix Factorization

$$\begin{array}{ccc} \text{Data} & & \text{Basis Vectors} \quad \text{Weights} \\ \left[\quad \mathbf{V} \quad \right] & \approx & \left[\ \mathbf{W} \ \right] \left[\quad \mathbf{H} \quad \right] \end{array}$$

- A matrix factorization where everything is non-negative
- $\mathbf{V} \in \mathrm{R}_{+}^{F \times T}$ - original non-negative data
- $\mathbf{W} \in \mathrm{R}_{+}^{F \times K}$ - matrix of basis vectors, dictionary elements
- $\mathbf{H} \in \mathrm{R}_{+}^{K \times T}$ - matrix of activations, weights, or gains
- $K < F < T$ (typically)
  - A compressed representation of the data
  - A low-rank approximation to $\mathbf{V}$

Non-Negative Matrix Factorization

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Interpretation of $\mathbf{V}$

$$\overset{\text{Data}}{\begin{bmatrix} & & \mathbf{V} & & \end{bmatrix}} \approx \overset{\text{Basis Vectors}}{\begin{bmatrix} & \mathbf{W} & \end{bmatrix}} \overset{\text{Weights}}{\begin{bmatrix} & & \mathbf{H} & & \end{bmatrix}}$$

- $\mathbf{V} \in \mathrm{R}_{+}^{F \times T}$ - original non-negative data
  - Each column is an F-dimensional data sample
  - Each row represents a data feature
  - We will use audio spectrogram data as $\mathbf{V}$

Interpretation of $\mathbf{W}$

$$
\begin{array}{ccccc}
\text{Data} & & \text{Basis Vectors} & \text{Weights} \\
\left[\quad \mathbf{V} \quad\right] & \approx & \left[\ \mathbf{W}\ \right] & \left[\quad \mathbf{H} \quad\right]
\end{array}
$$

- $\mathbf{W} \in \mathrm{R}_{+}^{F \times K}$ - matrix of basis vectors, dictionary elements
  - A single column is referred to as a basis vector
  - Not orthonormal, but commonly normalized to one

Interpretation of $\mathbf{H}$

$$\begin{array}{ccccc} \text{Data} & & \text{Basis Vectors} & \text{Weights} \\ \left[\quad\quad \mathbf{V} \quad\quad \right] & \approx & \left[\quad \mathbf{W} \quad \right] & \left[\quad\quad \mathbf{H} \quad\quad \right] \end{array}$$

- $\mathbf{H} \in \mathrm{R}_{+}^{K \times T}$ - matrix of activations, weights, or gains
  - A row represents the gain of corresponding basis vector
  - Not orthonormal, but commonly normalized to one

NMF With Spectrogram Data

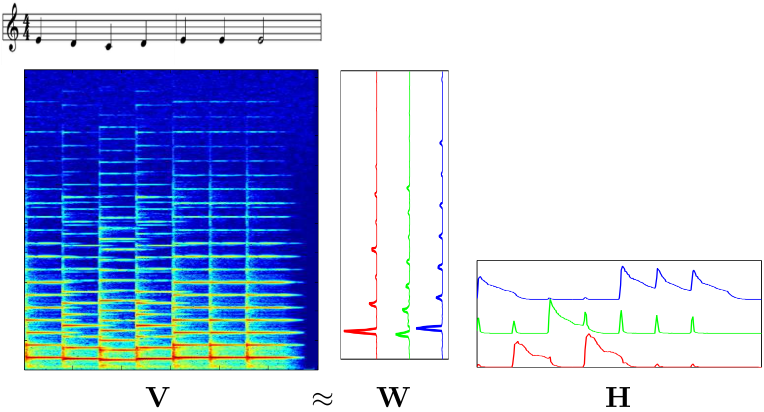


Figure : NMF of *Mary Had a Little Lamb* with $K = 3$

- The basis vectors capture prototypical spectra [SB03]
- The weights capture the gain of the basis vectors

NMF With Spectrogram Data

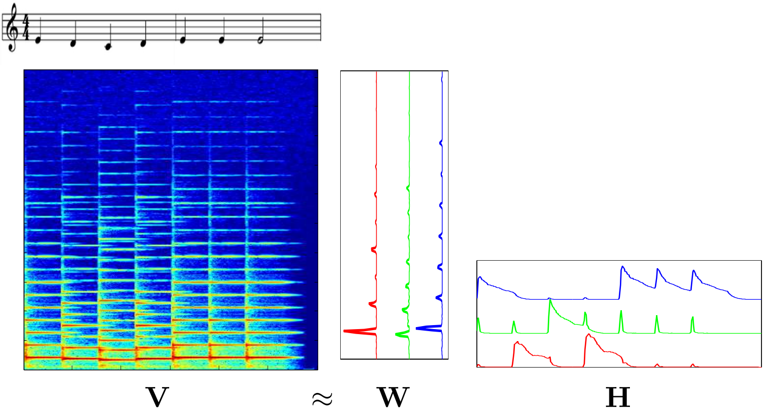
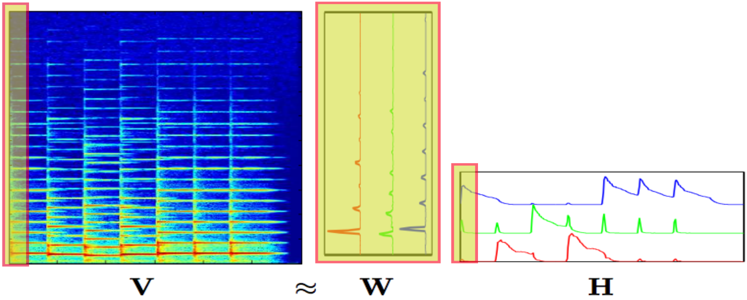


Figure : NMF of *Mary Had a Little Lamb* with $K = 3$ play stop

- The basis vectors capture prototypical spectra [SB03]
- The weights capture the gain of the basis vectors

Factorization Interpretation I

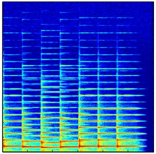
Columns of $\mathbf{V}$ $\approx$ as a weighted sum (mixture) of basis vectors



$$\begin{bmatrix} | & | & & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_T \\ | & | & & | \end{bmatrix} \approx \begin{bmatrix} \sum_{j=1}^{K} \mathbf{H}_{j1}\,\mathbf{w}_j & \sum_{j=1}^{K} \mathbf{H}_{j2}\,\mathbf{w}_j & \dots & \sum_{j=1}^{K} \mathbf{H}_{jT}\,\mathbf{w}_j \end{bmatrix}$$

Factorization Interpretation II

$\mathbf{V}$ is approximated as sum of matrix "layers"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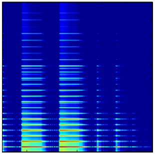
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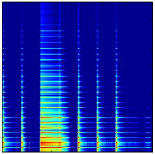
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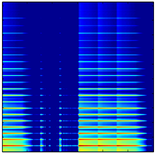

$$\begin{bmatrix} | & | & & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_T \\ | & | & & | \end{bmatrix} \approx \begin{bmatrix} | & | & & | \\ \mathbf{w}_1 & \mathbf{w}_2 & \dots & \mathbf{w}_K \\ | & | & & | \end{bmatrix} \begin{bmatrix} — & \mathbf{h}_1^{\mathrm{T}} & — \\ — & \mathbf{h}_2^{\mathrm{T}} & — \\ & \vdots & \\ — & \mathbf{h}_K^{\mathrm{T}} & — \end{bmatrix}$$

$$\mathbf{V} \approx \mathbf{w}_1\,\mathbf{h}_1^{\mathrm{T}} + \mathbf{w}_2\,\mathbf{h}_2^{\mathrm{T}} + \ldots + \mathbf{w}_K\,\mathbf{h}_K^{\mathrm{T}}$$

Questions

- How do we use $\mathbf{W}$ and $\mathbf{H}$ to perform separation?
- How do we solve for $\mathbf{W}$ and $\mathbf{H}$, given a known $\mathbf{V}$?

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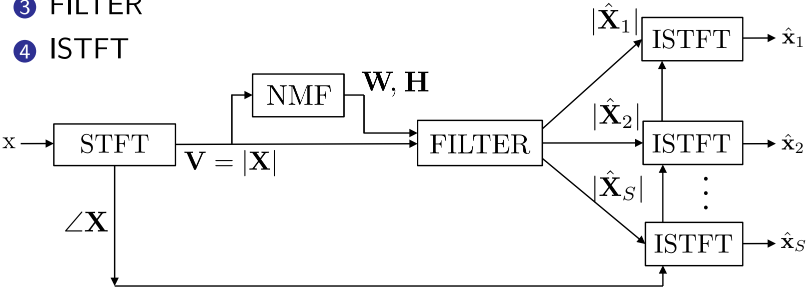
General Separation Pipeline

1. STFT
2. NMF
3. FILTER
4. ISTFT



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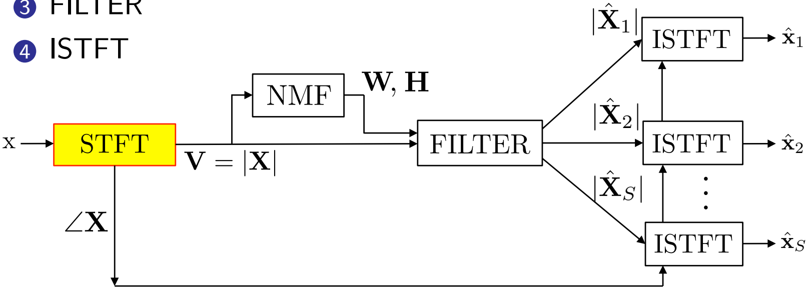
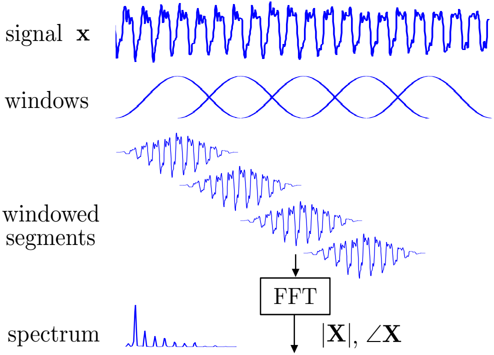


Short-Time Fourier Transform (STFT)



- Inputs time domain signal $\mathbf{x}$
- Outputs magnitude $|\,\mathbf{X}\,|$ and phase $\angle\,\mathbf{X}$ matrices

Short-Time Fourier Transform (STFT)

$$X_m(\omega_k) \quad = \quad e^{-j\omega_k mR} \sum_{n=-N/2}^{N/2-1} x(n+mR)w(n)e^{-j\omega_k n}$$

$$\begin{aligned}
x(n) &= \text{input signal at time } n \\
w(n) &= \text{length } M \text{ window function (e.g. Hann, etc.)} \\
N &= \text{DFT size, in samples} \\
R &= \text{hop size, in samples, between successive DFT} \\
M &= \text{window size, in samples} \\
w_k &= 2\pi k/N,\ k = 0, 1, 2, \ldots, N-1
\end{aligned}$$

- Choose window, window size, DFT size, and hop size
- Must maintain constant overlap-add COLA(R) [Smi11]

General Separation Pipeline

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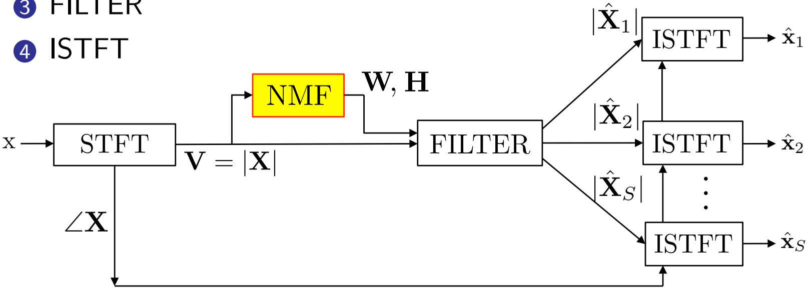

Non-Negative Matrix Factorization

- Inputs $|\,\mathbf{X}\,|$, outputs $\mathbf{W}$ and $\mathbf{H}$
- Algorithm to be discussed

General Separation Pipeline

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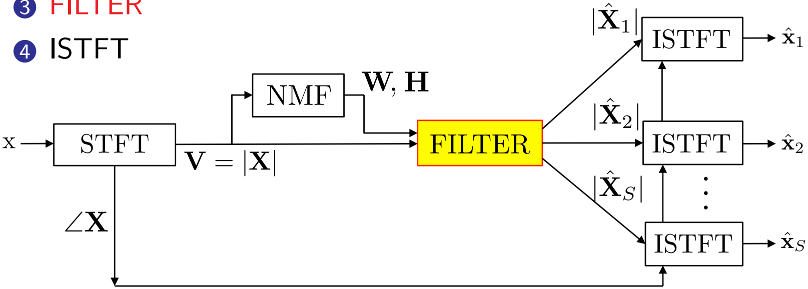
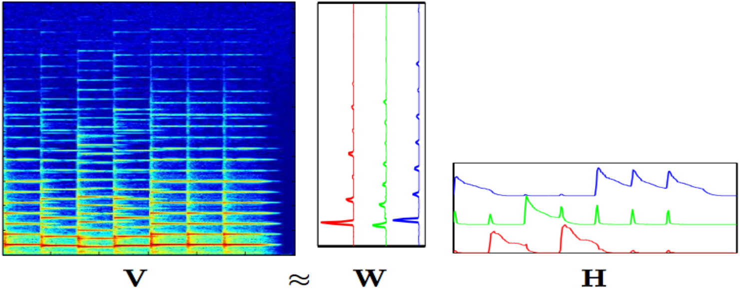


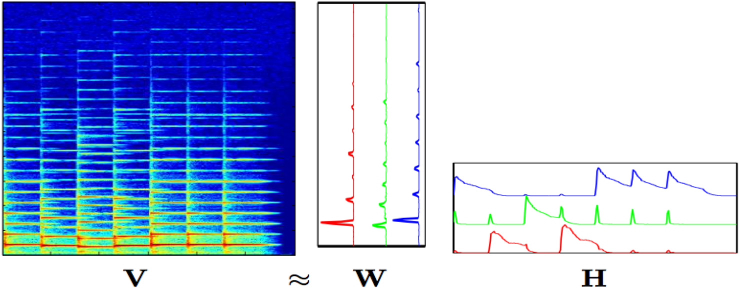
Source Synthesis I



- Choose a subset of basis vectors $\mathbf{W}_s$ and activations $\mathbf{H}_s$ to reconstruct source s
- Estimate the source s magnitude:

$$|\hat{\mathbf{X}}_s| = \mathbf{W}_s \mathbf{H}_s = \sum_{i \in s} (\mathbf{w}_i \mathbf{h}_i^T)$$

Source Synthesis I



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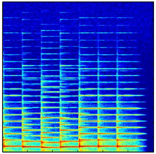
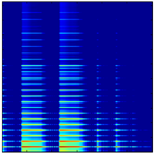
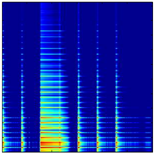
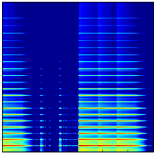
Source Synthesis II

Example 1: “D” pitches as a single source

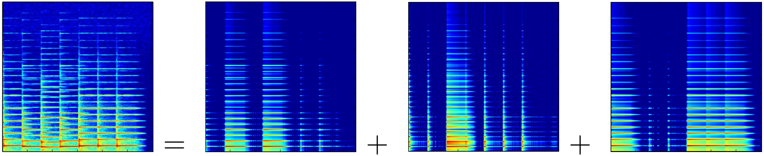
 $=$  $+$  $+$ 

$$\mathbf{V} \approx \color{red}{\mathbf{w}_1\, \mathbf{h}_1^{\mathrm{T}}} + \mathbf{w}_2\, \mathbf{h}_2^{\mathrm{T}} + \mathbf{w}_3\, \mathbf{h}_3^{\mathrm{T}}$$

- $|\hat{\mathbf{X}}_s| \approx \mathbf{w}_1\, \mathbf{h}_1^{\mathrm{T}}$
- Use one basis vector to reconstruct a source

Source Synthesis III

Example 2: "D" and "E" pitches as a source



$$\mathbf{V} \approx \color{red}{\mathbf{w}_1\,\mathbf{h}_1^{\mathrm{T}} + \mathbf{w}_2\,\mathbf{h}_2^{\mathrm{T}}} + \mathbf{w}_3\,\mathbf{h}_3^{\mathrm{T}}$$

- $|\hat{\mathbf{X}}_s| \approx \mathbf{w}_1\,\mathbf{h}_1^{\mathrm{T}} + \mathbf{w}_2\,\mathbf{h}_2^{\mathrm{T}}$
- Use two (or more) basis vector to reconstruct a source

Source Filtering I

Alternatively, we can estimate $|\hat{\mathbf{X}}_s|$ by filtering $|\,\mathbf{X}\,|$ via:

1. Generate a filter $\mathbf{M}_s,\ \forall s$

$$\mathbf{M}_s = \frac{(\mathbf{W}_s\,\mathbf{H}_s)^\alpha}{\sum_{i=1}^{K}(\mathbf{W}_i\,\mathbf{H}_i)^\alpha} = \frac{|\hat{\mathbf{X}}_s|^\alpha}{\sum_{i=1}^{K}|\hat{\mathbf{X}}_i|^\alpha} = \frac{\sum_{i\in s}(\mathbf{w}_i\,\mathbf{h}_i^{\mathrm{T}})^\alpha}{\sum_{i=1}^{K}(\mathbf{w}_i\,\mathbf{h}_i^{\mathrm{T}})^\alpha}$$

   where $\alpha \in \mathrm{R}_+$ is typically set to one or two.

2. Estimate the source s magnitude $|\,\mathbf{X}_s\,|$

$$|\hat{\mathbf{X}}_s| = \mathbf{M}_s \odot |\,\mathbf{X}\,|$$

   where $\odot$ is an element-wise multiplication

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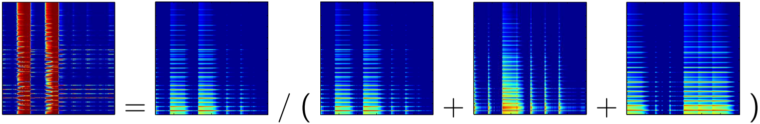
   where $\odot$ is an element-wise multiplication

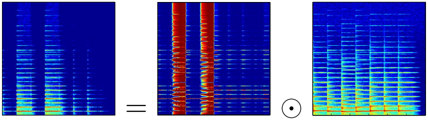
Source Filtering II

Example: Choose "D" pitches as a single source w/one basis vector

1. Compute filter $\mathbf{M}_s = \dfrac{\mathbf{w}_1\, \mathbf{h}_1^{\mathrm{T}}}{\sum_{i=1}^{K} \mathbf{w}_i\, \mathbf{h}_i^{\mathrm{T}}}$, with $\alpha = 1$



2. Multiply with $|\hat{\mathbf{X}}_s| = \mathbf{M}_s \odot |\,\mathbf{X}\,|$



Source Filtering III

- The filter $\mathbf{M}$ is referred to as a *masking filter* or *soft mask*
- Tends to perform better than the reconstruction method
- Similar to Wiener filtering discussed in Talk 1

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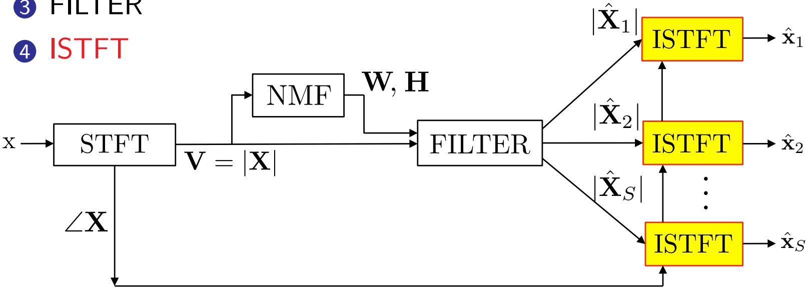
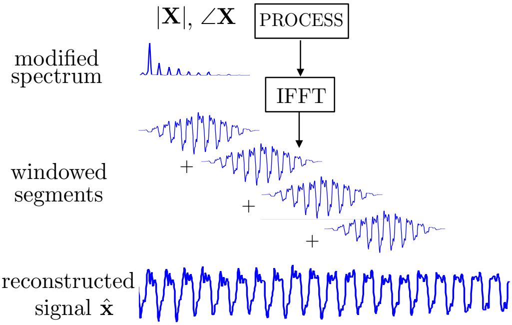


Inverse Short-Time Fourier Transform (ISTFT)



- Inputs $|\mathbf{X}|$ and phase $\angle\mathbf{X}$ matrices
- Outputs time domain signal $\mathbf{x}$

General Separation Pipeline

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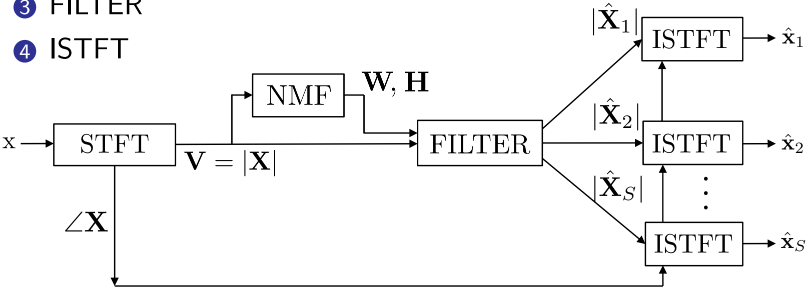

Algorithms for NMF

- Question: How do we solve for $\mathbf{W}$ and $\mathbf{H}$, given a known $\mathbf{V}$?
- Answer: Frame as optimization problem

$$\underset{\mathbf{W},\mathbf{H}\geq 0}{\text{minimize}} \quad D(\mathbf{V} \,||\, \mathbf{W}\,\mathbf{H})$$

where D is a measure of "divergence".

Algorithms for NMF

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where D is a measure of "divergence".

Algorithms for NMF

Some choices for D:

- **Euclidean**: $D(\mathbf{V}\,||\hat{\mathbf{V}}) = \sum_{i,j} (\mathbf{V}_{ij} - \hat{\mathbf{V}}_{ij})^2$
- **Kullback-Leibler**:
  $$D(\mathbf{V}\,||\hat{\mathbf{V}}) = \sum_{i,j} \left(\mathbf{V}_{ij} \log \frac{\mathbf{V}_{ij}}{\hat{\mathbf{V}}_{ij}} - \mathbf{V}_{ij} + \hat{\mathbf{V}}_{ij} \right)$$

We will focus on KL divergence in today's lecture.

Algorithms for NMF

Some choices for D:

- **Euclidean**: $D(\mathbf{V}\,||\hat{\mathbf{V}}) = \sum_{i,j}(\mathbf{V}_{ij} - \hat{\mathbf{V}}_{ij})^2$
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Tricks of the trade for minimizing a function $f(\mathbf{x})$.

- closed-form solutions: solve $\nabla f(\mathbf{x}) = 0$.
- gradient descent: iteratively move in steepest descent dir.

$$\mathbf{x}^{(\ell+1)} \leftarrow \mathbf{x}^{(\ell)} - \eta \nabla f(\mathbf{x}^{(\ell)}).$$

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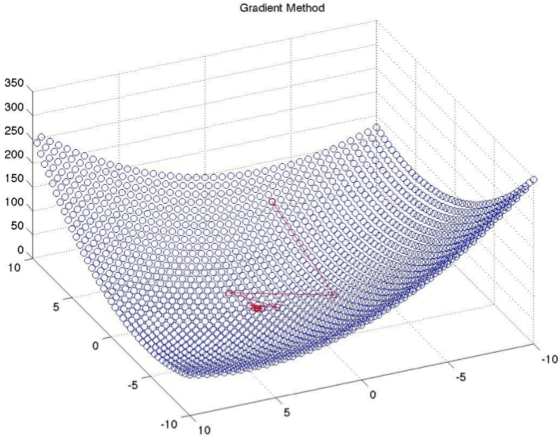
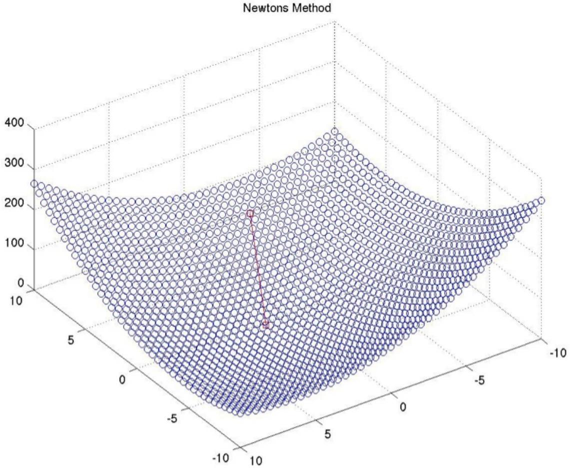
Gradient Descent



Newton's Method



Meta Algorithms

Coordinate descent

- Instead of minimizing $f(\mathbf{x})$, minimize $f(\mathbf{x}_i; \mathbf{x}_{-i}^{(\ell)})$ and cycle over i.
- Useful when $f(\mathbf{x}_i; \mathbf{x}_{-i}^{(\ell)})$ can be minimized in closed form.

Majorization-minimization

1. Find a majorizing function g for f at current iterate $\mathbf{x}^{(\ell)}$.
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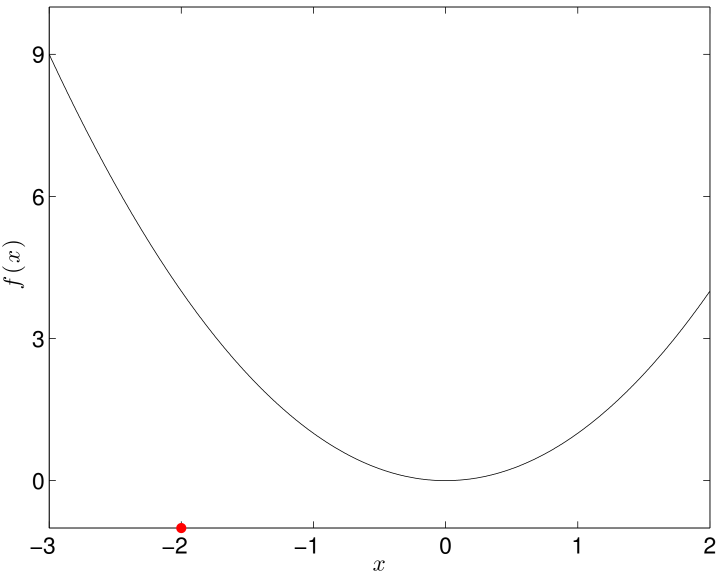

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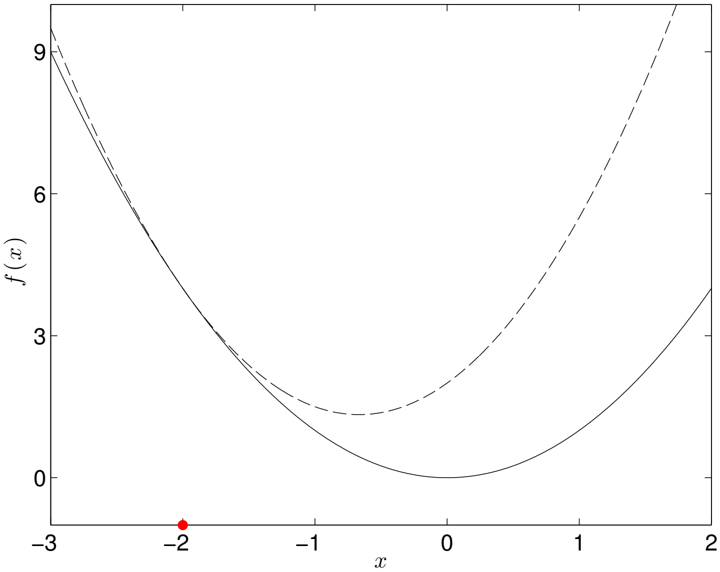

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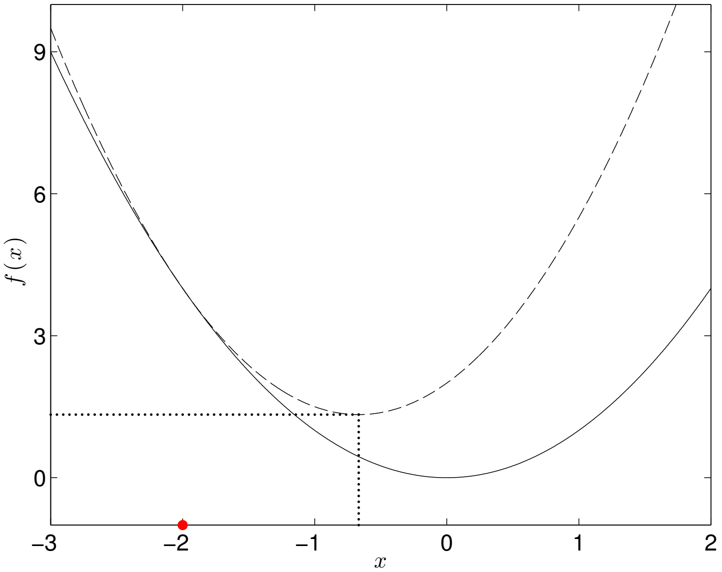

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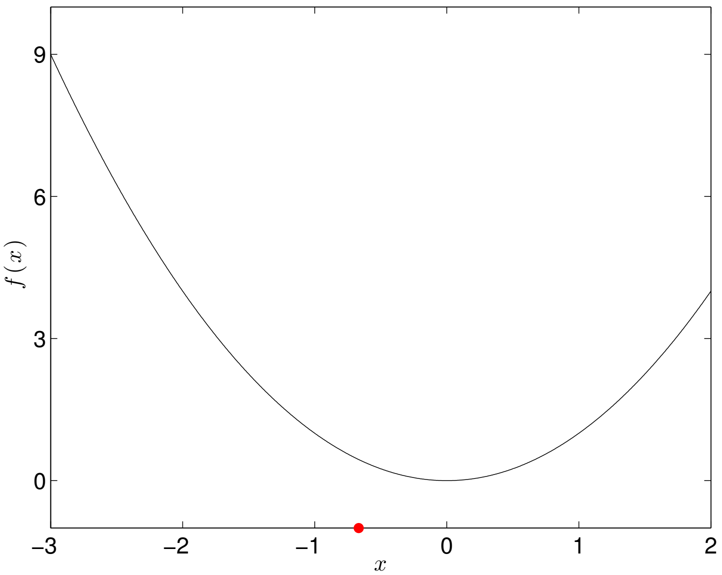

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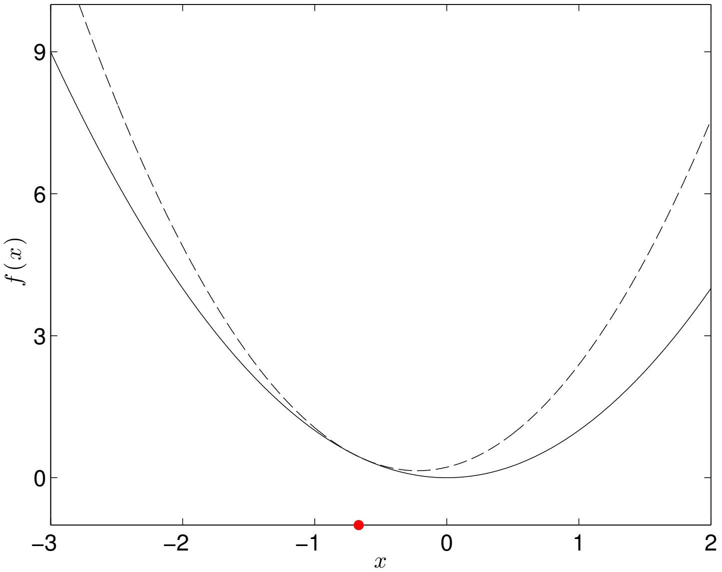

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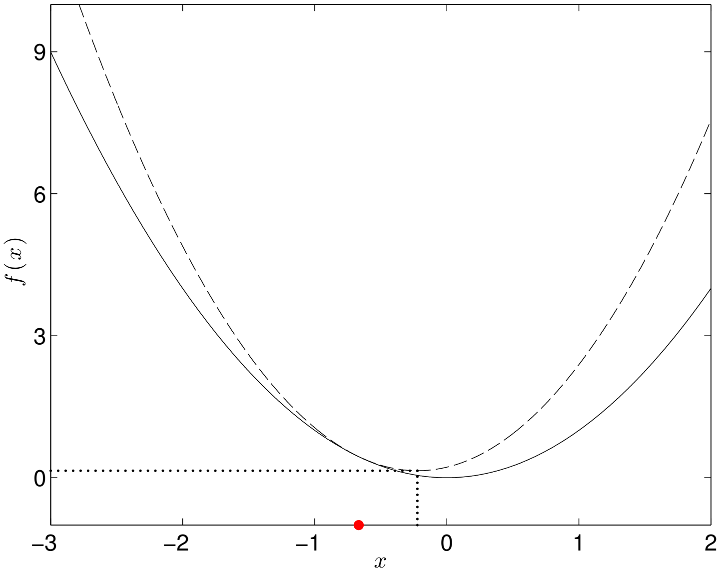

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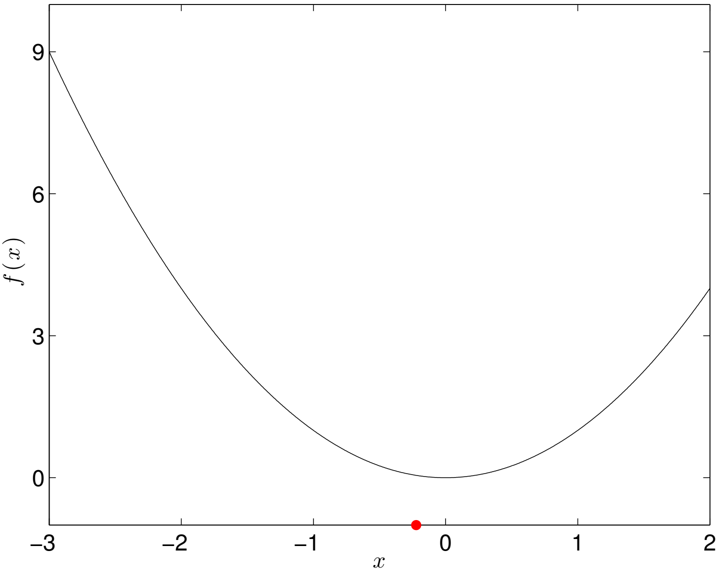

Algorithms for NMF

To minimize

$$D(\mathbf{V} \,||\, \mathbf{W}\,\mathbf{H}) = \sum_{i,j} \left(\mathbf{V}_{ij} \log \frac{\mathbf{V}_{ij}}{(\mathbf{W}\,\mathbf{H})_{ij}} - \mathbf{V}_{ij} + (\mathbf{W}\,\mathbf{H})_{ij} \right)$$

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we use **(block) coordinate descent**: optimize $\mathbf{H}$ for $\mathbf{W}$ fixed, then optimize $\mathbf{W}$ for $\mathbf{H}$ fixed (rinse and repeat).

Can we optimize this in closed form?

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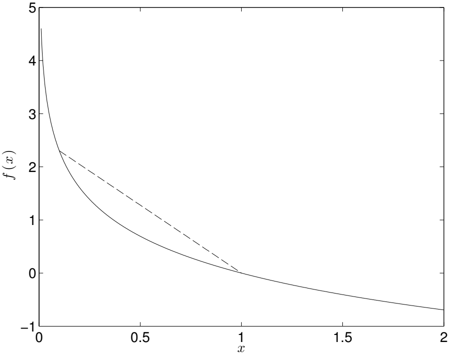
Not quite, so let's try to majorize the function. A useful tool is **Jensen's inequality**, which says that for **convex** functions f:

$$f(\text{average}) \leq \text{average of } f$$



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To apply Jensen's inequality, we introduce weights $\sum_k \pi_{ijk} = 1$.

$$= \sum_{i,j} \left(-\mathbf{V}_{ij} \log \sum_k \pi_{ijk} \frac{\mathbf{W}_{ik}\,\mathbf{H}_{kj}}{\pi_{ijk}} + \sum_k \mathbf{W}_{ik}\,\mathbf{H}_{kj} \right)$$
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Now this function *can* be minimized exactly!

$$\mathbf{H}^*_{kj} = \frac{\sum_i \mathbf{V}_{ij}\,\pi_{ijk}}{\sum_i \mathbf{W}_{ik}}$$

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If we substitute $\pi_{ijk} = \frac{\mathbf{W}_{ik}\,\mathbf{H}^{(\ell)}_{kj}}{\sum_k \mathbf{W}_{ik}\,\mathbf{H}^{(\ell)}_{kj}}$, we obtain the updates:

$$\mathbf{H}^{(\ell+1)}_{kj} \leftarrow \frac{\sum_i \mathbf{V}_{ij}\,\frac{\mathbf{W}_{ik}\,\mathbf{H}^{(\ell)}_{kj}}{\sum_k \mathbf{W}_{ik}\,\mathbf{H}^{(\ell)}_{kj}}}{\sum_i \mathbf{W}_{ik}}$$

$$= \mathbf{H}^{(\ell)}_{kj} \cdot \frac{\sum_i \left(\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}^{(\ell)}}\right)_{ij} \mathbf{W}_{ik}}{\sum_i \mathbf{W}_{ik}}$$

These are **multiplicative updates**. In matrix form:

$$\mathbf{H}^{(\ell+1)} \leftarrow \mathbf{H}^{(\ell)} \,.\!*\, \frac{\mathbf{W}^T\,\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}^{(\ell)}}}{\mathbf{W}^T\,\mathbf{1}}$$

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$$\mathbf{H}^{(\ell+1)} \leftarrow \mathbf{H}^{(\ell)} .* \frac{\mathbf{W}^T \, \frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}^{(\ell)}}}{\mathbf{W}^T\,\mathbf{1}}$$

Algorithms for NMF

If we substitute $\pi_{ijk} = \frac{\mathbf{W}_{ik}\,\mathbf{H}_{kj}^{(\ell)}}{\sum_k \mathbf{W}_{ik}\,\mathbf{H}_{kj}^{(\ell)}}$, we obtain the updates:

$$
\begin{aligned}
\mathbf{H}_{kj}^{(\ell+1)} &\leftarrow \frac{\sum_i \mathbf{V}_{ij}\,\frac{\mathbf{W}_{ik}\,\mathbf{H}_{kj}^{(\ell)}}{\sum_k \mathbf{W}_{ik}\,\mathbf{H}_{kj}^{(\ell)}}}{\sum_i \mathbf{W}_{ik}} \\
&= \mathbf{H}_{kj}^{(\ell)} \cdot \frac{\sum_i \left(\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}^{(\ell)}}\right)_{ij} \mathbf{W}_{ik}}{\sum_i \mathbf{W}_{ik}}
\end{aligned}
$$

These are **multiplicative updates**. In matrix form:

$$
\mathbf{H}^{(\ell+1)} \leftarrow \mathbf{H}^{(\ell)} \;.\!* \frac{\mathbf{W}^T\,\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}^{(\ell)}}}{\mathbf{W}^T\,\mathbf{1}}
$$

Algorithms for NMF

Using $D(\mathbf{V} \,||\, \mathbf{W}\,\mathbf{H}) = D(\mathbf{V}^T \,||\, \mathbf{H}^T\,\mathbf{W}^T)$, we obtain a similar update for $\mathbf{W}$.

Now we just iterate between:

1. Updating $\mathbf{W}$.
2. Updating $\mathbf{H}$.
3. Checking $D(\mathbf{V} \,||\, \mathbf{W}\,\mathbf{H})$. If the change since the last iteration is small, then declare convergence.

The algorithm is summarized below:

Algorithm KL-NMF

---

initialize $\mathbf{W}, \mathbf{H}$

repeat

$$\mathbf{H} \leftarrow \mathbf{H} \,.\!* \frac{\mathbf{W}^T \, \frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}}}{\mathbf{W}^T \, \mathbf{1}}$$

$$\mathbf{W} \leftarrow \mathbf{W} \,.\!* \frac{\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}} \, \mathbf{H}^T}{\mathbf{1}\,\mathbf{H}^T}$$

until convergence **return** $\mathbf{W}, \mathbf{H}$

Algorithms for NMF

Using $D(\mathbf{V} \,||\, \mathbf{W}\,\mathbf{H}) = D(\mathbf{V}^T \,||\, \mathbf{H}^T\,\mathbf{W}^T)$, we obtain a similar update for $\mathbf{W}$.

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The algorithm is summarized below:

Algorithm KL-NMF

initialize $\mathbf{W}, \mathbf{H}$

repeat

$$\mathbf{H} \leftarrow \mathbf{H} \,.\!*\, \frac{\mathbf{W}^T \frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}}}{\mathbf{W}^T\,\mathbf{1}}$$

$$\mathbf{W} \leftarrow \mathbf{W} \,.\!*\, \frac{\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}}\,\mathbf{H}^T}{\mathbf{1}\,\mathbf{H}^T}$$

until convergence **return** $\mathbf{W}, \mathbf{H}$

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until convergence **return** $\mathbf{W}, \mathbf{H}$

Algorithms for NMF

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The algorithm is summarized below:

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$$\mathbf{W} \leftarrow \mathbf{W} \,.\!* \frac{\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}}\,\mathbf{H}^T}{\mathbf{1}\,\mathbf{H}^T}$$

until convergence **return** $\mathbf{W}, \mathbf{H}$

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The algorithm is summarized below:

Algorithm KL-NMF

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$$\mathbf{W} \leftarrow \mathbf{W} \,.\!* \frac{\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}}\,\mathbf{H}^T}{\mathbf{1}\,\mathbf{H}^T}$$

until convergence **return** $\mathbf{W}, \mathbf{H}$

Algorithms for NMF

Using $D(\mathbf{V} \,||\, \mathbf{W}\,\mathbf{H}) = D(\mathbf{V}^T \,||\, \mathbf{H}^T\,\mathbf{W}^T)$, we obtain a similar update for $\mathbf{W}$.

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The algorithm is summarized below:

Algorithm KL-NMF

initialize $\mathbf{W}, \mathbf{H}$

repeat

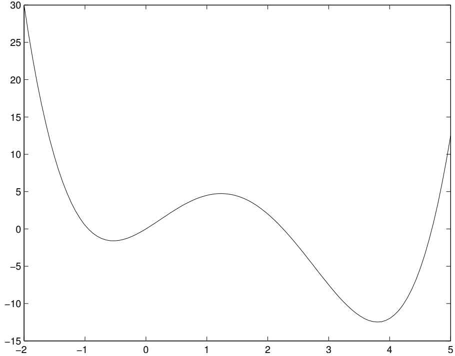
$$\mathbf{H} \leftarrow \mathbf{H} \, .^* \frac{\mathbf{W}^T \, \frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}}}{\mathbf{W}^T\,\mathbf{1}}$$

$$\mathbf{W} \leftarrow \mathbf{W} \, .^* \frac{\frac{\mathbf{V}}{\mathbf{W}\,\mathbf{H}}\,\mathbf{H}^T}{\mathbf{1}\,\mathbf{H}^T}$$

until convergence **return** $\mathbf{W}, \mathbf{H}$

Caveats

- The NMF problem is **non-convex**.



- The algorithm is only guaranteed to find a local optimum.
- The algorithm is sensitive to choice of initialization.

References I

- Jacob Benesty, Jingdong Chen, and Yiteng Huang, *Microphone array signal processing*, Springer, 2008.
- C. Févotte, N. Bertin, and J.-L. Durrieu, *Nonnegative matrix factorization with the itakura-saito divergence: With application to music analysis*, Neural Computation **21** (2009), no. 3, 793–830.
- C. Févotte and J. Idier, *Algorithms for nonnegative matrix factorization with the β-divergence*, Neural Computation **23** (2011), no. 9, 2421–2456.
- A. Hyvärinen and E. Oja, *Independent component analysis: algorithms and applications*, Neural Netw. **13** (2000), no. 4-5, 411–430.
- D. D. Lee and H. S. Seung, *Algorithms for non-negative matrix factorization*, Advances in Neural Information Processing Systems (NIPS), MIT Press, 2001, pp. 556–562.

References II

- P. Smaragdis and J.C. Brown, *Non-negative matrix factorization for polyphonic music transcription*, IEEE Workshop on Applications of Signal Processing to Audio and Acoustics (WASPAA), oct. 2003, pp. 177 – 180.
- J. O. Smith, *Spectral audio signal processing*, `http://ccrma.stanford.edu/~jos/sasp/`, 2011, online book.
- Avery Li-chun Wang, *Instantaneous and frequency-warped signal processing techniques for auditory source separation*, Ph.D. thesis, Stanford University, 1994.
- DeLiang Wang and Guy J. Brown, *Computational auditory scene analysis: Principles, algorithms, and applications*, Wiley-IEEE Press, 2006.