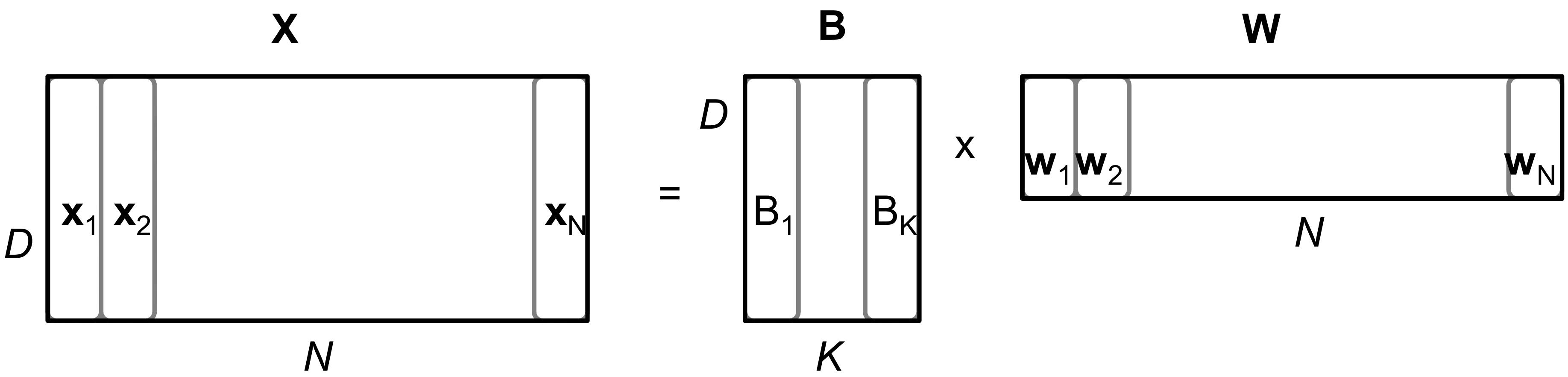
Machine Learning for Signal Processing

Non-negative Matrix Factorization

Instructor: Bhiksha Raj

With examples and slides from Paris Smaragdis

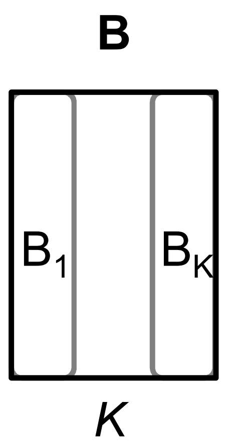
A Quick Recap

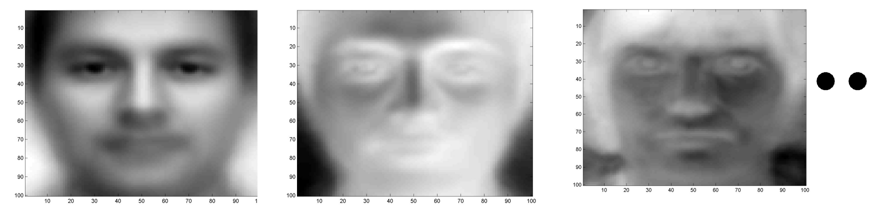


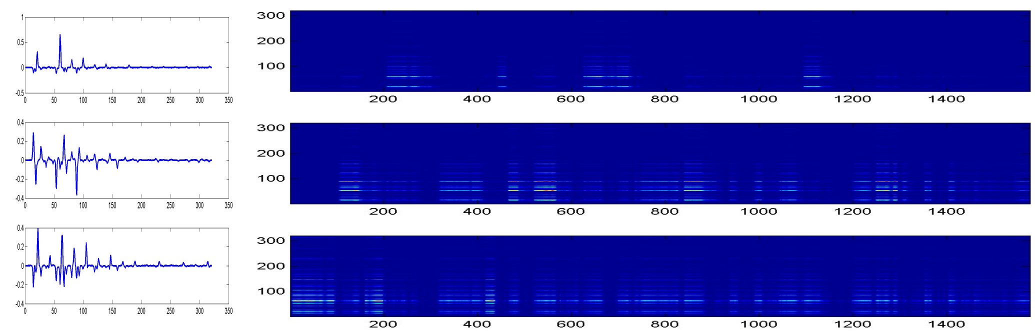
$$\boldsymbol{x}_i = \boldsymbol{B}\boldsymbol{w}_i \quad \Rightarrow \quad \boldsymbol{x}_i = w_{11}B_1 + \cdots + w_{1K}B_K$$

- **Problem:** Given a collection of data $\boldsymbol{X}$, find a set of "bases" $\boldsymbol{B}$, such that each vector $x_{\boldsymbol{i}}$ can be expressed as a weighted combination of the bases

A Quick Recap: Subproblem 1

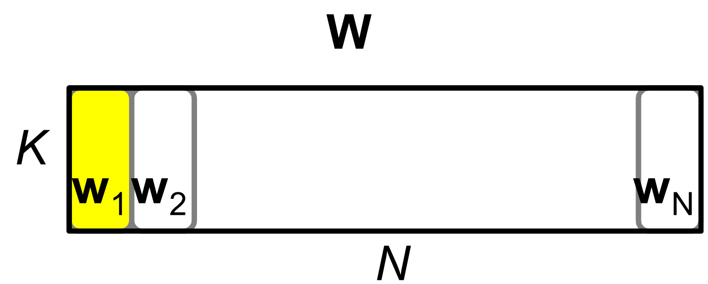


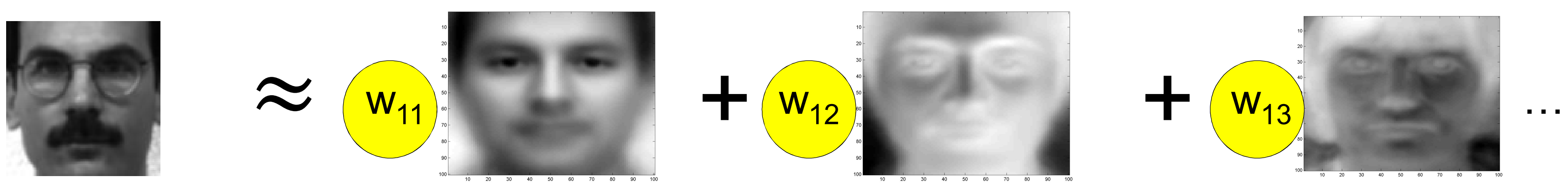




- **Problem 1:** Finding bases
  - – Finding typical faces
  - – Finding "notes" like structures

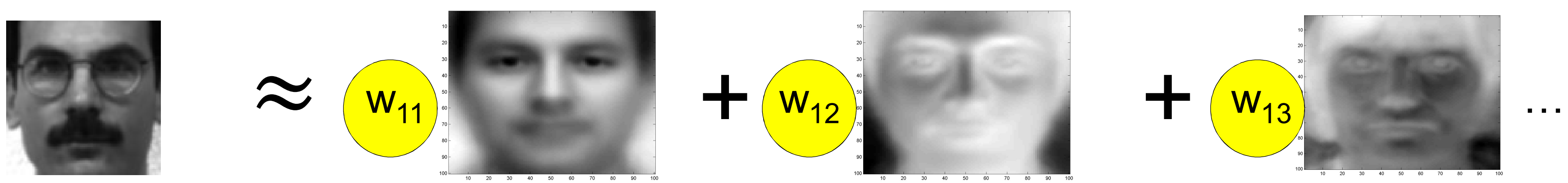
A Quick Recap: Subproblem 2





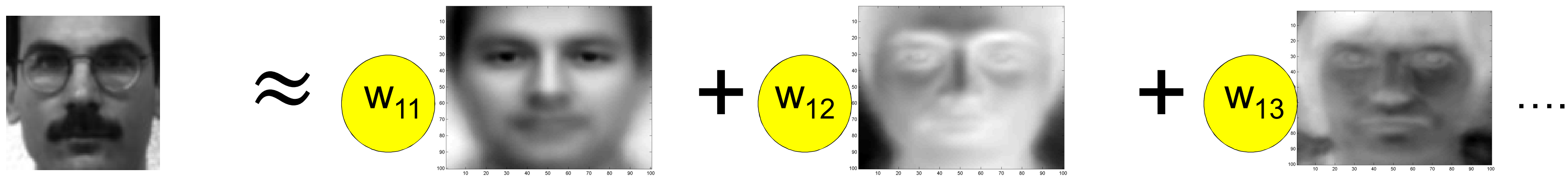
- **Problem 2:** Expressing instances in terms of these bases
  - Finding weights of typical faces
  - Finding weights of notes

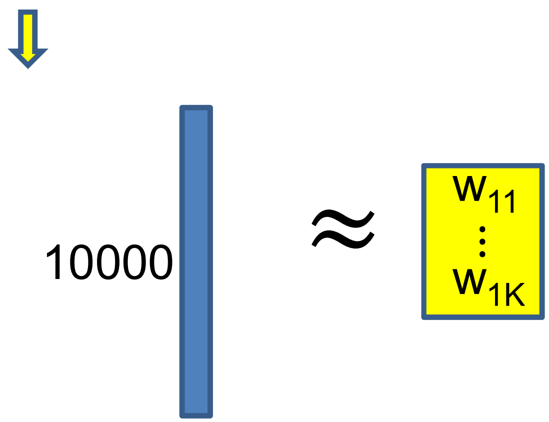
A Quick Recap: WHY? 1.

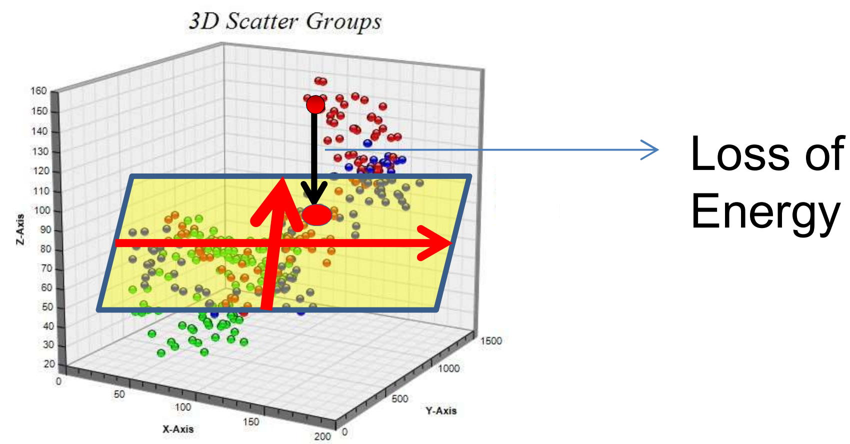


- ***Better Representation***: The weights $\{w_{ij}\}$ represent the vectors in a *meaningful* way
  - Better suited to semantically motivated operation
  - Better suited for specific statistical models

A Quick Recap: WHY? 2.

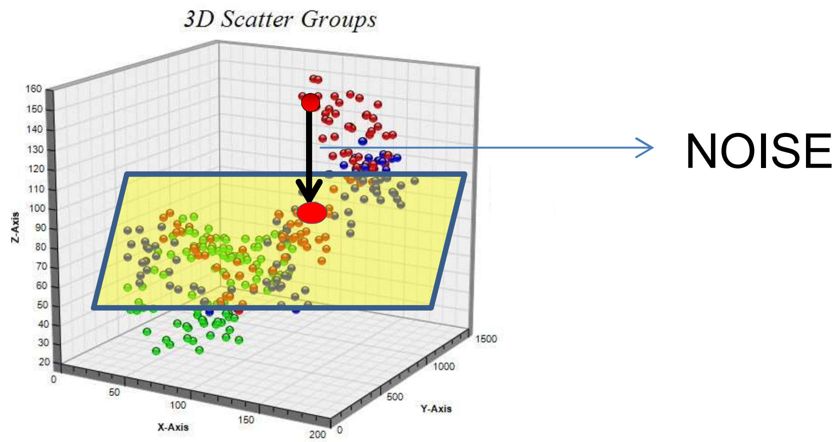






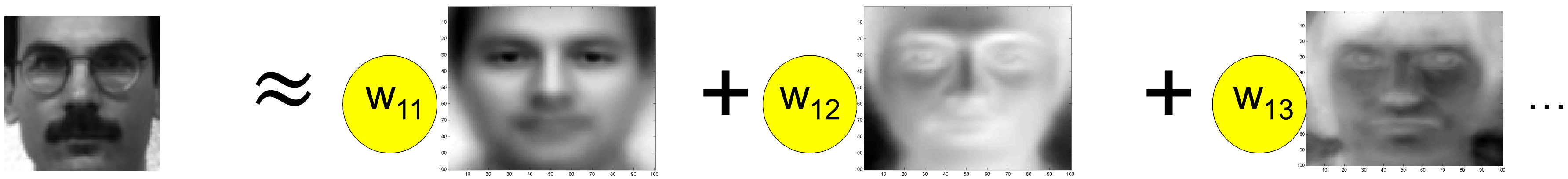
- ***Dimensionality Reduction:*** The number of Bases may be fewer than the dimensions of the vectors
  - Represent each Vector using fewer numbers
  - Expresses each vector within a *subspace*
    - Loses information / energy
    - **Objective**: Lose *least* energy

A Quick Recap: WHY? 3.



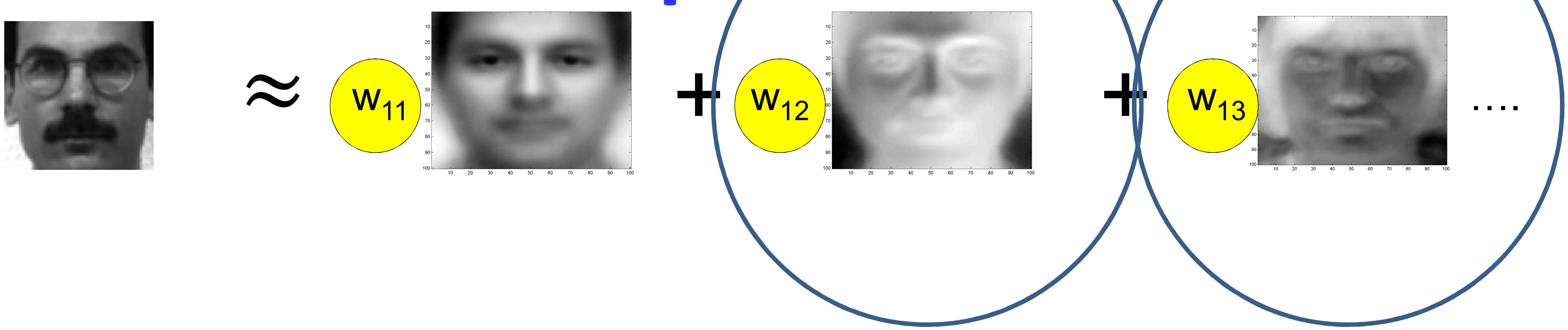
- ***Denoising:*** Reduced dimensional representation eliminates dimensions
- Can often eliminate *noise* dimensions
  - Signal-to-Noise ratio worst in dimensions where the signal has least energy/information
  - Removing them eliminates noise

A Quick Recap: HOW? PCA



- ***Find Eigenvectors of Correlation matrix***
  - These are our “eigen” bases
  - Capture information compactly and satisfy most of our requirements
- ***MOST***??

The problem?



- ***What is a negative face?***
  - And what does it mean to subtract one face from the other?
- Problem more obvious when applied to music
  - You would like bases to be notes
  - Weights to be scores
  - What is a negative note? What is a negative score?

Summary

- Decorrelation and Independence are statistically meaningful operations
- But may not be *physically* meaningful

- Next: A physically meaningful constraint
  - Non-negativity

The Engineer and the Musician

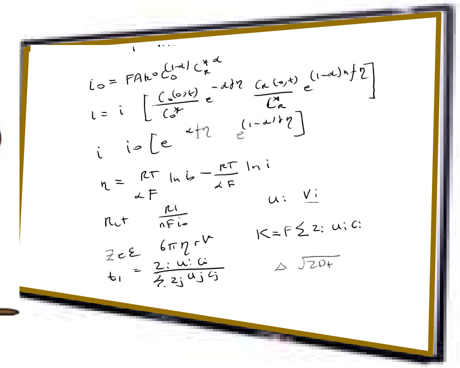
Once upon a time a rich potentate discovered a previously unknown recording of a beautiful piece of music. Unfortunately it was badly damaged.

He greatly wanted to find out what it would sound like if it were not.

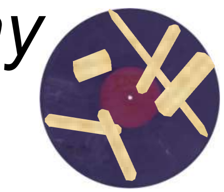
So he hired an engineer and a musician to solve the problem..

The Engineer and the Musician

The engineer worked for many years. He spent much money and published many papers.



Finally he had a somewhat scratchy restoration of the music..

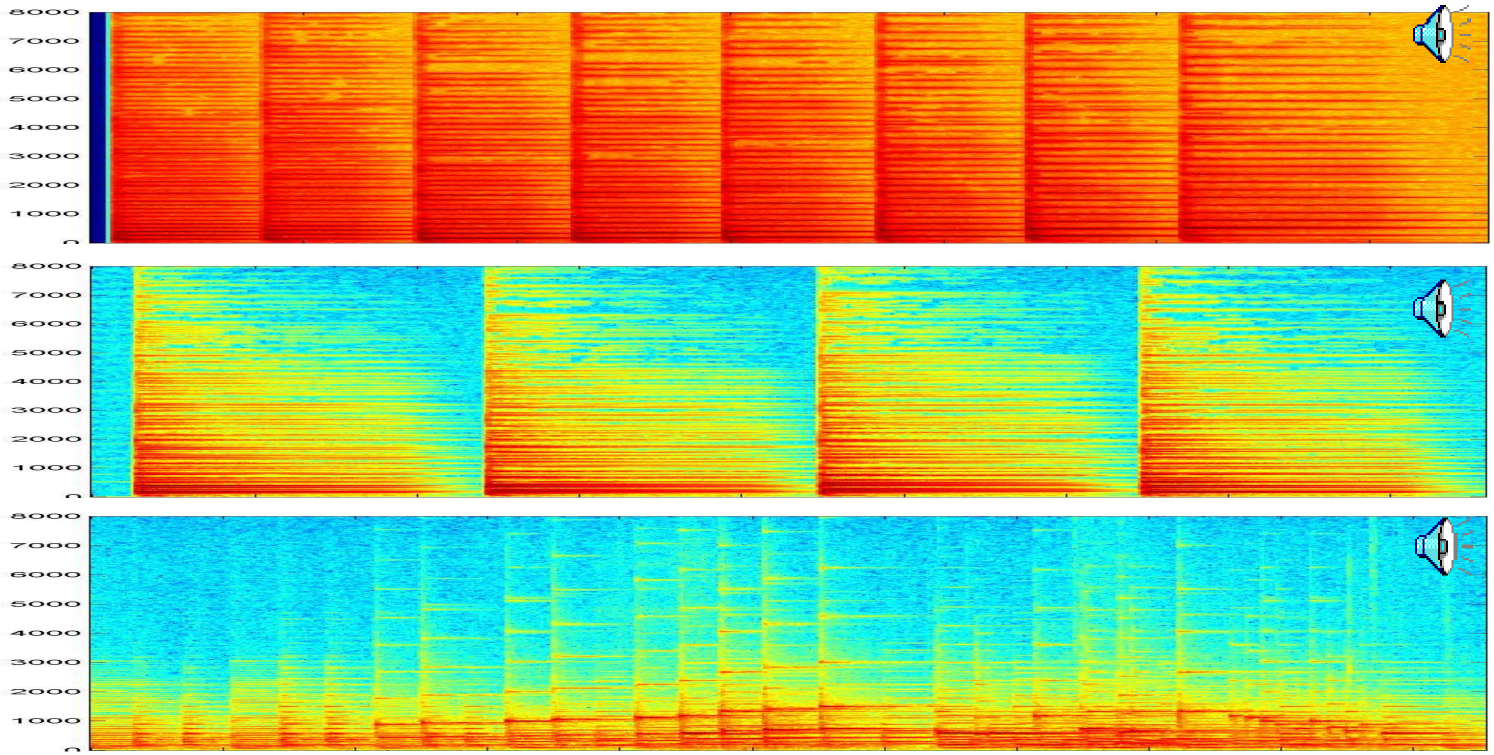


The musician listened to the music carefully for a day, transcribed it, broke out his trusty keyboard and replicated the music.

The Prize

Who do you think won the princess?

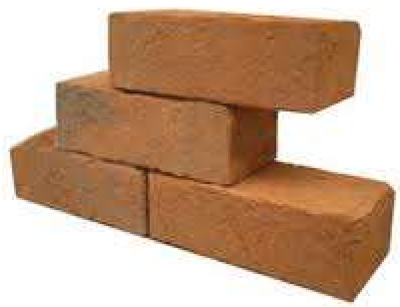
The search for building blocks



- What composes an audio signal?
  - E.g. notes compose music

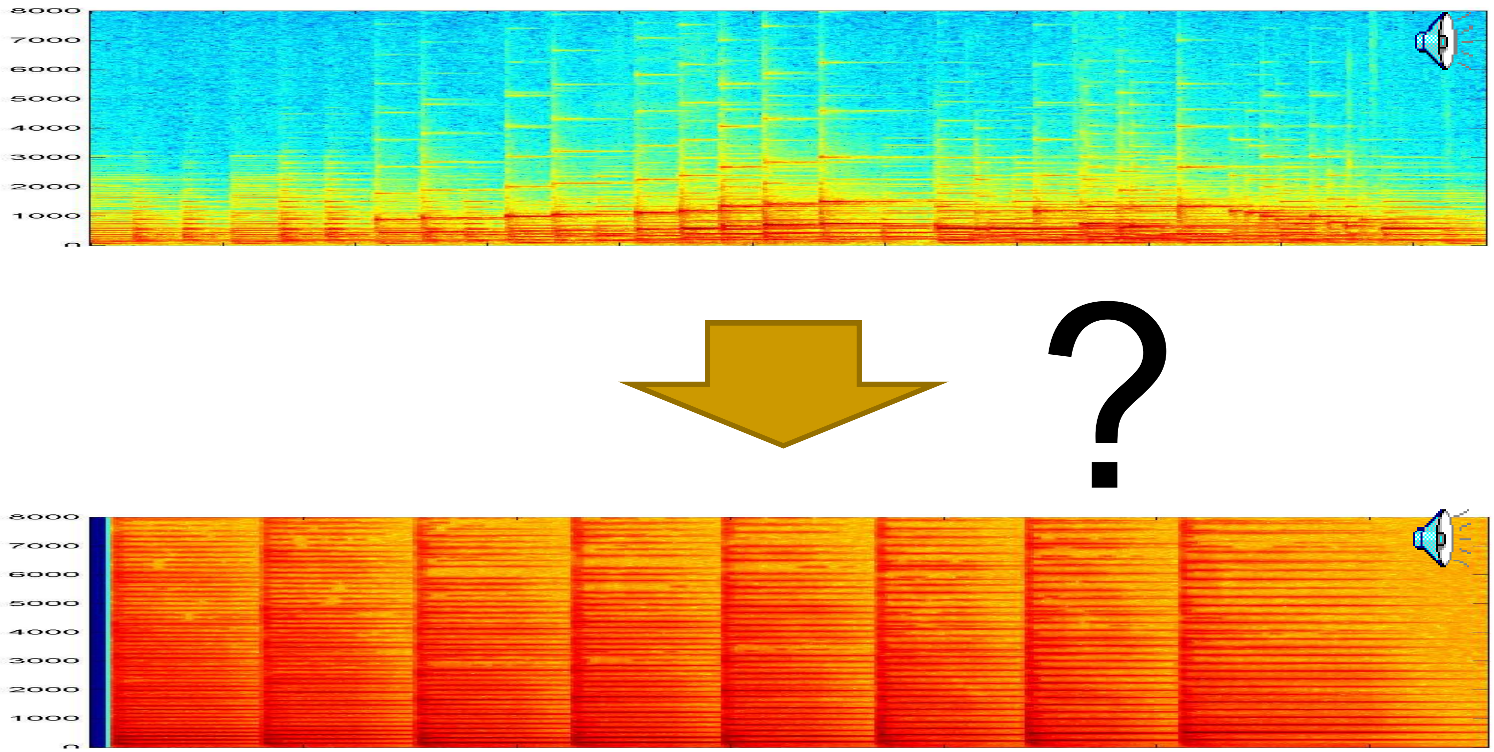
The properties of building blocks

- Constructive composition
  - A second note does not diminish a first note



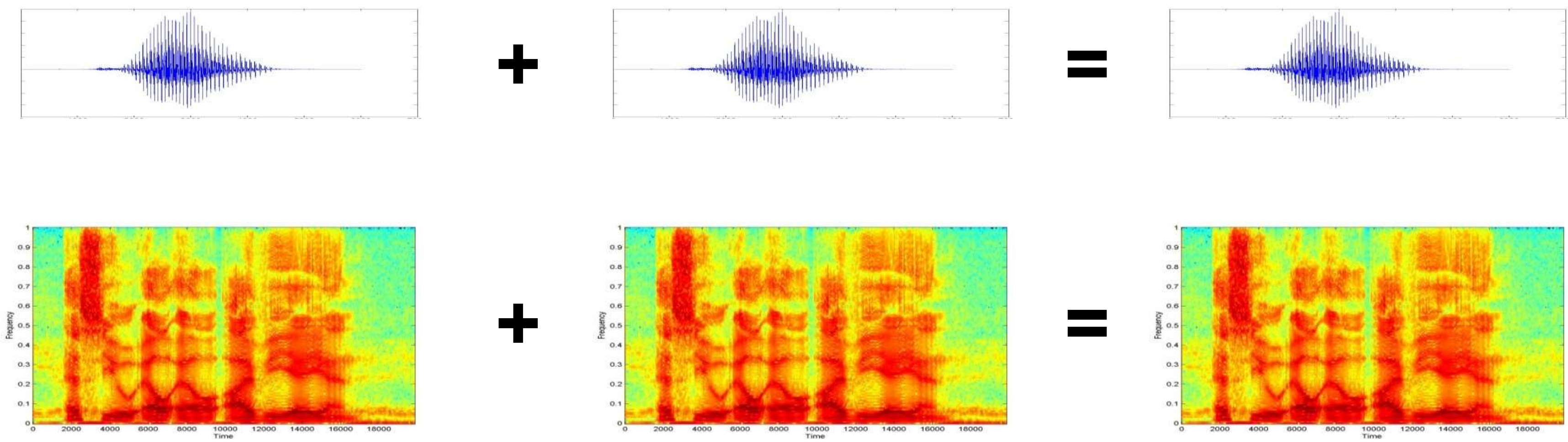
- Linearity of composition
  - Notes do not distort one another

Looking for building blocks in sound



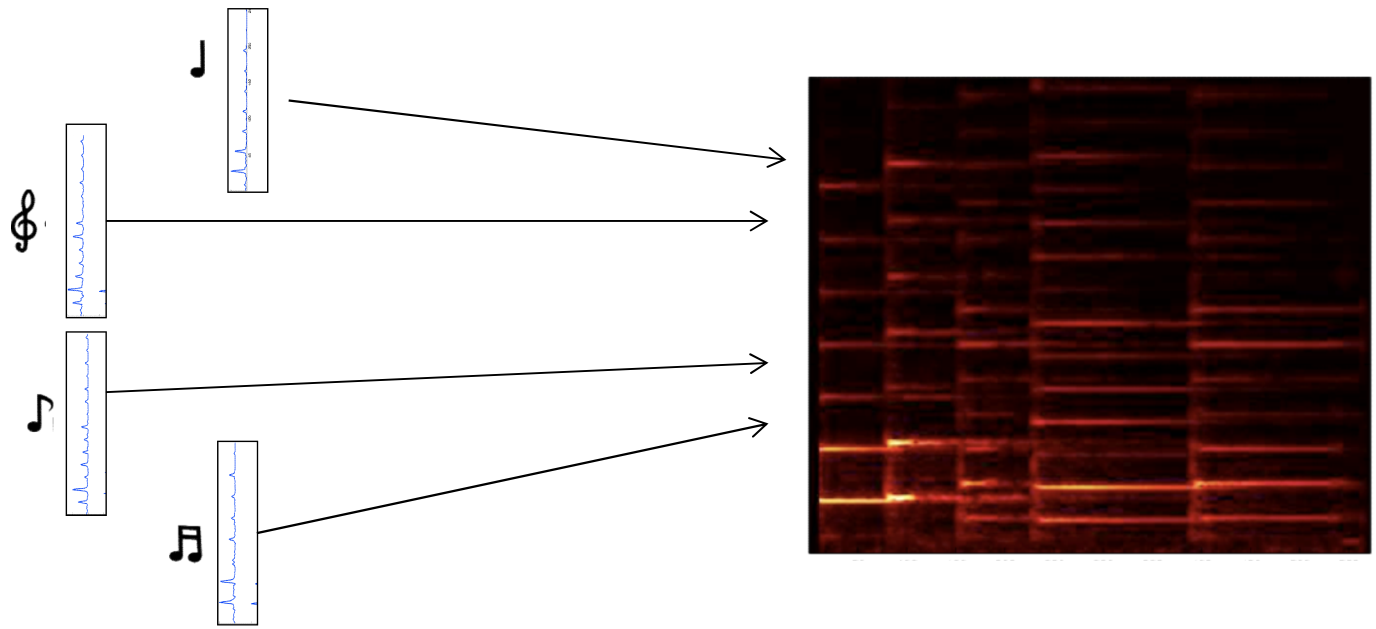
- Can we compute the building blocks from sound itself
  - *Can we learn the notes from the music?*

A property of power spectra



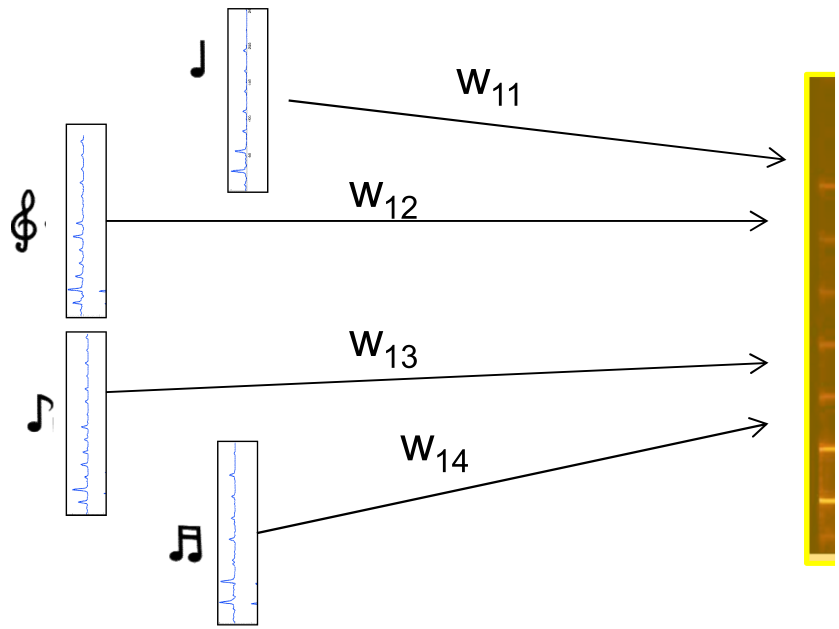
- When two or more independent signals are added, their power spectra (approximately) add
  - Their power spectrograms add as well

Building Blocks of Sound



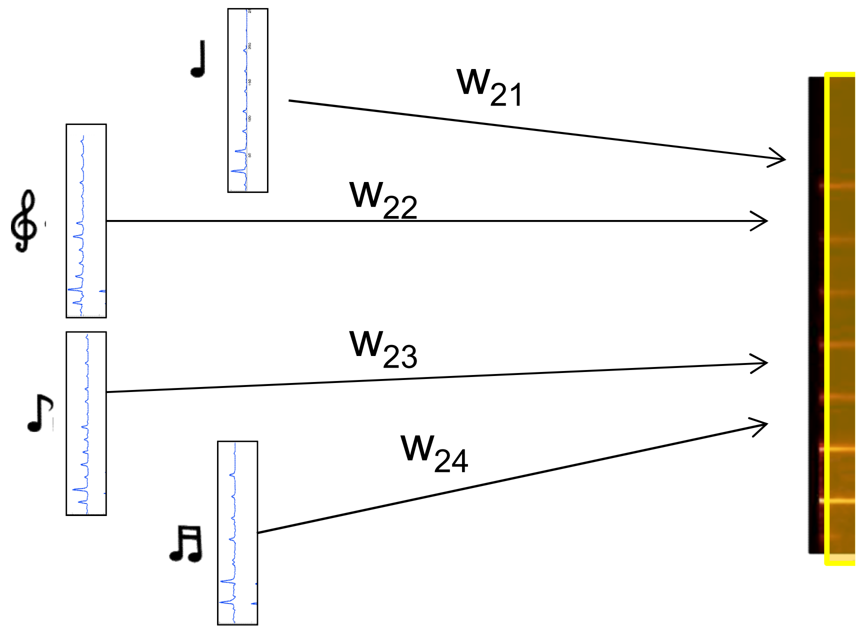
- The building blocks of sound are (power) spectral structures
  - E.g. notes build music
  - The spectra are entirely non-negative
- The complete sound is composed by *constructive* combination of the building blocks scaled to different non-negative gains
  - E.g. notes are played with varying energies through the music
  - The sound from the individual notes combines to form the final spectrogram
- The final spectrogram is also non-negative

Building Blocks of Sound



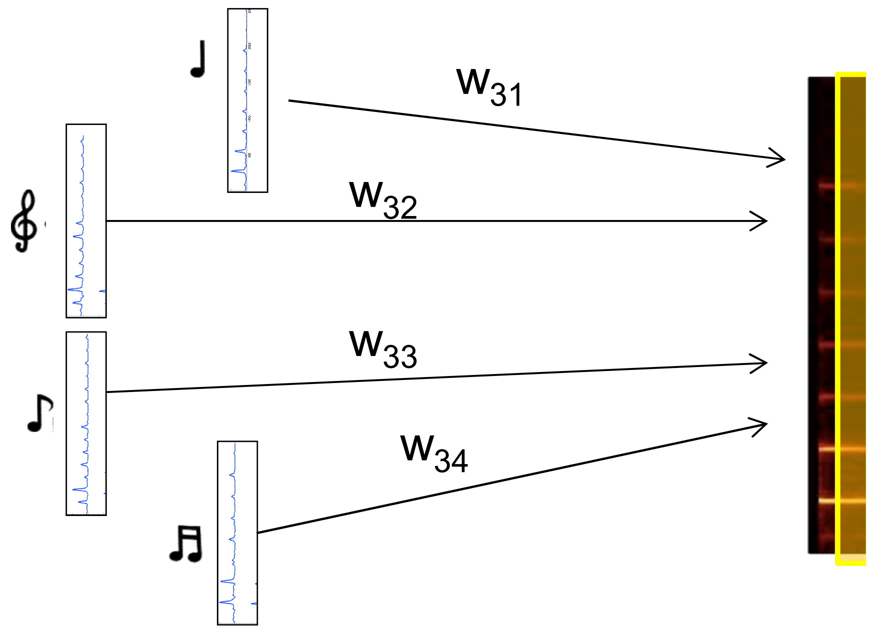
- Each frame of sound is composed by activating each spectral building block by a frame-specific amount
  - Individual frames are composed by activating the building blocks to different degrees
  - E.g. notes are strummed with different energies to compose the frame

Composing the Sound



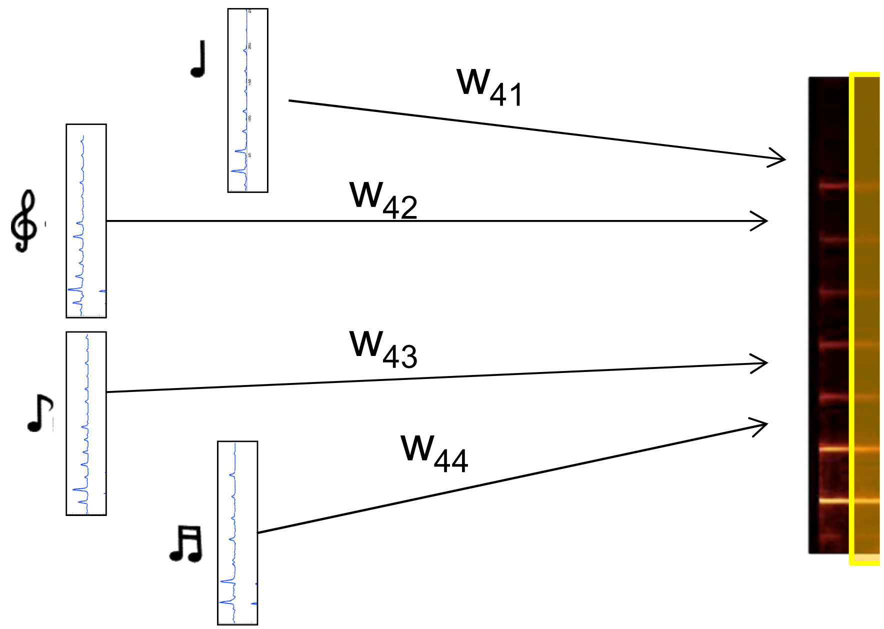
- Each frame of sound is composed by activating each spectral building block by a frame-specific amount
  - Individual frames are composed by activating the building blocks to different degrees
  - E.g. notes are strummed with different energies to compose the frame

Building Blocks of Sound



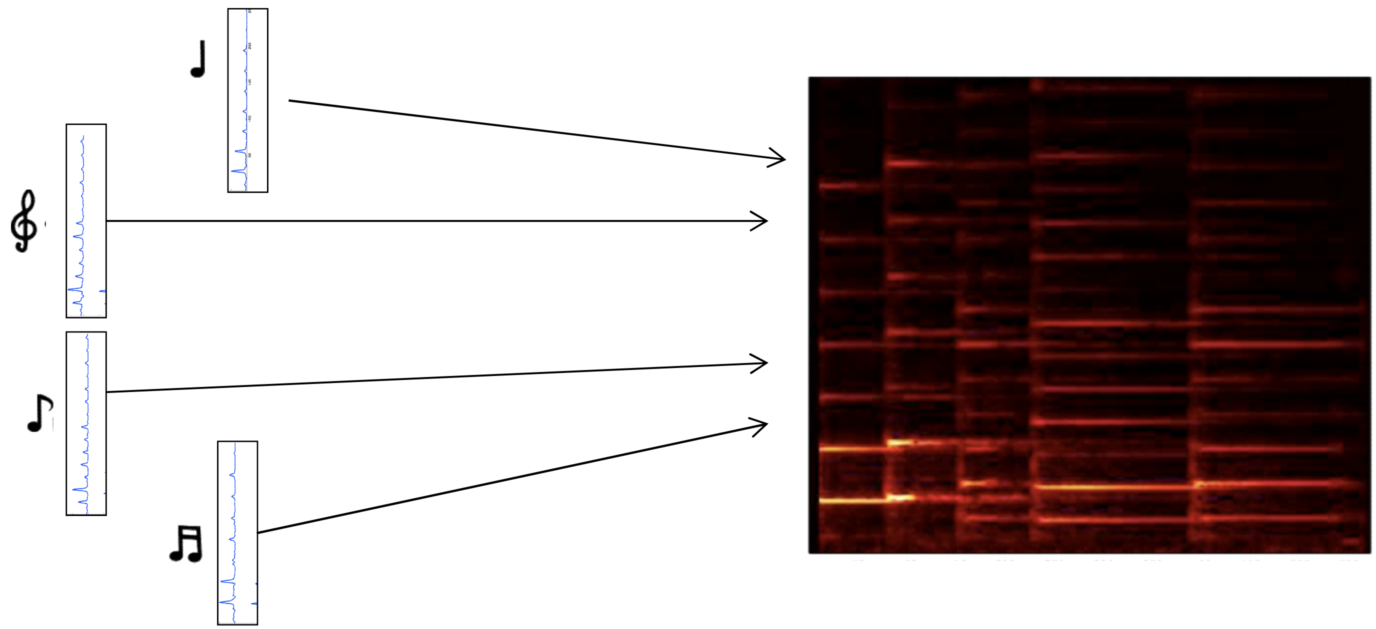
- Each frame of sound is composed by activating each spectral building block by a frame-specific amount
  - Individual frames are composed by activating the building blocks to different degrees
  - E.g. notes are strummed with different energies to compose the frame

Building Blocks of Sound



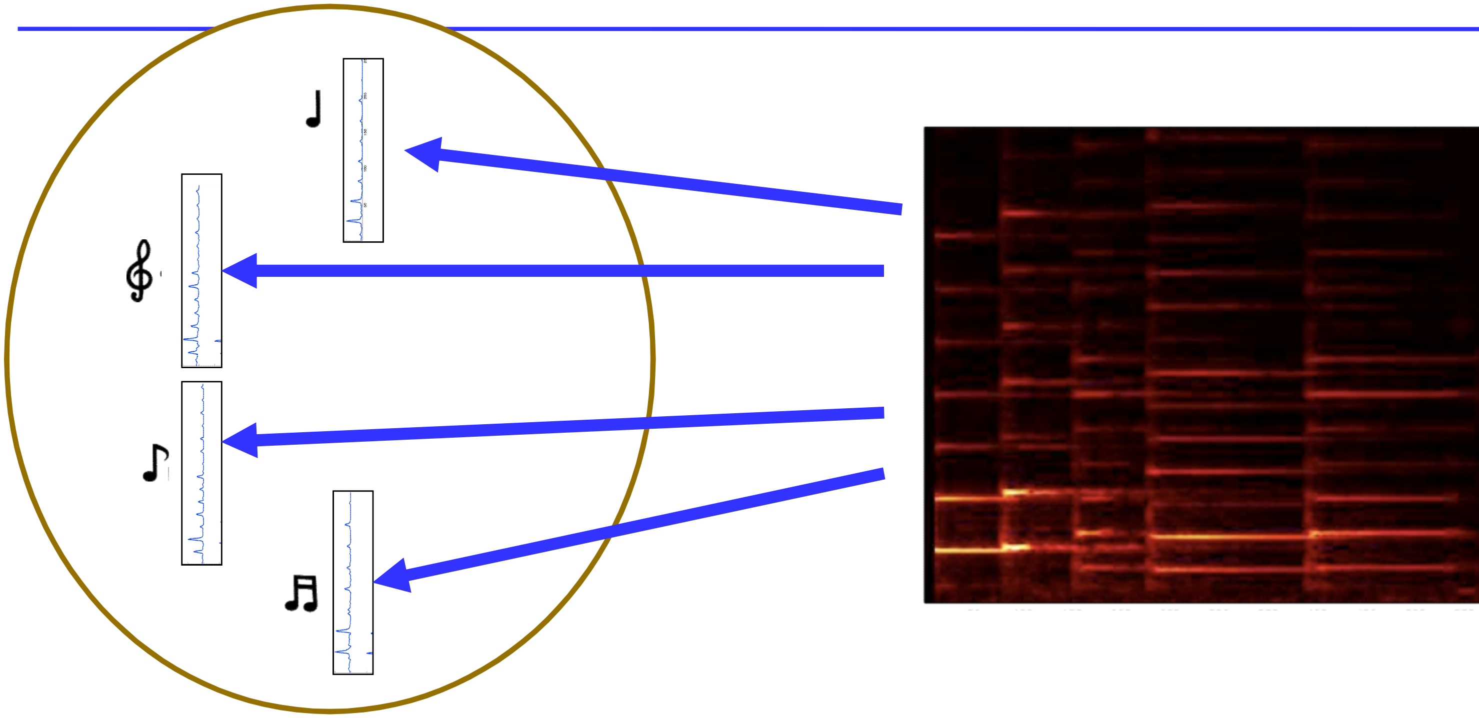
- Each frame of sound is composed by activating each spectral building block by a frame-specific amount
  - Individual frames are composed by activating the building blocks to different degrees
  - E.g. notes are strummed with different energies to compose the frame

Building Blocks of Sound



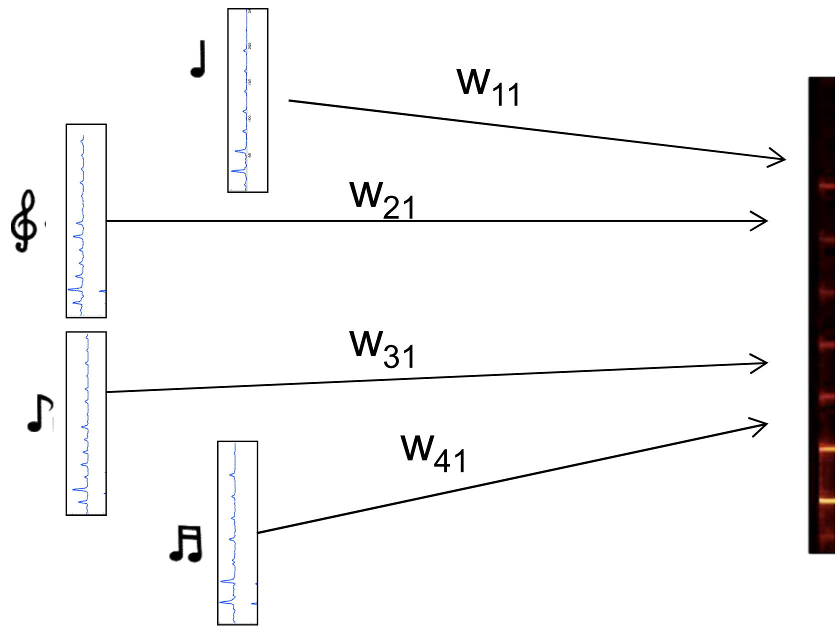
- Each frame of sound is composed by activating each spectral building block by a frame-specific amount
  - Individual frames are composed by activating the building blocks to different degrees
  - E.g. notes are strummed with different energies to compose the frame

The Problem of Learning



- Given only the final sound, determine its building blocks
  - From only listening to music, learn all about musical notes!

In Math



$$V_1 = w_{11}B_1 + w_{21}B_2 + w_{31}B_3 + \ldots$$

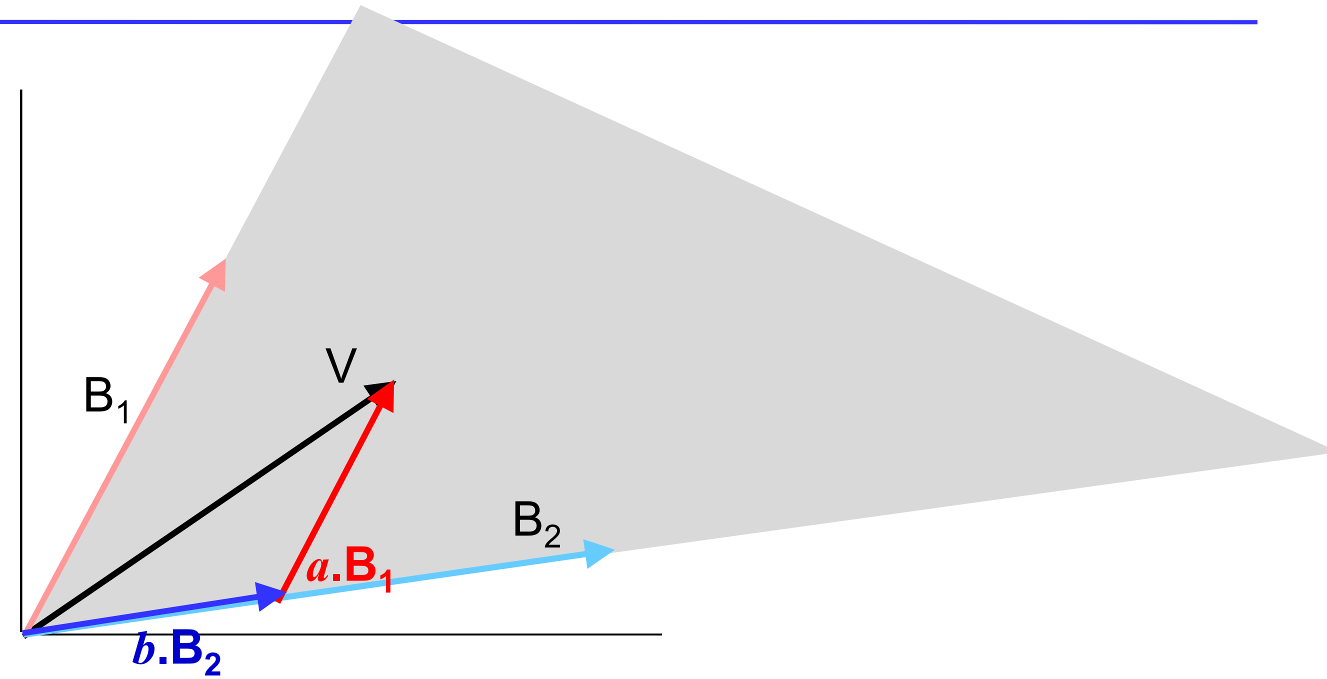
- Each frame is a non-negative power spectral vector
- Each note is a non-negative power spectral vector
- Each frame is a non-negative combination of the notes

Non-negative matrix factorization: Basics

- NMF is used in a *compositional* model
- Data are assumed to be non-negative
  - E.g. power spectra
- Every data vector is explained as a purely constructive linear composition of a set of bases
  - $V = \Sigma_i w_i B_i$
  - The bases B_i are in the same domain as the data
    - I.e. they are power spectra
- Constructive composition: no subtraction allowed
    - Weights w_i must all be non-negative
    - All components of bases B_i must also be non-negative

Understanding non-negative combination

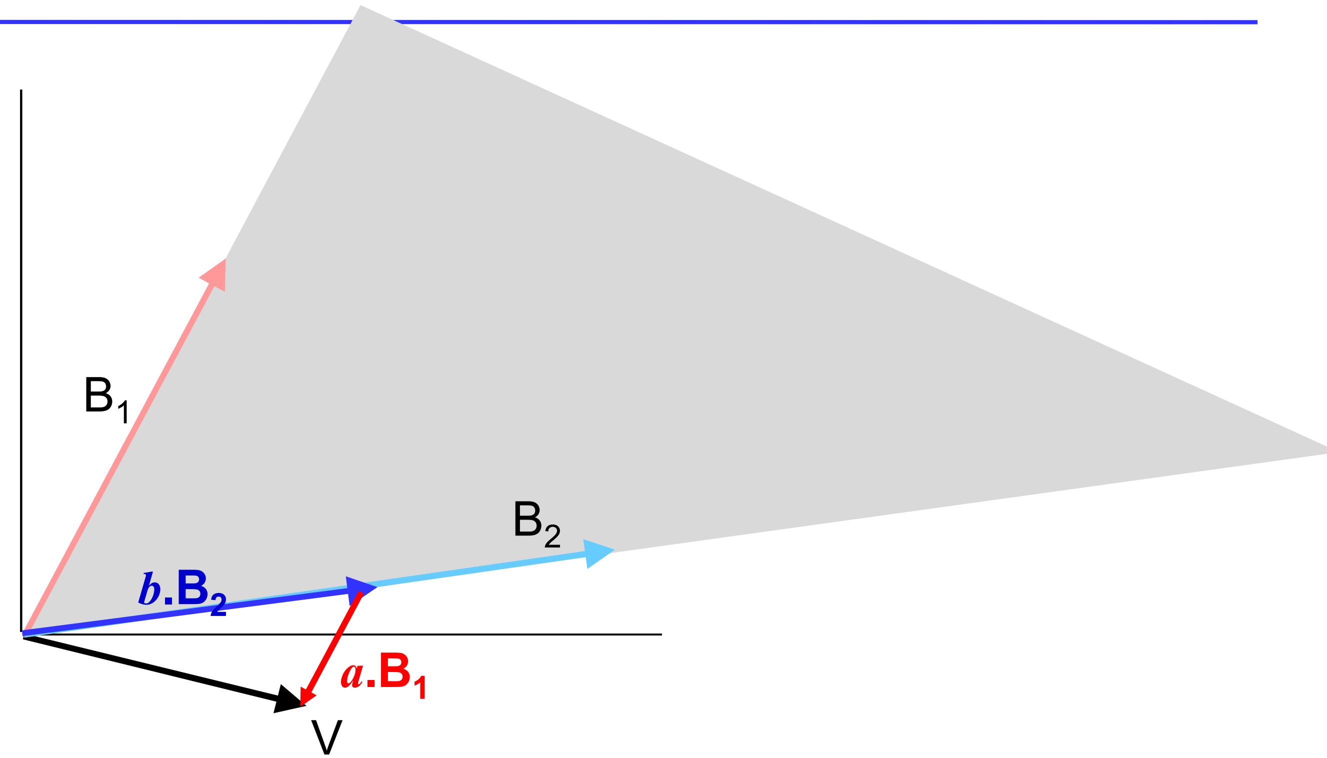
$$\boxed{V = aB_1 + bB_2}$$



- *Non-negative* combination: *a* and *b* are strictly non-negative
- Implies V must lie *inside the cone of B_1 and B_2*
  - V can be composed without reversing the directions of B_1 and B_2

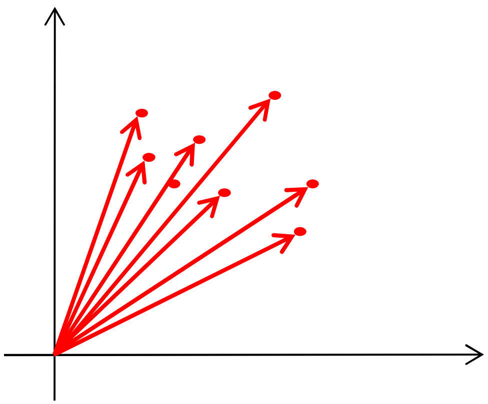
Understanding non-negative combination

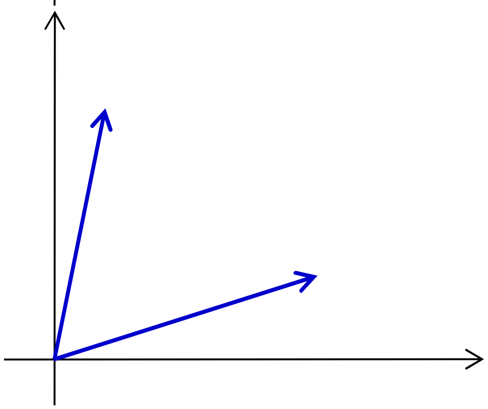
$$\boxed{V = aB_1 + bB_2}$$



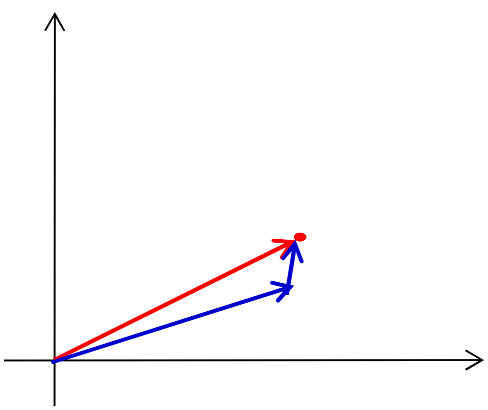
- If V lies outside the cone, at least one B_1 or B_2 must be reversed in direction to compose it
  - At least one of *a* and *b* must be negative

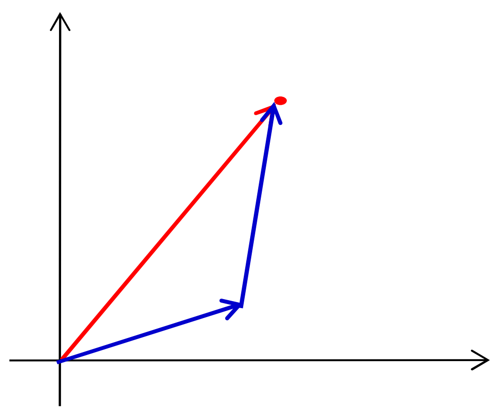
Learning building blocks: Restating the problem

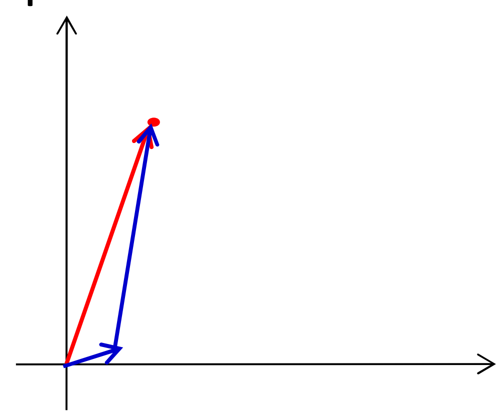




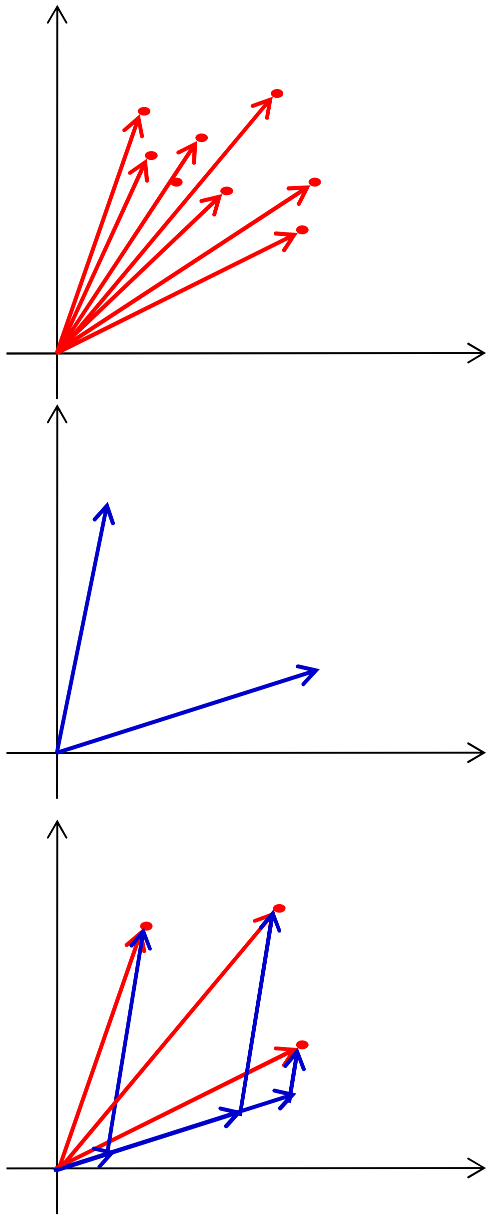
- Given a collection of spectral vectors (from the composed sound) …
- Find a set of “basic” sound spectral vectors such that …
- All of the spectral vectors can be composed through constructive addition of the bases
  - We never have to flip the direction of any basis







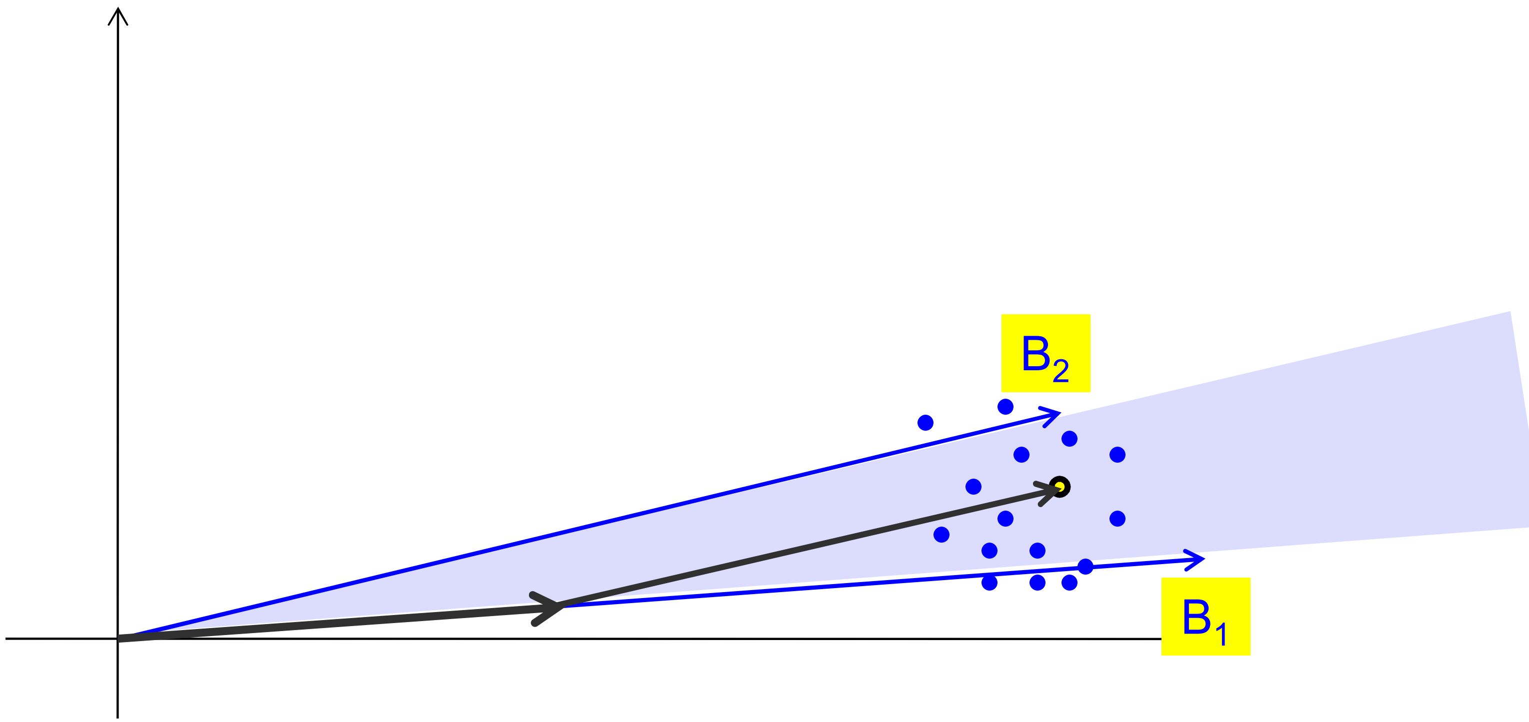
Learning building blocks: Restating the problem



$$\mathbf{V} = \mathbf{BW}$$

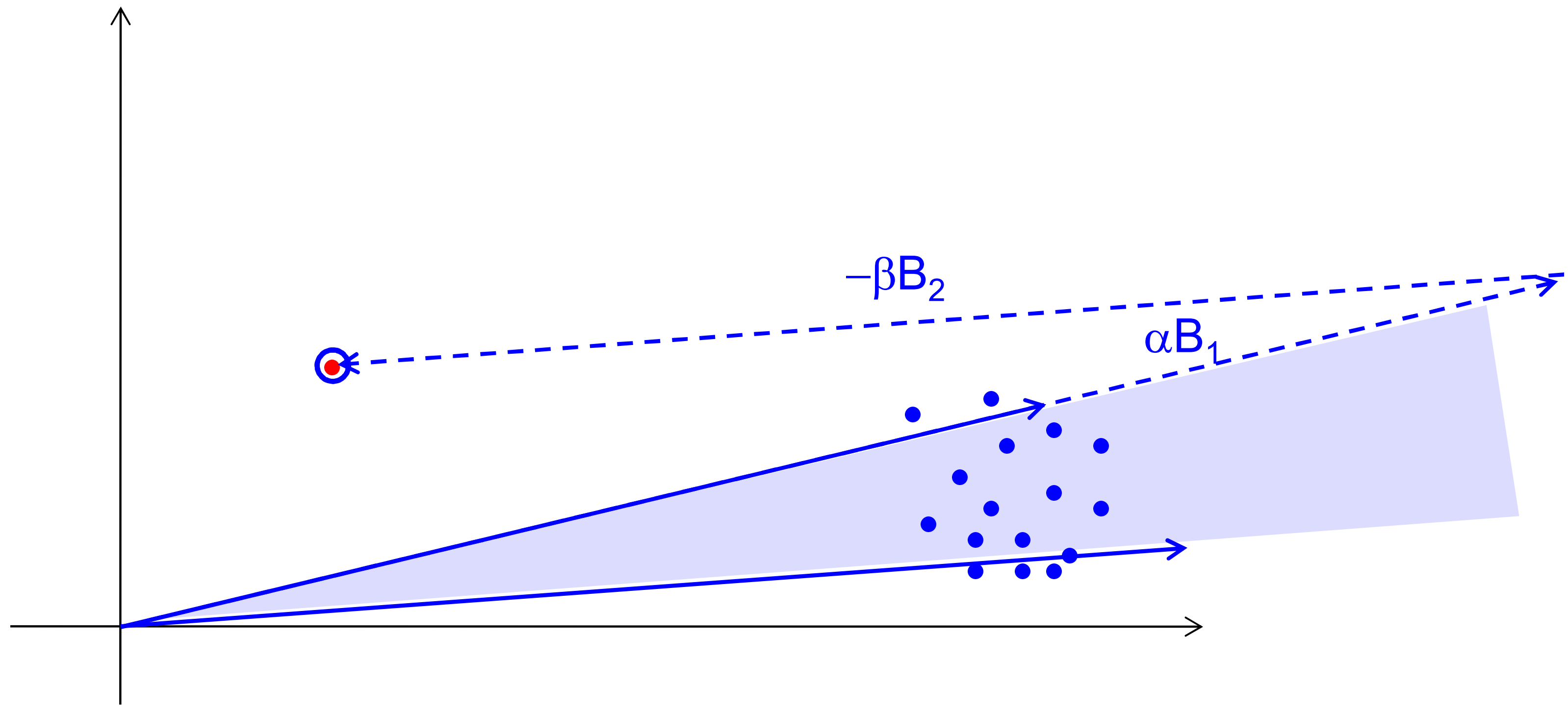
- Each column of **V** is one "composed" spectral vector
- Each column of **B** is one building block
  - One spectral basis
- Each column of **W** has the scaling factors for the building blocks to compose the corresponding column of **V**
- All columns of **V** are non-negative
- All entries of **B** and **W** must also be non-negative

Interpreting non-negative factorization



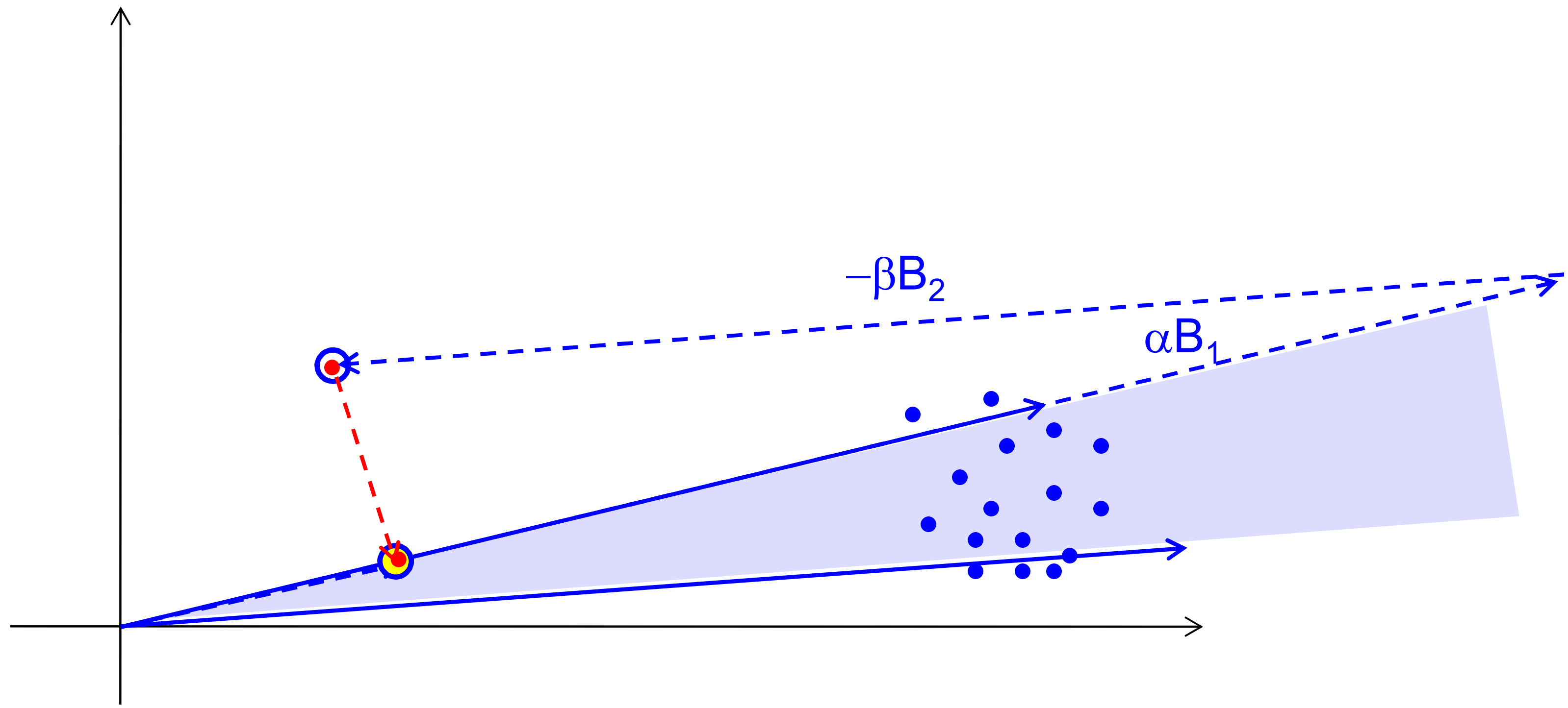
- Bases are non-negative, lie in the positive quadrant
- Blue lines represent bases, blue dots represent vectors
- Any vector that lies between the bases (highlighted region) can be expressed as a non-negative combination of bases
  - E.g. the black dot

Interpreting non-negative factorization



- Vectors outside the shaded enclosed area can only be expressed as a linear combination of the bases by reversing a basis
  - I.e. assigning a negative weight to the basis
  - E.g. the red dot
    - Alpha and beta are scaling factors for bases
    - Beta weighting is negative

Interpreting non-negative factorization



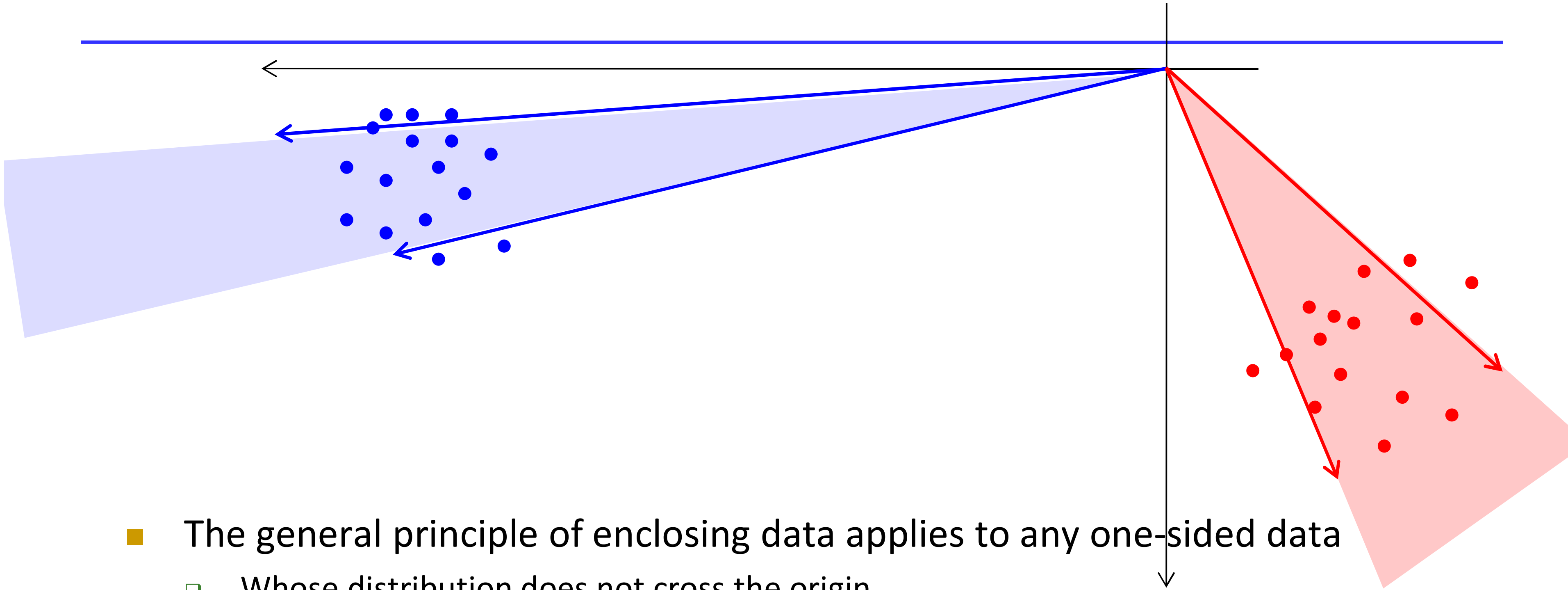
- If we approximate the red dot as a non-negative combination of the bases, the approximation will lie in the shaded region
  - On or close to the boundary
  - The approximation has error

The NMF representation

- The representation characterizes all data as lying within a compact convex region (a cone)
  - "Compact" → enclosing only a small fraction of the entire space
  - The more compact the enclosed region, the more it localizes the data within it
    - Represents the boundaries of the distribution of the data better
      - Conventional statistical models represent the mode of the distribution

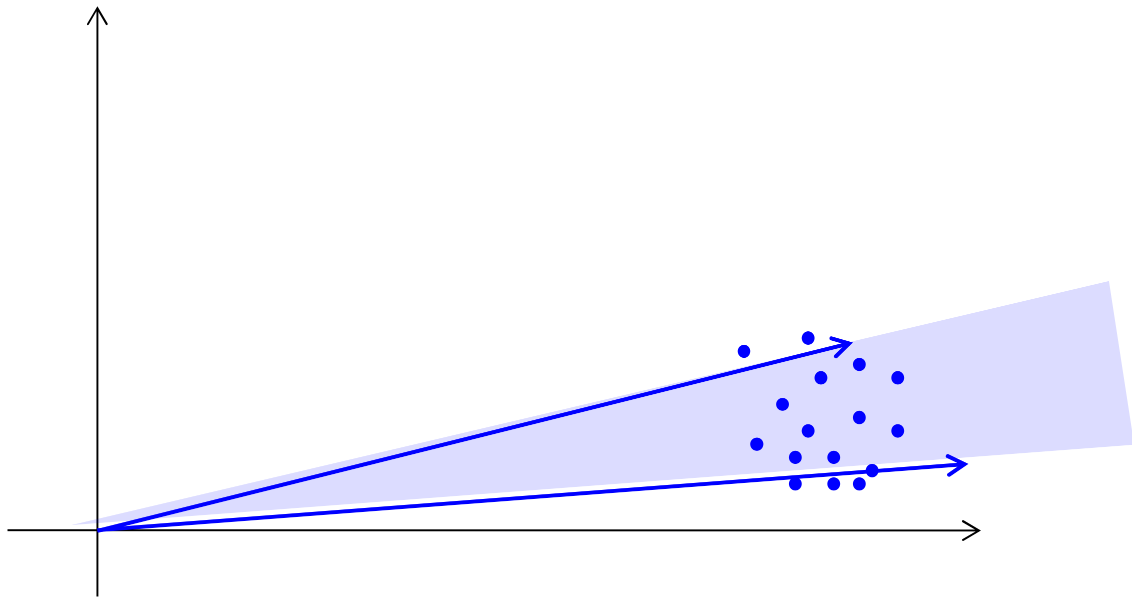
- The *bases* must be chosen to
  - Enclose the data as compactly as possible
  - And also enclose as much of the data as possible
    - Data that are not enclosed are not represented correctly

Data need not be non-negative



- The general principle of enclosing data applies to any one-sided data
  - Whose distribution does not cross the origin.
- The only part of the model that must be non-negative are the weights.
- Examples
  - Blue bases enclose blue region in negative quadrant
  - Red bases enclose red region in positive-negative quadrant
- Notions of compactness and enclosure still apply
  - This is a generalization of NMF
  - We wont discuss it further

NMF: Learning Bases

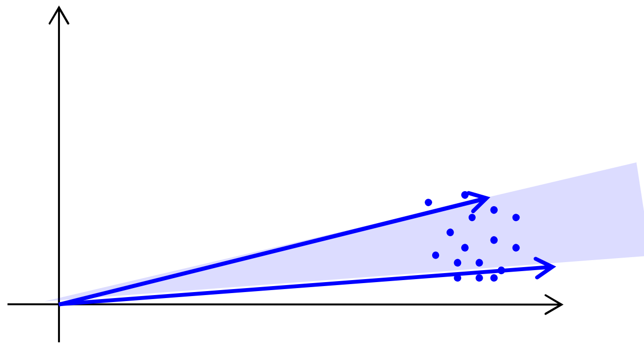


- Given a collection of data vectors (blue dots)
- Goal: find a set of bases (blue arrows) such that they enclose the data.
- Ideally, they must simultaneously enclose the smallest volume
  - *This “enclosure” constraint is usually not explicitly imposed in the standard NMF formulation*

NMF: Learning Bases

- Express every training vector as non-negative combination of bases
  - $V = \sum_i w_i B_i$
- In linear algebraic notation, represent:
  - Set of all training vectors as a data matrix **V**
    - A DxN matrix, D = dimensionality of vectors, N = No. of vectors
  - All basis vectors as a matrix **B**
    - A DxK matrix , K is the number of bases
  - The K weights for any vector V as a Kx1 column vector W
  - The weight vectors for all N training data vectors as a matrix **W**
    - KxN matrix
- Ideally **V** = **BW**
  - **All components of V, B and W are non-negative**

NMF: Learning Bases



- **V** = **BW** will only hold true if all training vectors in **V** lie inside the region enclosed by the bases

- Learning bases is an iterative algorithm
- Intermediate estimates of **B** do not satisfy **V = BW**
- Algorithm updates **B** until **V = BW** is satisfied as closely as possible

NMF: Minimizing Divergence

- Define a *Divergence* between data **V** and approximation **BW**
  - Divergence(**V**, **BW**) is the total error in approximating all vectors in **V** as **BW**
  - Must estimate *non-negative* **B** and **W** so that this error is minimized
- Divergence(**V**, **BW**) can be defined in different ways
  - L2: Divergence = $\Sigma_i\Sigma_j (V_{ij} - (BW)_{ij})^2$
    - Minimizing the L2 divergence gives us an algorithm to learn **B** and **W**
  - KL: Divergence(**V**,**BW**) = $\Sigma_i\Sigma_j V_{ij} \log(V_{ij} / (BW)_{ij}) + \Sigma_i\Sigma_j V_{ij} - \Sigma_i\Sigma_j (BW)_{ij}$
    - This is a *generalized* KL divergence that is minimum when **V** = **BW**
    - Minimizing the KL divergence gives us another algorithm to learn **B** and **W**
- Other divergence forms can also be used

NMF: Minimizing Divergence

- Define a *Divergence* between data **V** and approximation **BW**
  - Divergence(**V**, **BW**) is the total error in approximating all vectors in **V** as **BW**
  - Must estimate *non-negative* **B** and **W** so that this error is minimized

- Divergence(**V**, **BW**) can be defined in different ways
  - L2: Divergence = $\Sigma_i\Sigma_j (V_{ij} - (BW)_{ij})^2$
    - Minimizing the L2 divergence gives us an algorithm to learn **B** and **W**
  - KL: Divergence(**V**,**BW**) = $\Sigma_i\Sigma_j V_{ij} \log(V_{ij} / (BW)_{ij}) + \Sigma_i\Sigma_j V_{ij} - \Sigma_i\Sigma_j (BW)_{ij}$
    - This is a *generalized* KL divergence that is minimum when **V** = **BW**
    - Minimizing the KL divergence gives us another algorithm to learn **B** and **W**

- Other divergence forms can also be used

NMF: Minimizing L_2 Divergence

- Divergence(**V**, **BW**) is defined as
  - $E = ||\mathbf{V} - \mathbf{BW}||_F^2$
  - $E = \Sigma_i \Sigma_j (V_{ij} - (BW)_{ij})^2$

- Iterative solution: Minimize E such that **B** and **W** are strictly non-negative

NMF: Minimizing L_2 Divergence

- Learning both **B** and **W** with non-negativity
- Divergence(**V**, **BW**) is defined as
  - E = $||\mathbf{V} - \mathbf{BW}||_F^2$

$$\boldsymbol{V} \approx \boldsymbol{BW}$$

- Iterative solution:
  - **B = $[\mathbf{V}\ \mathrm{Pinv}(\mathbf{W})]_+$**
  - **W = $[\mathrm{Pinv}(\mathbf{B})\ \mathbf{V}]_+$**
  - Subscript + indicates thresholding –ve values to 0

NMF: Minimizing Divergence

- Define a *Divergence* between data **V** and approximation **BW**
  - Divergence(**V**, **BW**) is the total error in approximating all vectors in **V** as **BW**
  - Must estimate **B** and **W** so that this error is minimized

- Divergence(**V**, **BW**) can be defined in different ways
  - L2: Divergence = $\Sigma_i \Sigma_j (V_{ij} - (BW)_{ij})^2$
    - Minimizing the L2 divergence gives us an algorithm to learn **B** and **W**
  - KL: Divergence(**V**,**BW**) = $\Sigma_i \Sigma_j V_{ij} \log(V_{ij} / (BW)_{ij}) + \Sigma_i \Sigma_j V_{ij} - \Sigma_i \Sigma_j (BW)_{ij}$
    - This is a *generalized* KL divergence that is minimum when **V** = **BW**
    - Minimizing the KL divergence gives us another algorithm to learn **B** and **W**

- For many kinds of signals, e.g. sound, NMF-based representations work best when we minimize the KL divergence

NMF: Minimizing KL Divergence

- Divergence(**V**, **BW**) defined as
  - $E = \Sigma_i \Sigma_j V_{ij} \log(V_{ij} / (BW)_{ij}) + \Sigma_i \Sigma_j V_{ij} - \Sigma_i \Sigma_j (BW)_{ij}$

- Iterative update rules
- Number of iterative update rules have been proposed
- The most popular one is the multiplicative update rule..

NMF Estimation: Learning bases

- The algorithm to estimate **B** and **W** to minimize the KL divergence between **V** and **BW**:

- Initialize **B** and **W** (randomly)
- Iteratively update **B** and **W** using the following formulae

$$B = B \otimes \frac{\left(\frac{V}{BW}\right)W^T}{1W^T} \qquad W = W \otimes \frac{B^T\left(\frac{V}{BW}\right)}{B^T 1}$$

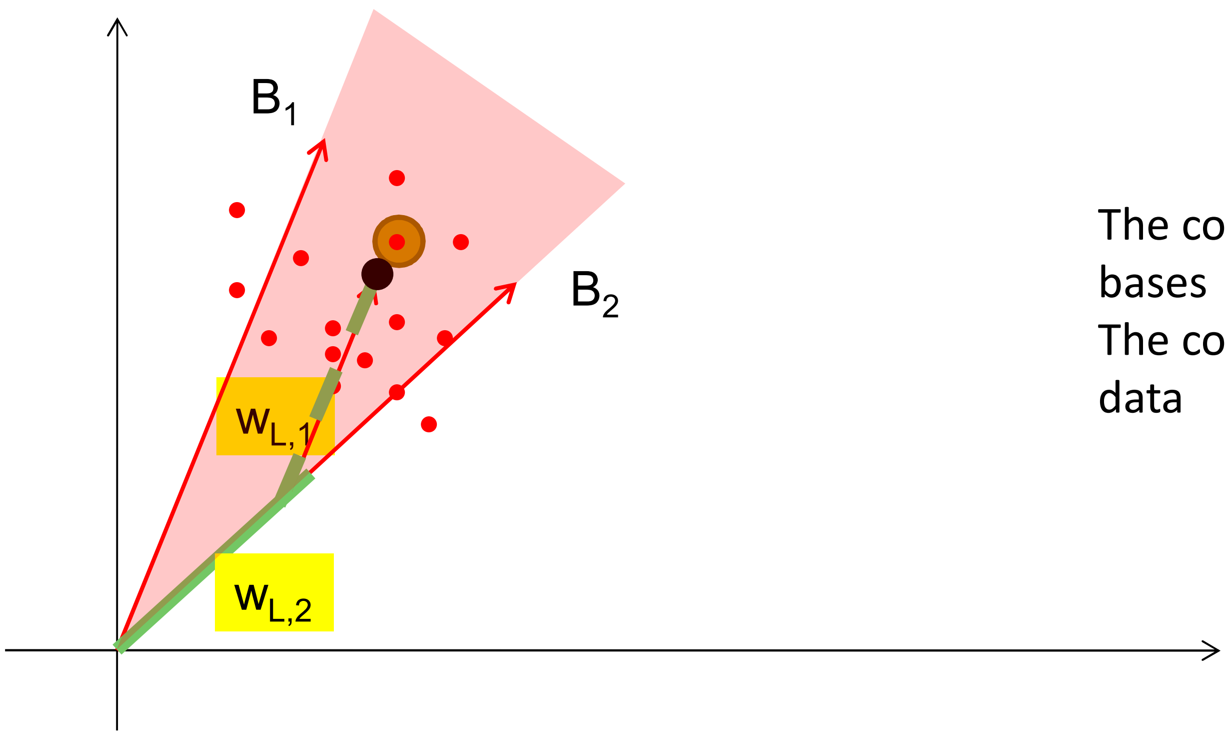
- Iterations continue until divergence converges
  - In practice, continue for a fixed no. of iterations

Reiterating

$$V_{D\times N} \approx B_{D\times K} W_{K\times N}$$

$$V_L \approx \sum_k w_{L,k} B_k$$

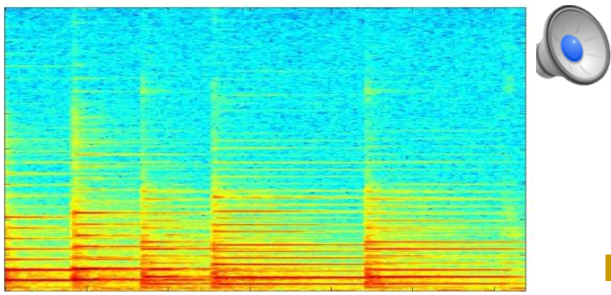
- NMF learns the *optimal set of basis vectors B_k* to approximate the data in terms of the bases
- It also learns how to compose the data in terms of these bases
  - Compositions can be inexact



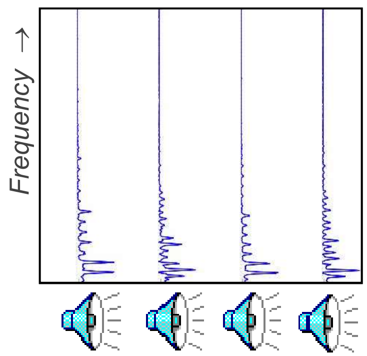
The columns of **B** are the bases
The columns of **V** are the data

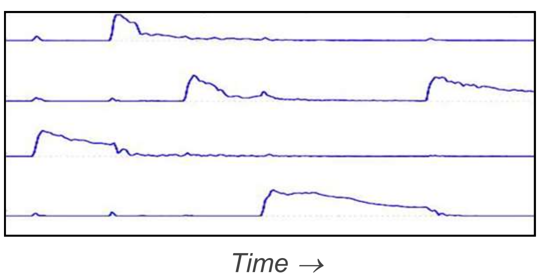
Learning building blocks of sound

From Bach's Fugue in Gm



bases



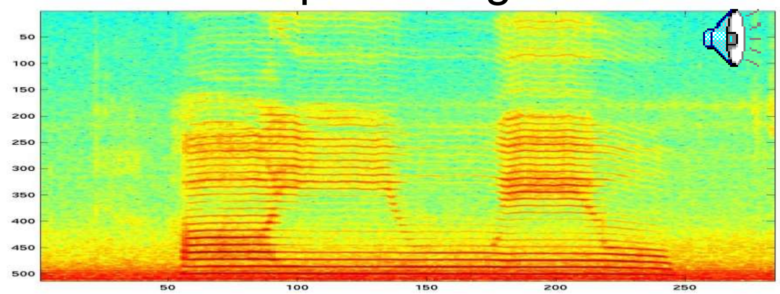


$$\mathbf{V} = \mathbf{BW}$$

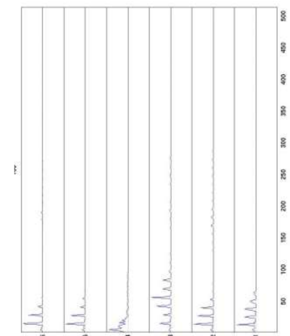
- Each column of **V** is one spectral vector
- Each column of **B** is one building block/basis
- Each column of **W** has the scaling factors for the bases to compose the corresponding column of **V**
- All terms are non-negative
- Learn **B** (and **W**) by applying NMF to **V**

Learning Building Blocks

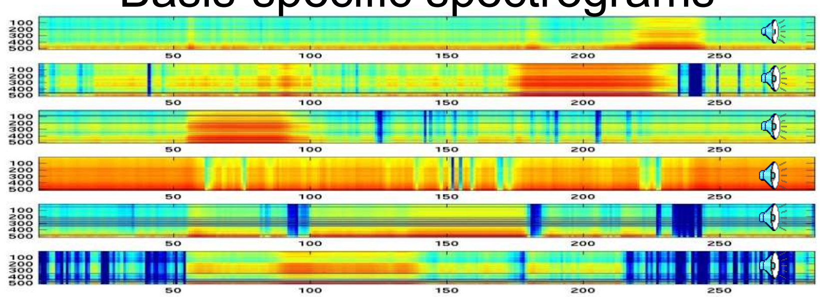
Speech Signal



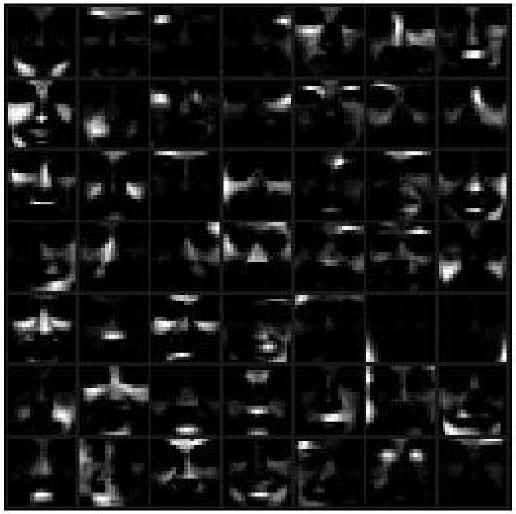
bases



Basis-specific spectrograms



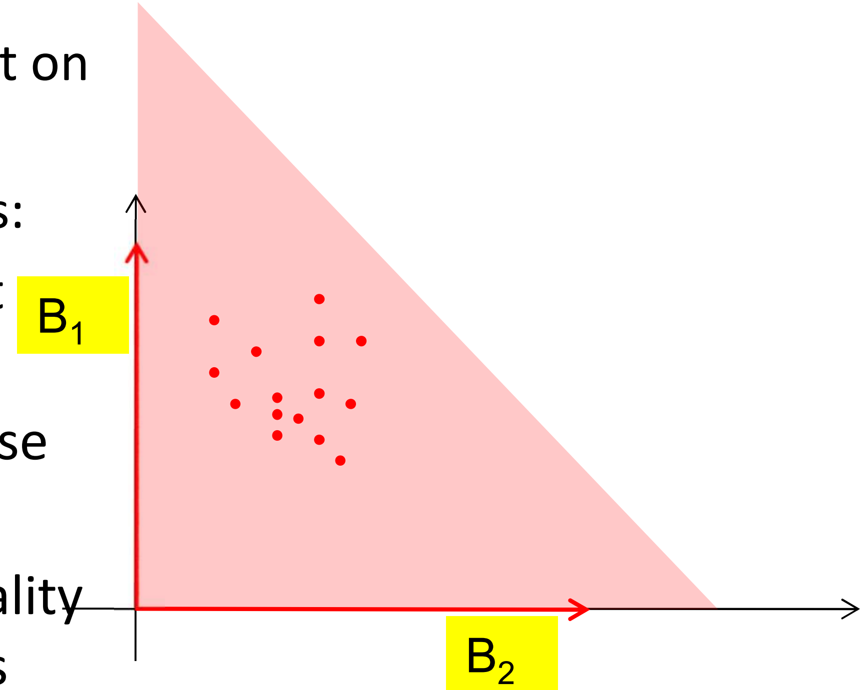
What about other data



- Faces
  - Trained 49 multinomial components on 2500 faces
    - Each face unwrapped into a 361-dimensional vector
  - Discovers parts of faces

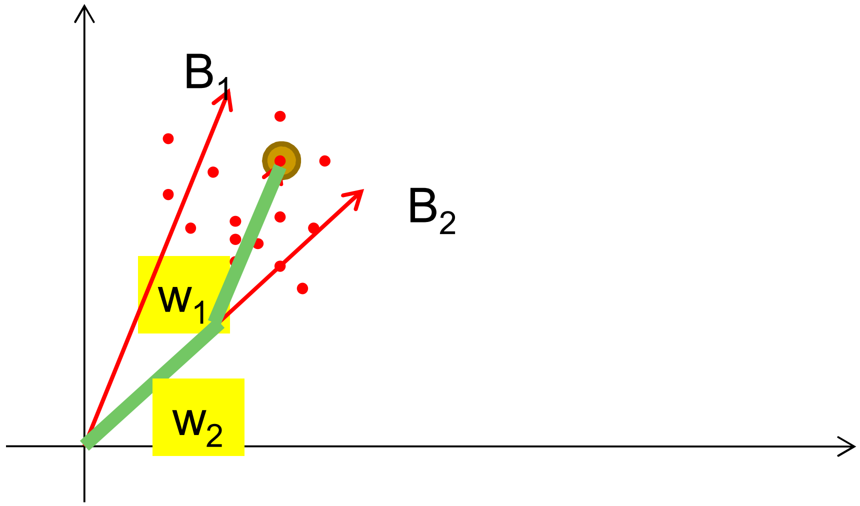
There is no "compactness" constraint

- No explicit "compactness" constraint on bases
- The red lines would be perfect bases:
  - Enclose all training data without error
  - Algorithm can end up with these bases
  - If no. of bases K >= dimensionality D, can get uninformative bases



- If K < D, we usually learn compact representations
  - NMF becomes a dimensionality reducing representation
    - Representing D-dimensional data in terms of K weights, where K < D

Representing Data using *Known* Bases



- If we already have bases B_k and are given a vector that must be expressed in terms of the bases: $V \approx \sum_k w_k B_k$

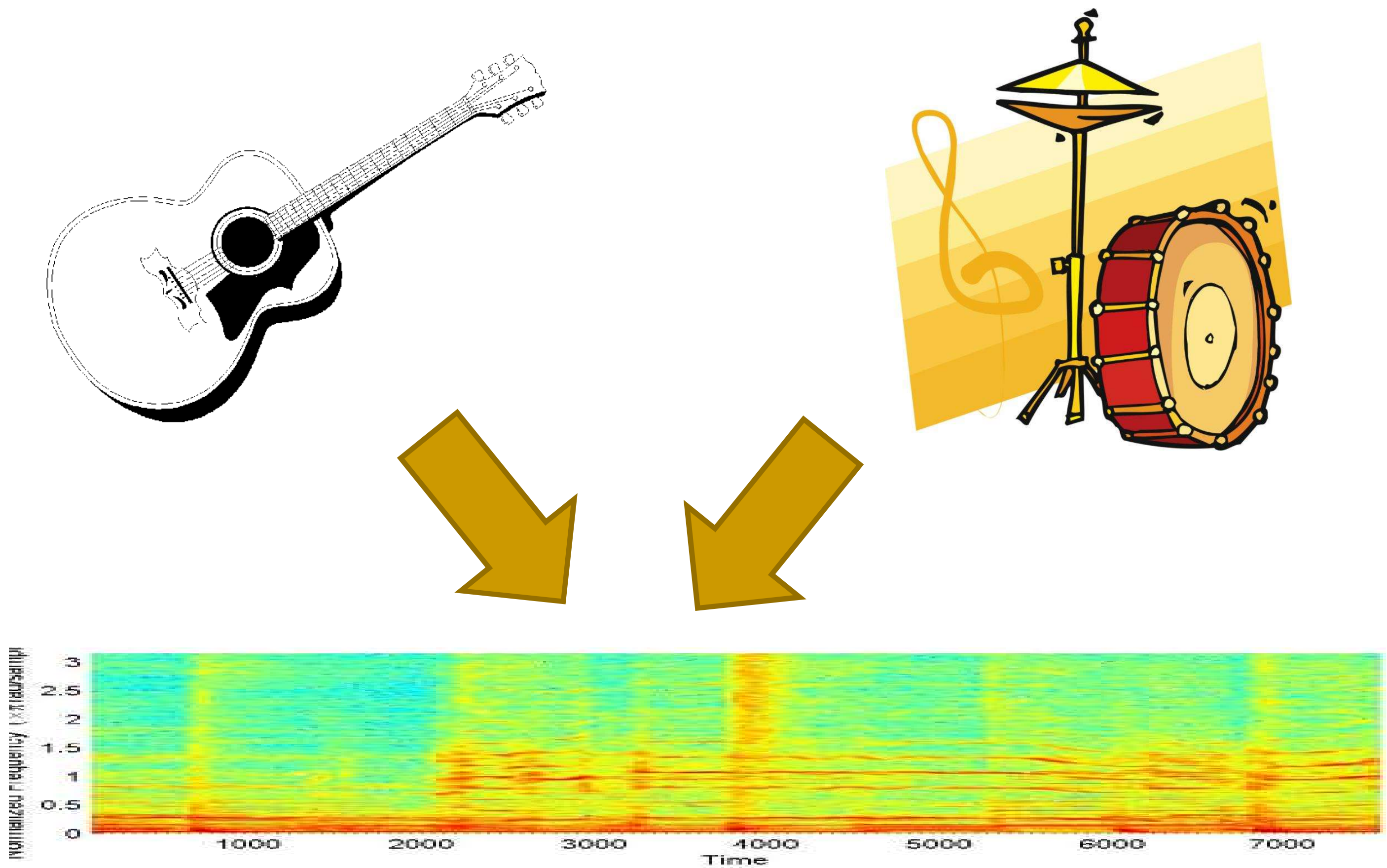
- Estimate weights as:
  - Initialize weights
  - Iteratively update them using

$$W = W \otimes \frac{B^T \left(\frac{V}{BW} \right)}{B^T 1}$$

What can we do knowing the building blocks

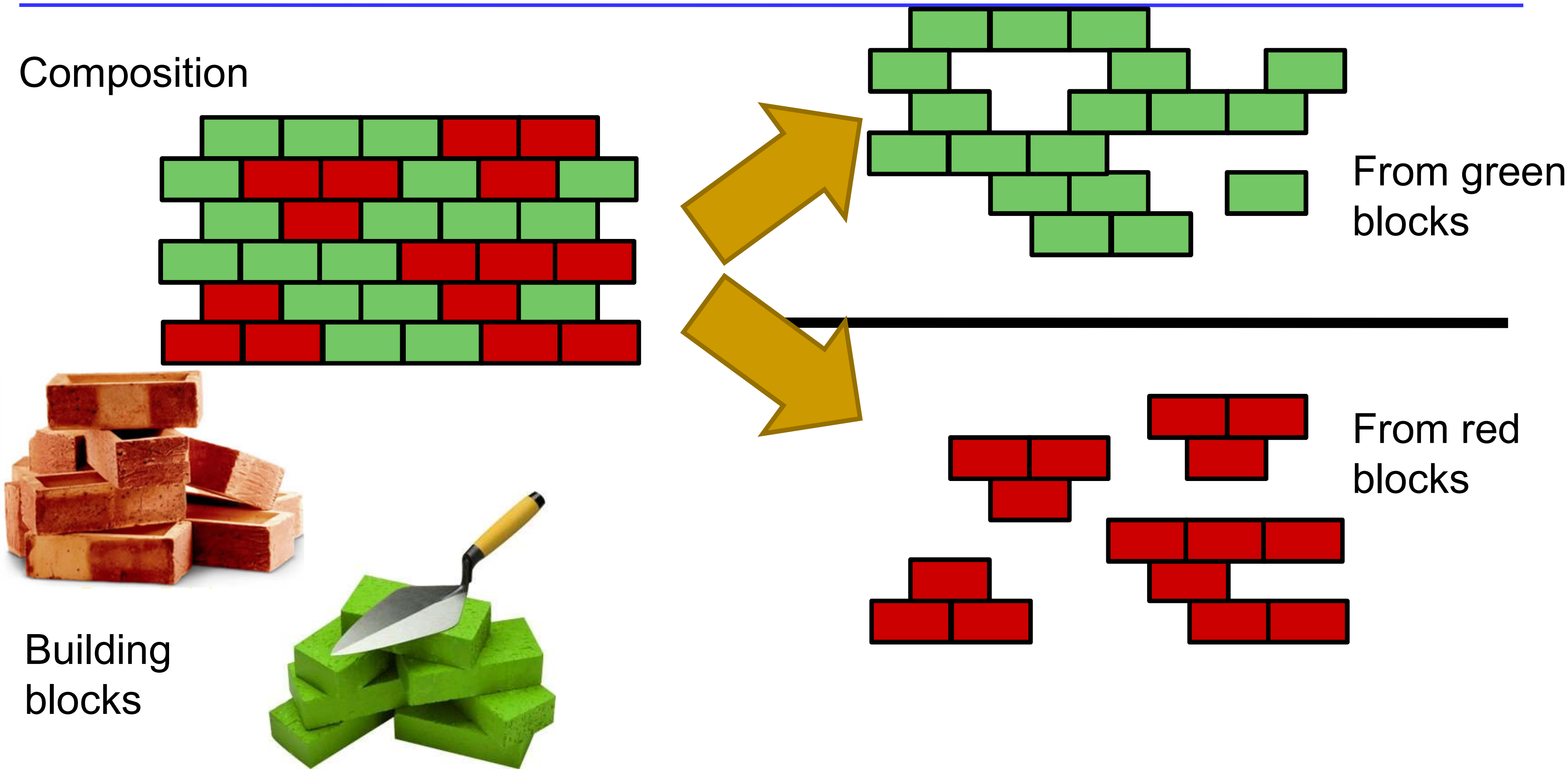
- *Signal Representation*
- *Signal Separation*
- *Signal Completion*
- Denoising
- Signal recovery
- Music Transcription
- Etc.

Signal Separation



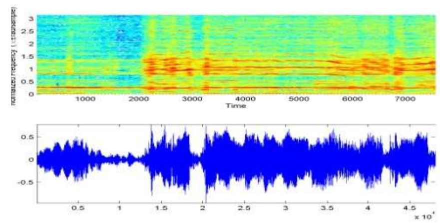
- Can we separate mixed signals?

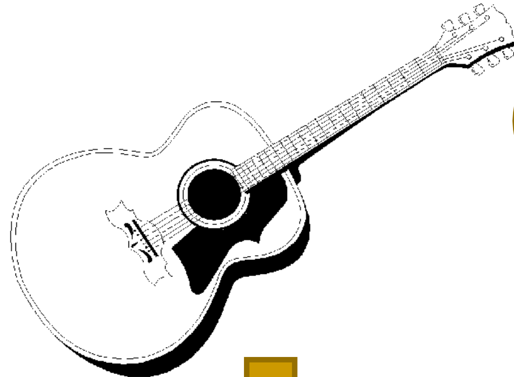
Undoing a Jigsaw Puzzle



- Given two distinct sets of building blocks, can we find which parts of a composition were composed from which blocks

Separating Sounds





$$\mathbf{V}_1 = \mathbf{B}_1 \mathbf{W}_1$$

estimate

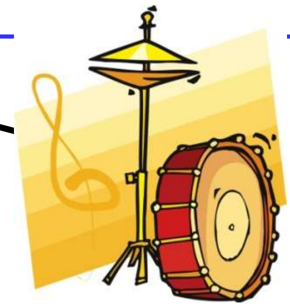
given estimate

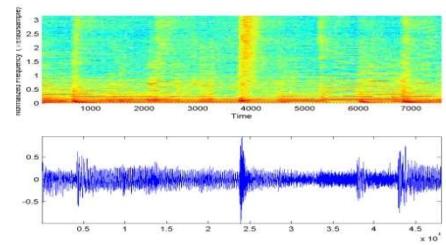
- From example of A, learn blocks A (NMF)

Separating Sounds

$$V_2 = B_2 W_2$$ estimate

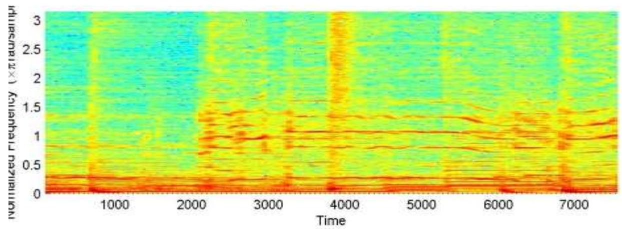
given estimate





- From example of A, learn blocks A (NMF)
- From example of B, learn B (NMF)

Separating Sounds



given

$$\mathbf{V} = \mathbf{B}\mathbf{W}$$

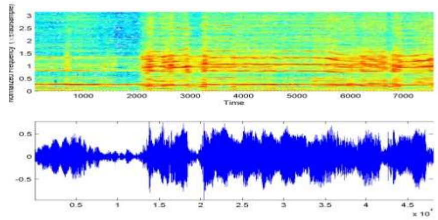
$$\begin{bmatrix} \mathbf{B}_1 & \mathbf{B}_2 \end{bmatrix} \begin{bmatrix} \mathbf{W}_1 \\ \mathbf{W}_2 \end{bmatrix}$$

given

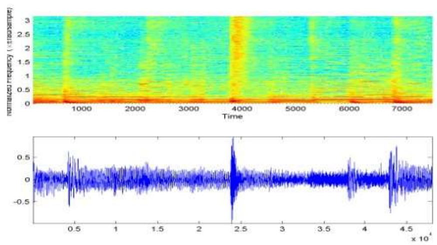
estimate

- From mixture, separate out (NMF)
  - Use known “bases” of both sources
  - Estimate the weights with which they combine in the mixed signal

Separating Sounds



estimate $\mathbf{B}_1\mathbf{W}_1$



estimate $\mathbf{B}_2\mathbf{W}_2$

$$\mathbf{V} = \mathbf{B}\mathbf{W}$$

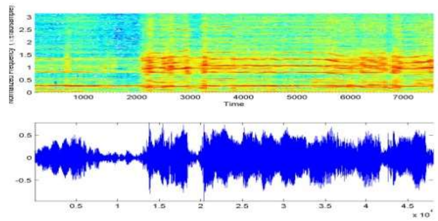
$$\begin{bmatrix}\mathbf{B}_1 & \mathbf{B}_2\end{bmatrix} \begin{bmatrix}\mathbf{W}_1 \\ \mathbf{W}_2\end{bmatrix}$$

given

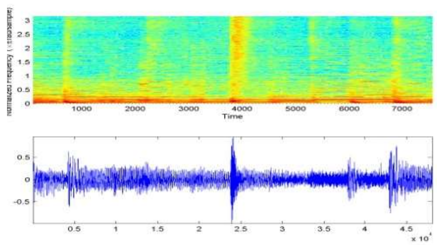
estimate

- Separated signals are estimated as the contributions of the source-specific bases to the mixed signal

Separating Sounds



estimate $\mathbf{B}_1\mathbf{W}_1$



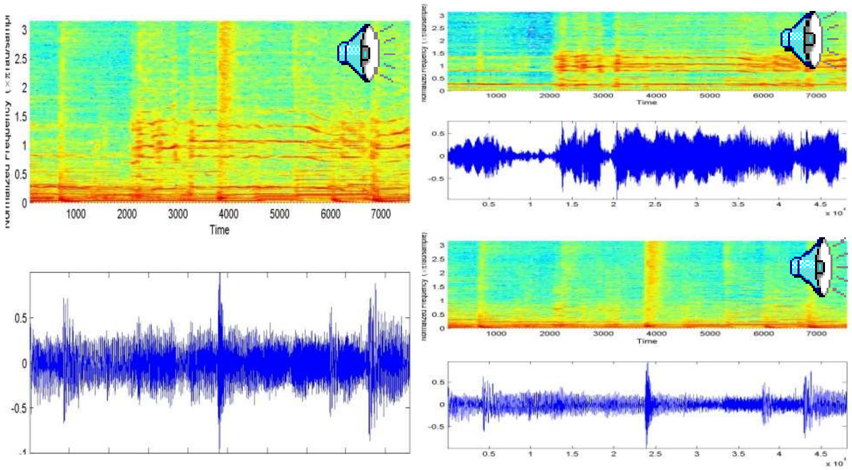
estimate $\mathbf{B}_2\mathbf{W}_2$

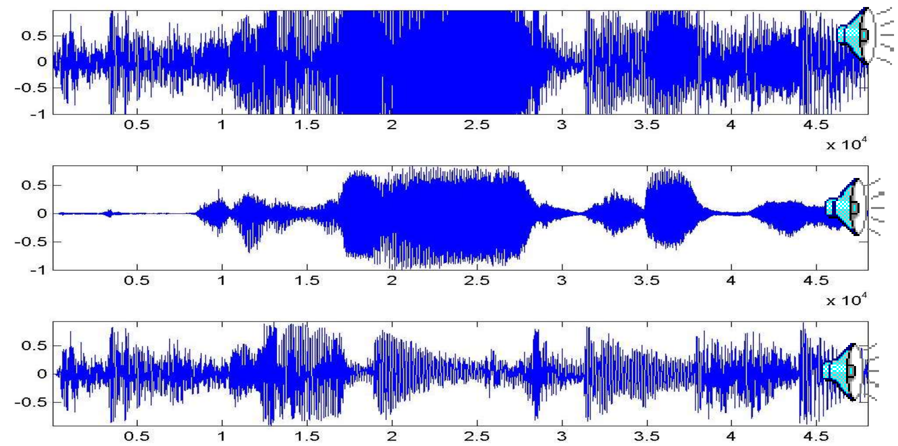
$$\mathbf{V} = \mathbf{B}\mathbf{W}$$

$$\underbrace{[\mathbf{B}_1}_{\text{given}} \quad \underbrace{\boxed{\mathbf{B}_2}]}_{\text{estimate}} \underbrace{\begin{bmatrix} \mathbf{W}_1 \\ \mathbf{W}_2 \end{bmatrix}}_{\text{estimate}}$$

- It is sometimes sufficient to know the bases for only one source
  - The bases for the other can be estimated from the mixed signal itself

Separating Sounds

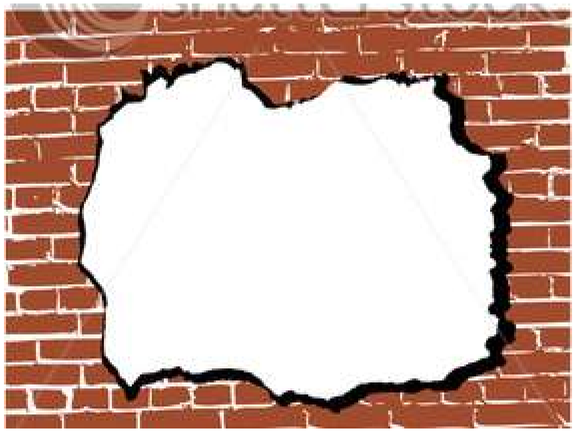


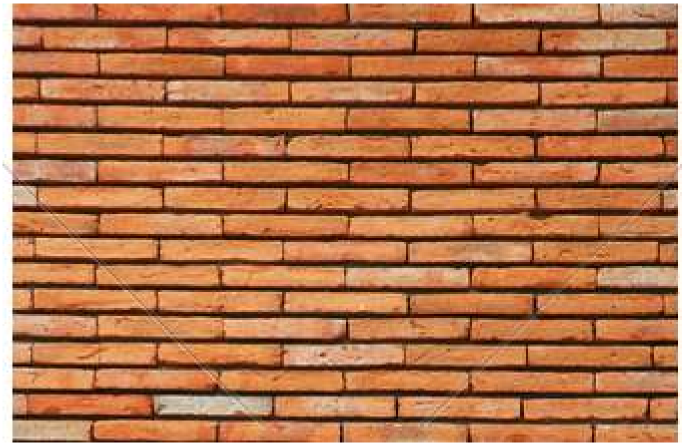


- "Raise my rent" by David Gilmour
- Background music "bases" learnt from 5-seconds of music-only segments within the song
- Lead guitar "bases" bases learnt from the rest of the song

- Norah Jones singing "Sunrise"
- Background music bases learnt from 5 seconds of music-only segments

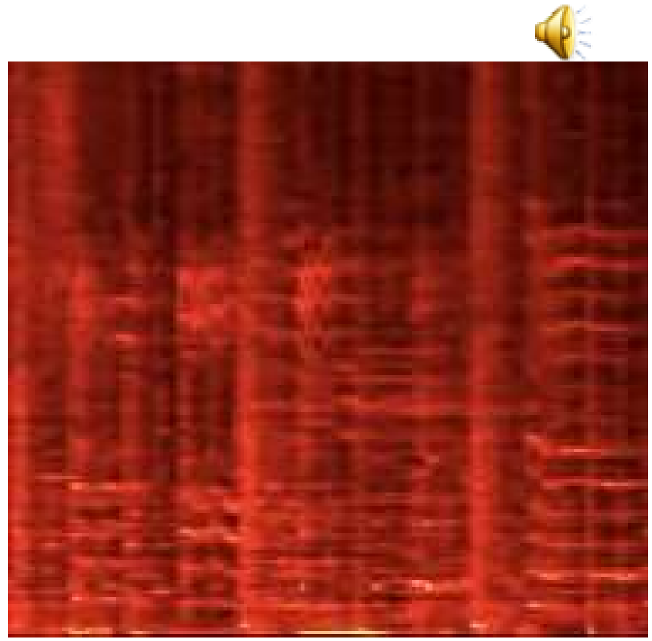
Predicting Missing Data





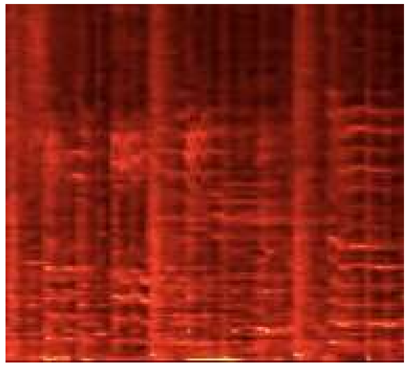
- Use the building blocks to fill in “holes”

Filling in



- Some frequency components are missing (left panel)
- We know the bases
  - But not the mixture weights for any particular spectral frame
- We must "fill in" the holes in the spectrogram
  - To obtain the one to the right

Learn building blocks

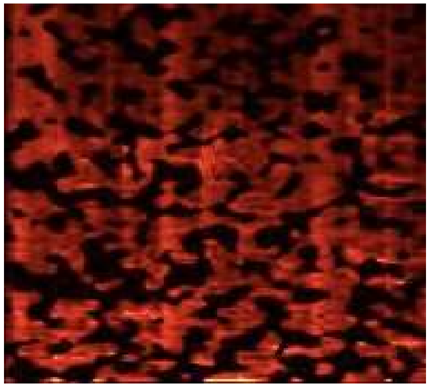


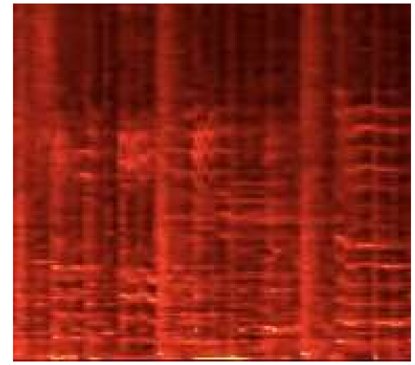
$$\mathbf{V_2} = \mathbf{B_2}\mathbf{W_2}$$ estimate

given estimate

- Learn the building blocks from other examples of similar sounds
  - E.g. music by same singer
  - E.g. from undamaged regions of same recording

Predict data





$$\hat{\mathbf{V}} = \hat{\mathbf{B}}\mathbf{W}$$

estimate

Modified bases (given)

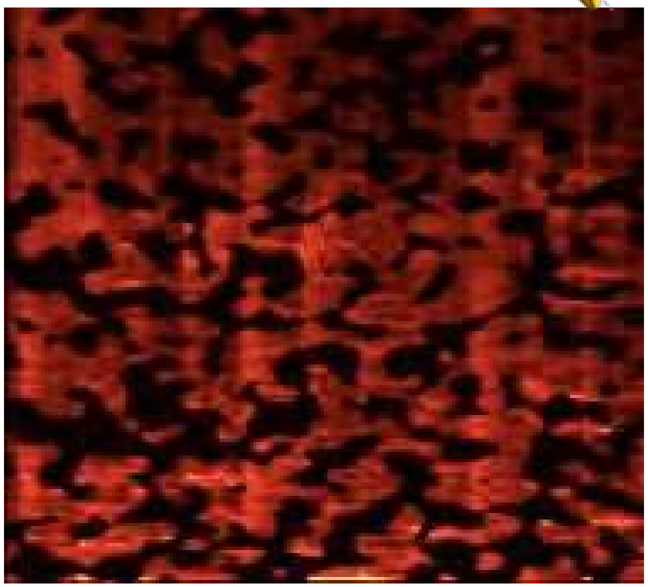
estimate

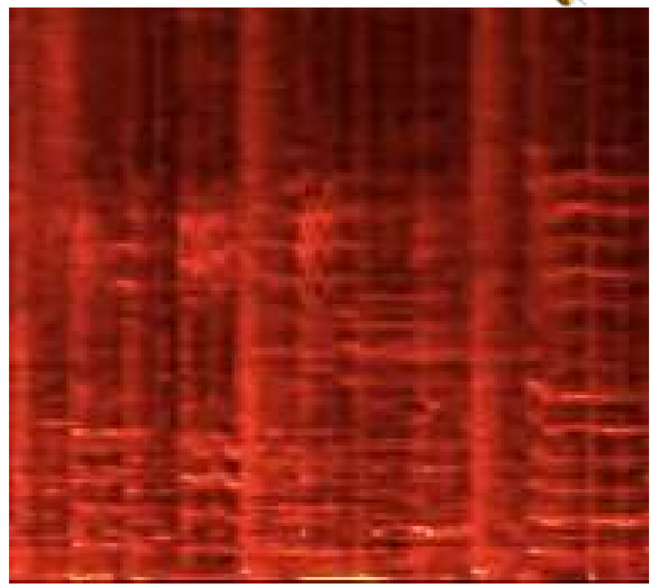
$$\mathbf{V} = \mathbf{B}\mathbf{W}$$

Full bases

- "Modify" bases to look like damaged spectra
  - Remove appropriate spectral components
- Learn how to compose damaged data with modified bases
- Reconstruct missing regions with complete bases

Filling in : An example

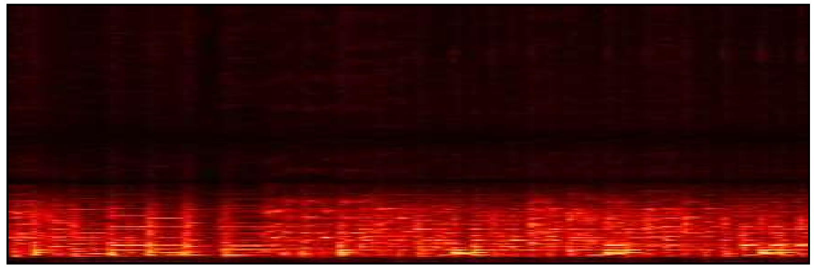




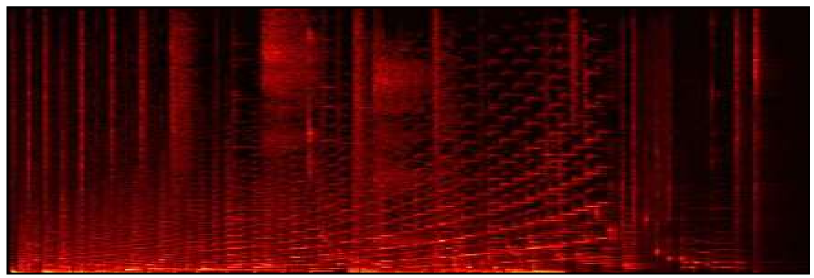
- Madonna…
- Bases learned from other Madonna songs

A more fun example

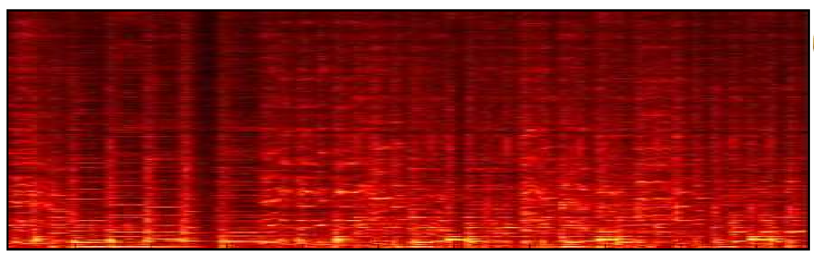
•Reduced BW data



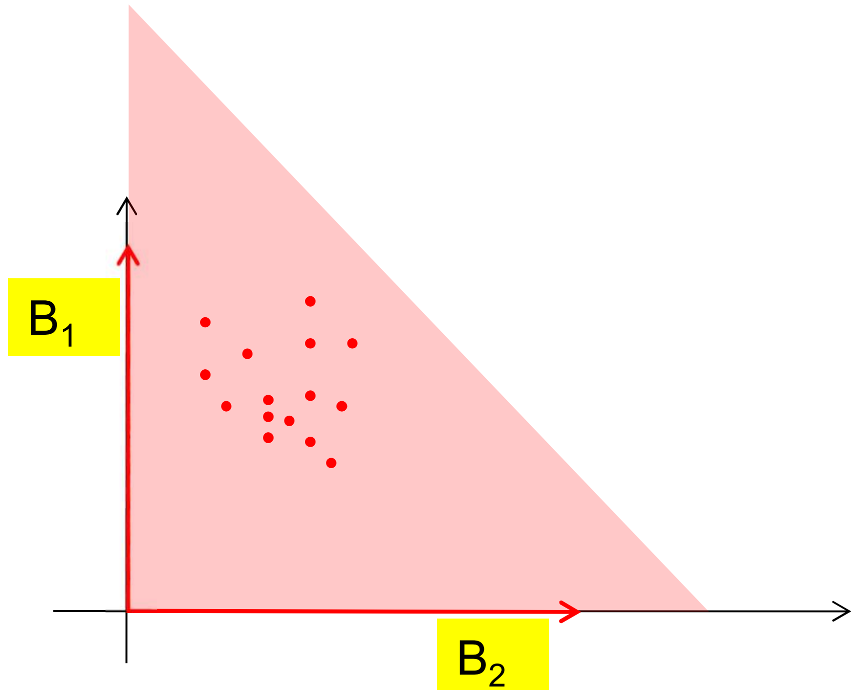
•Bases learned from this



•Bandwidth expanded version



A Natural Restriction

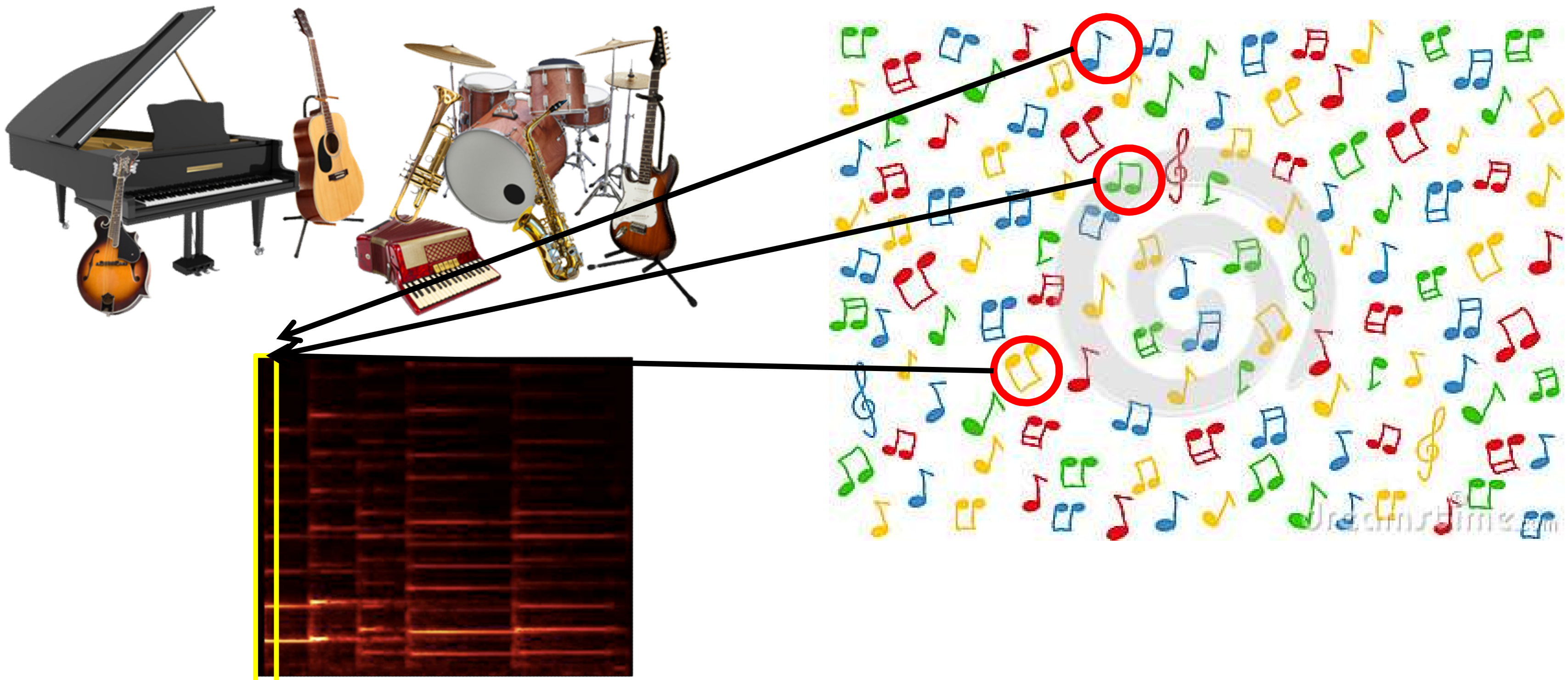


- For K-dimensional data, can learn no more than K-1 bases meaningfully
  - At K bases, simply select the axes as bases
  - The bases will represent *all* data exactly

Its an unnatural restriction

- For K-dimensional spectra, can learn no more than K-1 bases
- Nature does not respect the dimensionality of your spectrogram
- E.g. Music: There are tens of instruments
  - Each can produce dozens of unique notes
  - Amounting to a total of many thousands of notes
  - Many more than the dimensionality of the spectrum
- E.g. images: a 1024 pixel image can show millions of recognizable pictures!
  - Many more than the number of pixels in the image

Fixing the restriction: Updated model

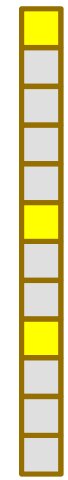


- Can have a *very large* number of building blocks (bases)
  - E.g. notes
- But any *particular* frame is composed of only a small subset of bases
  - E.g. any single frame only has a small set of notes

The Modified Model

$$\mathbf{V} = \mathbf{B}\mathbf{W} \qquad V = \mathbf{B}W$$

For one vector



- **Modification 1:**
  - In any column of **W**, only a small number of entries have non-zero value
  - I.e. the columns of **W** are *sparse*
  - These are *sparse* representations
- **Modification 2:**
  - **B** may have more columns than rows
  - These are called *overcomplete* representations

- Sparse representations need not be overcomplete, but the reverse will generally not provide useful decompositions

Imposing Sparsity

$$\mathbf{V} = \mathbf{BW}$$

$$E = Div(\mathbf{V}, \mathbf{BW})$$

$$Q = Div(\mathbf{V}, \mathbf{BW}) + \lambda \,|\, \mathbf{W} \,|_0$$

- Minimize a modified objective function
- Combines divergence and ell-0 norm of **W**
  - The number of non-zero elements in **W**
- Minimize Q instead of E
  - Simultaneously minimizes both divergence and number of active bases at any time

Imposing Sparsity

$$\mathbf{V} = \mathbf{BW}$$

$$Q = Div(\mathbf{V}, \mathbf{BW}) + \cancel{\lambda |\mathbf{W}|_0}$$

$$Q = Div(\mathbf{V}, \mathbf{BW}) + \lambda |\mathbf{W}|_1$$

- Minimize the ell-0 norm is hard
  - Combinatorial optimization
- Minimize ell-1 norm instead
  - The sum of all the entries in W
  - *Relaxation*
- Is equivalent to minimize ell-0
  - We cover this equivalence later
- Will also result in sparse solutions

Update Rules

- Modified Iterative solutions
  - In gradient based solutions, gradient w.r.t any W term now includes λ
  - I.e. if $\mathrm{d}Q/\mathrm{d}W = \mathrm{d}E/\mathrm{d}W + \lambda$

- For KL Divergence, results in following modified update rules

$$B = B \otimes \frac{\left(\frac{V}{BW}\right) W^T}{1 W^T} \qquad W = W \otimes \frac{B^T \left(\frac{V}{BW}\right)}{B^T 1 + \lambda}$$

- Increasing λ makes the weights increasingly sparse

Update Rules

- Modified Iterative solutions
  - In gradient based solutions, gradient w.r.t any W term now includes λ
  - I.e. if $\mathrm{d}Q/\mathrm{d}W = \mathrm{d}E/\mathrm{d}W + \lambda$

- Both **B** and **W** can be made sparse

$$B = B \otimes \frac{\left(\frac{V}{BW}\right)W^T}{1W^T + \lambda_b}$$

$$W = W \otimes \frac{B^T\left(\frac{V}{BW}\right)}{B^T 1 + \lambda_w}$$

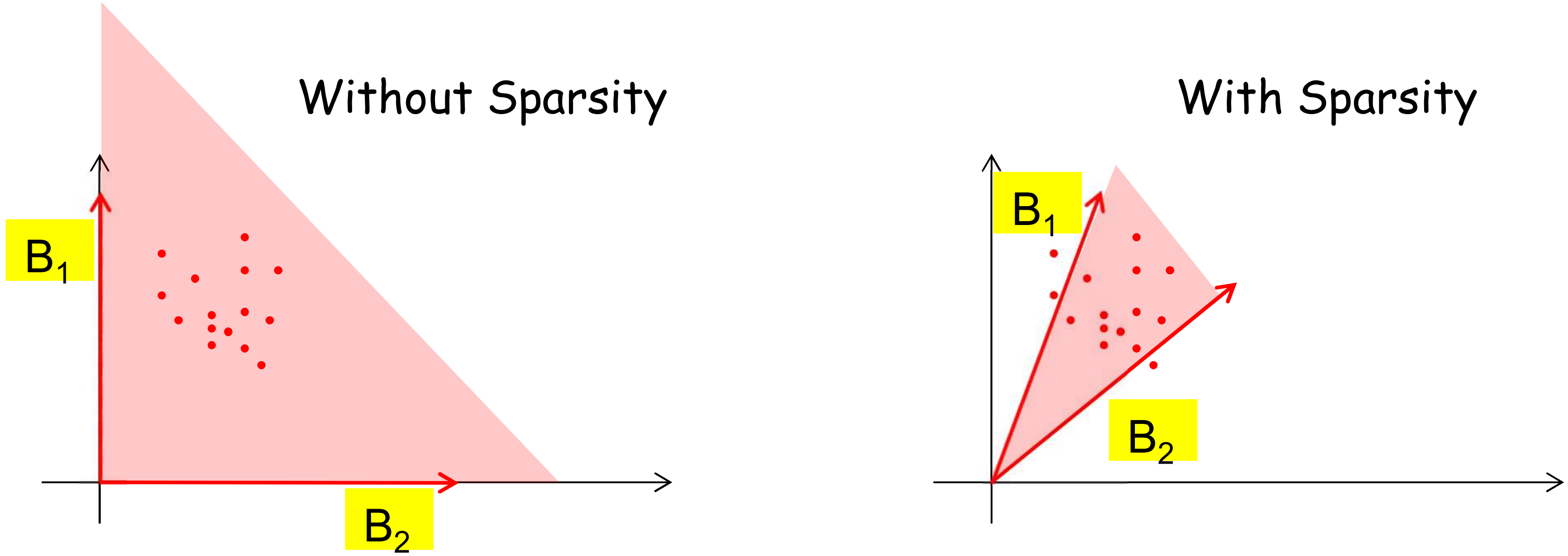
What about Overcompleteness?

- Use the same solutions
- Simply make **B** wide!
  - **W** must be made sparse

$$B = B \otimes \frac{\left(\frac{V}{BW}\right) W^T}{1 W^T}$$

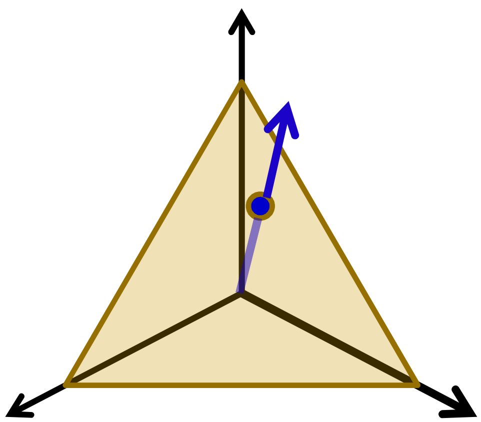
$$W = W \otimes \frac{B^T \left(\frac{V}{BW}\right)}{B^T 1 + \lambda_w}$$

Sparsity: What do we learn

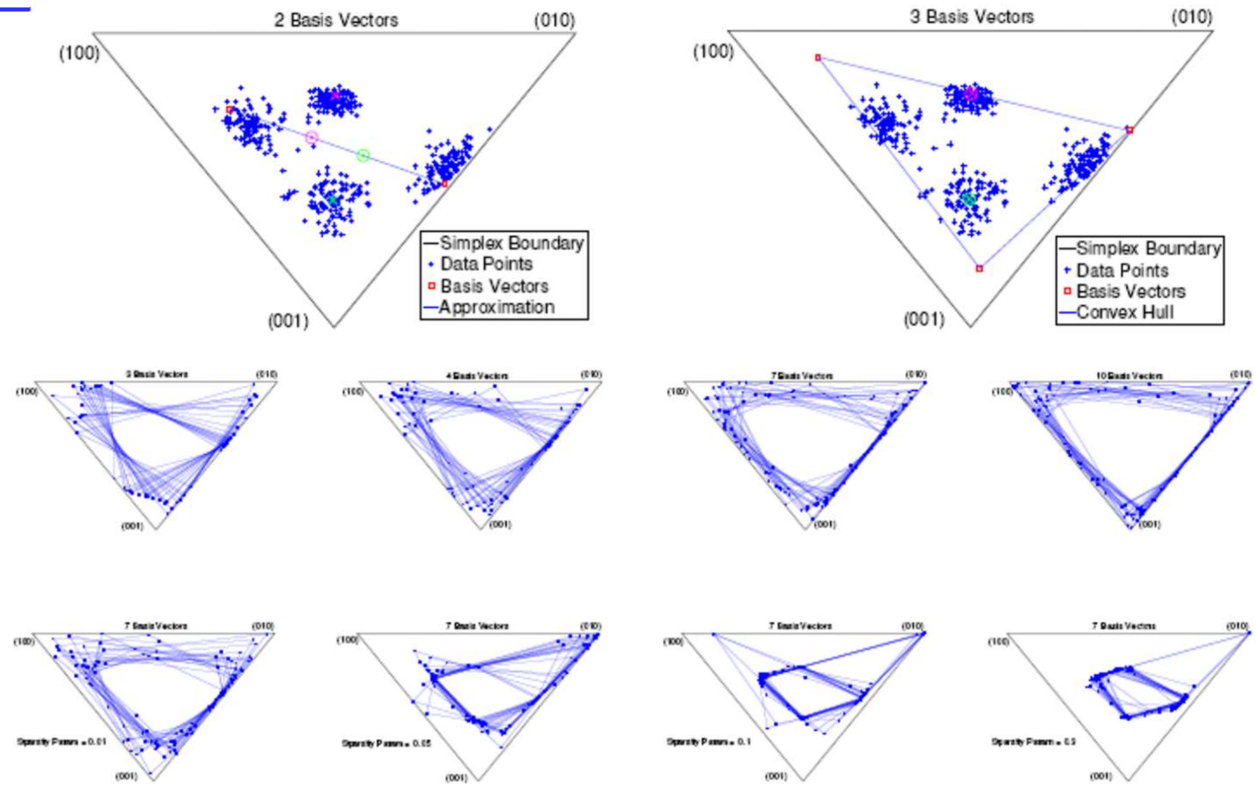


- Without sparsity: The model has an implicit limit: can learn no more than D-1 useful bases
  - If K >= D, we can get uninformative bases
- Sparsity: The bases are "pulled towards" the data
  - Representing the distribution of the data much more effectively

Sparsity: What do we learn

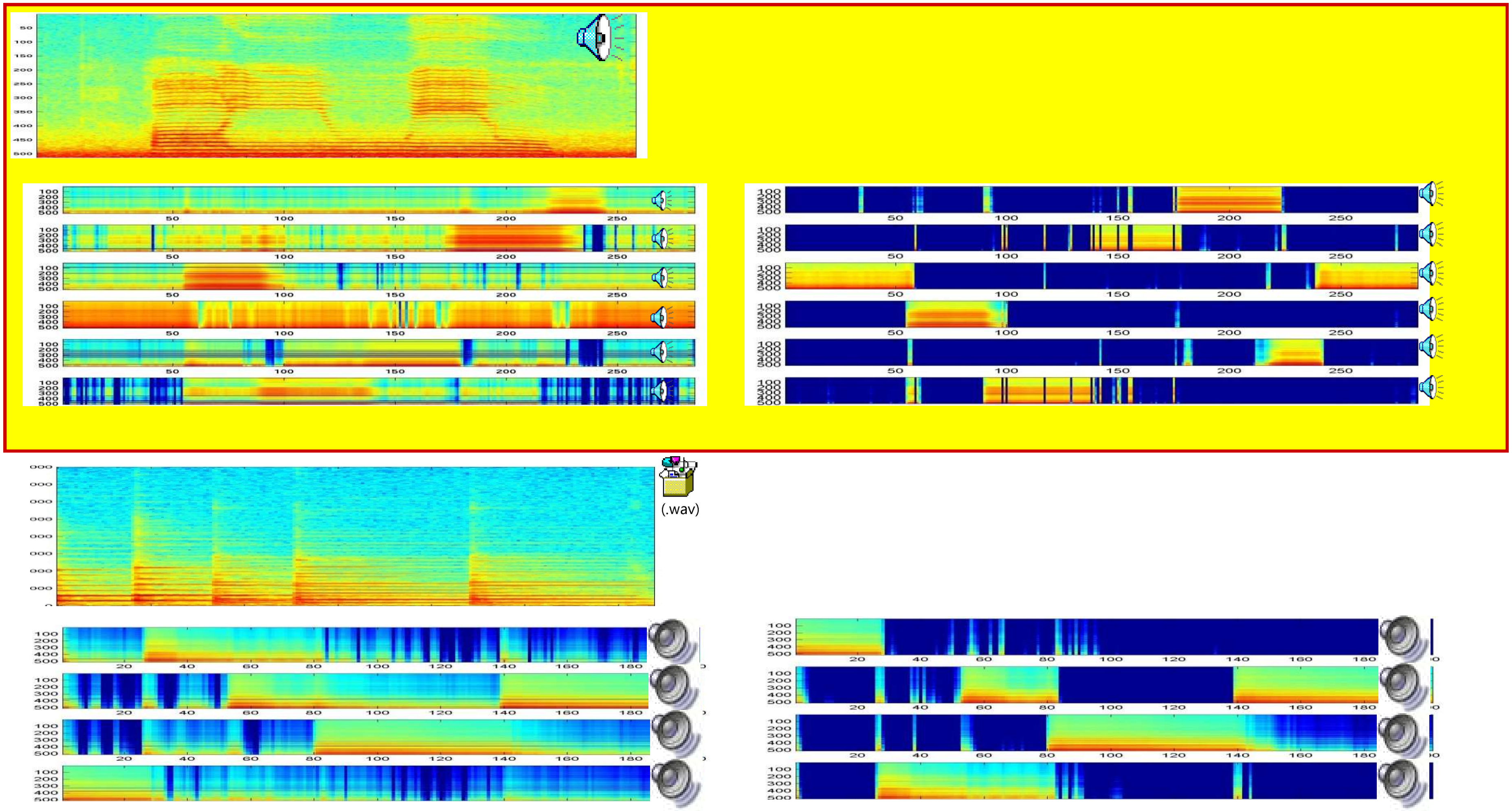


Each dot represents a location where a vector "pierces" the simplex



- Top and middle panel: Compact (non-sparse) estimator
  - As the number of bases increases, bases migrate towards corners of the orthant
- Bottom panel: Sparse estimator
  - Cone formed by bases shrinks to fit the data

The Vowels and Music Examples

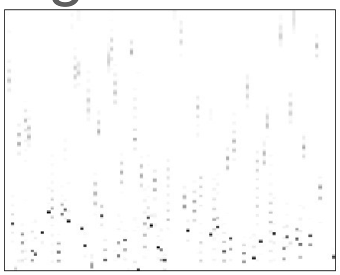


- Left panel, Compact learning: most bases have significant energy in all frames
- Right panel, Sparse learning: Fewer bases active within any frame
  - Decomposition into basic sounds is cleaner

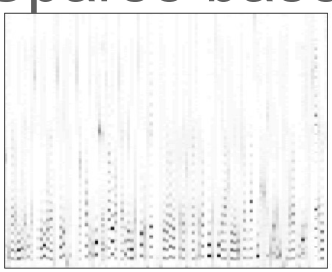
Sparse Overcomplete Bases: Separation

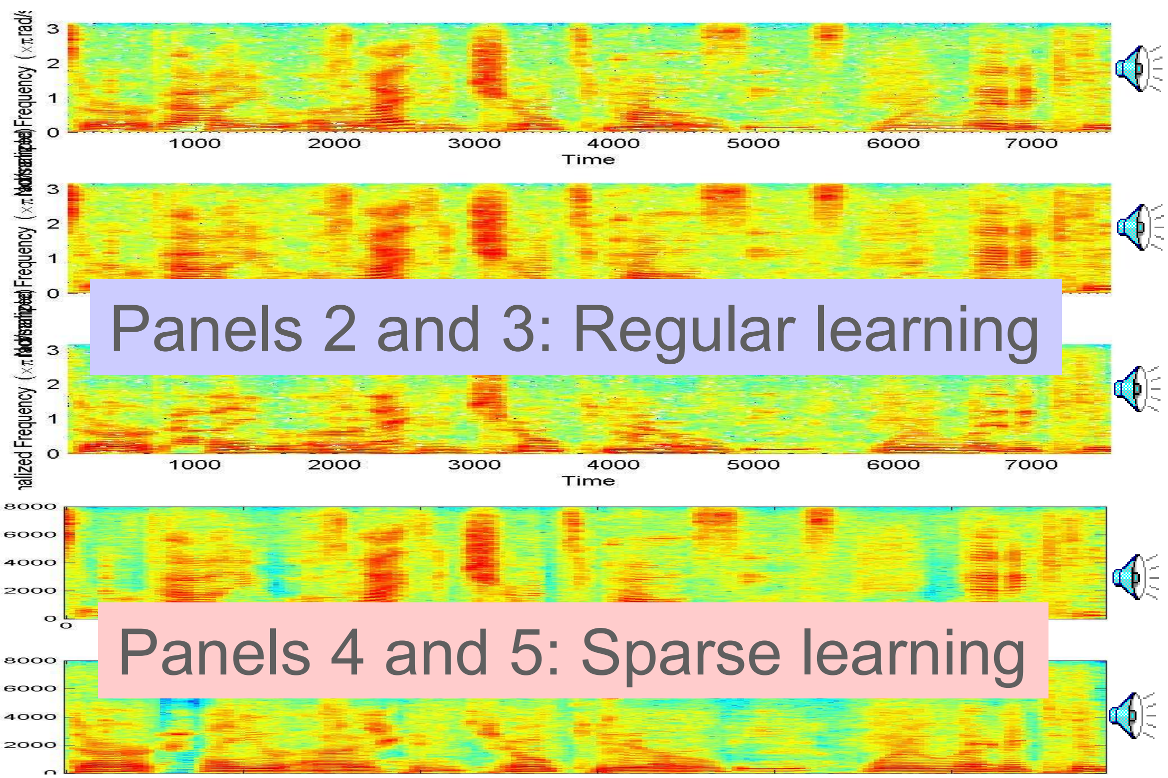
- 3000 bases for each of the speakers
  - The speaker-to-speaker ratio typically doubles (in dB) w.r.t compact bases

Regular bases



Sparse bases



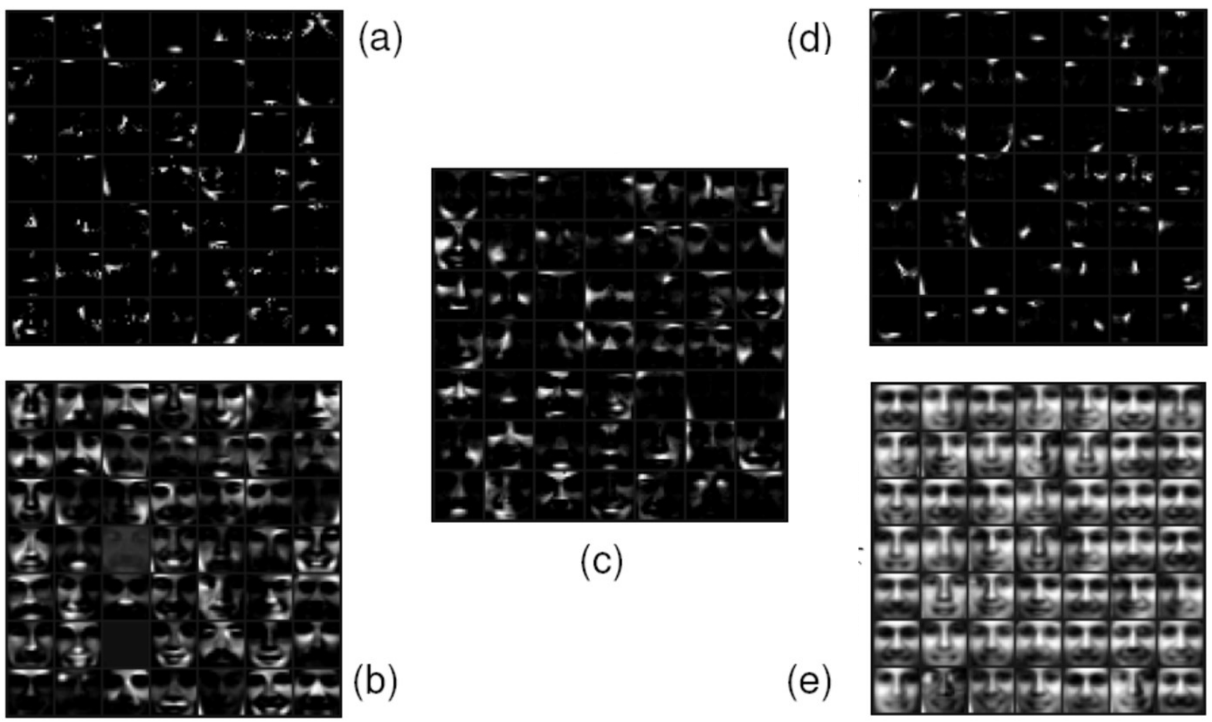


Sparseness: what do we learn

- As solutions get more sparse, bases become more informative
  - In the limit, each basis is a complete face by itself.
  - Mixture weights simply select face

Sparse bases

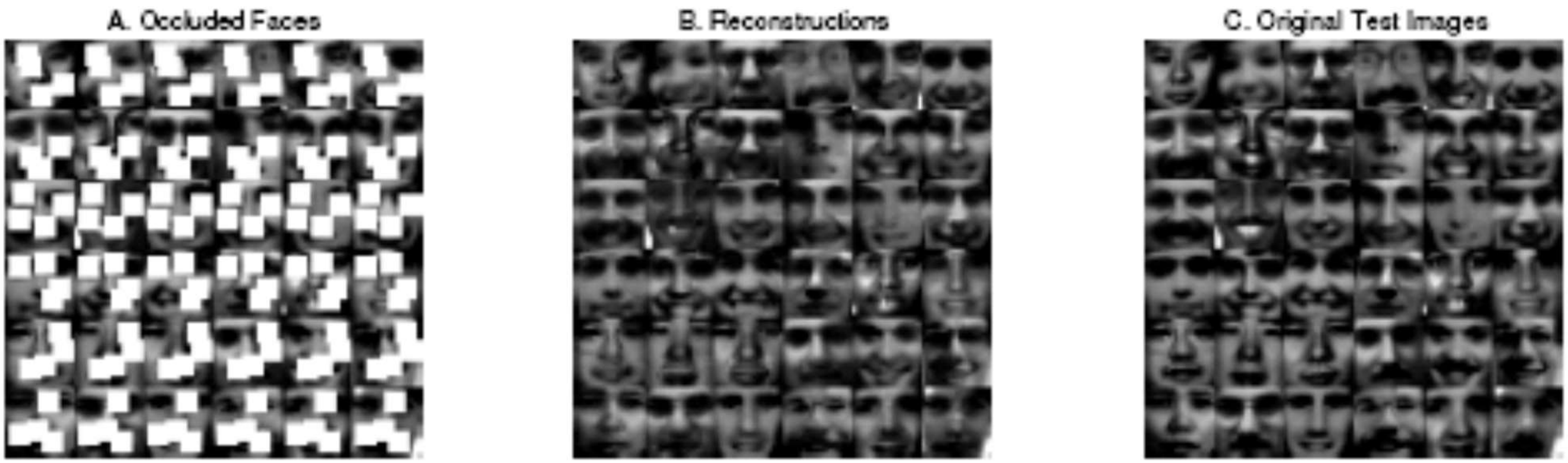
“Dense” weights

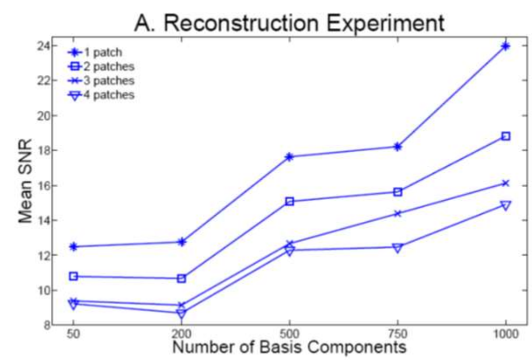


Dense bases

Sparse weights

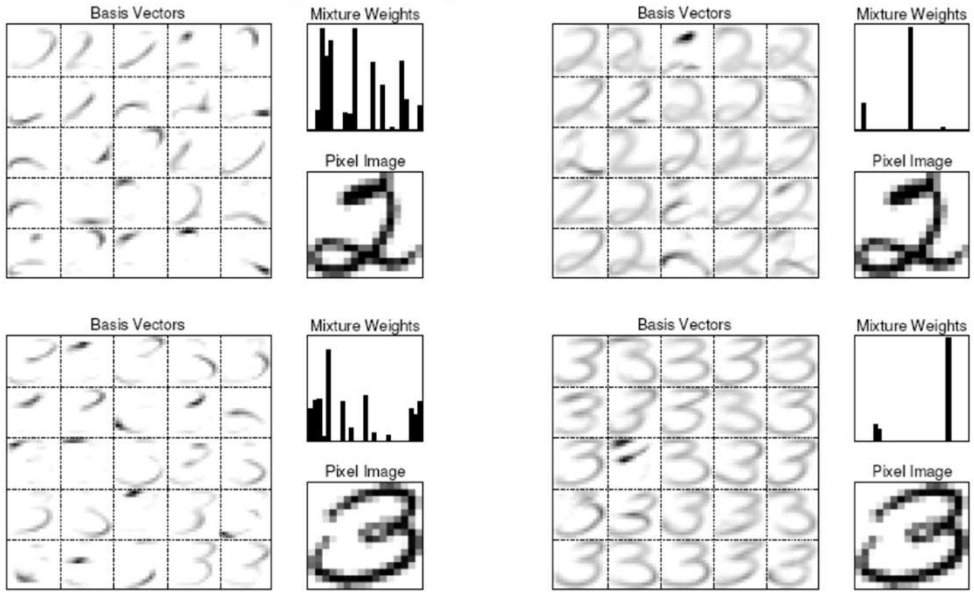
Filling in missing information

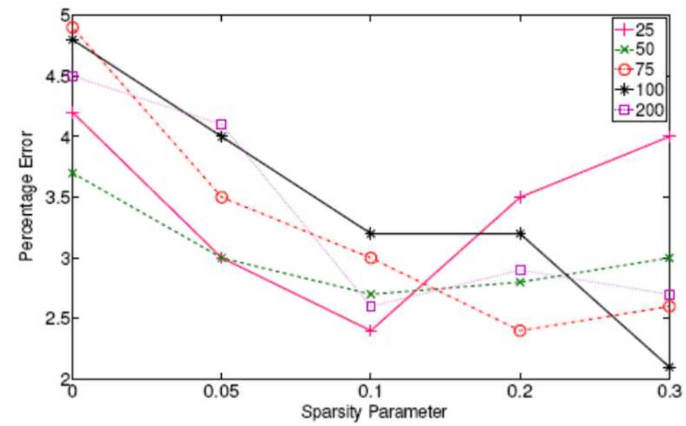




- 19x19 pixel images (361 pixels)
- 1000 bases trained from 2000 faces
- SNR of reconstruction from overcomplete basis set more than 10dB better than reconstruction from corresponding “compact” (regular) basis set

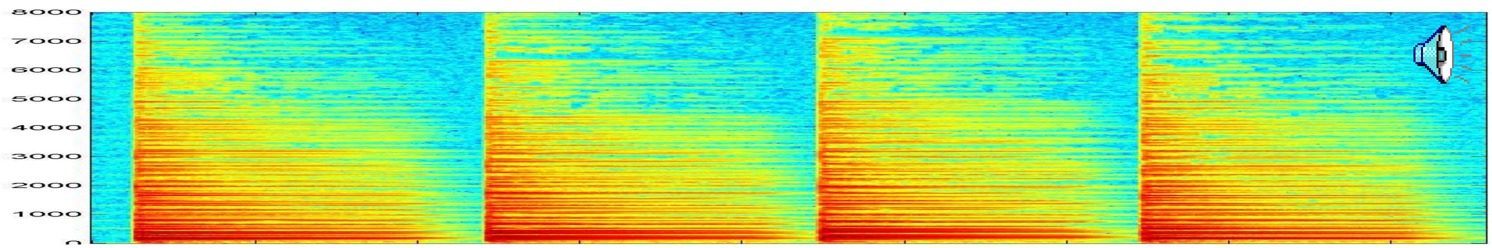
Sparse decomposition for





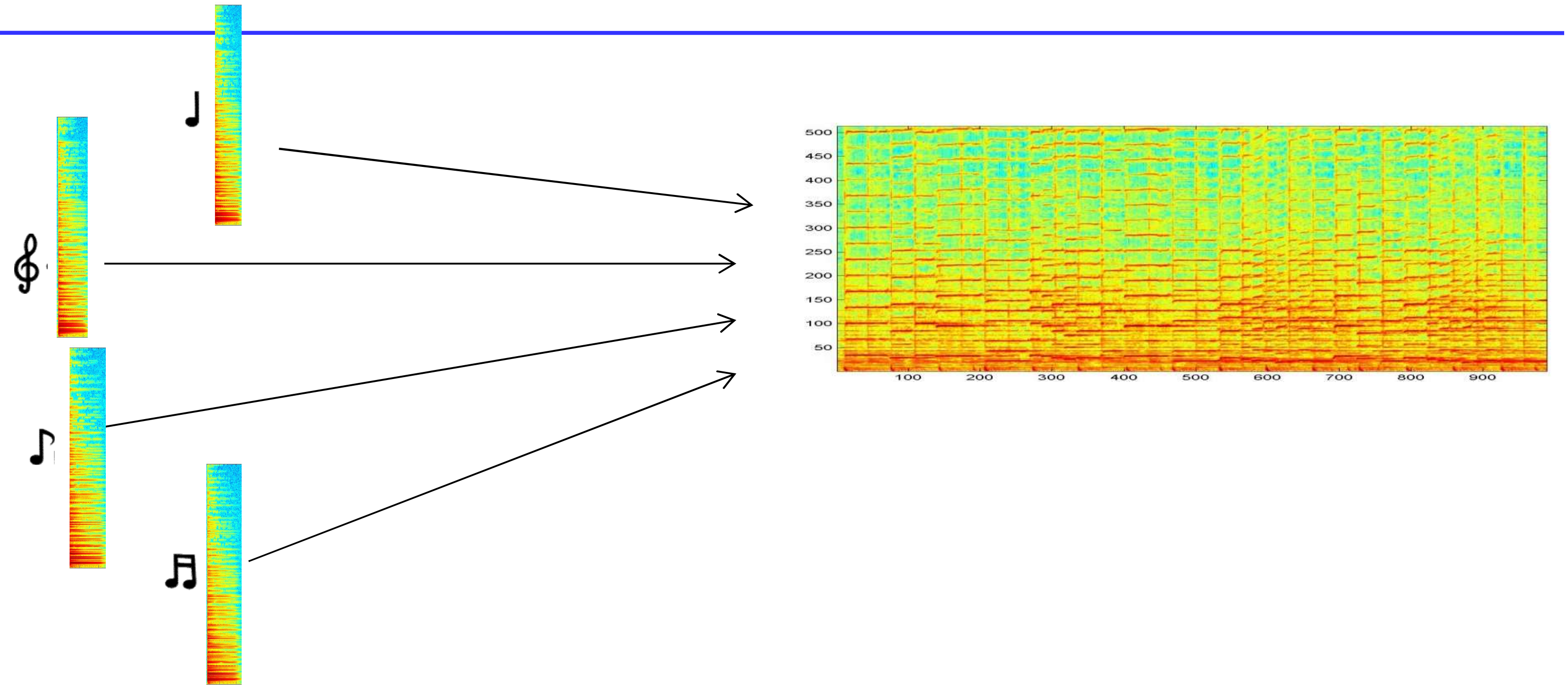
- Given a number of examples of handwritten instances of numbers “2” and “3”
  - Find bases for “2” and “3”
- For any test instance, attempt to construct it using the bases for 2 and (separately) the bases for 3
- The set whose bases result in the better reconstruction is selected
- Accuracy improves with increasing sparsity

Extending the model



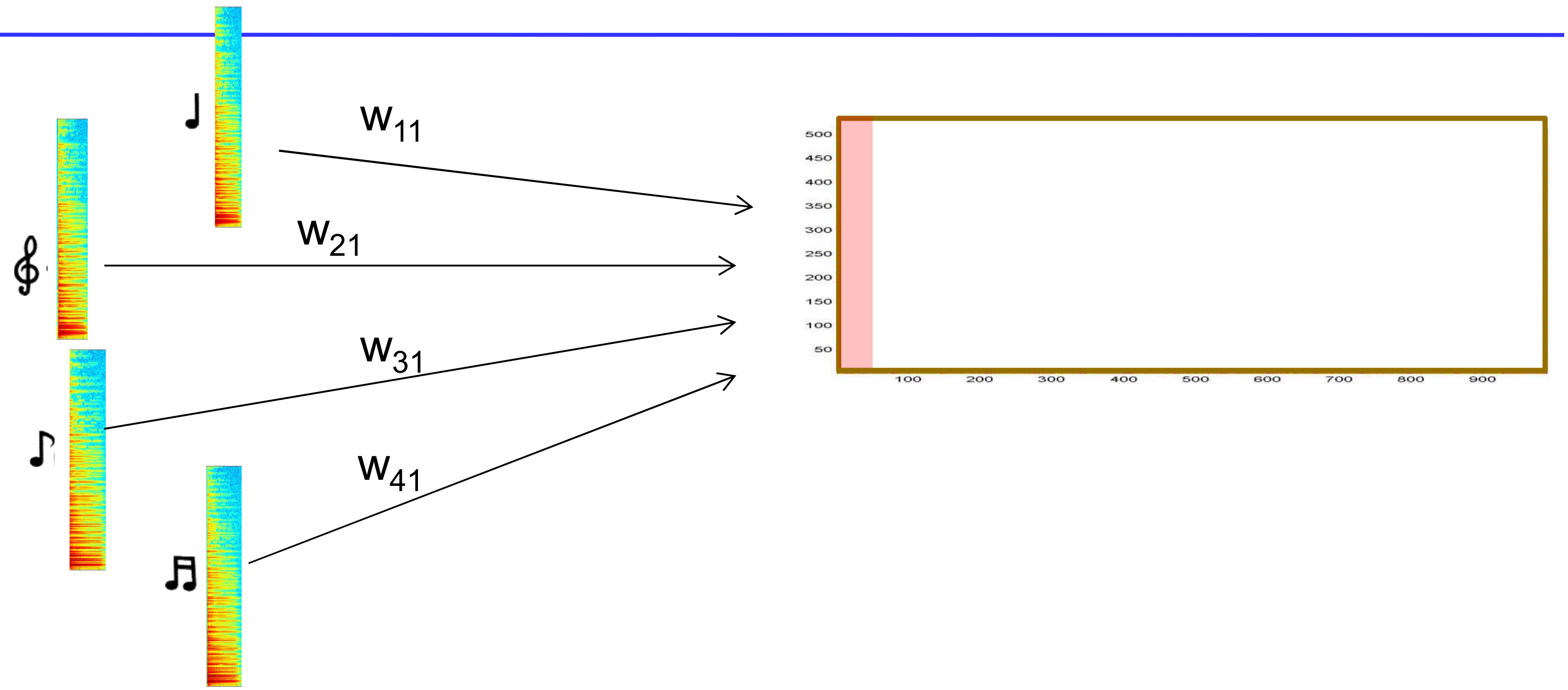
- In reality our building blocks are not spectra
- They are spectral patterns!
  - Which change with time

Convolutive NMF



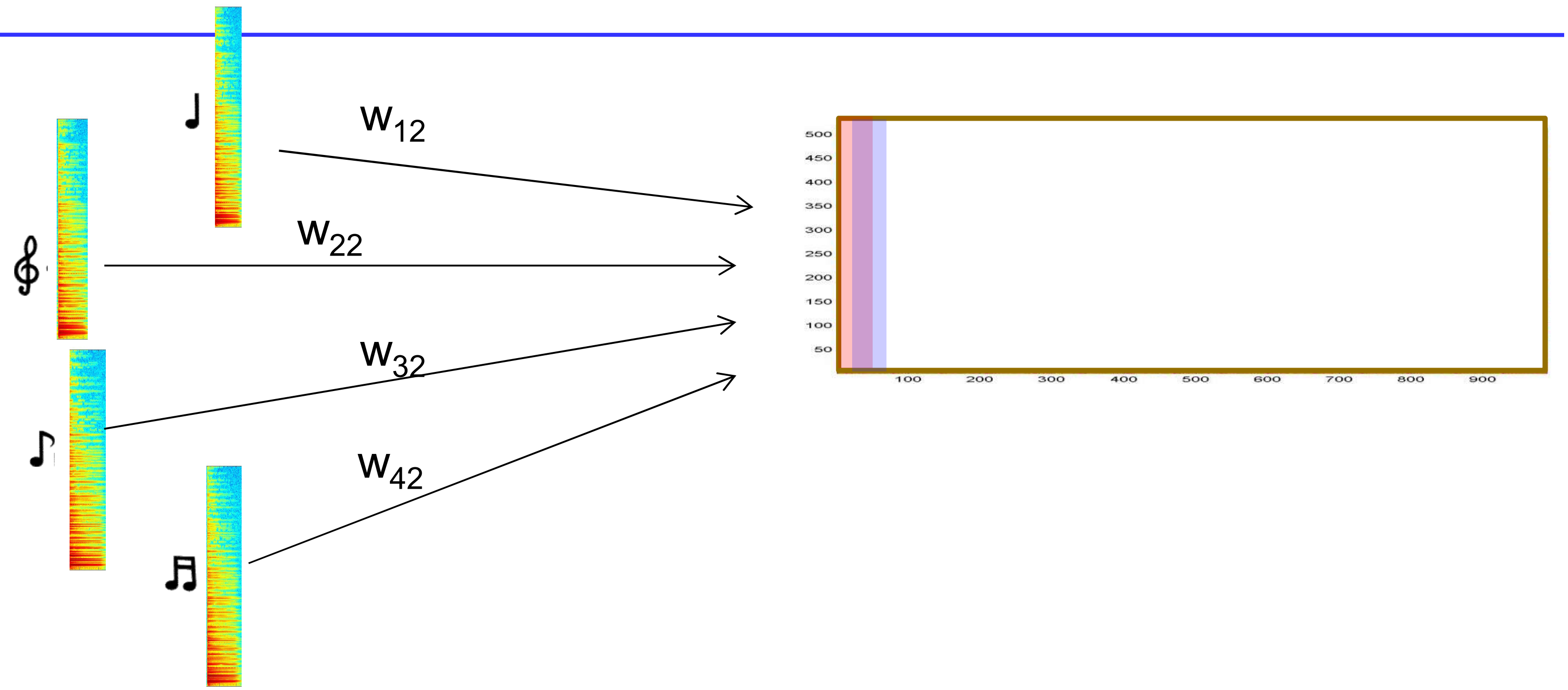
- The building blocks of sound are spectral patches!

Convolutive NMF



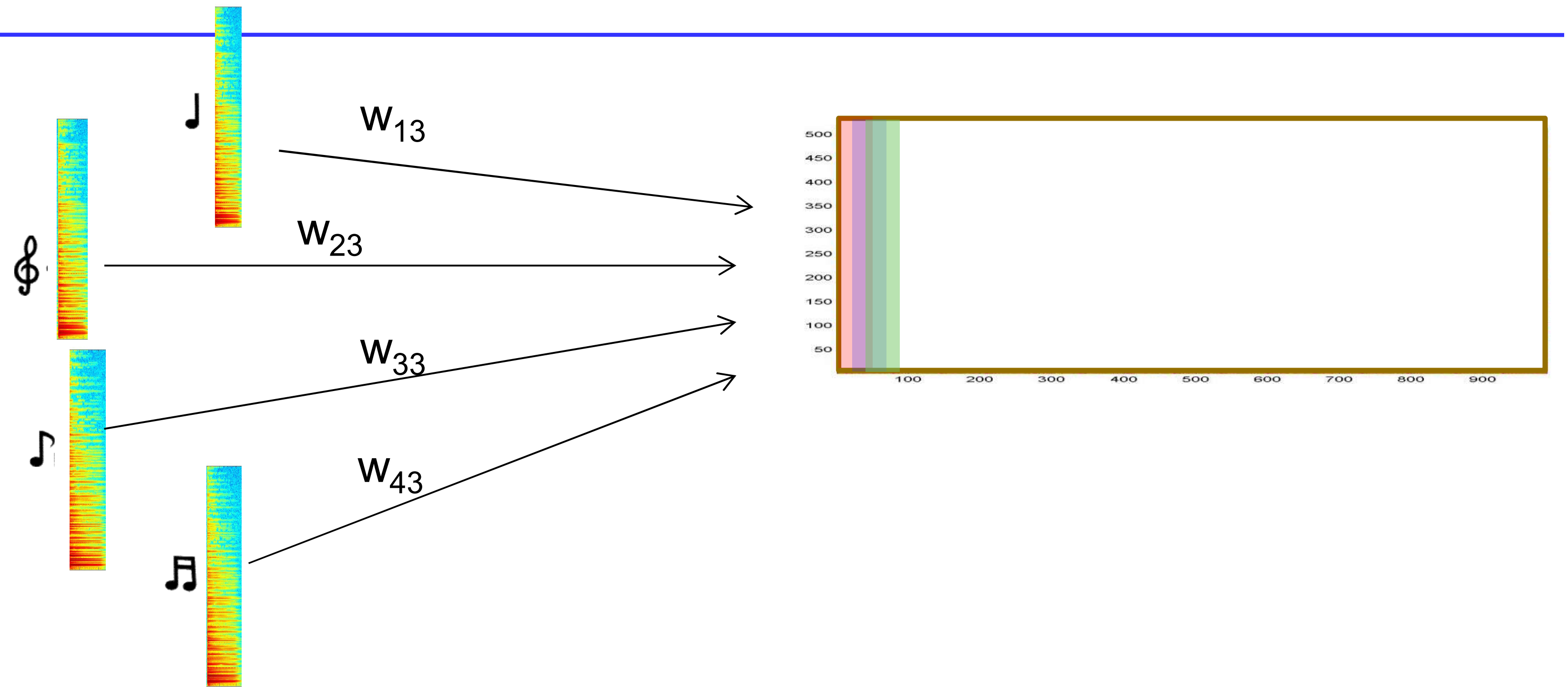
- The building blocks of sound are spectral patches!
- At each time, they combine to compose a patch starting from that time
- Overlapping patches *add*

Convolutive NMF



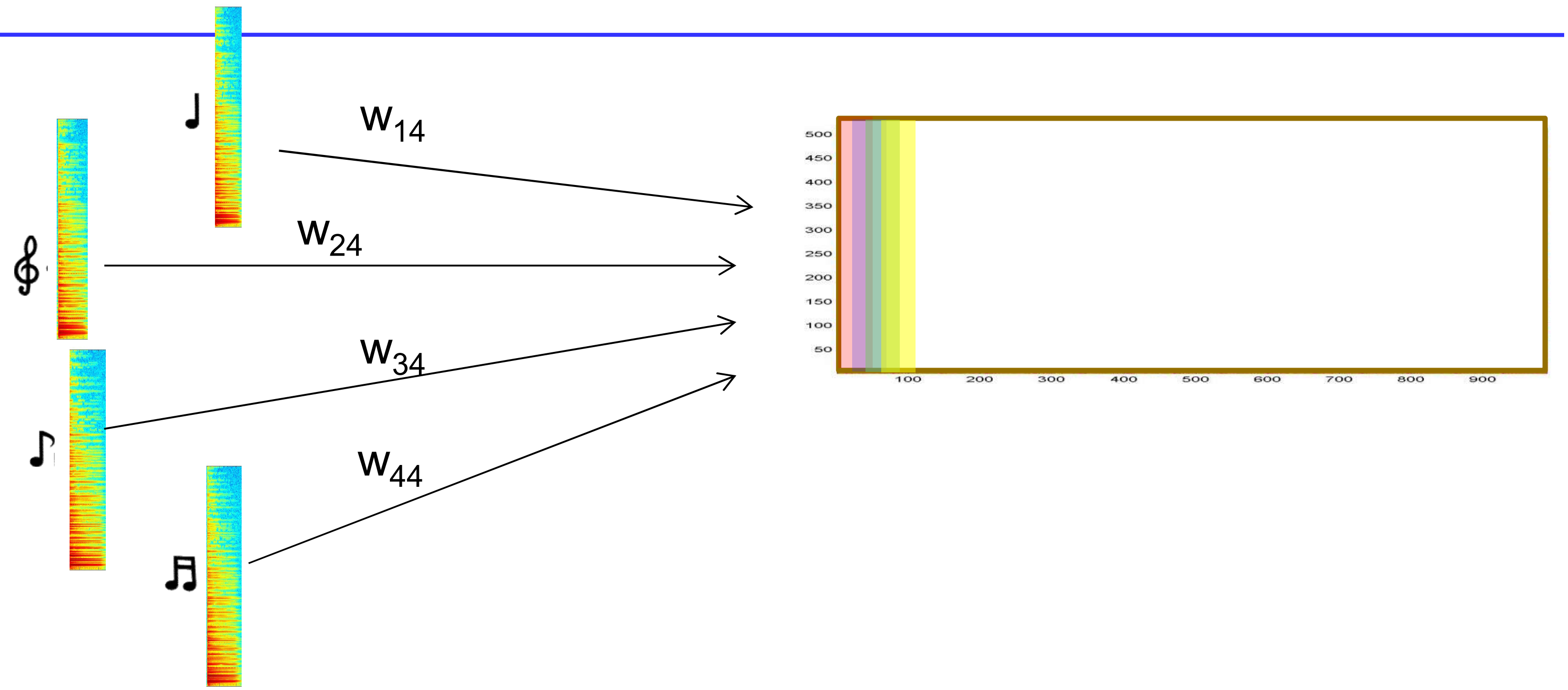
- The building blocks of sound are spectral patches!
- At each time, they combine to compose a patch starting from that time
- Overlapping patches *add*

Convolutive NMF



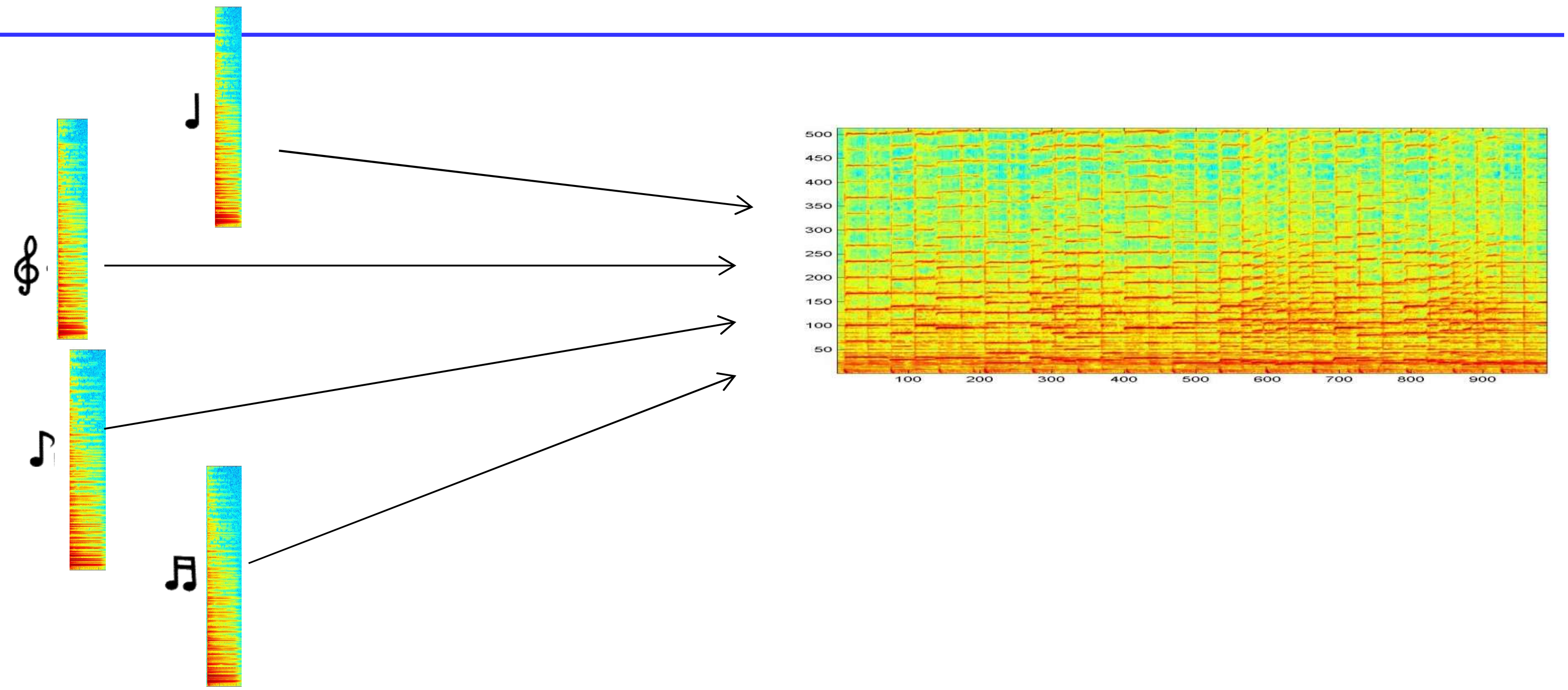
- The building blocks of sound are spectral patches!
- At each time, they combine to compose a patch starting from that time
- Overlapping patches *add*

Convolutive NMF



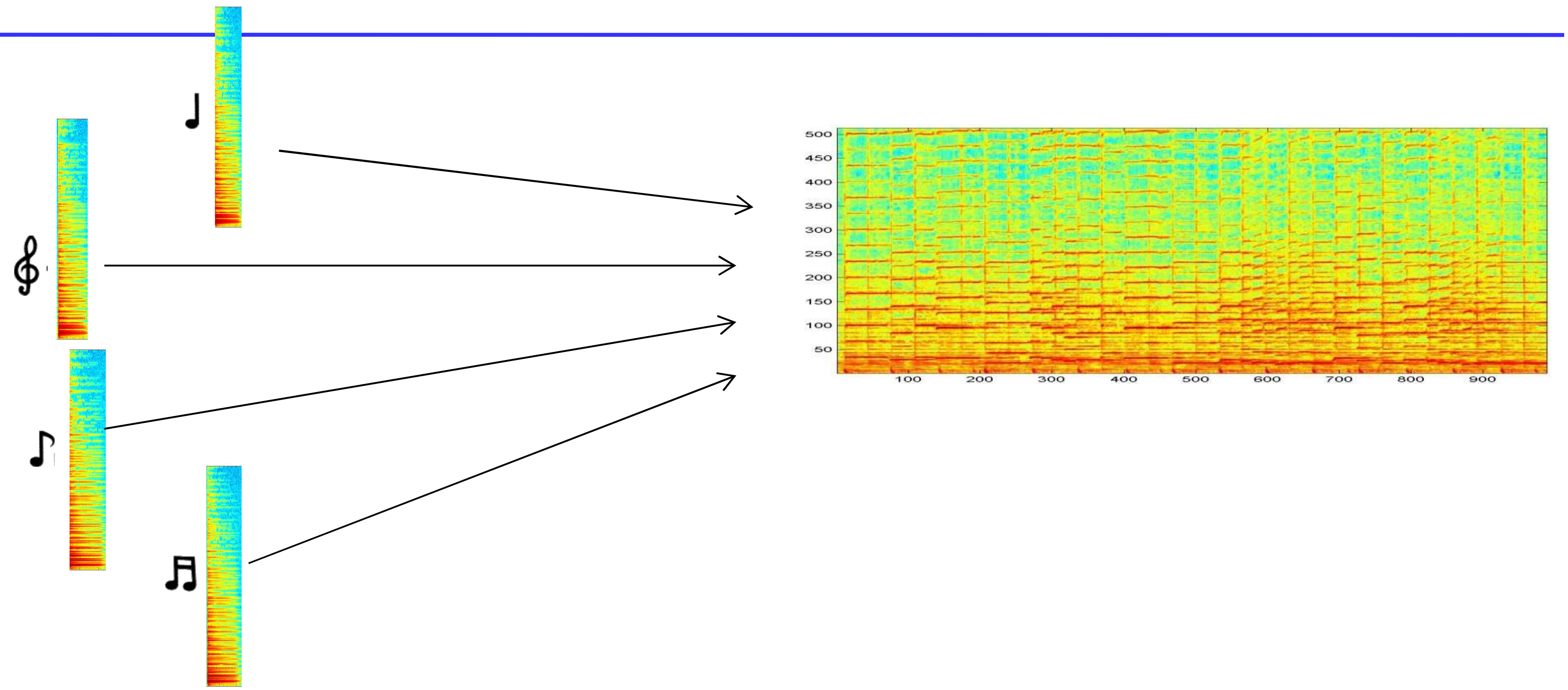
- The building blocks of sound are spectral patches!
- At each time, they combine to compose a patch starting from that time
- Overlapping patches *add*

Convolutive NMF



- The building blocks of sound are spectral patches!
- At each time, they combine to compose a patch starting from that time
- Overlapping patches *add*

In Math

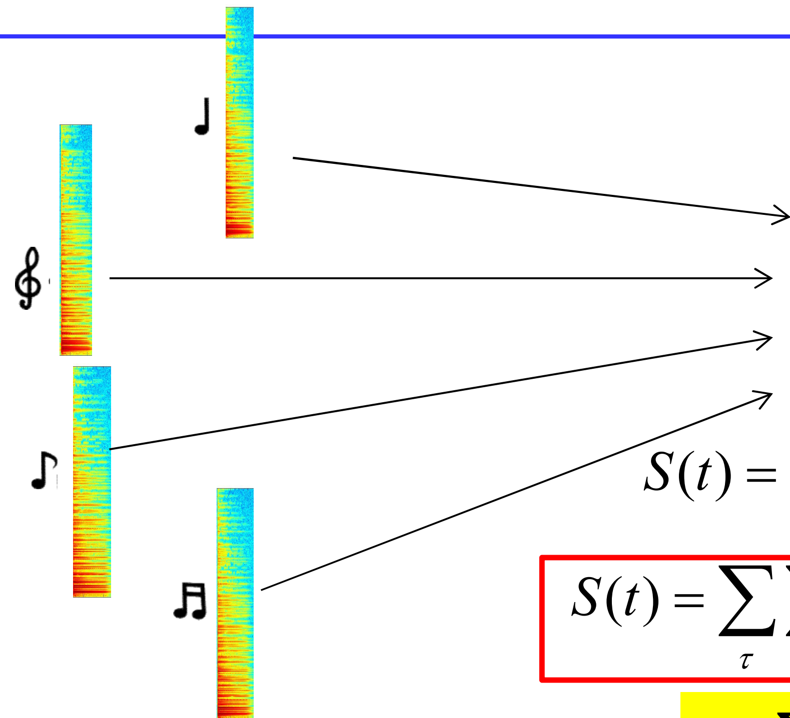


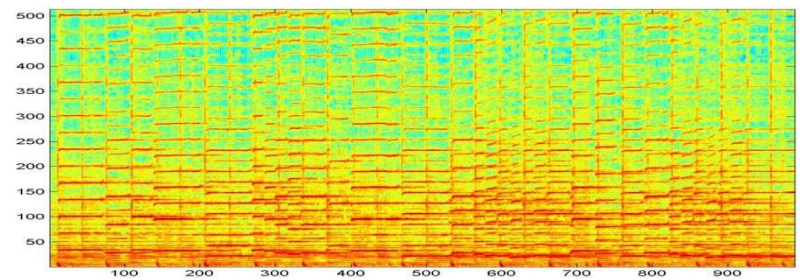
$$S(t)=\sum_i w_i(0)B_i(t)+\sum_i w_i(1)B_i(t-1)+\sum_i w_i(2)B_i(t-2)+\ldots.=\sum_i\sum_\tau w_i(\tau)B_i(t-\tau)$$

$$S(t)=\sum_i B_i(t)\otimes w_i(t)$$

- Each spectral frame has contributions from several previous shifts

An Alternate Repesentation





$$S(t) = \sum_i \sum_\tau w_i(\tau) B_i(t-\tau) = \sum_i \sum_\tau w_i(t-\tau) B_i(\tau)$$

$$\boxed{S(t) = \sum_\tau \sum_i B_i(\tau) w_i(t-\tau)}$$

$$\mathbf{S} = \sum_\tau \mathbf{B}(\tau) \overset{\tau\rightarrow}{\mathbf{W}}$$

- $\mathbf{B}(t)$ is a matrix composed of the t-th columns of all bases
  - The i-th column represents the i-th basis
- W is a matrix whose i-th row is sequence of weights applied to the i-th basis
  - The superscript t→ represents a right shift by t

Convolutive NMF

$$\hat{\mathbf{S}} = \sum_{\tau} \mathbf{B}(\tau)\overrightarrow{\mathbf{W}}$$

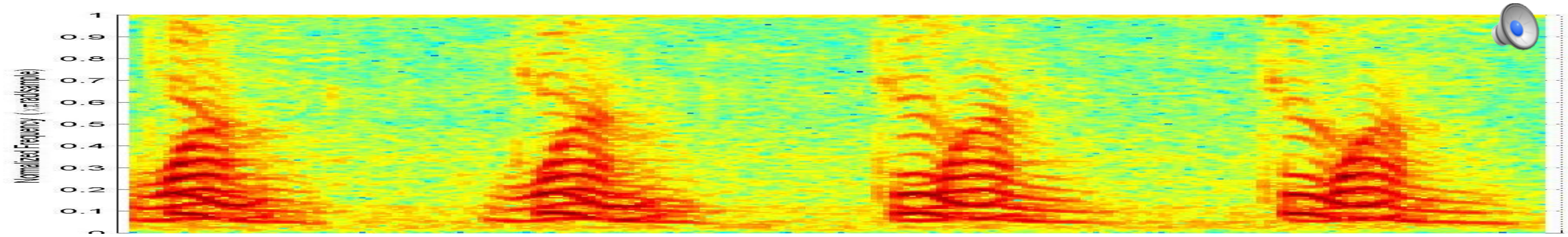
$$\mathbf{B}(t) = \mathbf{B}(t) \otimes \frac{\frac{\mathbf{S}}{\hat{\mathbf{S}}} \overset{t}{\overrightarrow{\mathbf{W}}}^{T}}{\mathbf{1}.\overset{t}{\overrightarrow{\mathbf{W}}}^{T}} \qquad \mathbf{W} = \frac{1}{T}\sum_{t} \mathbf{W} \otimes \frac{\mathbf{B}(t)\overset{t}{\overleftarrow{\left[\frac{\mathbf{S}}{\hat{\mathbf{S}}}\right]}}}{\mathbf{B}(t)^{T}\mathbf{1}}$$

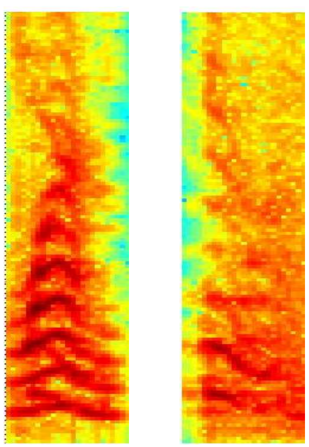
- Simple learning rules for **B** and **W**
- Identical rules to estimate **W** given **B**
  - Simply don’t update **B**
- Sparsity can be imposed on **W** as before if desired

The Convolutive Model

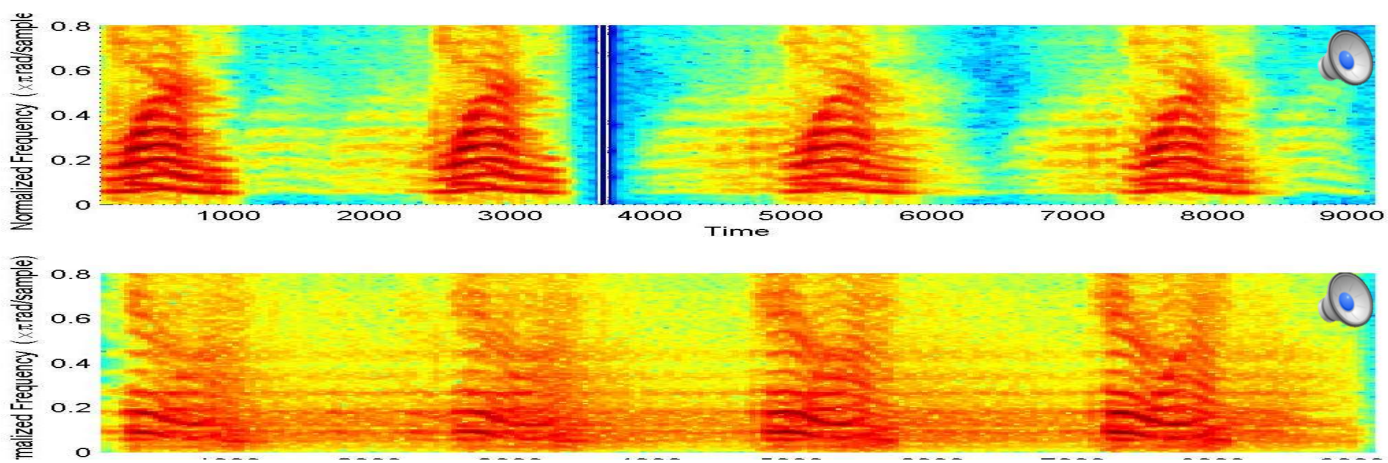
- An Example: Two distinct sounds occurring with different repetition rates within a signal
  - Each sound has a time-varying spectral structure

INPUT SPECTROGRAM



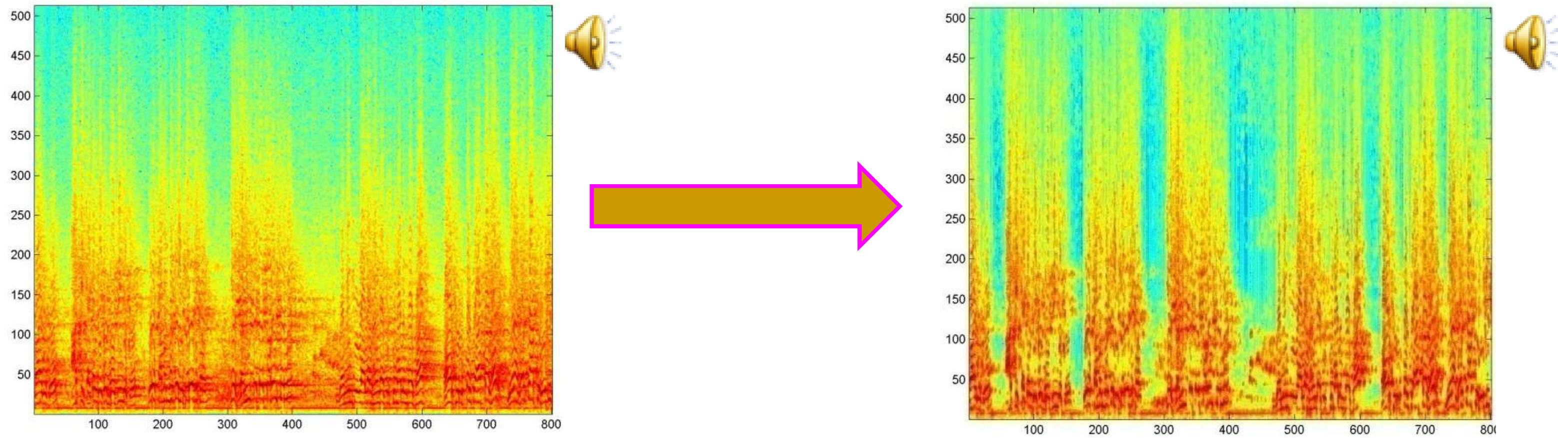


Discovered “patch” bases



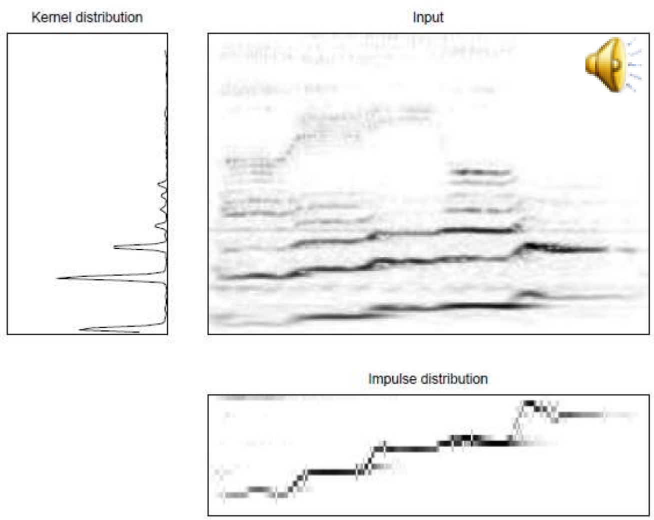
Contribution of individual bases to the recording

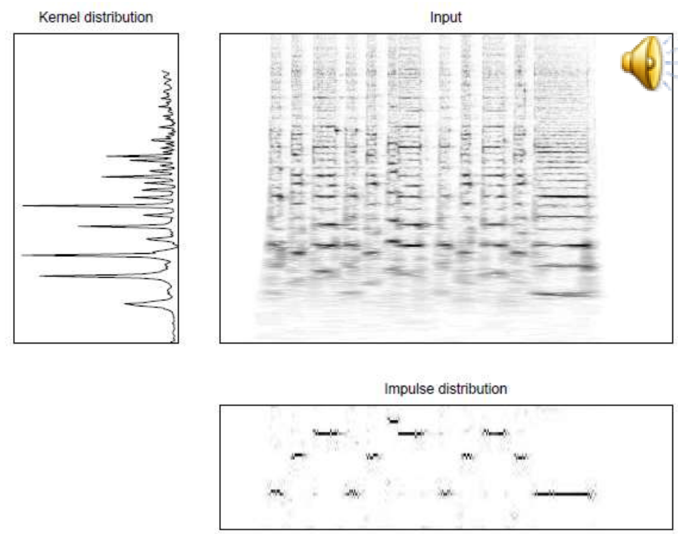
Example applications: Dereverberation



- From "Adrak ke Panje" by Babban Khan
- Treat the reverberated spectrogram as a composition of many shifted copies of a "clean" spectrogram
  - "Shift-invariant" analysis
- NMF to estimate clean spectrogram

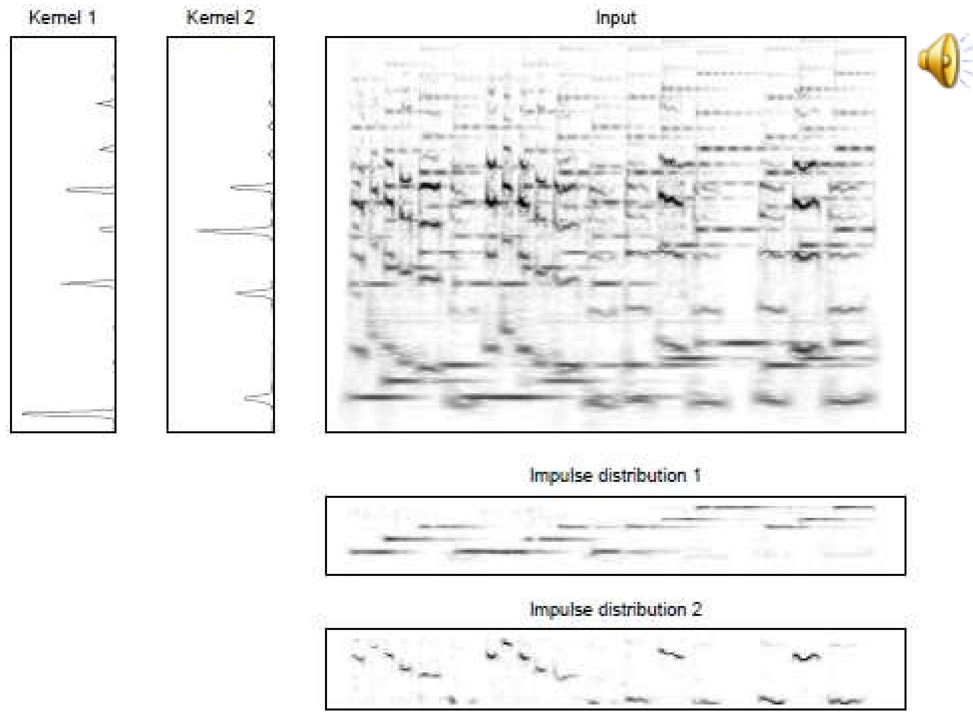
Pitch Tracking





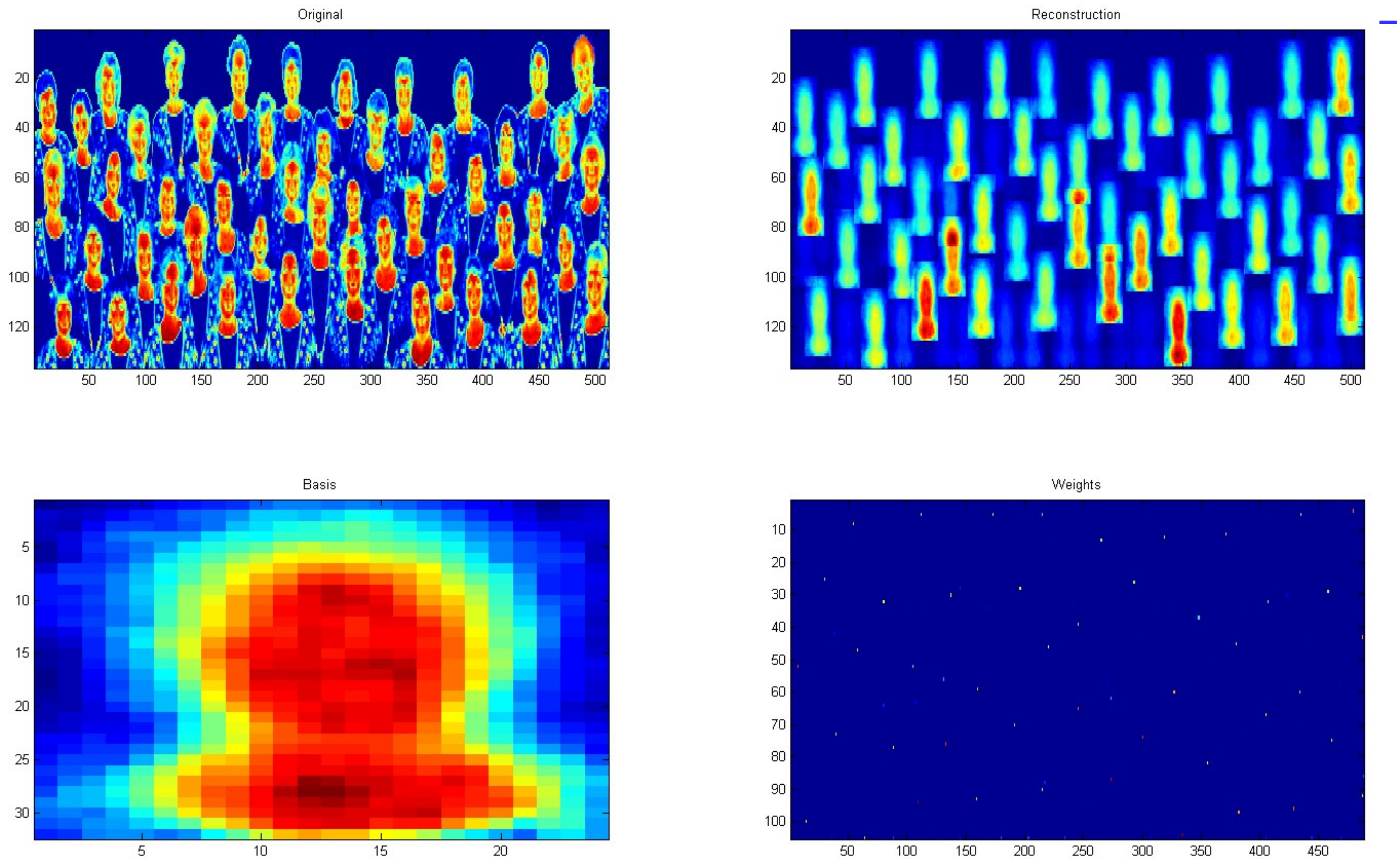
- Left: A segment of a song
- Right: Smoke on the water
  - “Impulse” distribution captures the “melody”!

Pitch Tracking



- Simultaneous pitch tracking on multiple instruments
- Can be used to find the velocity of cars on the highway!!
  - "Pitch track" of sound tracks Doppler shift (and velocity)

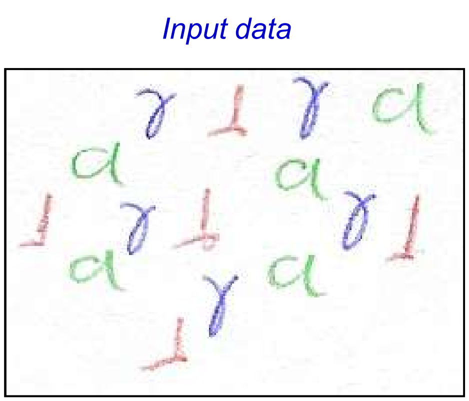
Example: 2-D shift invariance

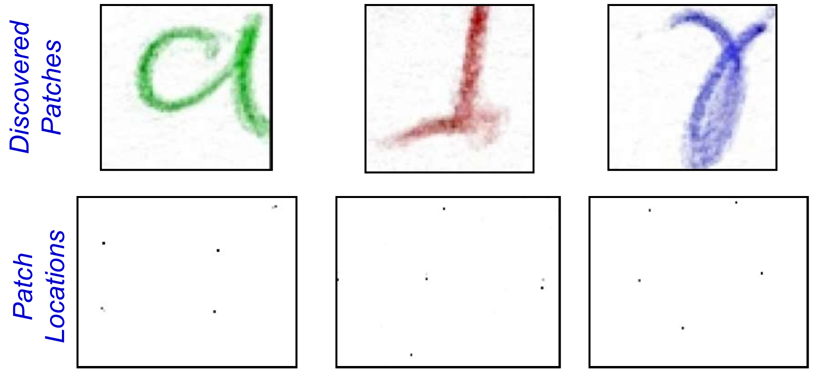


- Sparse decomposition employed in this example
  - Otherwise locations of faces (bottom right panel) are not precisely determined

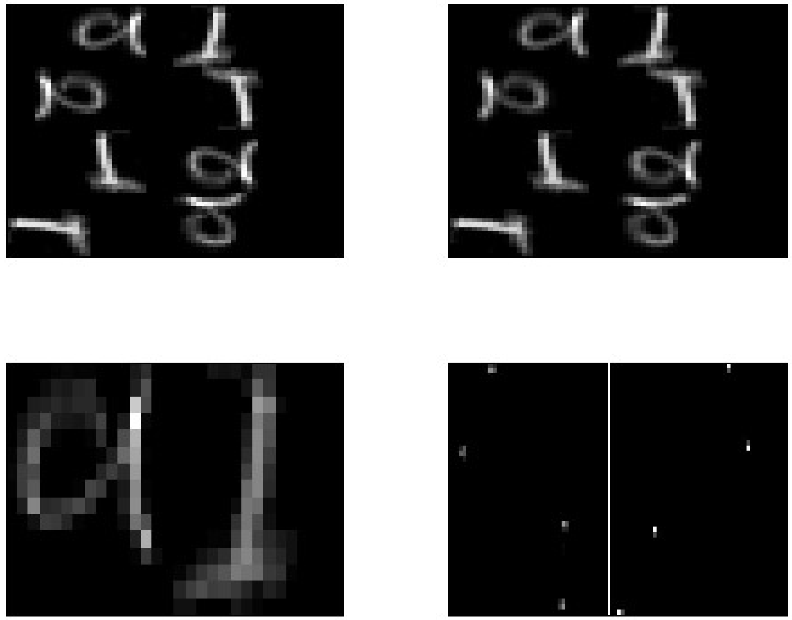
Example: 2-D shift invarince

- The original figure has multiple handwritten renderings of three characters
  - In different colours
- The algorithm learns the three characters and identifies their locations in the figure





Example: Transform Invariance

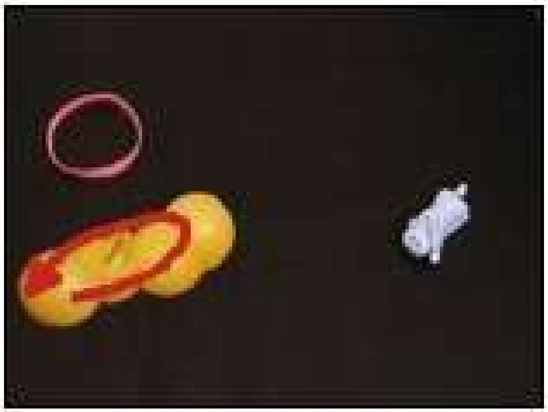


- Top left: Original figure
- Bottom left – the two bases discovered
- Bottom right –
  - Left panel, positions of “a”
  - Right panel, positions of “l”
- Top right: estimated distribution underlying original figure

Example: Higher dimensional data

- Video example

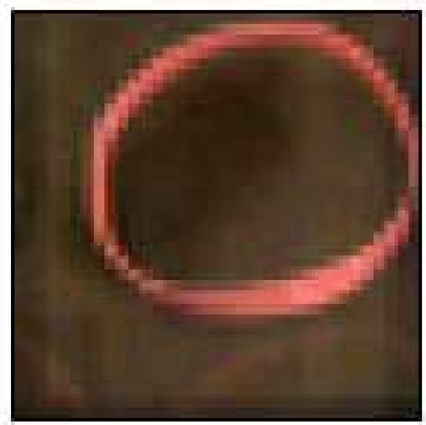
Description of Input



Kernel 1

Kernel 2

Kernel 3



Lessons learned

- Linear decomposition when constrained with semantic constraints e.g. non-negativity can result in semantically meaningful bases
- NMF: Useful *compositional* model of data
- Really effective when the data obey compositional rules..