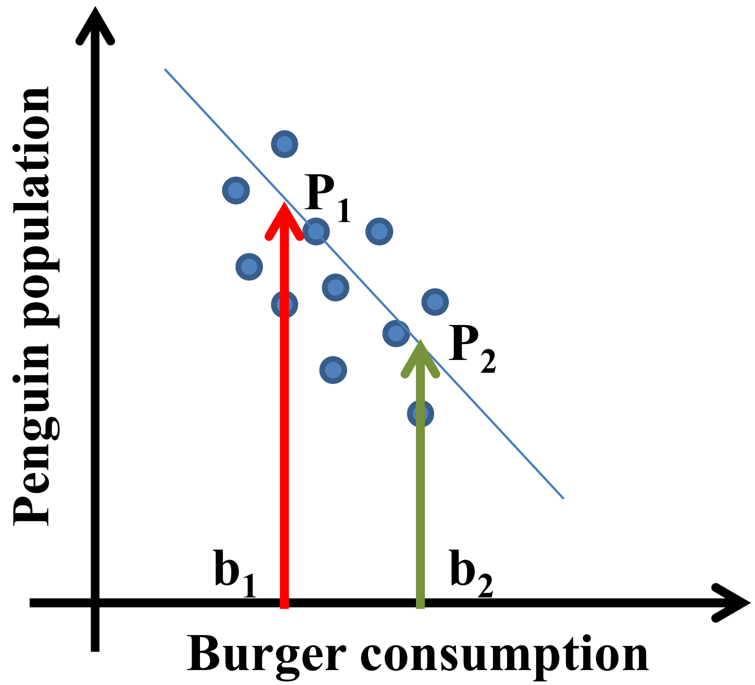
Machine Learning for Signal Processing

Independent Component Analysis

Instructor: Bhiksha Raj

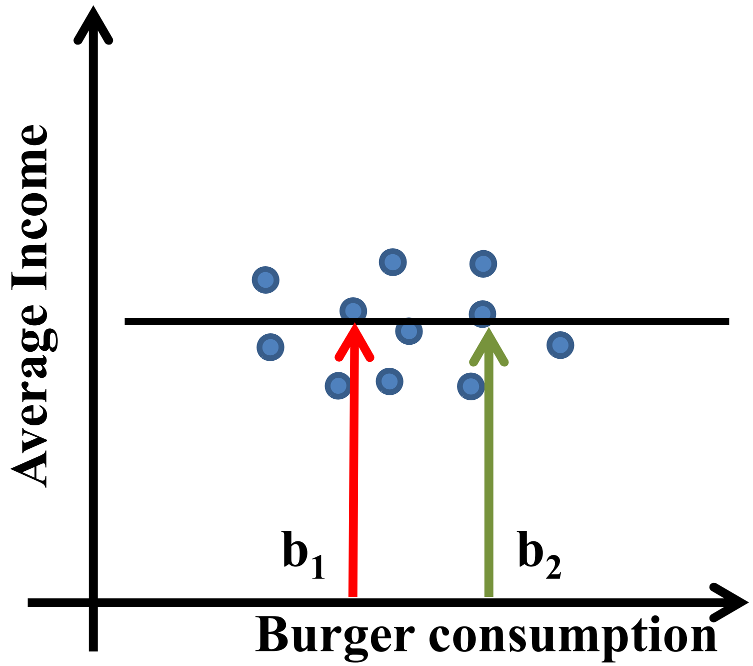
Slides (the good ones) are by Patrick Conrey

Recap: Correlated Variables



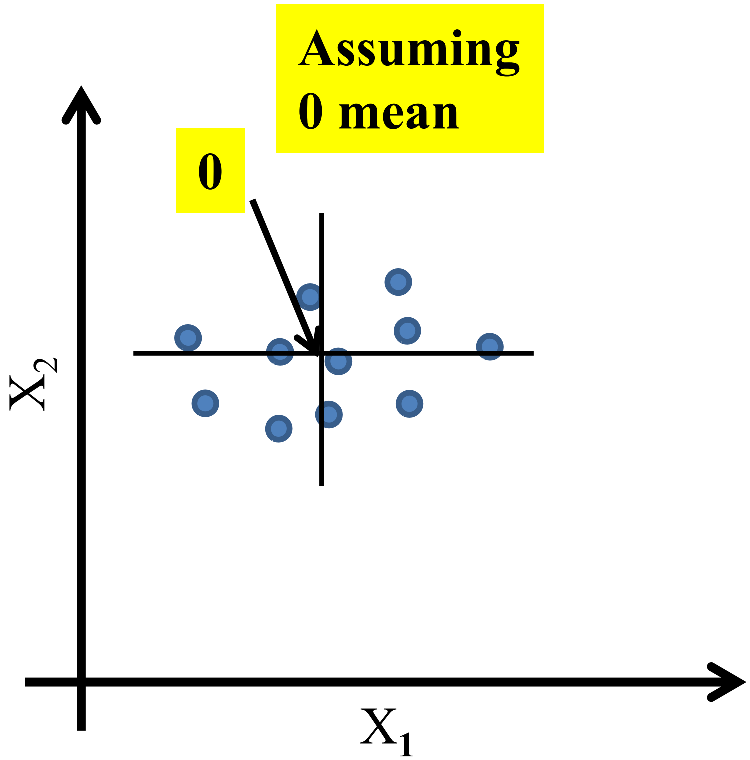
- Expected value of Y given X varies with X
  - And vice versa

Uncorrelatedness



- Knowing X does not tell you what the *average* value of Y is
  – And vice versa

Recap: Uncorrelatedness



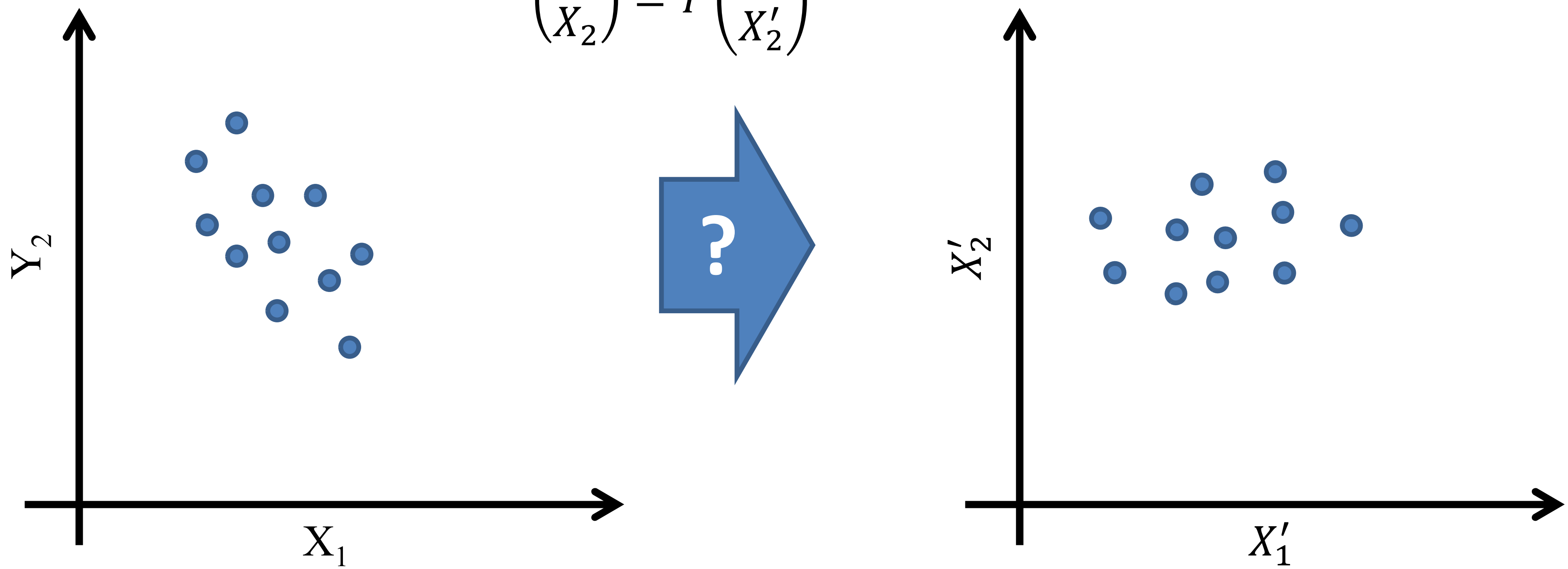
- $E[X_1] = constant$
- $E[X_2] = constant$
- $E[X_2|X_1] = constant$
- $E[X_1 X_2] = E[X_1]E[X_2]$
- All will be 0 for centered data

$$E\left[\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} (X_1 \quad X_2)\right] = E\begin{pmatrix} X_1^2 & X_2 X_1 \\ X_1 X_2 & X_2^2 \end{pmatrix} = \begin{pmatrix} E[X_1^2] & 0 \\ 0 & E[X_2^2] \end{pmatrix} = diagonal\ matrix$$

- If $\mathbf{X}$ is a matrix of vectors, $\mathbf{XX}^T$ = diagonal

Recap: Decorrelation

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = T \begin{pmatrix} X_1' \\ X_2' \end{pmatrix}$$



- So how does one transform the correlated variables (X_1, X_2) to the uncorrelated (X_1', X_2')

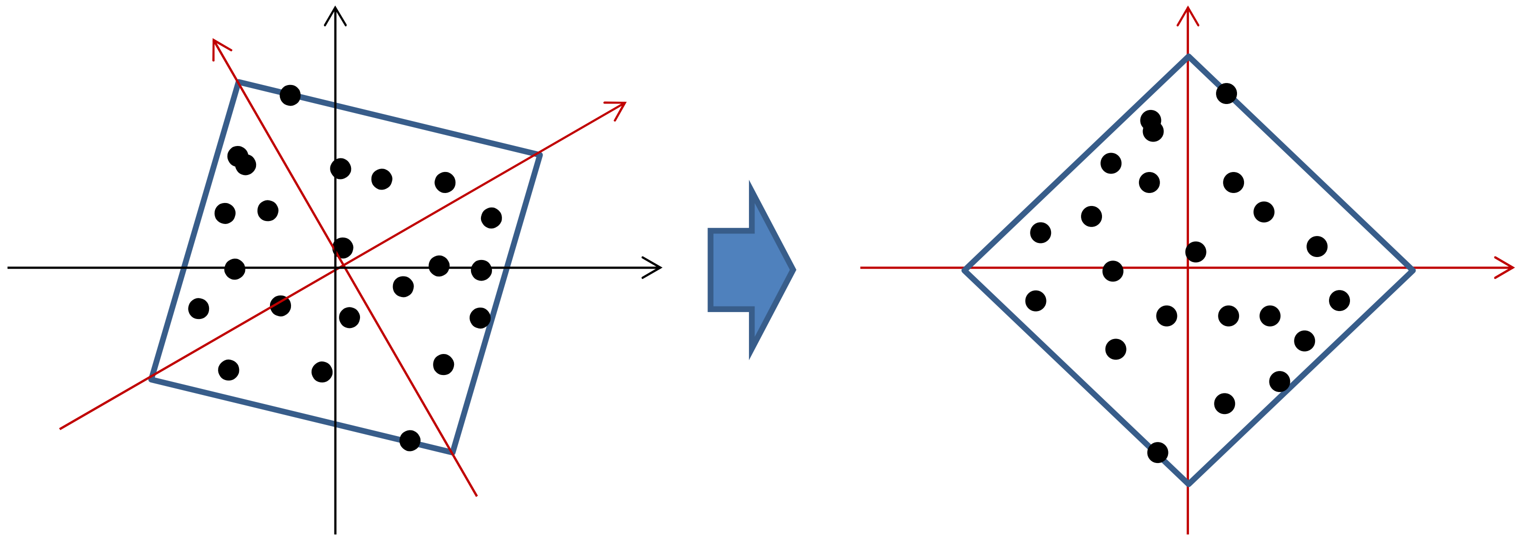
Recap: PCA

- Let $\mathbf{X}$ be the matrix of correlated data vectors
  - Each component of $\mathbf{X}$ informs us of the mean trend of other components

- Need a transform $\mathbf{T}$ such that if $\mathbf{Y} = \mathbf{TX}$, the covariance of $\mathbf{Y}$ is diagonal
  - $\mathbf{YY}^{\mathrm{T}}$ is diagonal

- **PCA:** $\mathbf{T}$ is the (transposed) matrix of Eigenvectors of the covariance matrix $\mathbf{XX}^{\mathrm{T}}$

Recap: Decorrelating by PCA



- PCA finds the principal axes of the scatter of the data
  - The Eigen vectors of the covariance matrix
- The PCA transformation transforms the principal axes of the data scatter to the main axes of the space
- This also has the *side effect* of decorrelating the data

PCA decorrelates data

- For centered (zero-mean) data $\mathbf{X}$
- The Eigenvectors of the covariance matrix are identical to the left singular vectors

$$\text{SVD: } \mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T$$

- We can write $\mathbf{Y} = \mathbf{S}\mathbf{V}^{\mathbf{T}}$ and

$$\mathbf{X} = \mathbf{U}\mathbf{Y} \quad (\text{and } \mathbf{Y} = \mathbf{U}^T\mathbf{X})$$

  - i.e. we're setting the transform $\mathbf{T} = \mathbf{U}^T$ and $\mathbf{Y} = \mathbf{T}\mathbf{X}$
- $\mathbf{Y}$ is the representation of $\mathbf{X}$ in terms of the columns of $\mathbf{U}$
- But

$$\mathbf{Y}\mathbf{Y}^T = (\mathbf{S}\mathbf{V}^{\mathbf{T}}\mathbf{V}\mathbf{S}^{\mathbf{T}}) = \mathbf{S}\mathbf{S}^{\mathbf{T}} = \text{Diagonal}$$

- I.e. the new representations $\mathbf{Y}$ are uncorrelated

Recap: The statistical concept of *Independence*

- Two variables X and Y are *dependent* if If knowing X gives you *any information about* Y

- X and Y are *independent* if knowing X tells you nothing at all of Y

Recap: Independence

- ***Independence:*** Two random variables X and Y are independent iff:
  - Their joint probability equals the product of their individual probabilities
- $P(X,Y) = P(X)P(Y)$
- Independence implies uncorrelatedness
  - The average value of X is the same regardless of the value of Y
    - $E[X|Y] = E[X]$
  - But uncorrelatedness does not imply independence

Recap: Independence

- *Independence:* Two random variables X and Y are independent iff:
- The average value of ***any function*** *of* X is the same regardless of the value of Y
  - Or any function of Y
- **E[f(X)g(Y)] = E[f(X)] E[g(Y)] for all f(), g()**

Poll 1

- The objective of PCA is to decorrelate the data
  - True
  - False

- If two random values x and y are independent, then which of the following is true of $E[x^2y^2]$?
  - $E[x^2y^2] = E[x]^2E[y]^2$
  - $E[x^2y^2] = E[x^2]E[y^2]$

Poll 1

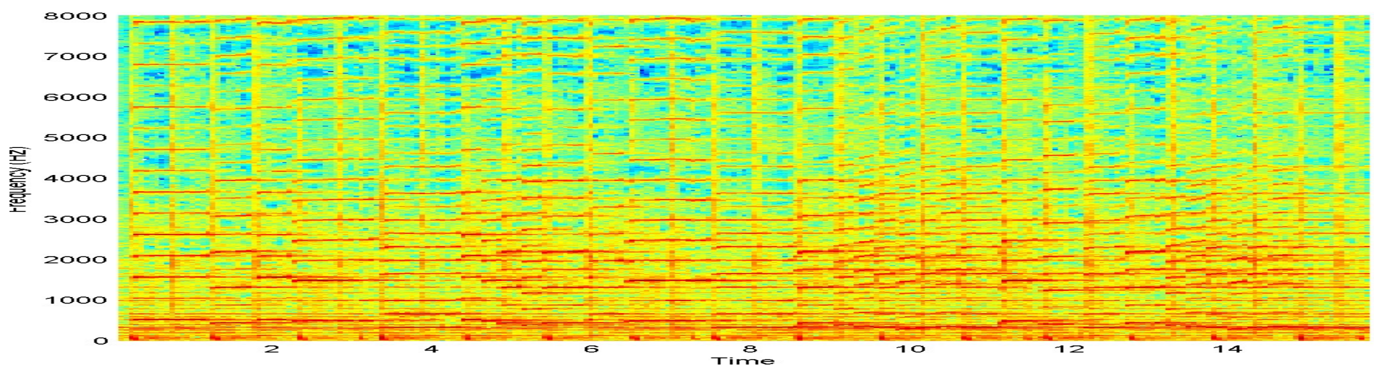
- The objective of PCA is to decorrelate the data
  - True
  - **False**

- If two random values x and y are independent, then which of the following is true of $E[x^2y^2]$?
  - $E[x^2y^2] = E[x]^2E[y]^2$
  - **$E[x^2y^2] = E[x^2]E[y^2]$**

Moving on: Finding bases…

Recap: Finding bases, aka building blocks..

M =



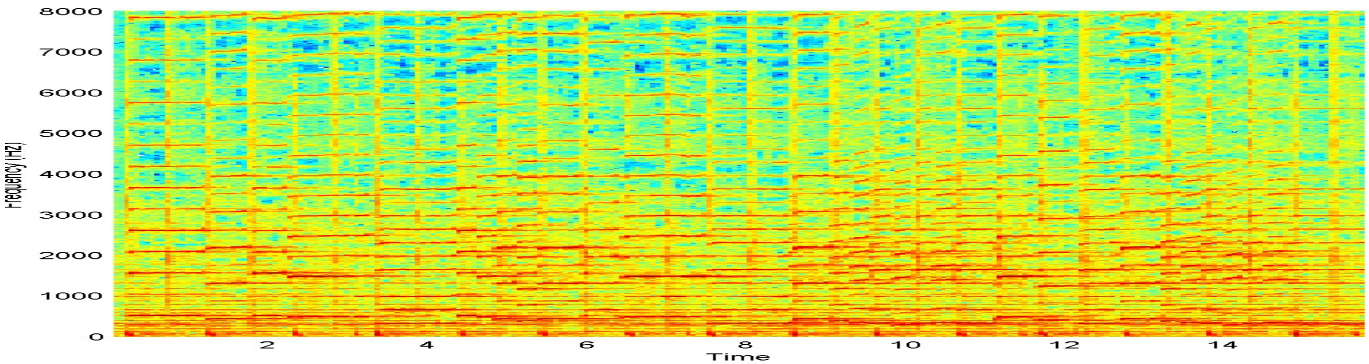
H = ?

W = ?

U = ?

- Find the bases **W** that best explain the data *in a meaningful way*

Recap: Finding bases, aka building blocks..

M = 

H = **?**

W = **?**

U = **?**

- Meaningful – try1: The bases are ***orthogonal***

A least squares solution

$$\mathbf{W}, \mathbf{H} = \arg\min_{\overline{\mathbf{W}}, \overline{\mathbf{H}}} \| \mathbf{M} - \overline{\mathbf{W}}\overline{\mathbf{H}} \|_F^2 + \Lambda(\overline{\mathbf{W}}^T \overline{\mathbf{W}} - \mathbf{I})$$

- Constraint: $\mathbf{W}$ is orthogonal
  - $\mathbf{W}^{\mathrm{T}}\mathbf{W} = \mathbf{I}$
- The solution:
  - $\mathbf{W}$ are the Eigen vectors of $\mathbf{M}\mathbf{M}^{\mathbf{T}}$
  - PCA!!

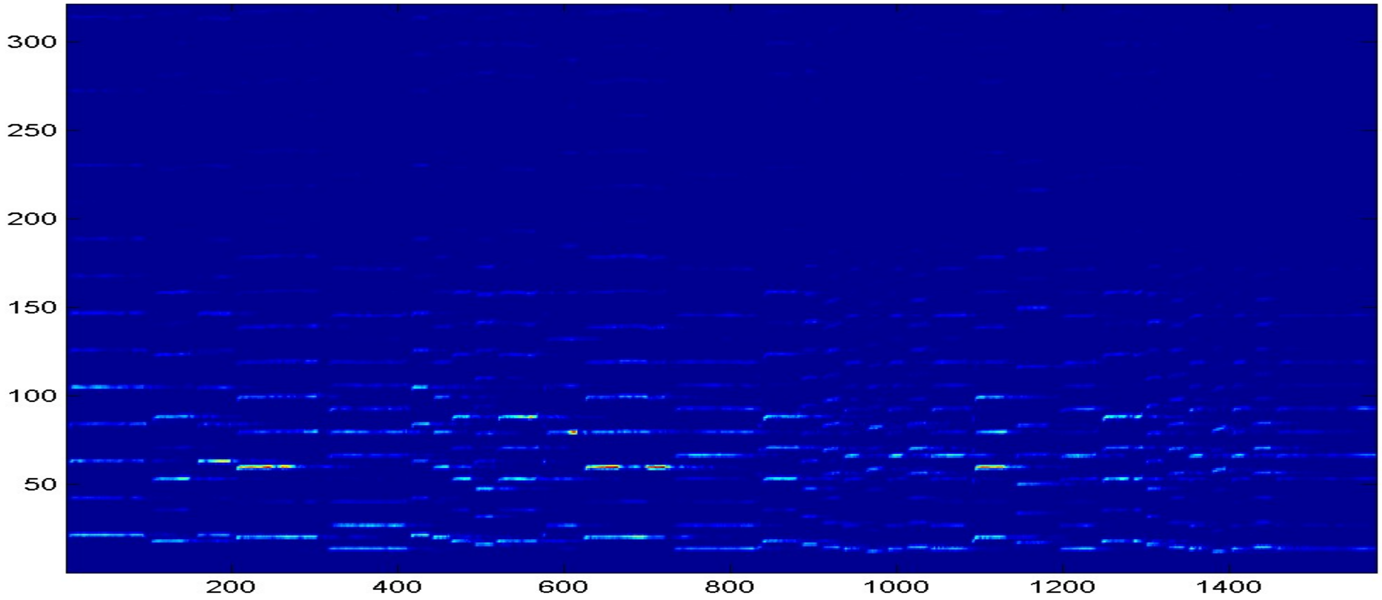
- $\mathbf{M} \sim \mathbf{W}\mathbf{H}$ is an approximation
- Also, the rows of $\mathbf{H}$ are *decorrelated*

PCA

$$\mathbf{M} = \mathbf{WH}$$

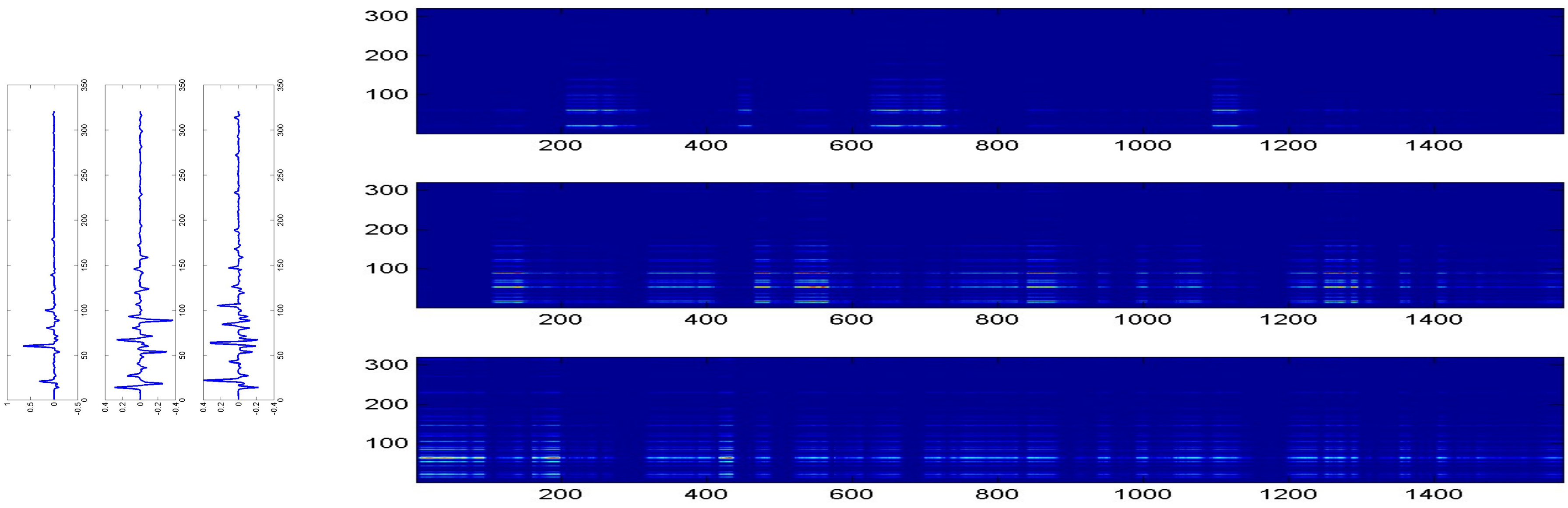
- The orthogonal columns of $\mathbf{W}$ are the bases we have learned
  - The linear “building blocks” that compose the music
- They represent “learned” notes
  - $\mathbf{w}_i \mathbf{h}_i$ is the contribution of the ith note to the music
    - $\mathbf{w}_i$ is the ith column of $\mathbf{W}$
    - $\mathbf{h}_i$ is the ith row of $\mathbf{H}$

So how does that work?



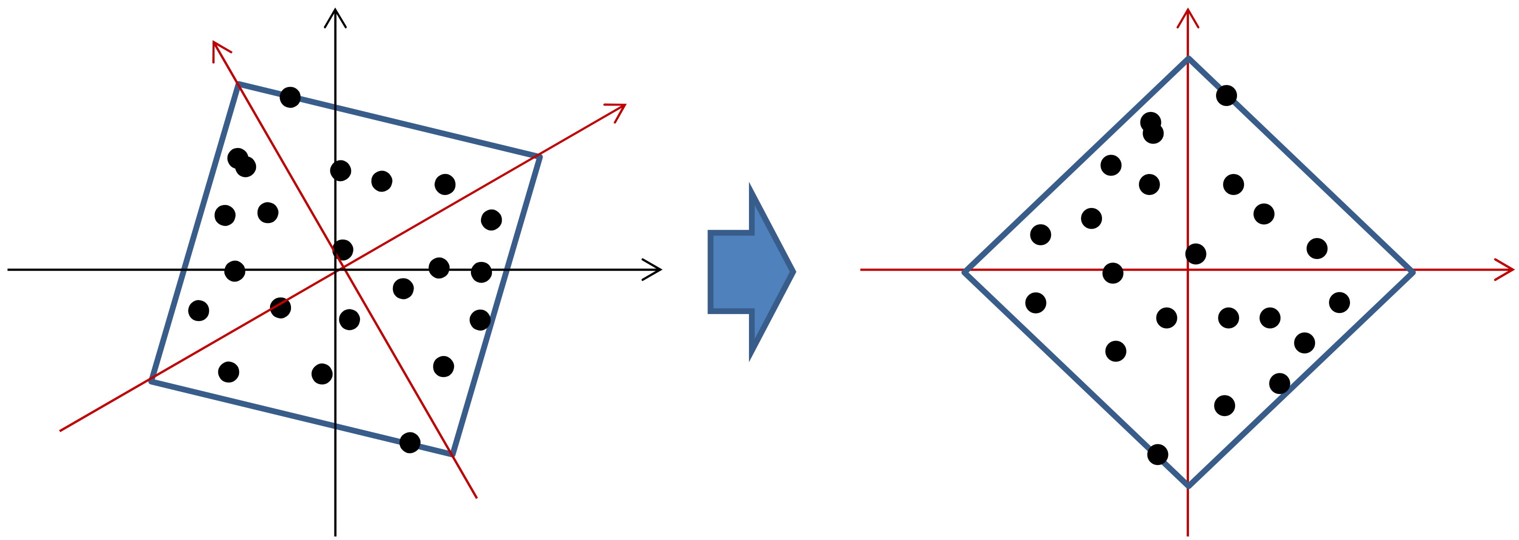
- There are 12 notes in the segment, hence we try to estimate 12 notes..

So how does that work?



- There are 12 notes in the segment, hence we try to estimate 12 notes..
- Results are not good

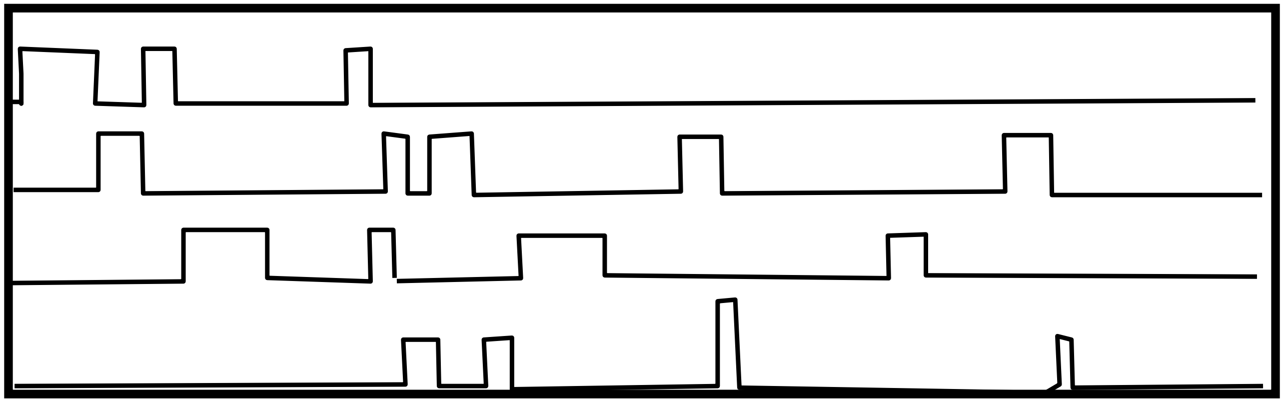
Recap: Decorrelating by PCA



- PCA decorrelates the data *incidentally*
- The focus is on the orthogonality of the axes, decorrelated representations is a side effect
- What if we focus, instead, on *decorrelating* the data directly?

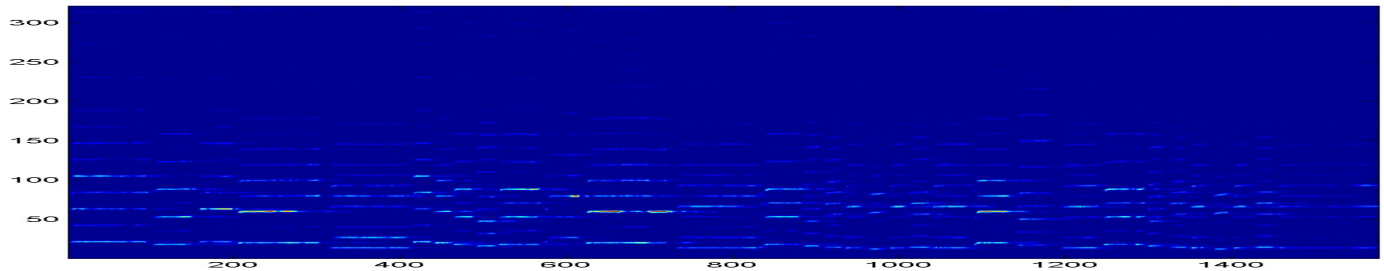
PCA through decorrelation of notes

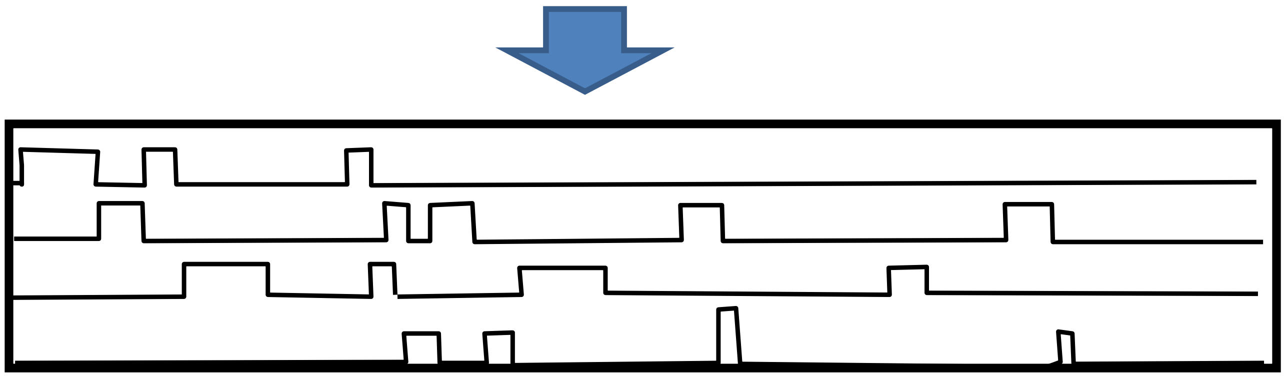
$$\mathbf{W},\mathbf{H} = \arg\min_{\overline{\mathbf{W}},\overline{\mathbf{H}}} \|\mathbf{M} - \overline{\mathbf{H}}\|_F^2 + \Lambda(\overline{\mathbf{H}}\overline{\mathbf{H}}^T - \mathbf{D})$$



- Different constraint: Constraint $\mathbf{H}$ to be decorrelated
  - $\mathbf{H}\mathbf{H}^{\mathrm{T}} = \mathbf{D}$

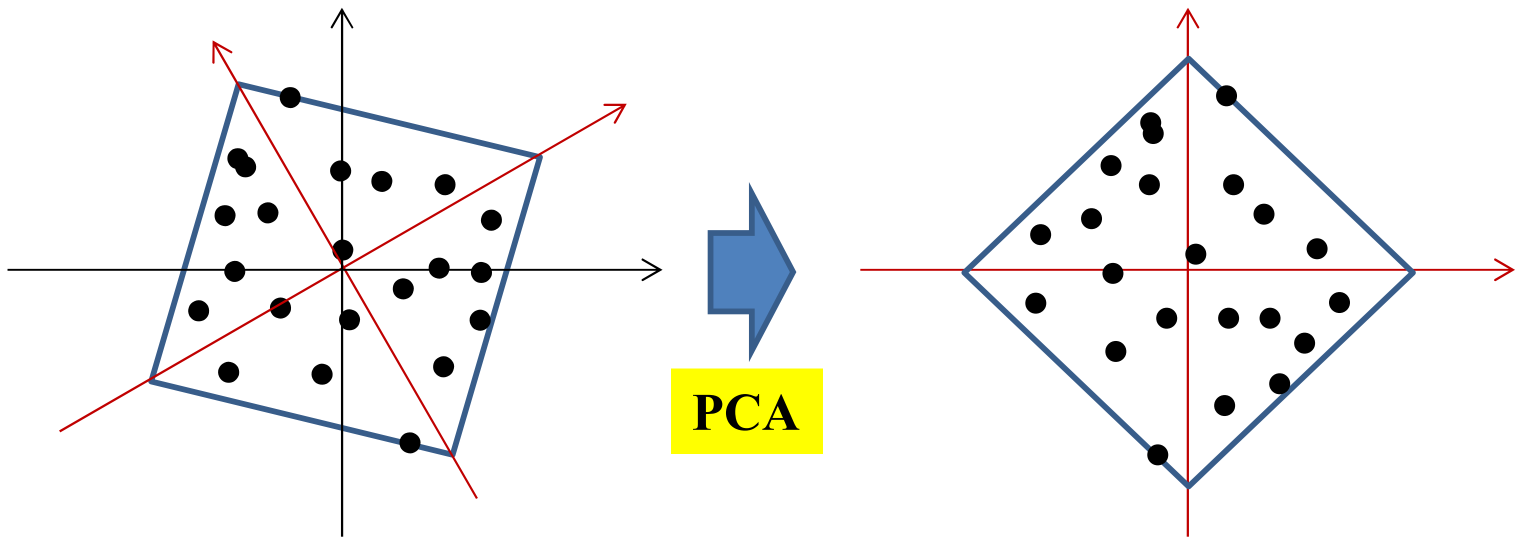
Decorrelation





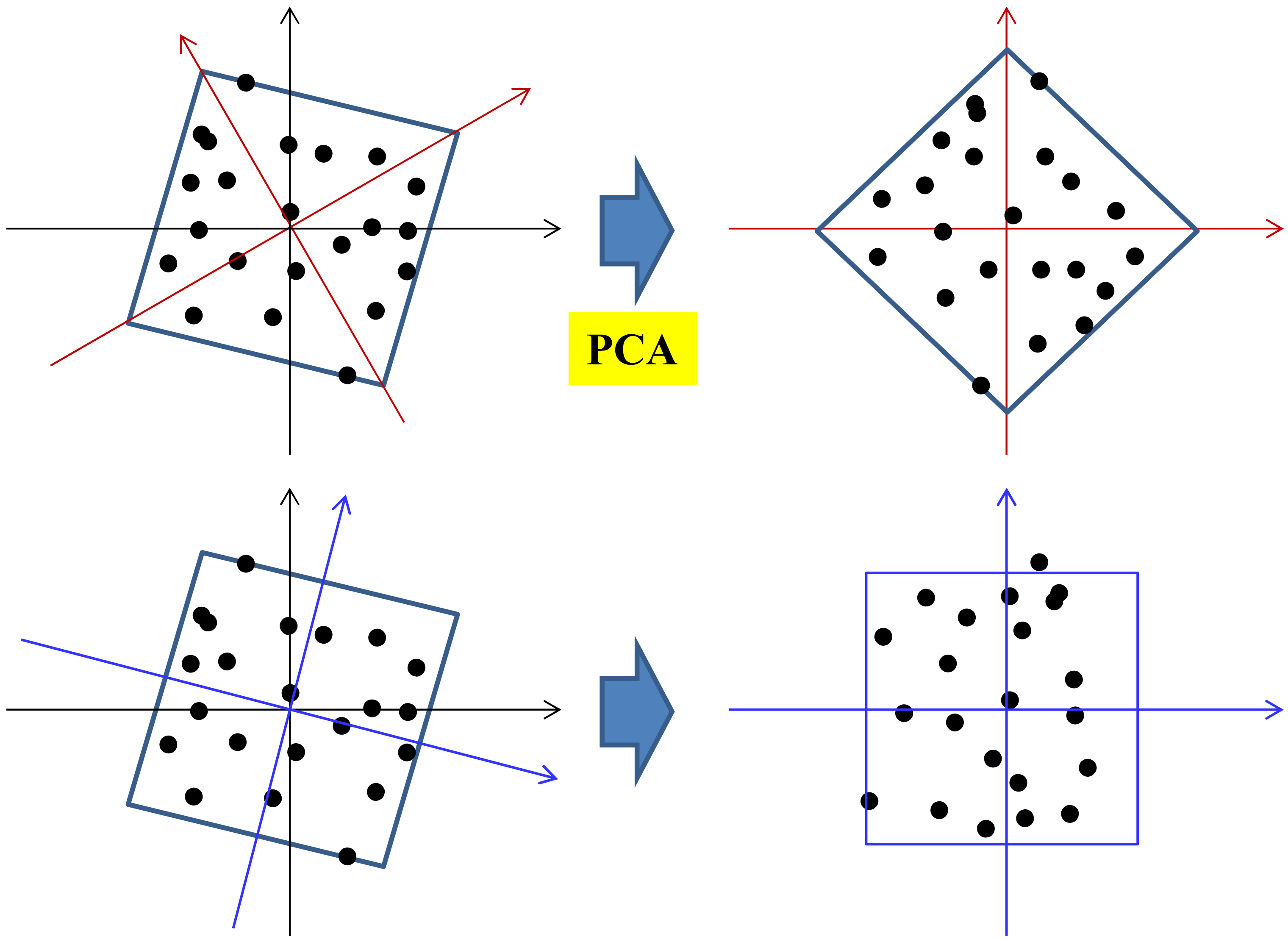
- Alternate view: Find a matrix $\mathbf{B}$ such that the rows of $\mathbf{H}=\mathbf{B}\mathbf{M}$ are uncorrelated
- PCA is one solution already
- **Are there others?**

Decorrelating the data



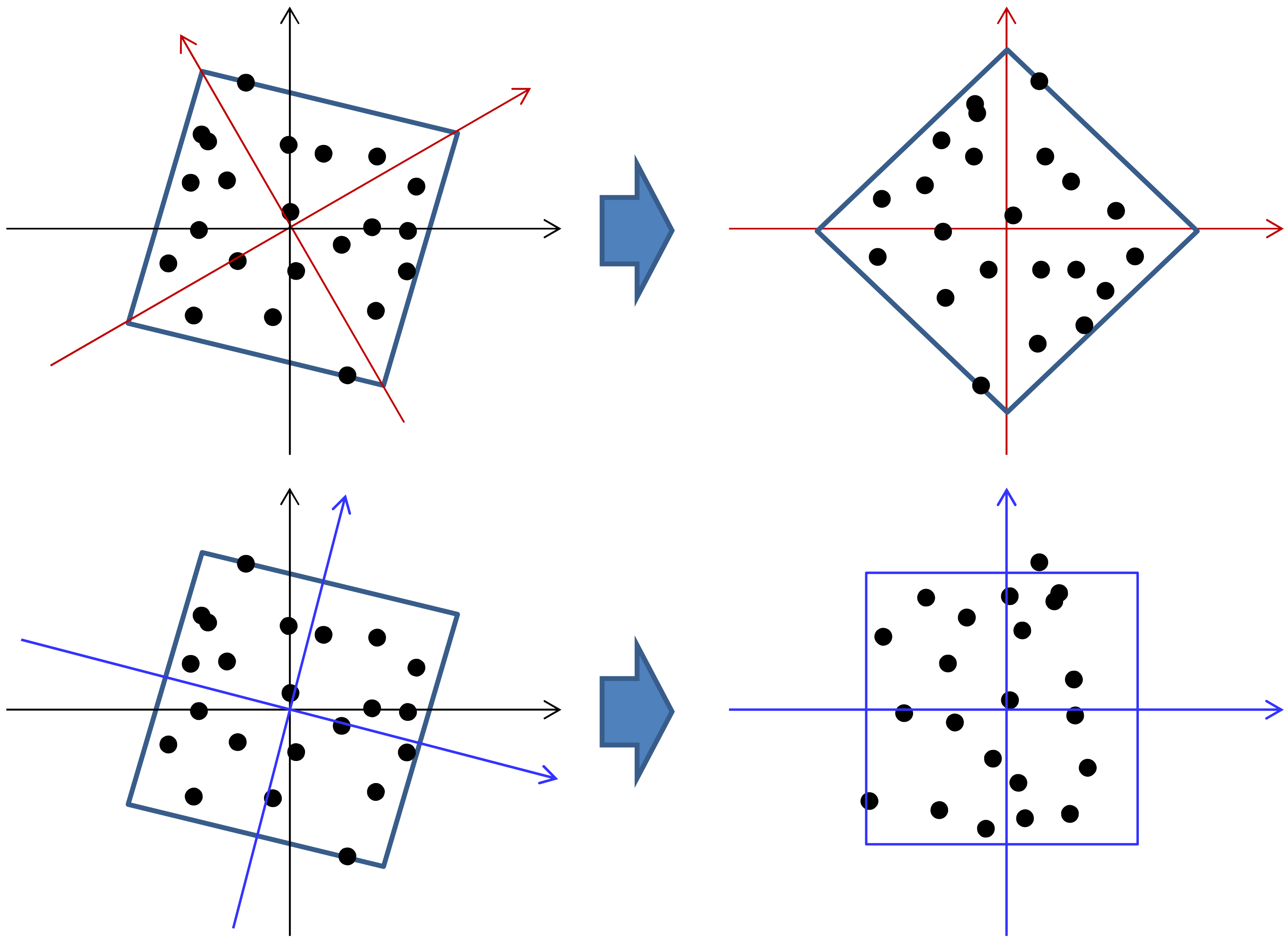
- Are there other decorrelating axes?

Decorrelating the data



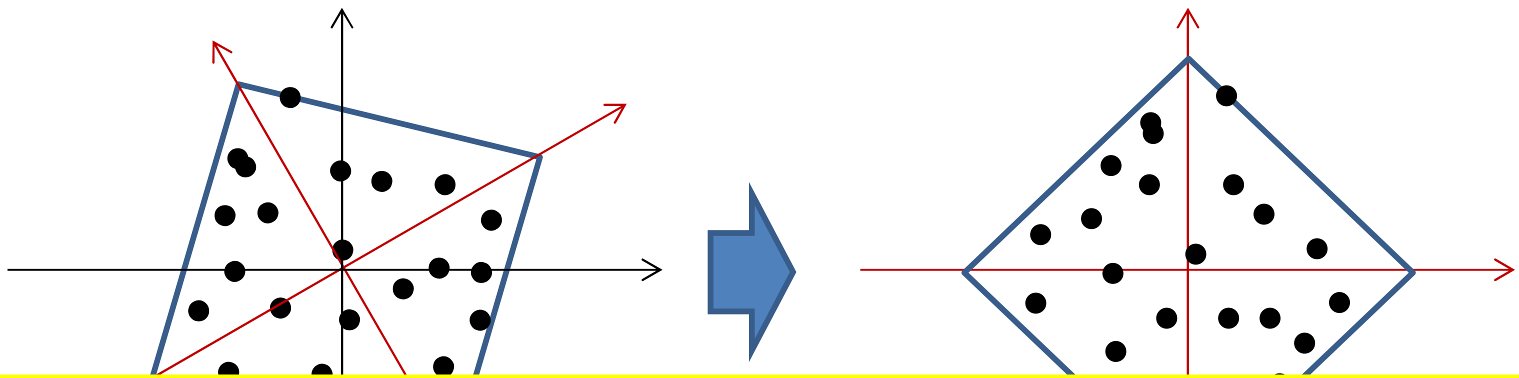
- But PCA will find only one of them, why?

Decorrelating the data

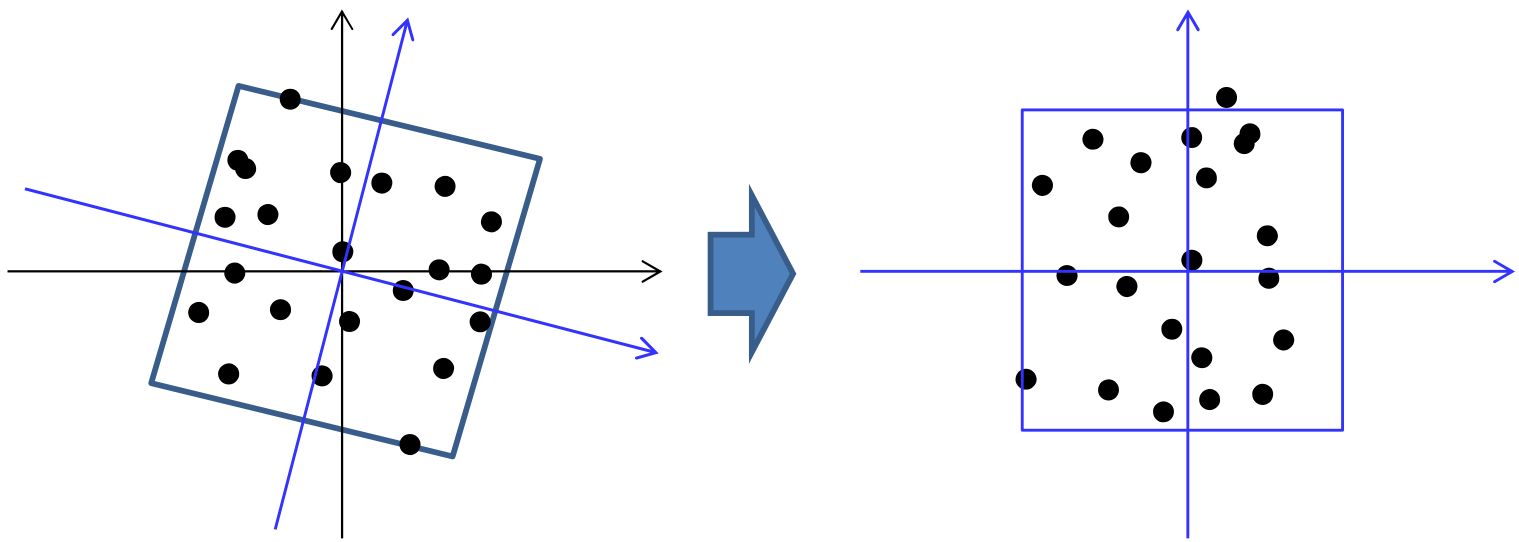


A decorrelation-based decomposition can find either of them.
The solution is non-unique

Decorrelating the data



What is special about the blue axes,
and how can we modify our decomposition to find them instead



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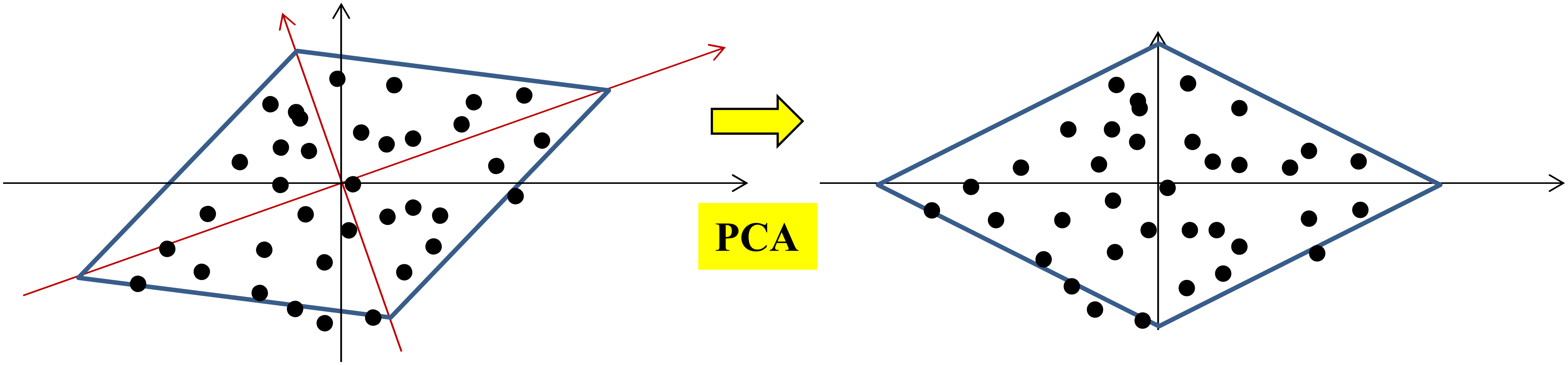
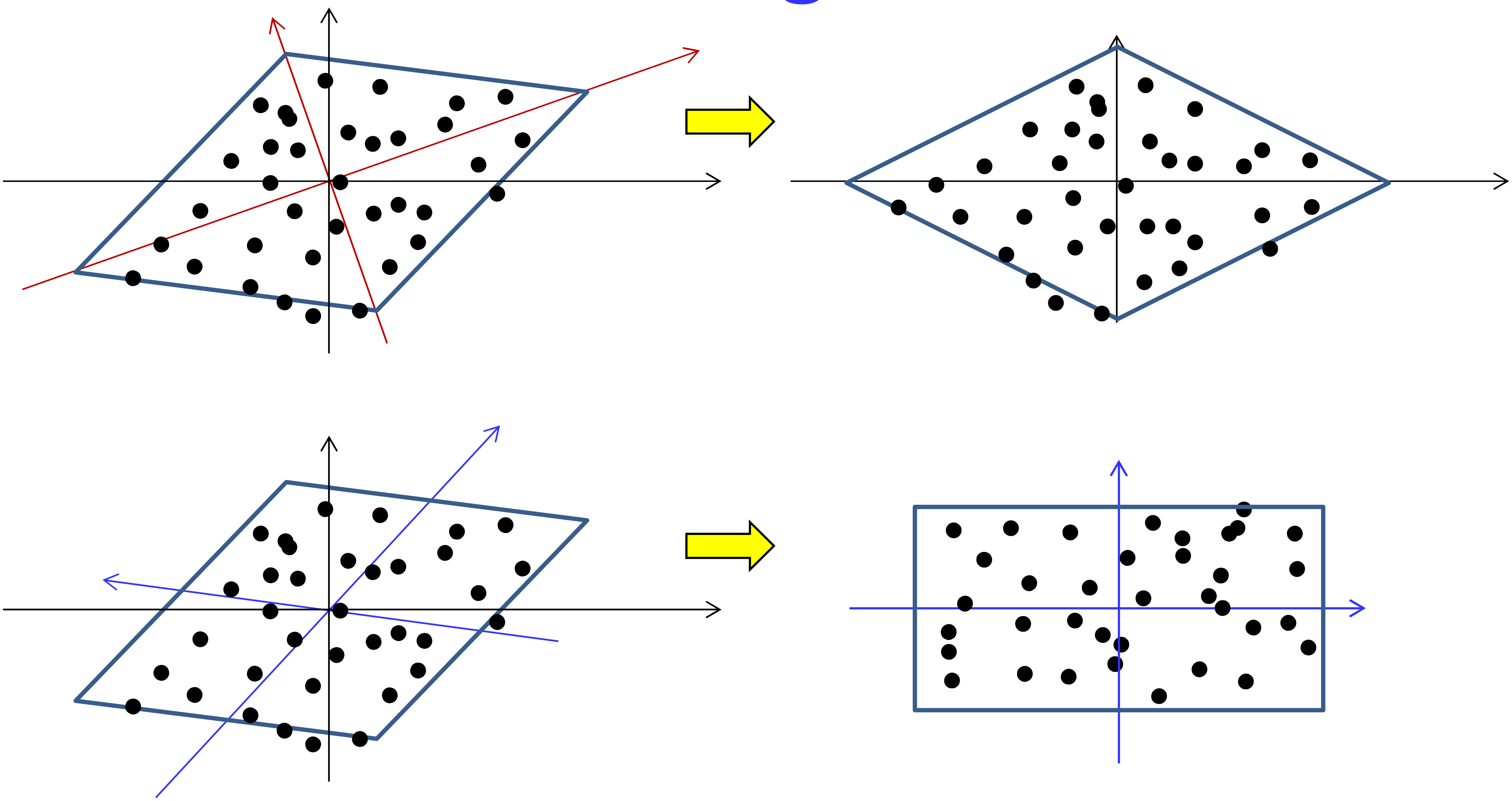


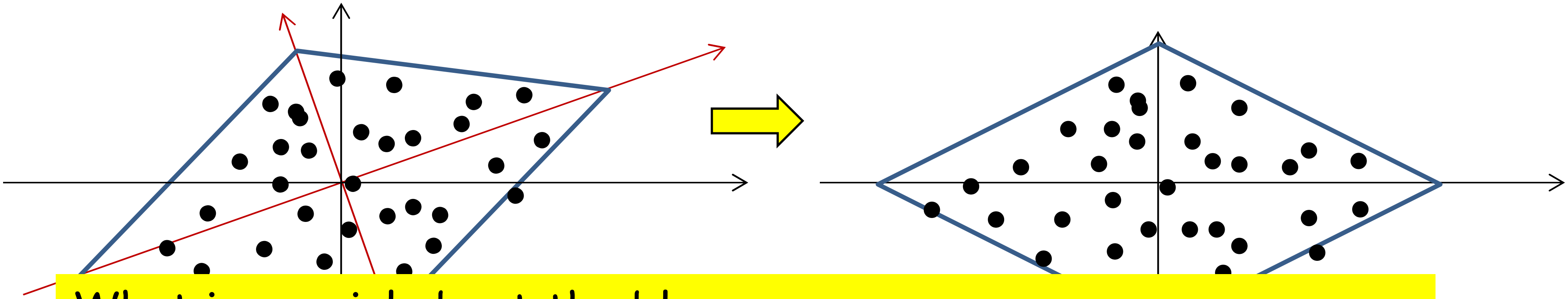
- Are there other decorrelating axes?

Decorrelating the data



- The decorrelation-based decomposition has multiple solutions, but PCA will find only one of them

Decorrelating the data



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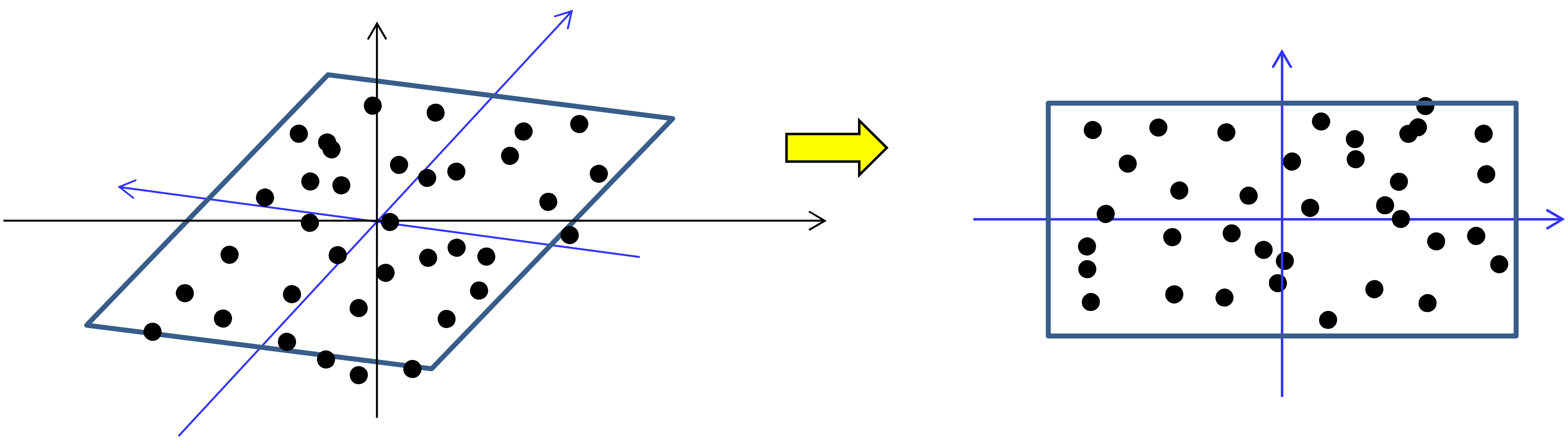
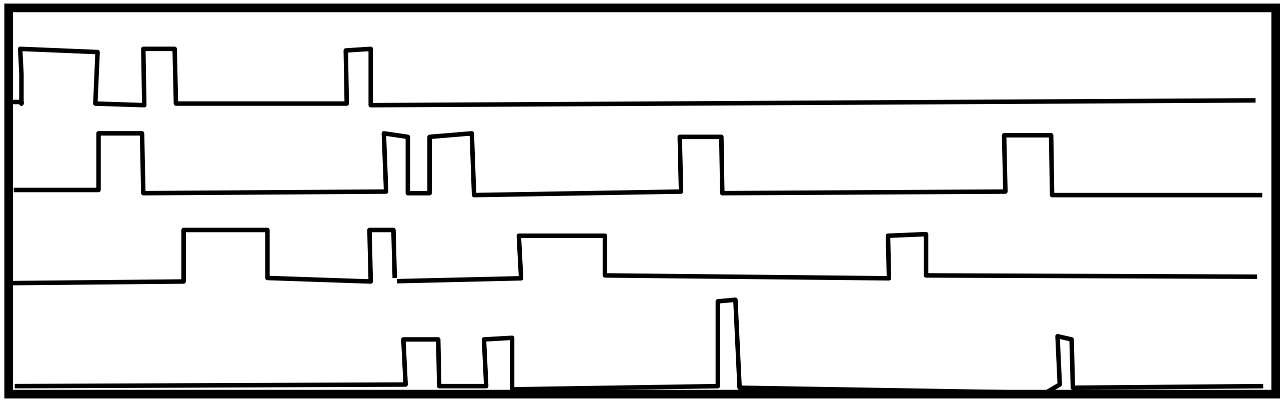


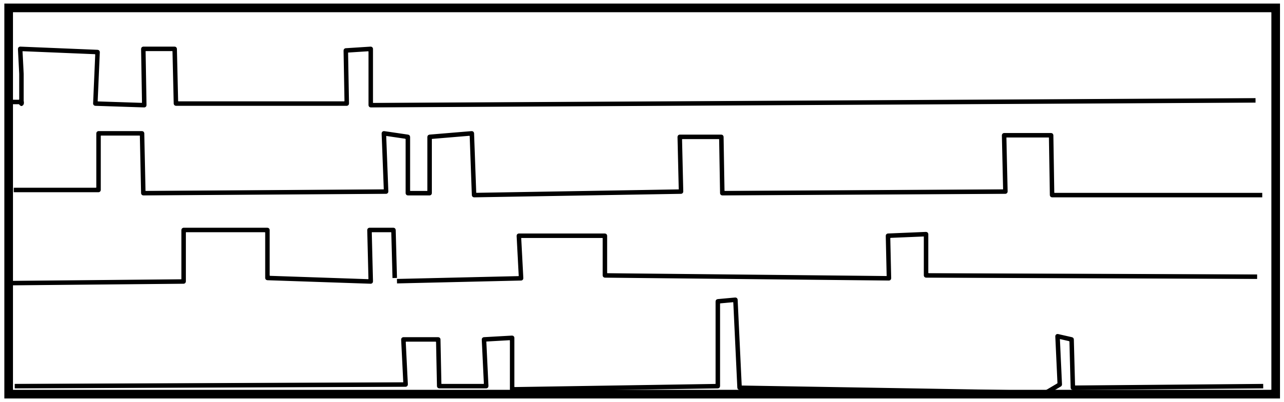
- The decorrelation-based decomposition has multiple solutions, but PCA will find only one of them

What *else* can we look for?



- Assume: The "transcription" of one note does not depend on what else is playing
  - Or, in a multi-instrument piece, instruments are playing independently of one another
- Not strictly true, but still..

What *else* can we look for?



- Assume: The “transcription” of one note does not depend on what else is playing
  - Or, in a multi-instrument piece, instruments are playing independently of one another

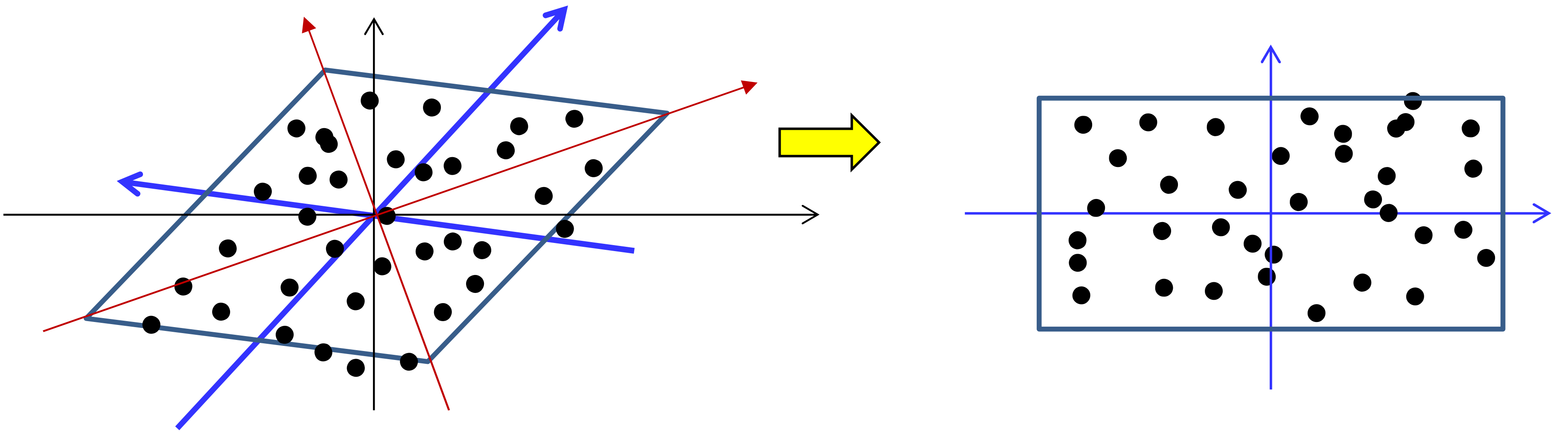
- **Attempting to find statistically independent components of the mixed signal**
  - ***Independent Component Analysis***

Formulating it with Independence

$$\mathbf{W}, \mathbf{H} = \arg\min_{\overline{\mathbf{W}}, \overline{\mathbf{H}}} \| \mathbf{M} - \overline{\mathbf{W}}\overline{\mathbf{H}} \|_F^2 + \Lambda(\textit{rows of } \mathbf{H} \textit{ are independent})$$

- Impose statistical independence constraints on decomposition

Independent Component Analysis



- **Independent Component Analysis** searches through all possible combinations of bases to find the set that makes the representations in terms of these bases maximally independent

Poll 2

- If there are multiple decorrelating axes, the solution to PCA will always be indeterminate
  - True
  - False

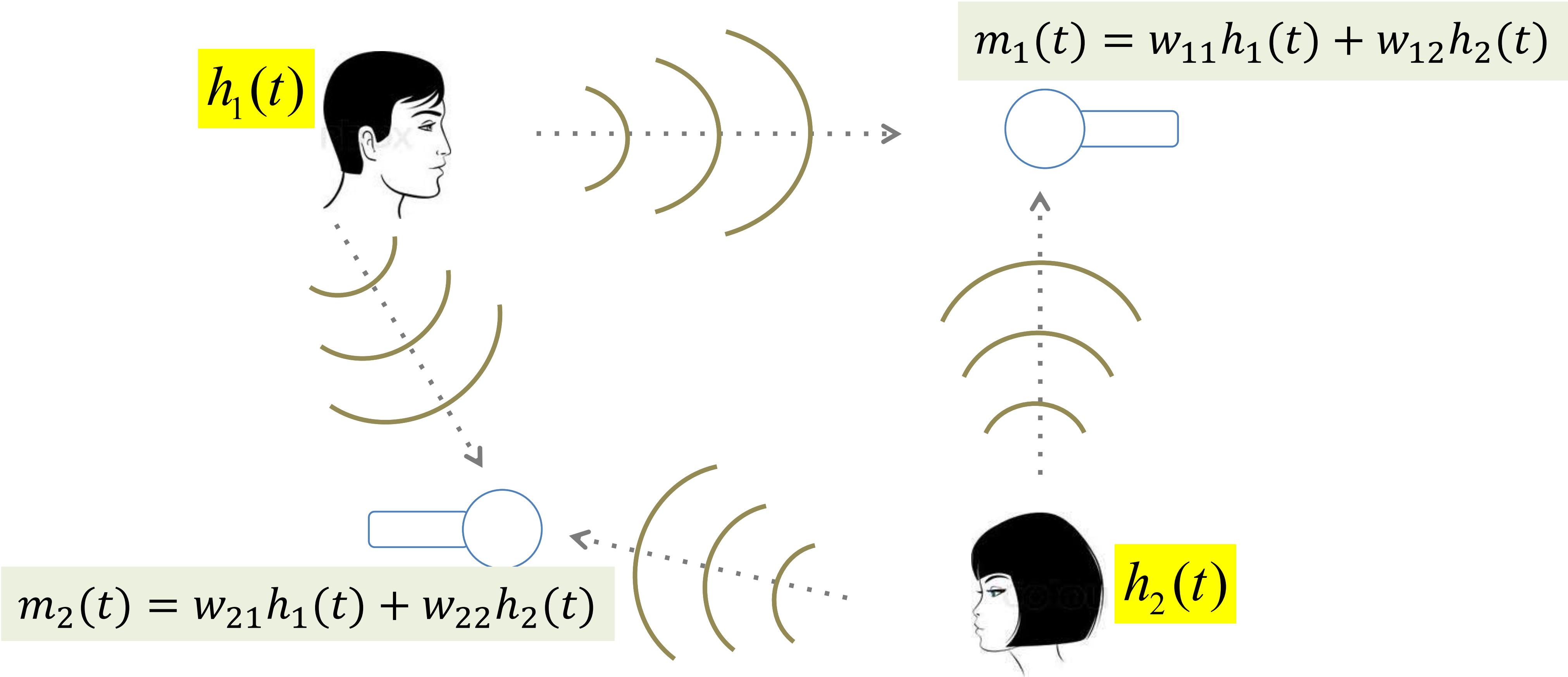
- Independent Component Analysis attempts to decompose a data matrix into the product of a bases matrix and a weights matrix, such that the components of the weights vectors are statistically independent
  - True
  - False

Poll 2

- If there are multiple decorrelating axes, the solution to PCA will always be indeterminate
  - True
  - **False**

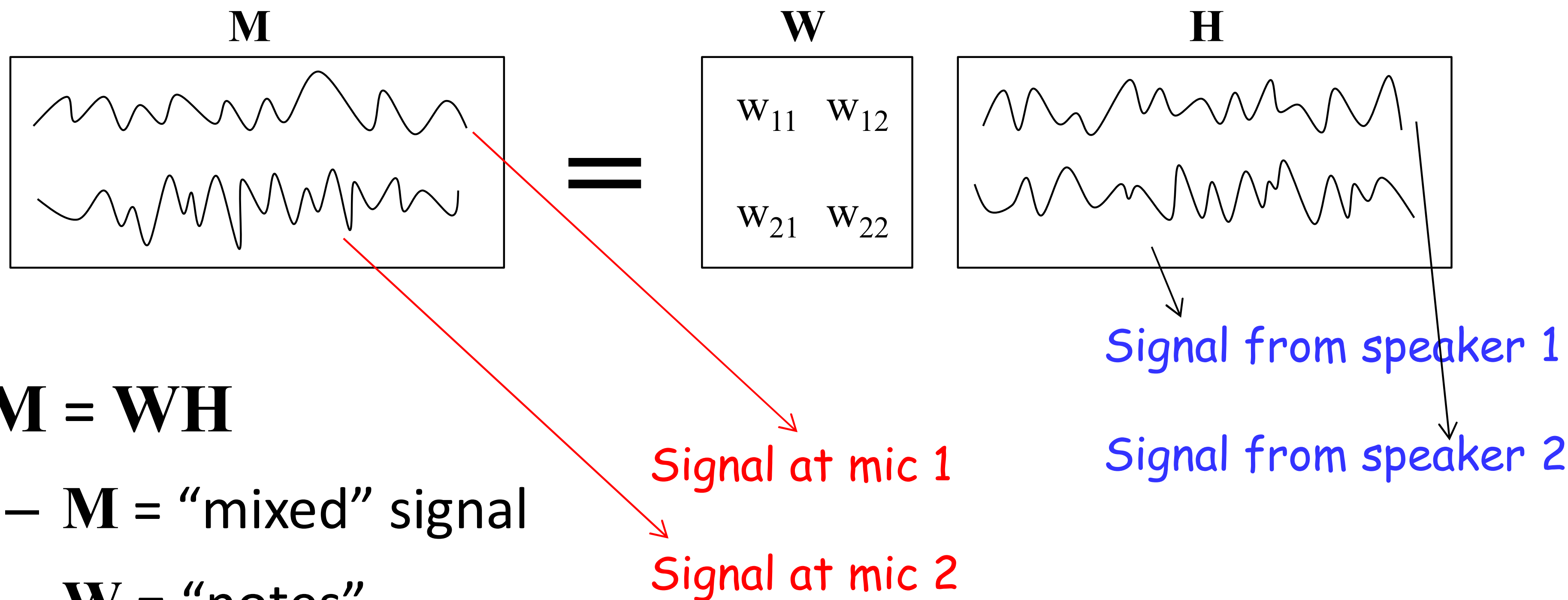
- Independent Component Analysis attempts to decompose a data matrix into the product of a bases matrix and a weights matrix, such that the components of the weights vectors are statistically independent
  - **True**
  - False

Changing problems for a bit



- Two people speak simultaneously
- Recorded by two microphones
- Each recorded signal is a mixture of both signals

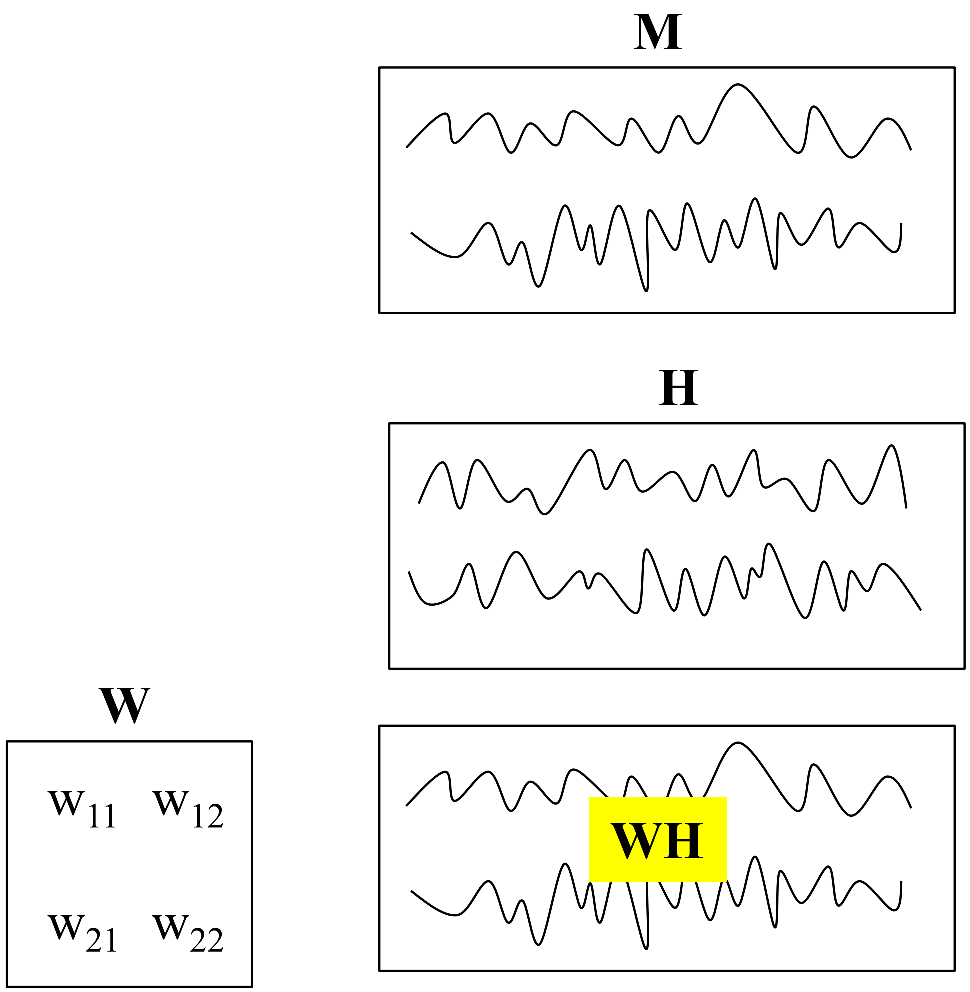
A Separation Problem



- **M** = **WH**
  - **M** = "mixed" signal
  - **W** = "notes"
  - **H** = "transcription"

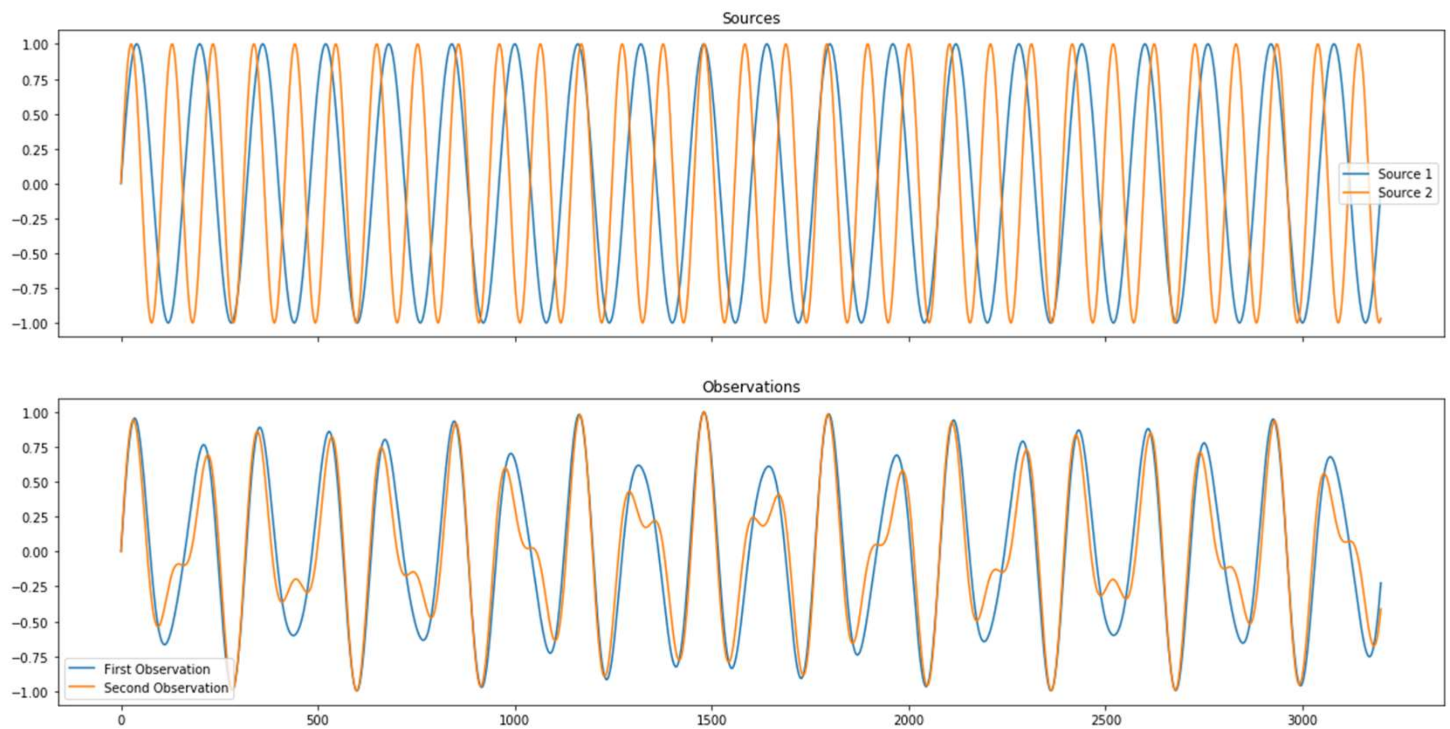
- Separation challenge: Given only **M** estimate **H**
- Identical to the problem of "finding scores (and notes)"

A Separation Problem



- Separation challenge: Given only $\mathbf{M}$ estimate $\mathbf{H}$
- **Identical to the problem of "finding scores"**

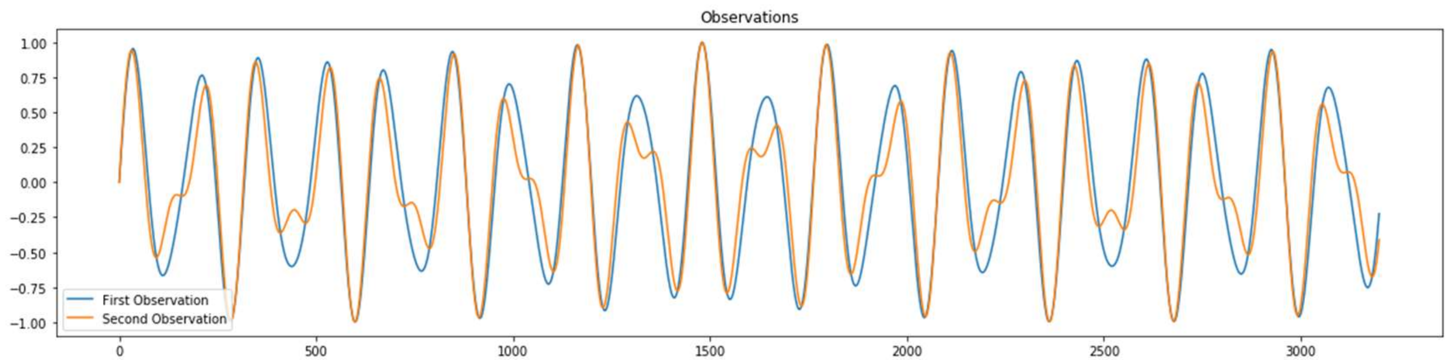
Example: Sources & Mixing



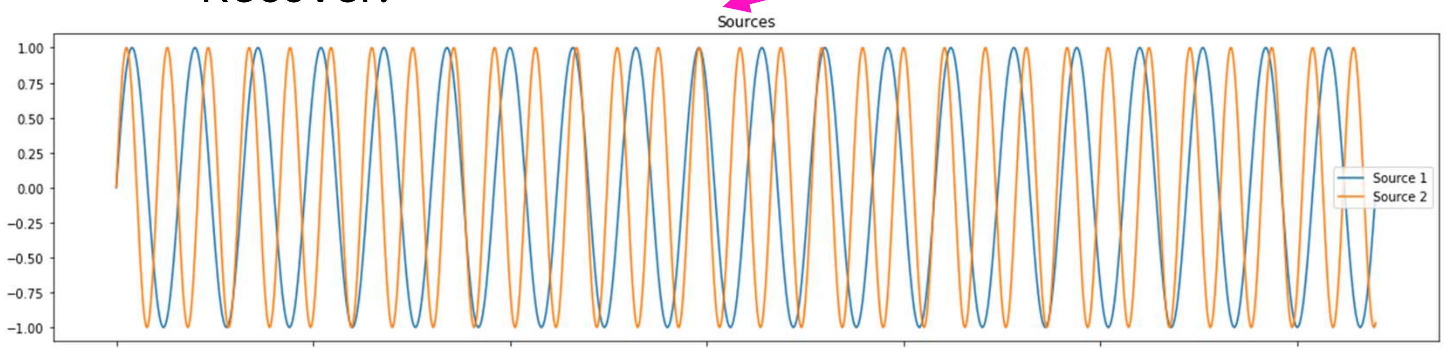
$$W = \begin{bmatrix} 0.8 & 0.2 \\ 0.6 & 0.4 \end{bmatrix}$$

Problem Statement

Given:

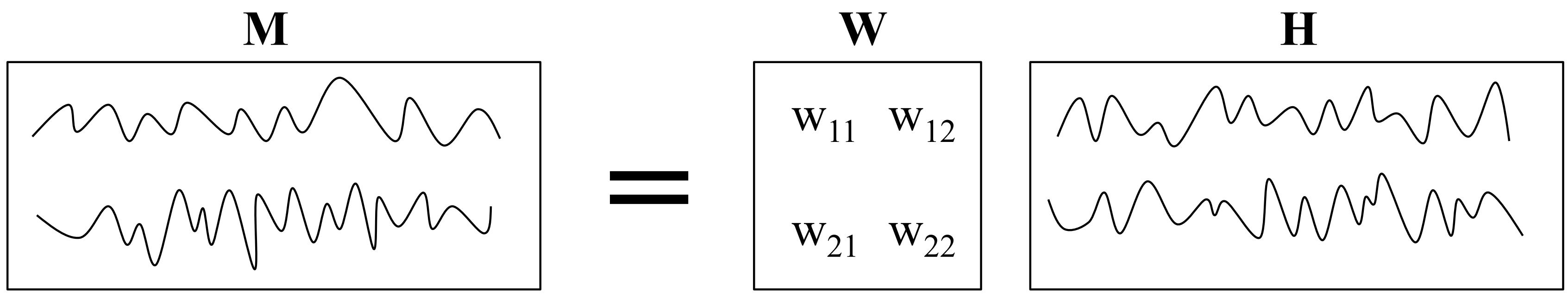


Recover:



$$W = \begin{bmatrix} 0.8 & 0.2 \\ 0.6 & 0.4 \end{bmatrix}$$

Imposing Statistical Constraints



- $\mathbf{M} = \mathbf{WH}$
- Given only $\mathbf{M}$ estimate $\mathbf{H}$
- $\mathbf{H} = \mathbf{W}^{-1}\mathbf{M} = \mathbf{AM}$
- Only known constraint: The rows of $\mathbf{H}$ are independent
- Estimate $\mathbf{A}$ such that the components of $\mathbf{AM}$ are statistically independent
  - $\mathbf{A}$ is the *unmixing* matrix

Statistical Independence

- $\mathbf{M = WH}$ $\quad \boxed{\mathbf{H = AM}}$

Remember this form

In order to recover the original unmixed signals H from the mixed signal M

An ugly algebraic solution

$$\mathbf{M} = \mathbf{W}\mathbf{H} \xrightarrow{\textbf{decorrelate}} \mathbf{H} = \mathbf{A}\mathbf{M}$$

- **Solution 1**: "Recover" $\mathbf{H}$ by decorrelating $\mathbf{M}$
  - We know uncorrelated signals have diagonal correlation matrix
- Find a transform $\mathbf{A}$ such that the rows of $\mathbf{H}=\mathbf{A}\mathbf{M}$ are decorrelated
  - i.e. $\mathbf{H}\mathbf{H}^T$ = Diagonal (assuming 0 mean signals)
  - $\mathbf{A}$ was obtained by eigen decomposition of the correlation matrix of $\mathbf{M}$
    - I.e. by Eigen decomposition of $\mathbf{M}\mathbf{M}^T$

- We know this does not work, however
- Can we do the same for independence
  - Is there a linear transform that will enforce independence?

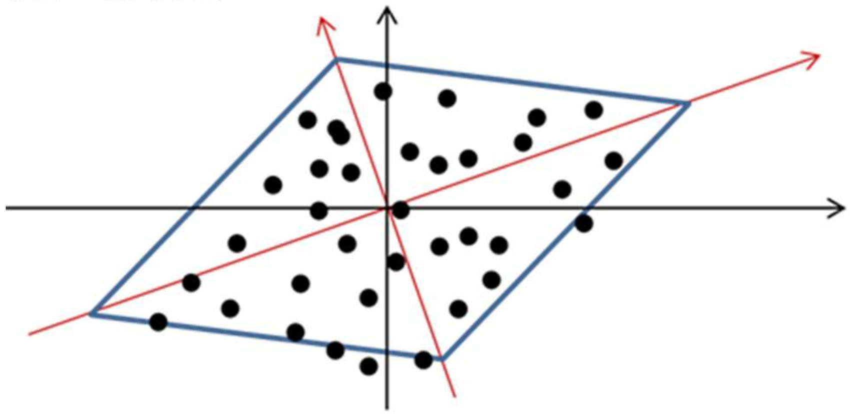
An ugly algebraic solution

- We *decorrelated* signals by diagonalizing the covariance matrix through Eigen decomposition

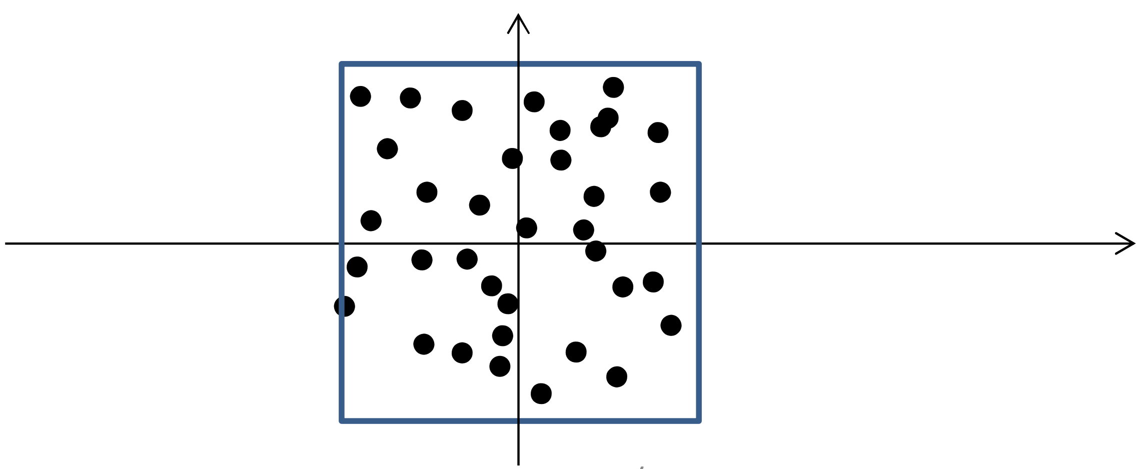
- *Is there a simple matrix we could just similarly diagonalize to make them independent?*
  - Some matrix whose Eigenvector matrix gives us the transform $\mathbf{A}$ such that the rows of $\mathbf{AM}$ are independent

Actual question

- Is there a linear transform that can transform a scatter like this



- To something like this:



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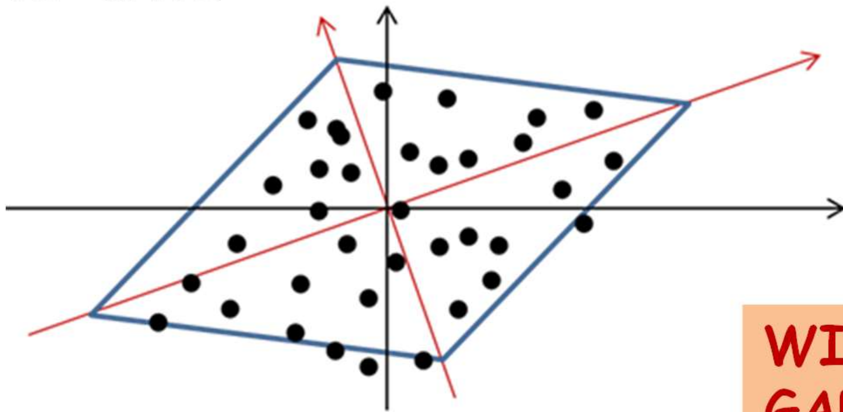

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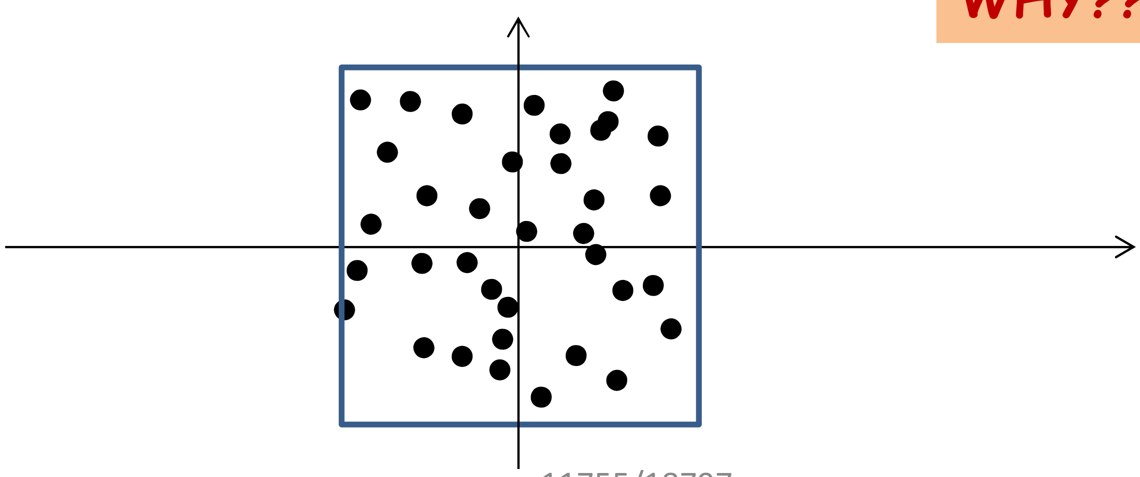
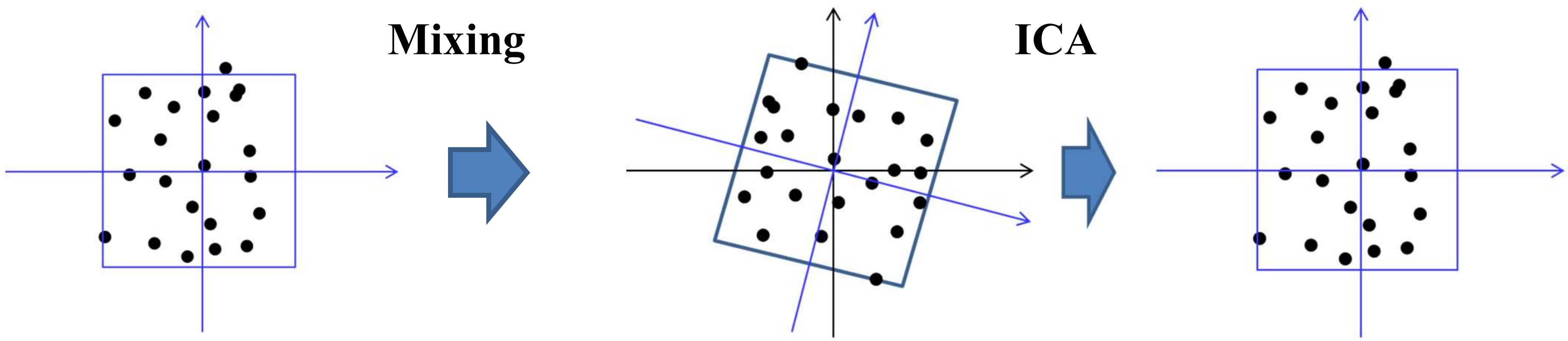


WILL NOT WORK FOR GAUSSIAN DATA

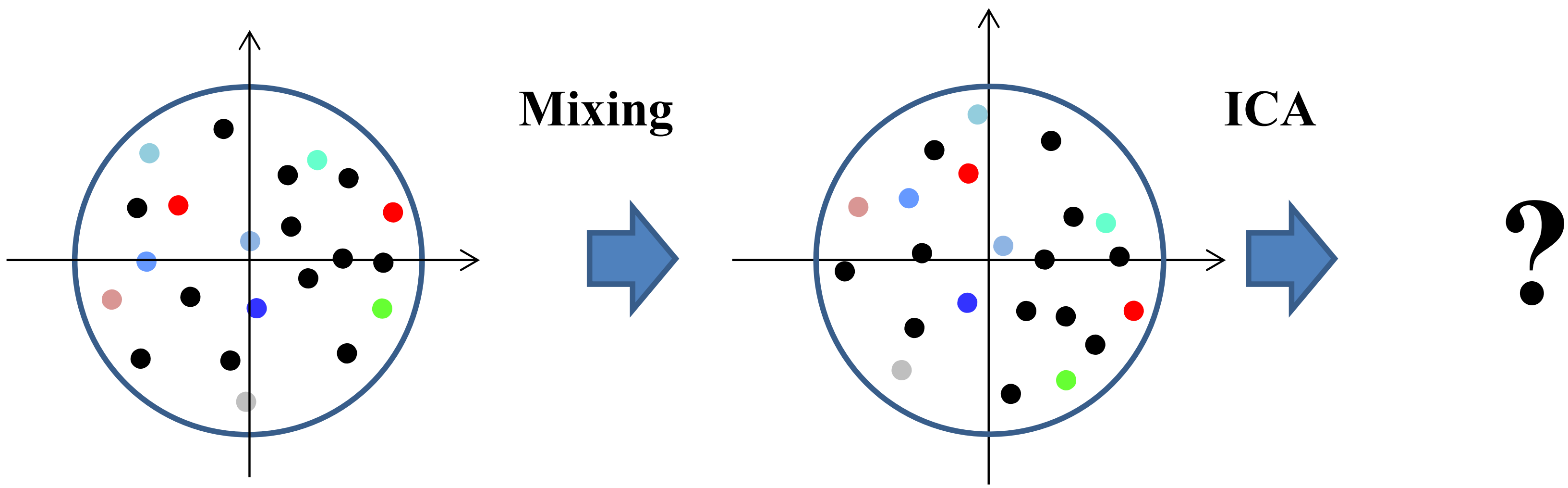
WHY??

Will not work for Gaussian data



- Concept behind ICA:
  - Original sources had some independent distribution
    - Assume all had identical variance
  - "Mixing" rotated the joint distribution
  - ICA finds the axes that "unmixes" the distribution
    - In principle, searches through all rotations such that the distribution is axis parallel again
      - This should give us back the original independent distribution

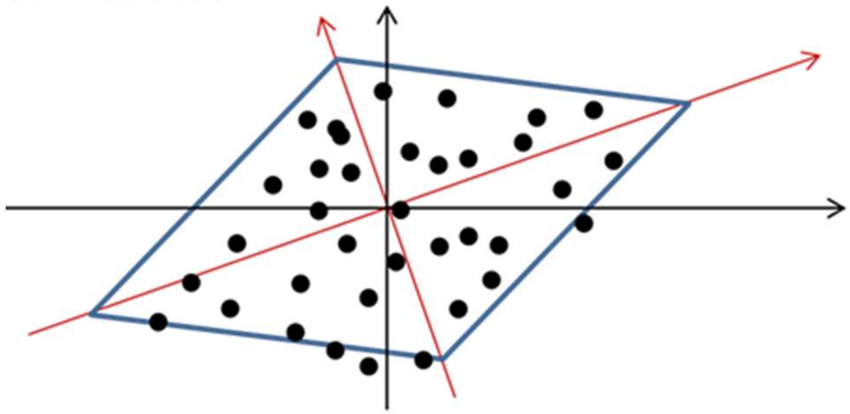
Will not work for Gaussian data



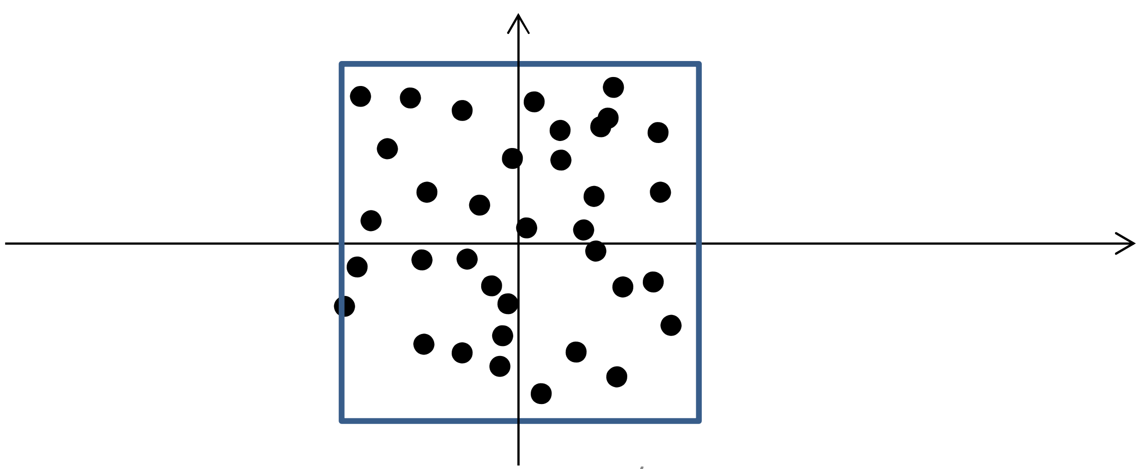
- For independent Gaussian RVs of equal variance, a mixing rotation results in an effectively unchanged distribution
  - The unmixing rotation cannot be determined through inspection of the distribution

Returning to our problem

- Is there a linear transform that can transform a scatter like this



- To something like this:



Zero Mean

- Usual to assume *zero mean* processes
  - Otherwise, some of the math doesn't work well

- $\mathbf{M} = \mathbf{W}\mathbf{H} \qquad \mathbf{H} = \mathbf{A}\mathbf{M}$

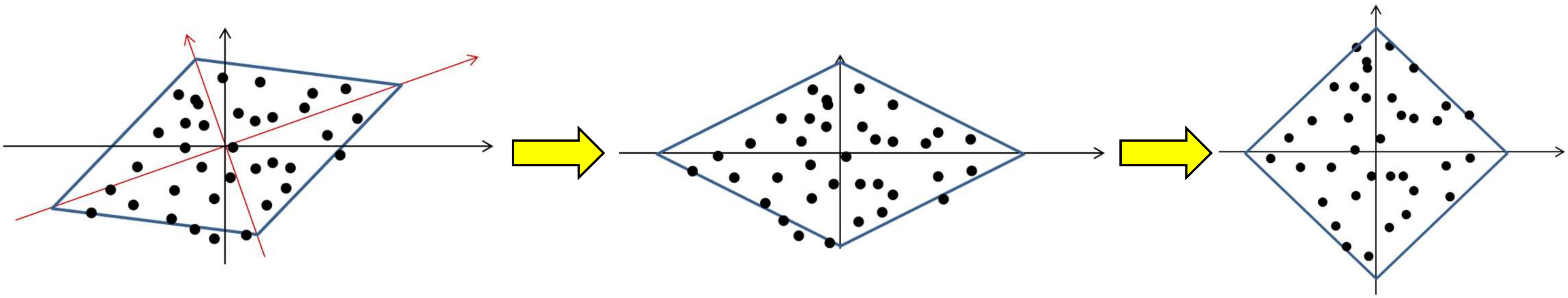
- If mean($\mathbf{M}$) = 0 => mean($\mathbf{H}$) = 0
  - $\mathrm{E}[\mathbf{H}] = \mathbf{A}.\mathrm{E}[\mathbf{M}] = \mathbf{A0} = \mathbf{0}$
  - First step of ICA: Set the mean of $\mathbf{M}$ to 0

$$\mu_{\mathbf{m}} = \frac{1}{cols(\mathbf{M})} \sum_i \mathbf{m}_i$$

$$\mathbf{m}_i = \mathbf{m}_i - \mu_{\mathbf{m}} \qquad \forall i$$

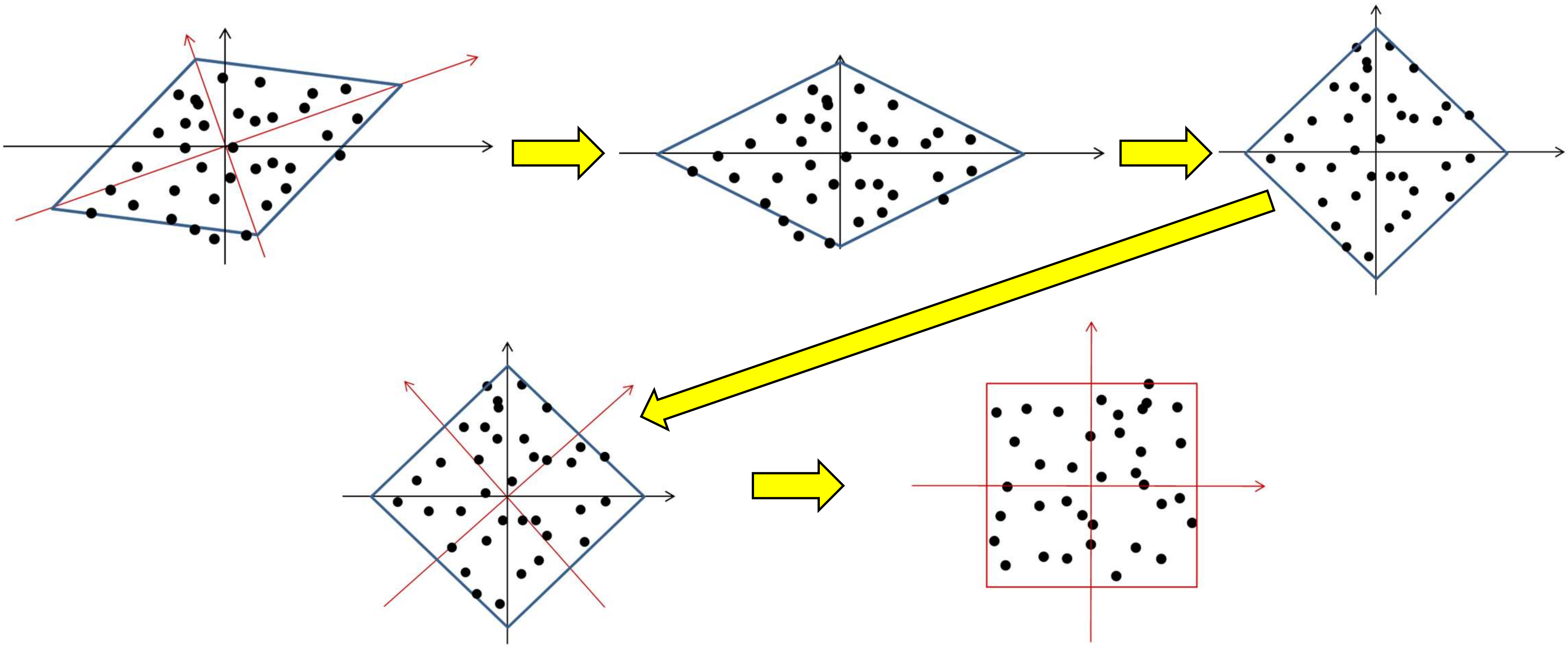
  - $\mathbf{m}_i$ are the columns of $\mathbf{M}$

Actual process



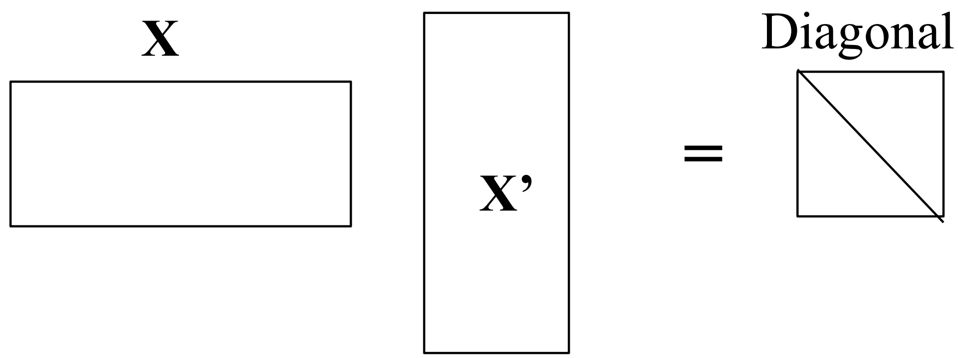
- To simplify the process, we will first *decorrelate* the data and *whiten* it
  - So that the variance is the same along all dimensions

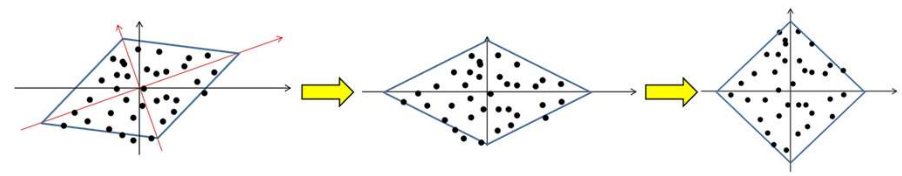
Actual process



- To simplify the process, we will first *decorrelate* the data and *whiten* it
  - So that the variance is the same along all dimensions
- *Then* we search for the axes that make the data independent

Decorrelating and Whitening





- Eigen decomposition $\mathbf{MM}^T = \mathbf{E\Lambda E}^T$
- $\mathbf{C} = \Lambda^{-1/2}\mathbf{E}^T$
- $\mathbf{X} = \mathbf{CM}$

- Not merely decorrelated but ***whitened***
  - $\mathbf{XX}^T = \mathbf{CMM}^T\mathbf{C}^T = \Lambda^{-1/2}\mathbf{E}^T\,\mathbf{E\Lambda E}^T\mathbf{E}\Lambda^{-1/2} = \mathbf{I}$

- $\mathbf{C}$ is the ***whitening matrix***

Uncorrelated != Independent

- Whitening merely ensures that the resulting signals are uncorrelated, i.e.

$$E[\mathbf{x}_i\mathbf{x}_j] = 0 \text{ if } i \mathrel{!}= j$$

- This does not ensure higher order moments are also decoupled, e.g. it does not ensure that

$$E[\mathbf{x}_i^2\mathbf{x}_j^2] = E[\mathbf{x}_i^2]E\,[\mathbf{x}_j^2]$$

- This is *one* of the signatures of independent RVs
- Lets explicitly decouple the fourth order moments

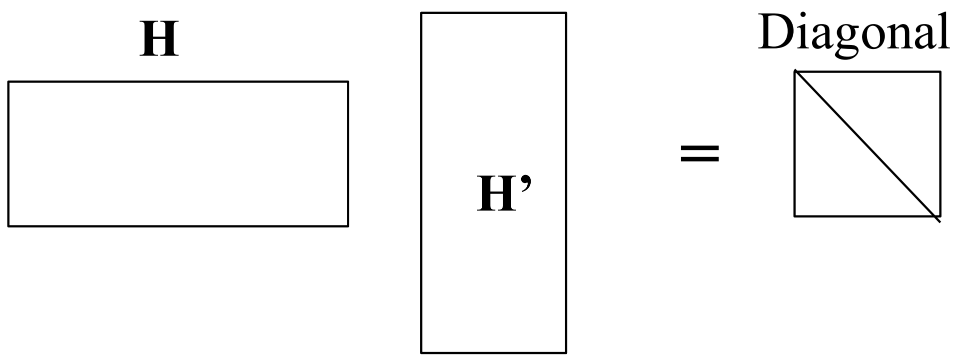
Decorrelating

$\mathbf{H{=}BX}$

$\mathbf{H{=}BCM}$

$\mathbf{A{=}BC}$

$\mathbf{H{=}AM}$



- $\mathbf{X} = \mathbf{CM}$
- $\mathbf{XX}^T = \mathbf{I}$

- **Our objective:** Find the matrix $\mathbf{B}$ that makes the rows of $\mathbf{BX}$ independent
  - $\mathbf{H} = \mathbf{BX}$
- Will multiplying $\mathbf{X}$ by $\mathbf{B}$ *re-correlate* the components?
- Not if $\mathbf{B}$ is *unitary*
  - $\mathbf{BB}^T = \mathbf{B}^T\mathbf{B} = \mathbf{I}$
- $\mathbf{HH}^T = \mathbf{BXX}^T\mathbf{B}^T = \mathbf{BB}^T = \mathbf{I}$
  - Because $\mathbf{XX}^T = \mathbf{I}$
- So we want to find a *unitary* matrix
  - Since the rows of $\mathbf{H}$ are uncorrelated
    - Because they are independent

An ugly algebraic solution

- We *decorrelated* signals by diagonalizing the covariance matrix through Eigen decomposition

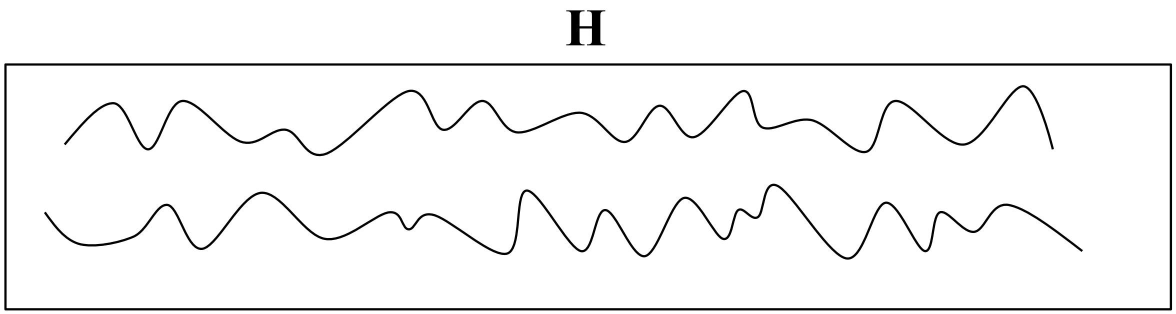
- *Is there a simple matrix we could just similarly diagonalize to make them independent?*
  - Some matrix whose Eigenvector matrix gives us the transform $\mathbf{A}$ such that the rows of $\mathbf{AM}$ are independent

An ugly algebraic solution

- We *decorrelated* signals by diagonalizing the covariance matrix through Eigen decomposition

- *Is there a simple matrix we could just similarly diagonalize to make them independent?*
  - Not really, but there is a matrix we can diagonalize to make *fourth-order* moments independent
    - Just as decorrelation made second-order moments independent

Emulating Independence



- The rows of $\mathbf{H}$ are uncorrelated
  - $E[\mathbf{h}_i\mathbf{h}_j] = E[\mathbf{h}_i]E[\mathbf{h}_j]$
  - $\mathbf{h}_i$ and $\mathbf{h}_j$ are the i^th^ and j^th^ components of any vector in $\mathbf{H}$

- The fourth order moments are independent
  - $E[\mathbf{h}_i\mathbf{h}_j\mathbf{h}_k\mathbf{h}_l] = E[\mathbf{h}_i]E[\mathbf{h}_j]E[\mathbf{h}_k]E[\mathbf{h}_l]$
  - $E[\mathbf{h}_i^2\mathbf{h}_j\mathbf{h}_k] = E[\mathbf{h}_i^2]E[\mathbf{h}_j]E[\mathbf{h}_k]$
  - $E[\mathbf{h}_i^2\mathbf{h}_j^2] = E[\mathbf{h}_i^2]E[\mathbf{h}_j^2]$
  - Etc.

FOBI: Freeing Fourth Moments

- Find $\mathbf{B}$ such that the rows of $\mathbf{H} = \mathbf{BX}$ are independent

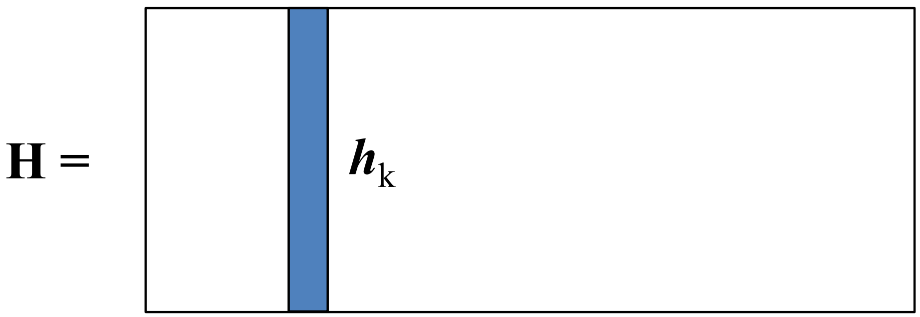
- The fourth moments of $\mathbf{H}$ have the form:
  $\mathrm{E}[\mathbf{h}_i\ \mathbf{h}_j\ \mathbf{h}_k\ \mathbf{h}_l]$

- If the rows of $\mathbf{H}$ were independent
  $\mathrm{E}[\mathbf{h}_i\ \mathbf{h}_j\ \mathbf{h}_k\ \mathbf{h}_l] = \mathrm{E}[\mathbf{h}_i]\ \mathrm{E}[\mathbf{h}_j]\ \mathrm{E}[\mathbf{h}_k]\ \mathrm{E}[\mathbf{h}_l]$

- Solution: Compute $\mathbf{B}$ such that the fourth moments of $\mathbf{H} = \mathbf{BX}$ are decoupled
  - While ensuring that $\mathbf{B}$ is Unitary

- **FOBI: Fourth Order Blind Identification**

ICA: Freeing Fourth Moments



Objective: Find a matrix B such that the rows of H=BX are statistically independent

Define a matrix D that *would* be diagonal if the rows of BX are independent

Compute B such that this matrix becomes diagonal

- Create a matrix of fourth moment terms that would be diagonal if the rows of $\mathbf{H}$ were independent, and diagonalize it

- A good candidate: the weighted correlation matrix of $\mathbf{H}$

$$\boldsymbol{D} = E\left[\|\boldsymbol{h}\|^2 \boldsymbol{h}\boldsymbol{h}^{\mathrm{T}}\right] = \sum_k \|\boldsymbol{h}_k\|^2 \boldsymbol{h}_k \boldsymbol{h}_k^{\mathrm{T}}$$

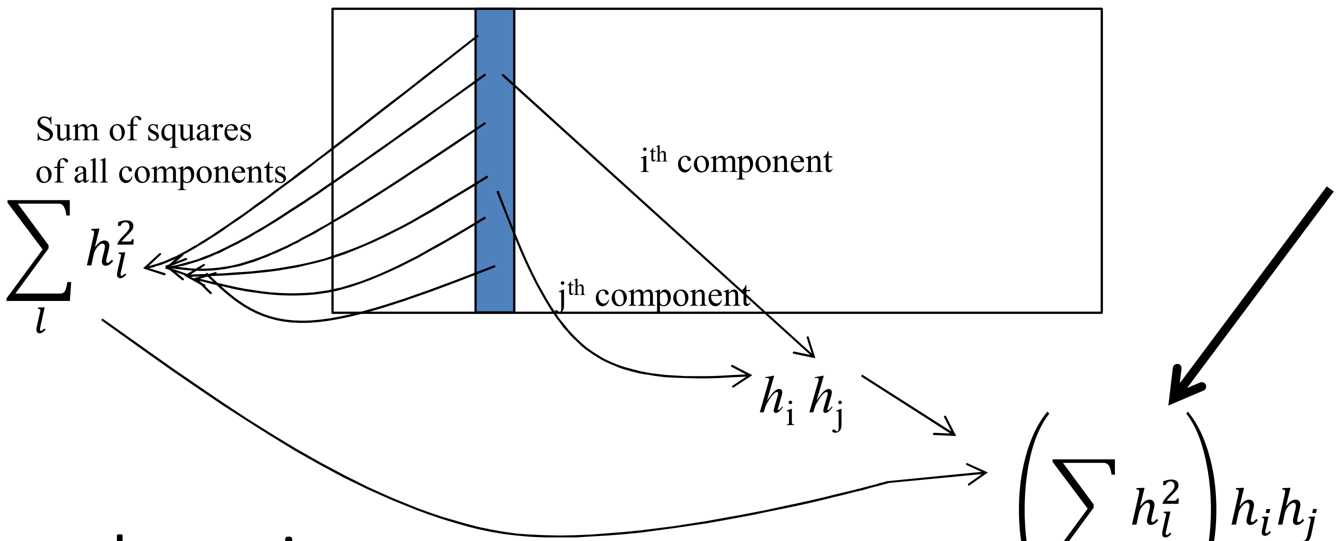
  - $\boldsymbol{h}$ are the columns of $\mathbf{H}$
  - Assuming $\boldsymbol{h}$ is real, else replace transposition with Hermitian

ICA: The D matrix

$$D = \begin{bmatrix} d_{11} & d_{12} & d_{13} & .. \\ d_{21} & d_{22} & d_{23} & .. \\ .. & .. & .. & .. \end{bmatrix}$$

$$\boldsymbol{D} = \boldsymbol{E}\left[\|\boldsymbol{h}\|^2 \boldsymbol{h}\boldsymbol{h}^{\mathrm{T}}\right]$$

$$d_{ij} = \boldsymbol{E}\left[\left(\sum_l h_l^2\right) h_i h_j\right]$$



$$\left(\sum_l h_l^2\right) h_i h_j$$

On the actual matrix

$$\boldsymbol{D} = \frac{\mathbf{1}}{cols(\boldsymbol{H})} \sum_{\boldsymbol{k}} \|\boldsymbol{h}_k\|^2 \boldsymbol{h}_k \boldsymbol{h}_k^{\mathrm{T}}$$

$$d_{ij} = \frac{1}{cols(\mathbf{H})} \sum_k \left(\sum_l h_{kl}^2\right) h_{ki} h_{kj}$$

ICA: The D matrix

$$D = \begin{bmatrix} d_{11} & d_{12} & d_{13} & .. \\ d_{21} & d_{22} & d_{23} & .. \\ .. & .. & .. & .. \end{bmatrix}$$

$$d_{ij} = \frac{1}{cols(\mathbf{H})} \sum_k \left(\sum_l h_{kl}^2 \right) h_{ki} h_{kj}$$

- If the h_i terms were independent and zero mean
- For i != j (off-diagonal elements)

$$E\left[h_i h_j \sum_l h_l^2\right] = E[h_i^3]E[h_j] + E[h_i]E\left[h_j^3\right] + E[h_i]E[h_j] \sum_{l \neq i, l \neq j} E[h_l^2] = \mathbf{0}$$

- For $i = j$ (diagonal elements)
  - $E[h_i h_j \sum_l h_l^2] = E[h_i^4] + E[h_i^2] \sum_{l \neq i} E[h_l^2] \neq \mathbf{0}$

- i.e., if h_i were independent, D would be a diagonal matrix
  - **Let us diagonalize *D***

Diagonalizing D

- Recall: $\mathbf{H} = \mathbf{BX}$
  - $\mathbf{B}$ is what we're trying to learn to make $\mathbf{H}$ independent
  - Assumption: $\mathbf{B}$ is unitary, i.e. $\mathbf{B}^T\mathbf{B} = \mathbf{I}$

Objective: Find a matrix B such that the rows of H=BX are statistically independent

Define a matrix D that *would* be diagonal if the rows of BX are independent

Compute B such that this matrix becomes diagonal

- Note: if $\mathbf{H} = \mathbf{BX}$, then each vector $\mathbf{h} = \mathbf{Bx}$
- The fourth moment matrix of $\mathbf{H}$ is
- $\mathbf{D} = E[\mathbf{h}^T\mathbf{h}\ \mathbf{h}\ \mathbf{h}^T] = E[\mathbf{x}^T\mathbf{B}^T\mathbf{Bx}\ \mathbf{Bx}\ \mathbf{x}^T\ \mathbf{B}^T]$

$$= E[\mathbf{x}^T\mathbf{x}\ \mathbf{Bx}\ \mathbf{x}^T\ \mathbf{B}^T]$$

$$= \mathbf{B}\ E[\mathbf{x}^T\mathbf{x}\ \mathbf{xx}^T]\mathbf{B}^T$$

$$= \mathbf{B}\ E[||\mathbf{x}||^2\ \mathbf{xx}^T]\mathbf{B}^T$$

Diagonalizing D

- Objective: Estimate $\mathbf{B}$ such that the fourth moment of $\mathbf{H} = \mathbf{BX}$ is diagonal

- Compose $\mathbf{D_x} = \sum_{\boldsymbol{k}} \|\mathbf{x}_k\|^2 \mathbf{x_k x}_k^{\mathrm{T}}$

- Diagonalize $\mathbf{D_x}$ via Eigen decomposition

  $\mathbf{D_x} = \mathbf{U}\Lambda_{\mathrm{H}}\mathbf{U}^{\mathrm{T}}$

- $\mathbf{B} = \mathbf{U}^{\mathrm{T}}$
  - **That's it!!!!**

B frees the fourth moment

$$\mathbf{D_x} = \mathbf{U}\Lambda\mathbf{U}^T \;\; ; \quad \mathbf{B} = \mathbf{U}^T$$

- $\mathbf{U}$ is a unitary matrix, i.e. $\mathbf{U}^T\mathbf{U} = \mathbf{U}\mathbf{U}^T = \mathbf{I}$ (identity)
- $\mathbf{H} = \mathbf{B}\mathbf{X} = \mathbf{U}^T\mathbf{X}$
  - $\mathbf{h} = \mathbf{U}^T\mathbf{x}$

- The fourth moment matrix of $\mathbf{H}$ is

$$\mathbf{D} = E[||\mathbf{h}||^2 \, \mathbf{h}^T]$$

$$\begin{aligned}\mathbf{D} &= \mathbf{U}^T E[||\mathbf{x}||^2 \, \mathbf{x}\mathbf{x}^T]\mathbf{U} \\ &= \mathbf{U}^T \mathbf{D_x} \mathbf{U} \\ &= \mathbf{U}^T \mathbf{U} \Lambda_H \mathbf{U}^T \mathbf{U} = \Lambda_H\end{aligned}$$

- The fourth moment matrix of $\mathbf{H} = \mathbf{U}^T\mathbf{X}$ is Diagonal!!

Overall Solution

- Objective: Estimate A such that the rows of $\mathbf{H} = \mathbf{AM}$ are independent
- Step 1: *Whiten M*
  - $\mathbf{C} = \Lambda^{-1/2}\mathbf{E}^T$ where Λ and $\mathbf{E}$ are the eigen value and eigen vector matrices of $\mathbf{MM}^T$
  - $\mathbf{X} = \mathbf{CM}$
- Step 2: Free up fourth moments on $\mathbf{X}$
  - $\mathbf{B}$ is the (transpose of the) matrix of Eigenvectors of $\mathbf{X}.diag(\mathbf{X}^T\mathbf{X}).\mathbf{X}^T$
  - $\mathbf{A} = \mathbf{BC}$

FOBI for ICA

- Goal: to derive a matrix $\mathbf{A}$ such that the rows of $\mathbf{AM}$ are independent
- Procedure:
  1. "Center" $\mathbf{M}$
  2. Compute the autocorrelation matrix $\boldsymbol{R}_{MM}$ of $\mathbf{M}$
  3. Compute whitening matrix $\mathbf{C}$ via Eigen decomposition
     $\boldsymbol{R}_{\mathrm{MM}} = \mathbf{E}\Lambda\mathbf{E}^{\mathrm{T}}, \quad \mathbf{C} = \Lambda^{-1/2}\mathbf{E}^{\mathrm{T}}$
  4. Compute $\mathbf{X} = \mathbf{CM}$
  5. Compute the fourth moment matrix $\mathbf{D}' = E[\|\mathbf{x}\|^2\mathbf{x}\mathbf{x}^{\mathrm{T}}]$
  6. Diagonalize $\mathbf{D}'$ via Eigen decomposition
  7. **$\mathbf{D}' = \mathbf{U}\Lambda_{\mathrm{H}}\mathbf{U}^{\mathrm{T}}$**
  8. Compute $\mathbf{A} = \mathbf{U}^{\mathrm{T}}\boldsymbol{C}$
- The fourth moment matrix of $\mathbf{H{=}AM}$ is diagonal
  – **Note that the autocorrelation matrix of $\mathbf{H}$ will also be diagonal**

ICA by diagonalizing moment matrices

- FOBI is not perfect
  - Only a subset of fourth order moments are considered
    - Diagonalizing the particular fourth-order moment matrix we have chosen is not guaranteed to diagonalize every other fourth-order moment matrix
- JADE: (Joint Approximate Diagonalization of Eigenmatrices), J.F. Cardoso
  - Jointly diagonalizes multiple fourth-order cumulant matrices

Poll 3

- Which of the following statements are true of FOBI
  - It computes a transform that makes *all* fourth-order moments independent
  - It requires a first pre-whitening step
  - The transform is the Eigenvector matrix of the fourth-order moment matrix
  - The transform is the product of the Eigenvector matrix of the fourth-order moment matrix of the whitened data, and the whitening matrix obtained through PCA

Poll 3

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  - It computes a transform that makes *all* fourth-order moments independent
  - **It requires a first pre-whitening step**
  - The transform is the Eigenvector matrix of the fourth-order moment matrix
  - **The transform is the product of the Eigenvector matrix of the fourth-order moment matrix of the whitened data, and the whitening matrix obtained through PCA**

Lets try a different tack

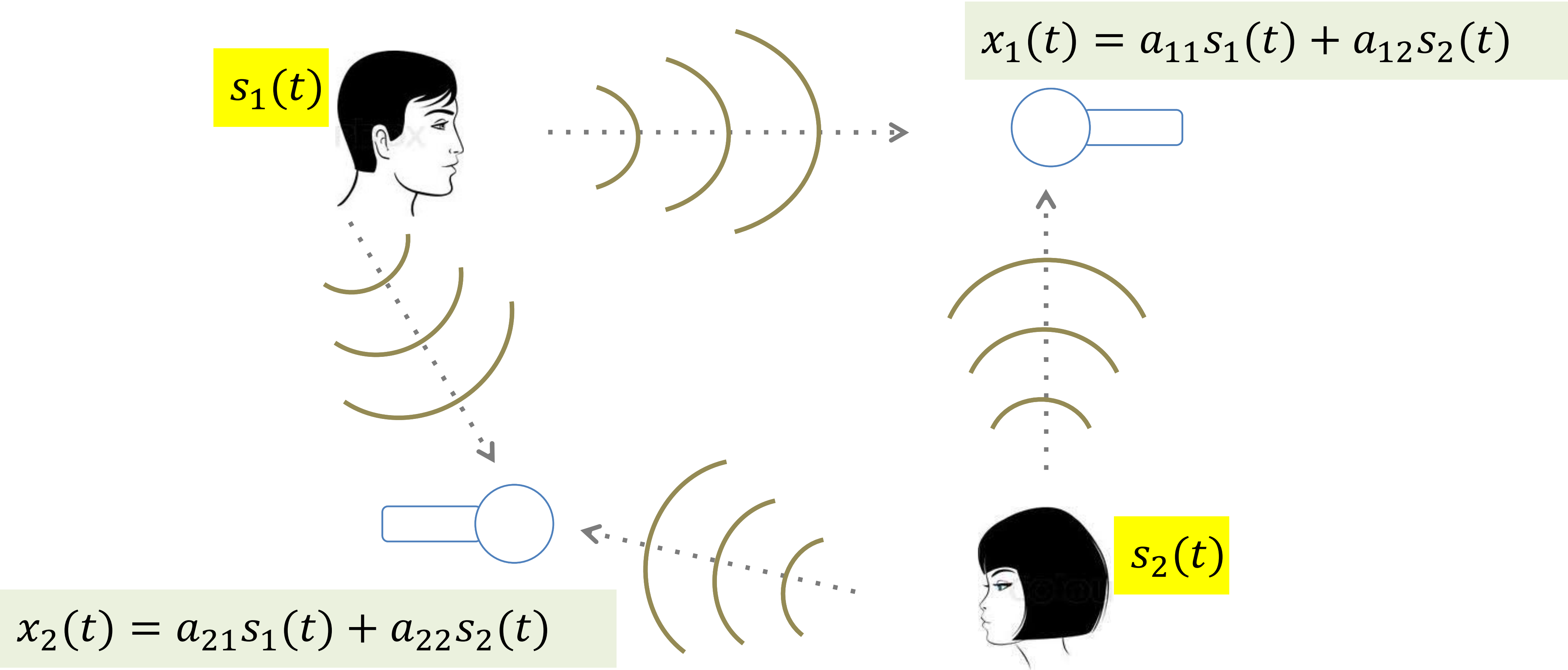
- Use the statistical properties of mixing…

The Central Limit Theorem

- Sum of independent random variables will tend toward a Gaussian distribution
- Even if the independent random variables don't have a Gaussian distribution!

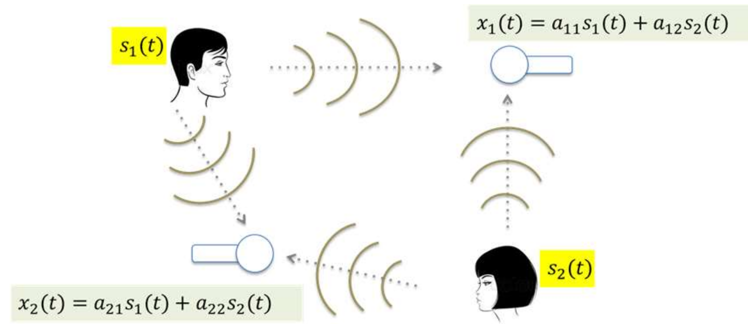
- The sum will *almost always* be *"more"* Gaussian than the component signals
  - Even if the independent RVs are not Gaussian

Changing notation for a bit



- Two people speak simultaneously are recorded by two microphones
  - Each recorded signal is a mixture of both signals
- Find a linear transform that unmixes them

Problem setting and notation



- Independent signals $s_1 \ldots s_N$ (arranged as a vector $\boldsymbol{s}$) have been mixed by mixing matrix $\boldsymbol{A}$ to generate mixed output $\boldsymbol{x}$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{22} & a_{22} \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \end{bmatrix}$$

$$\boldsymbol{x} = \boldsymbol{A}\boldsymbol{s}$$

- We need to find a matrix $\boldsymbol{W}$ that will unmix $\boldsymbol{x}$ to recover $\boldsymbol{s}$

$$\boldsymbol{y} = \boldsymbol{W}^\top \boldsymbol{x} \qquad \boldsymbol{s.t.}\ \boldsymbol{y} \approx \boldsymbol{x}$$

The Central Limit Theorem & ICA

Let each s_i be identically distributed

Let's obtain one of the sources

$$y = w^T \boldsymbol{x}$$

Here, $\boldsymbol{w}$ is a column of $\boldsymbol{W}$

The Central Limit Theorem & ICA

$$y = w^T \boldsymbol{x}$$

Suppose, w^T is a row of the mixing matrix's inverse ($W^T = A^{-1}$) . Then y would be one of the independent sources:

$$\boldsymbol{x} = A\boldsymbol{s} \ \rightarrow \boldsymbol{s} = A^{-1}\boldsymbol{x}$$

The Central Limit Theorem & ICA

Useful Relations: $\boldsymbol{x} = A\boldsymbol{s}$ $\boldsymbol{y} = W^T\boldsymbol{x}$

$y = w^T\boldsymbol{x}$

Let's define a convenient variable:

$$z = A^T w$$

And let's do some substitutions:

$$y = w^T\boldsymbol{x} \rightarrow y = w^T A\boldsymbol{s} \rightarrow y = (w^T A)\boldsymbol{s} \rightarrow y = (A^T w)^T\boldsymbol{s} \rightarrow y = z^T\boldsymbol{s}$$

The Central Limit Theorem & ICA

Useful Relations:

$$x = A\boldsymbol{s}$$
$$y = w^T\boldsymbol{x}$$
$$y = z^T\boldsymbol{s}$$

What does this last relation mean?

We want y to be ONE OF the independent sources

The Central Limit Theorem & ICA

Useful Relations: $x = A\boldsymbol{s}$

$$y = w^T \boldsymbol{x}$$

$$y = z^T \boldsymbol{s}$$

1. y is a linear combination of sources

What does this do for us?

The Central Limit Theorem & ICA

Useful Relations: $x = A\boldsymbol{s}$

$$y = w^T\boldsymbol{x}$$

$$y = z^T\boldsymbol{s}$$

1. $\boldsymbol{y}$ is a linear combination of sources
2. If $\boldsymbol{y}$ is one of the sources, then $\boldsymbol{z} = [\mathbf{0}, \ldots, \mathbf{1}, \ldots, \mathbf{0}]$.

What does this do for us?

The Central Limit Theorem & ICA

Useful Relations:

$$x = A\boldsymbol{s}$$

$$y = w^T \boldsymbol{x}$$

$$y = z^T \boldsymbol{s}$$

1. $\boldsymbol{y}$ is a linear combination of sources
2. If $\boldsymbol{y}$ is one of the sources, then $\boldsymbol{z} = [0, \ldots, 1, \ldots, 0]$.

$$s_3 = z^T \begin{bmatrix} s_1 \\ s_2 \\ s_3 \end{bmatrix} \rightarrow s_3 = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \\ s_3 \end{bmatrix}$$

What does this do for us?

The Central Limit Theorem & ICA

Useful Relations:

$$x = A\boldsymbol{s}$$
$$y = w^T\boldsymbol{x}$$
$$y = z^T\boldsymbol{s}$$

1. $\boldsymbol{y}$ is a linear combination of sources
2. If $\boldsymbol{y}$ is one of the sources, then $\boldsymbol{z} = [0, \ldots, 1, \ldots, 0]$.
3. Since the sources are independent R.V.'s, any ***mixed*** $\boldsymbol{y}$ is "more Gaussian" than any of the sources

What does this do for us?

The Central Limit Theorem & ICA

Useful Relations:

$$x = A\boldsymbol{s}$$
$$y = w^T\boldsymbol{x}$$
$$y = z^T\boldsymbol{s}$$

1. $\boldsymbol{y}$ is a linear combination of sources
2. If $\boldsymbol{y}$ is one of the sources, then $\boldsymbol{z} = [0, \ldots, 1, \ldots, 0]$.
3. Since the sources are independent R.V.'s, any ***mixed*** $\boldsymbol{y}$ is "more Gaussian" than any of the sources
4. If $\boldsymbol{y}$ is one of the sources, $\boldsymbol{y}$ is the *least Gaussian!*

What does this do for us?

The Central Limit Theorem & ICA

Useful Relations:

$$\boldsymbol{x} = A\boldsymbol{s}$$

$$y = w^T\boldsymbol{x} \qquad y = z^T\boldsymbol{s}$$

Recall: we are given *x*.

Recall: we are not given *s*.

Recall: *z* is a variable we defined for convenience

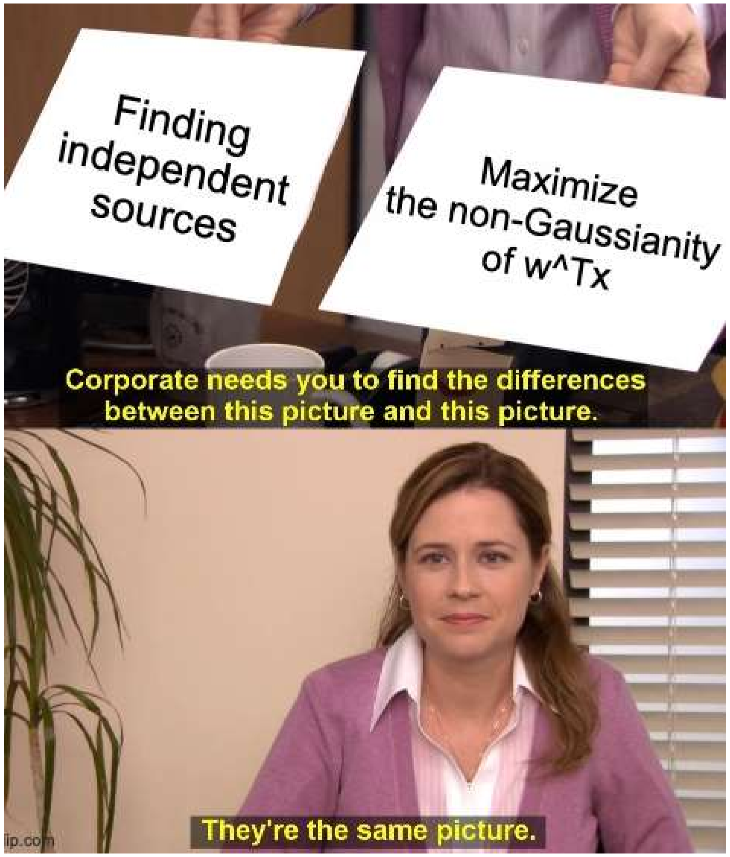
Let's pick a *w* that maximizes the non-Gaussianity of *y*.

This should force *z* to have just one non-zero component

***y* will then be one of the independent sources.**

BIG GOAL™

MAXIMIZE THE NON-GAUSSIANITY OF $y = w^T x$



What they are and what they proxy

CONTRAST FUNCTIONS

“more Gaussian” & “least Gaussian”

- How can we measure Gaussianity
- If we can measure Gaussianity, can we produce a way to optimize over that?
- If we can optimize non-Gaussianity, can we solve ICA?

Fortunately, there are lots of ways to measure non-Gaussianity!

Kurtosis

A very clear formula:

$$Kurt[X] = E\left[\left(\frac{X - \mu}{\sigma}\right)^4\right] = \frac{E[(X - \mu)^4]}{(E[(X - \mu)^2]^2)}$$

$$Kurt[X] = E\left[X^4\right] - 3\left(E\left[X^2\right]\right)^2)$$

Kurtosis

$$Kurt[X] = E[X^4] - 3\left(E[X^2]\right)^2)$$

Note: For a multivariate normal distribution with unit variance, $E[X^4] = 3\left(E[X^2]\right)^2 = 3$.

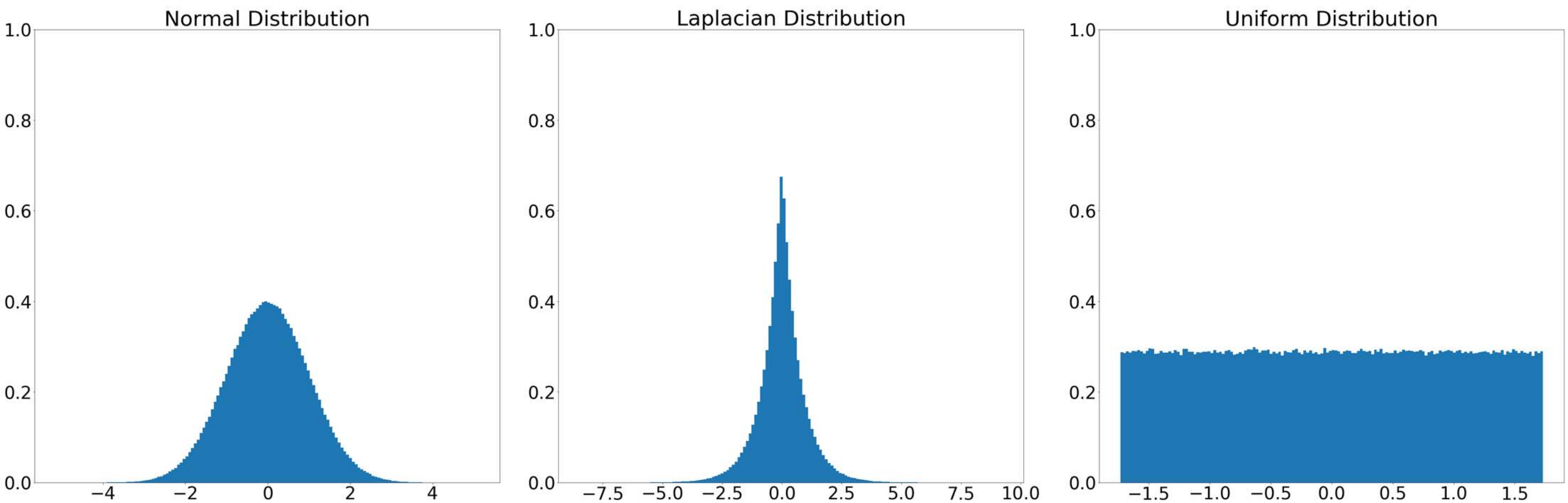
Note: for a multivariate normal distribution with unit variance, $3\left(E[X^2]\right)^2 = 3(1)^2 = 3.$

So, if $X \sim N(0,1)$, $Kurt[X] = 0.$

Kurtosis

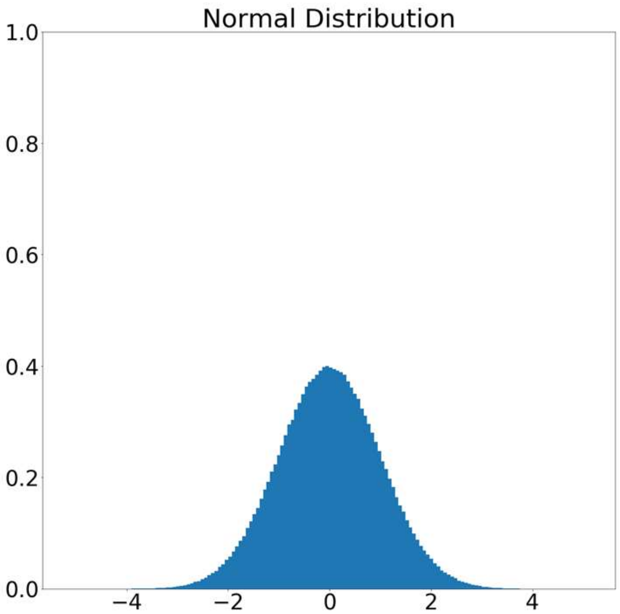
- A measure of how heavy the tails of a distribution are

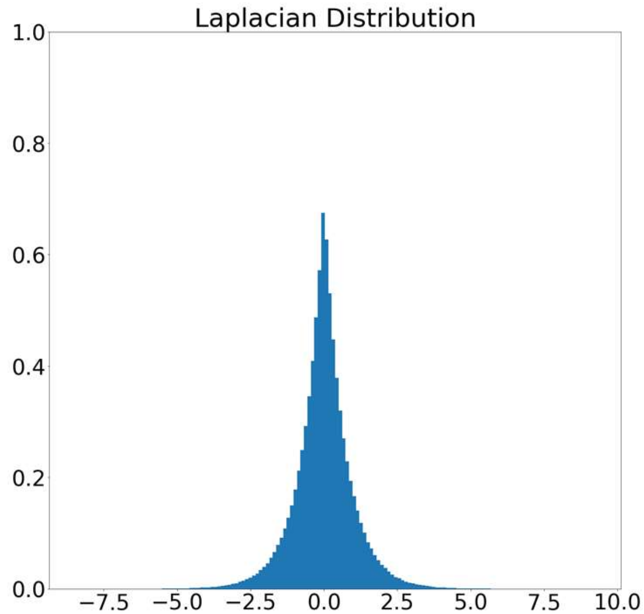
Generated with 1,000,000 samples.

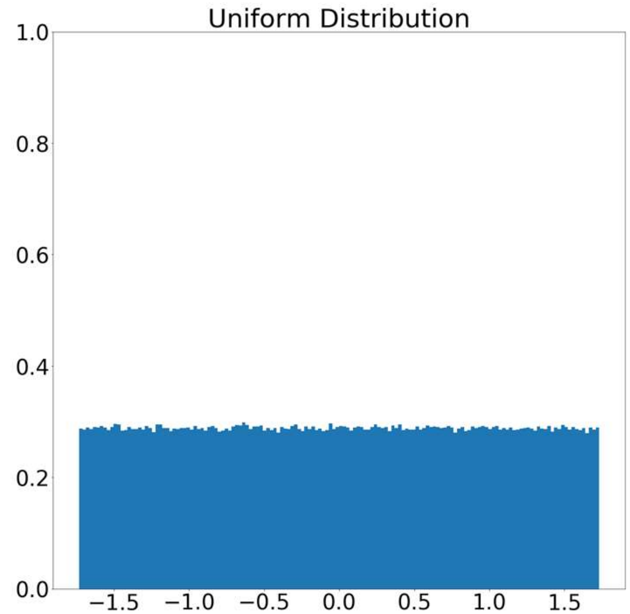


Ground Truth Kurt[X] = 0.0 **Ground Truth Kurt[X] = 3.0** **Ground Truth Kurt[X] = -1.2**

Generated with 1,000,000 samples.







Ground Truth Kurt[X] = 0.0

Calculated Kurt[X] = 0.0

Ground Truth Kurt[X] = 3.0

Calculated Kurt[X] = 3.023

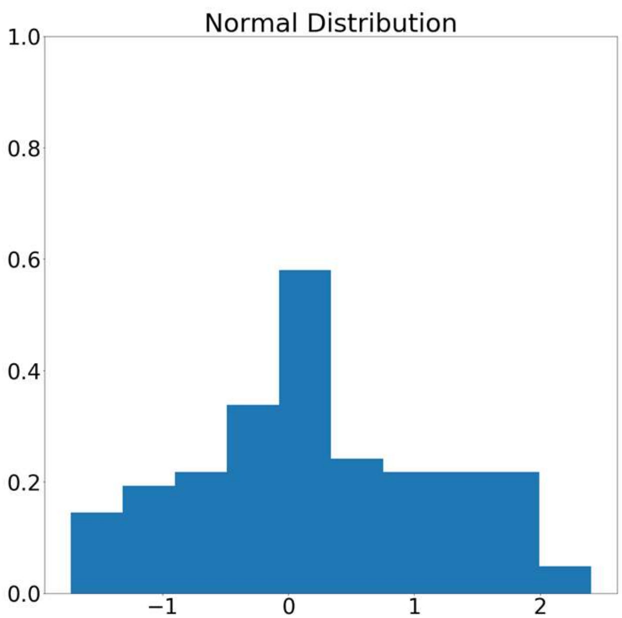
Ground Truth Kurt[X] = -1.2

Calculated Kurt[X] = -1.199

Kurtosis

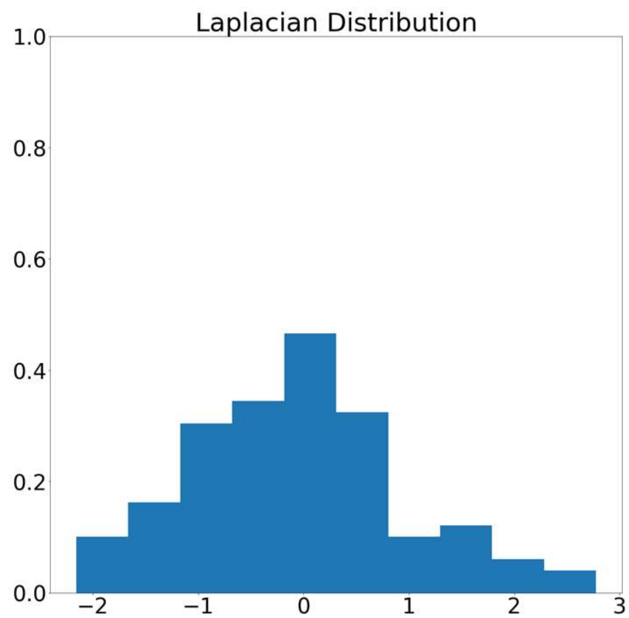
- How would we optimize?
- Use the absolute value of kurtosis
- For a Gaussian R.V., its kurtosis is 0
- Therefore, we want to maximize the kurtosis of the distribution

Generated with 100 samples.



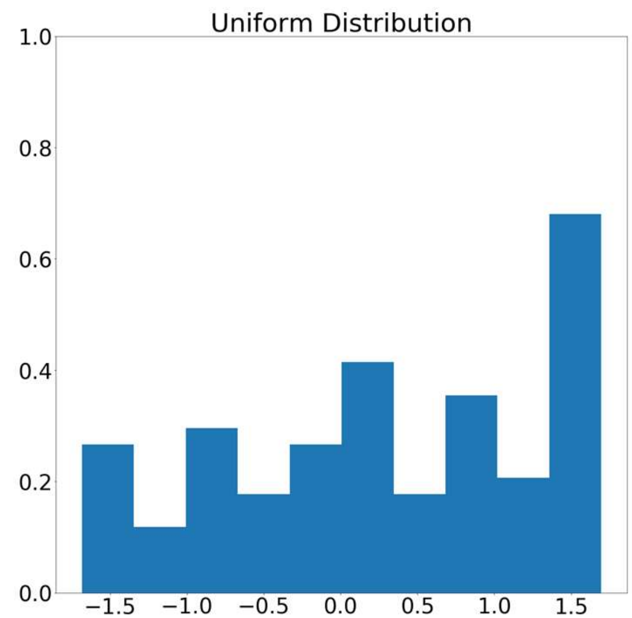
Ground Truth Kurt[X] = 0.0

Calculated Kurt[X] = -0.54



Ground Truth Kurt[X] = 3.0

Calculated Kurt[X] = 0.121



Ground Truth Kurt[X] = -1.2

Calculated Kurt[X] = 1.15

Kurtosis

- Benefits
  - computationally easy
  - some nice linearity properties
  - widely used!
- Disadvantages
  - Susceptible to outliers
  - Few data points leads to bad estimate

Not a robust measure of Gaussianity!

Negentropy

- Entropy:

$$H(X) = -\sum_{i=1}^{n} P(x_i) \log P(x_i)$$

From last lecture: minimal number of bits sent for an optimal code

Negentropy

- Entropy: a measure of surprise
- R.V. that is “more random” will have a larger entropy
  - More bits needed to send
- R.V. that is “less random” will have a smaller entropy
  - Fewer bits needed to send
  - Spiky PDFs

What is the entropy of a Gaussian random variable?

Negentropy

- Entropy of a Gaussian: depends but it's the largest possible value of any distribution with equal variance

How does this help us?

Negentropy

Define:

$$J(X) = H(X_{gauss}) - H(X)$$

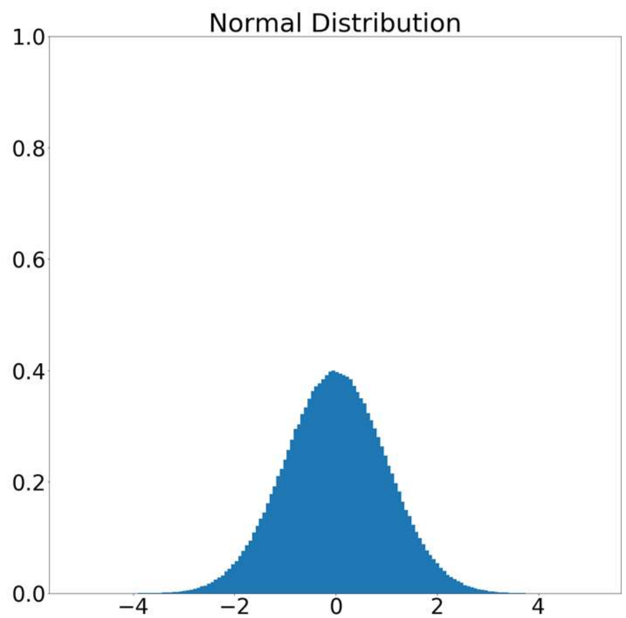
X_{gauss} is a Gaussian with the same covariance matrix as ***X.***

With this definition: ***J(X)*** > 0 and ***J(X) = 0*** if ***X*** is Gaussian

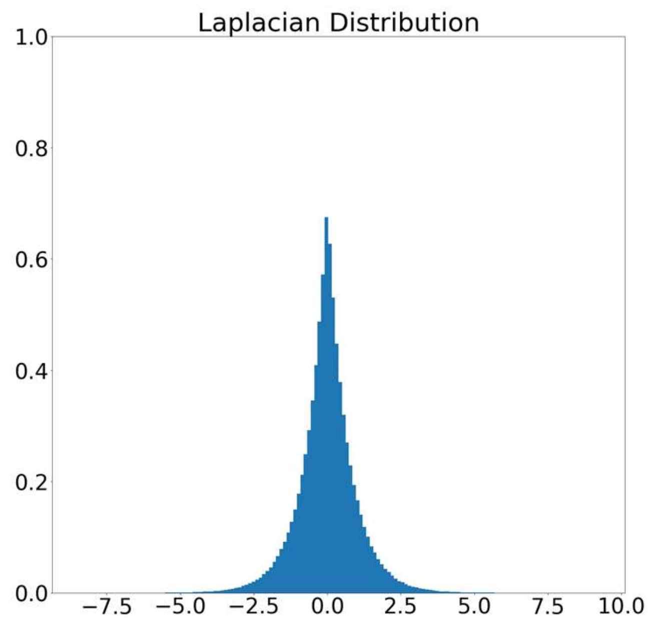
So, to minimize Gaussianity, we want to maximize negentropy!

Negentropy

Generated with 1,000,000 samples.



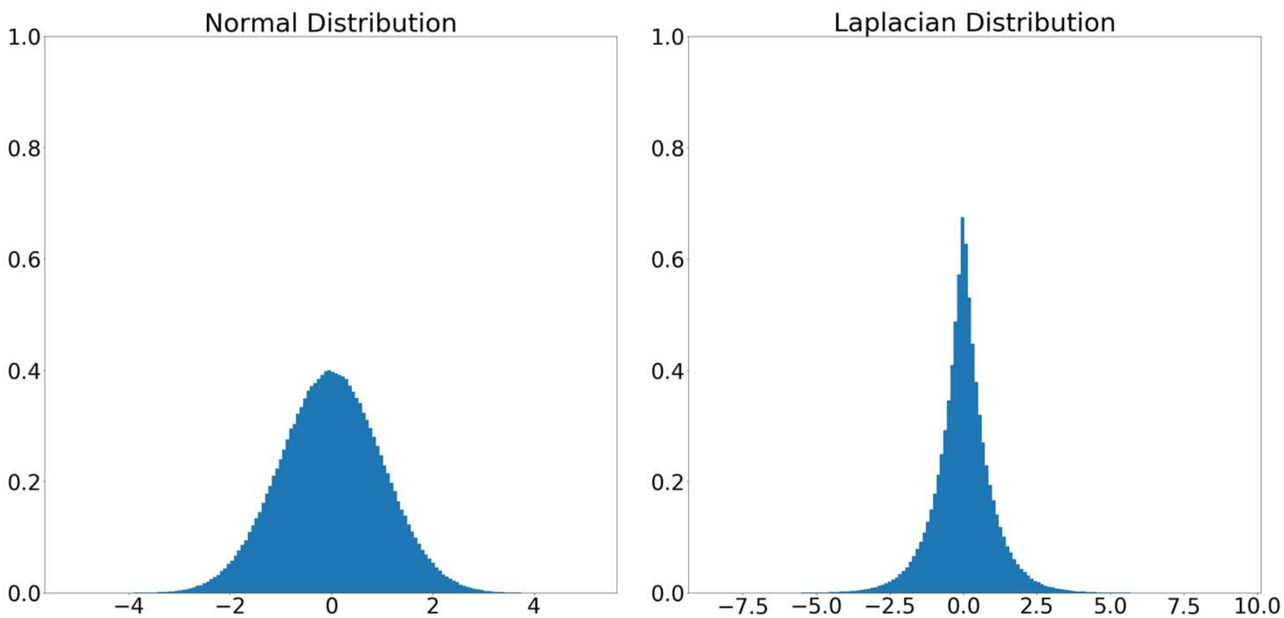
Ground Truth J[X] = 0.0



Ground Truth J[X] = 1.07

Negentropy

Generated with 1,000,000 samples.



Ground Truth J[X] = 0.0
Calculated J[X] = 0.08

Ground Truth J[X] = 1.07
Calculated J[X] = 0.717

Negentropy

- Advantages:
  - Very well justified measure of Gaussianity
  - *Optimal* measure of Gaussianity
- Disadvantages
  - Computationally hard
  - Must estimate the PDF of a R.V.: *always a fun thing to do :/*

We will usually approximate negentropy and maximize over that

When you’re tired of looking at math slides and want to build something

ALGORITHMS

Maximizing an approximation to negentropy.

FASTICA

General principle

- Want to maximize $H(\nu) - H(X)$
  - Where ν is a 0 mean unit variance Gaussian RV and the variance of X is 1 (whitened)

$$\max(E[-\log P(\nu)] - E[-\log P(X)])$$
$$= \max(E[\log P(X)] - E[\log P(\nu)])$$

- Taking expectations requires knowledge of $\log P(X)$
  - Which we do not know

- Instead we will take a different approach to maximize the difference between $P(X)$ and a Gaussian
- Ensure that the expected value of *every moment of X is maximally different from the corresponding moment of ν*
  - $\max div(E[X^n], E[\nu^n])$ for every n

Maximizing the gap

$$\max div(E[X^n], E[\nu^n]) \,\forall\, n \;\approx$$
$$\max \mathrm{a}_1 div(E[X], E[\nu]) + \mathrm{a}_2 div\left(E[X]^2, E\left[\nu^2\right]\right) + \mathrm{a}_3 div\left(E\left[X^3\right], E\left[\nu^3\right]\right) + \cdots$$

- Not tractable: will require explicit computation or estimation of all inifinite moments
  - Or at least a whole lot of high-order moments
  - Which are verrrrrrrrrrrry noisy to estimate

- Instead do the following

$$\max div\left(E\left[\mathrm{a}_1 X + a_2 X^2 + a_3 X^3 + \cdots\right], E\left[a_1 \nu + a_2 \nu^2 + a_3 \nu^3 \ldots.\right]\right)$$

- Or alternately

$$\max \;\; div(G(X), G(\nu))$$

- Where $G(X)$ is any function that has a fast convergent Power series expansion:

$$G(X) = \sum_{n=0}^{\infty} (x - x_0)^n$$

  - The power series must include at least four terms to be meaningful
- Using the squared L2 divergence we get
  - $\max J(X) \;\; where \;\; J(X) \propto \left[E[G(X)] - E[G(\nu)]\right]^2$

FastICA

- Hyvärinen 2000
- Uses an approximation of negentropy:

$$J(X) \propto \left[E[G(X)] - E[G(\nu)] \right]^2$$

ν is a Gaussian variable with zero-mean and unit-variance

G are nonquadratic functions

FastICA: the *G* function

- *G* just needs to be non-quadratic
  - Ideally a function whose polynomial expansion includes all higher powers of the argument
    - Maximizing negentropy will "free" up the moments of those higher powers
- Some weird forms:

$$G(u) = \frac{1}{a_1} \log\cosh(a_1 u)$$

$$G(u) = -\frac{1}{a_2} \exp\left(-\frac{a_2 u^2}{2}\right)$$

$$G(u) = \frac{1}{4} u^4$$

FastICA: comments

- Maximize $J(X) = \left[E[G(X)] - E[G(\nu)]\right]^2$ while ensuring $var(X) = 1$
  - Pre-whiten the data
- Taking actual expectations is not possible
- Instead use the empirical average over samples
- Can be performed in online manner

FastICA

1. Pre-whiten the data
2. Choose an initial $\boldsymbol{w}$
3. Let $w^{+} = E\left[xG'\left(w^{T}x\right)\right] - E\left[G''\left(w^{T}x\right)\right]w$
4. Normalize: $w = w^{+}/\ \|w^{+}\|$
5. Check convergence, head back to 3!

- Normalization of w maintains variance = 1

FastICA: Derivation

- Newton's Method
- Maximize:

$$J(y) \propto \left[E[G(y)] - E[G(v)]\right]^2$$

- Constrain:

$$\|w\|^2 = 1$$

FastICA: Industry Standard

- Basically the industry standard implementation of ICA:
  - https://github.com/scikit-learn/scikit-learn/blob/0fb307bf3/sklearn/decomposition/_fastica.py#L304

Poll 4

- Which of the following are true of FastICA
  - It derives a linear transform that frees up fourth moments
  - It finds the independent directions along which the distributions of the data are maximally non-Gaussian
  - It is a *batch* algorithm
  - It is an *online* algorithm

Poll 4

- Which of the following are true of FastICA
  - It derives a linear transform that frees up fourth moments
  - **It finds the independent directions along which the distributions of the data are maximally non-Gaussian**
  - It is a *batch* algorithm
  - **It is an *online* algorithm**

Speech-Music Example

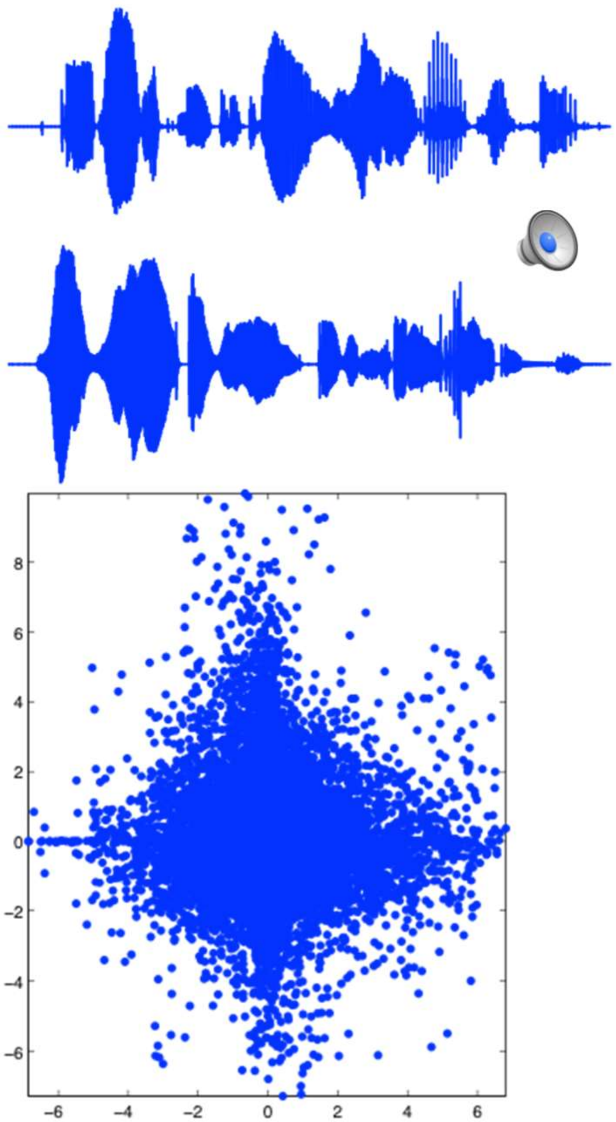
- Te-Won Lee @ UCSD

Mixed

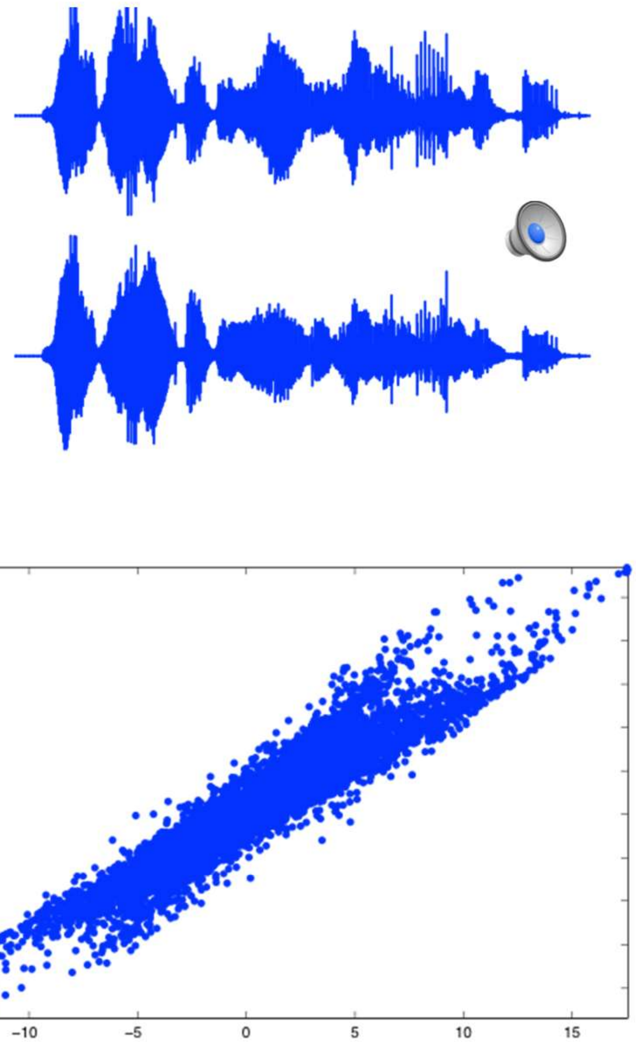
Separated

Another example!

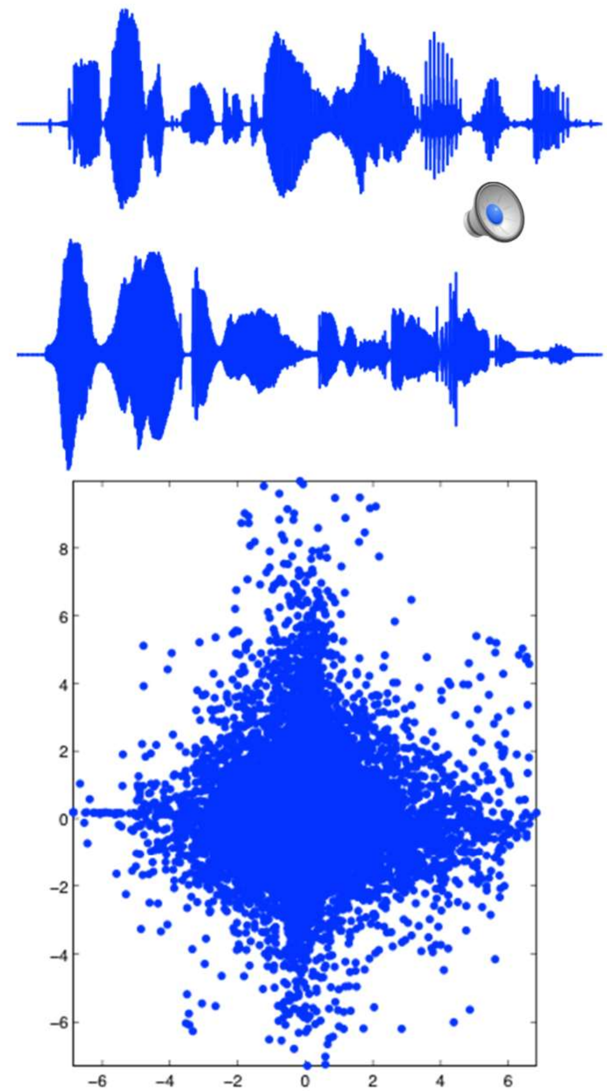
Input



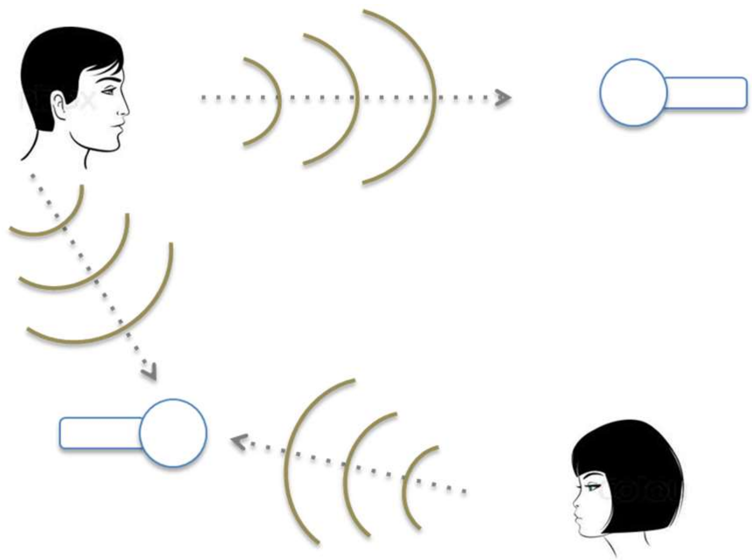
Mix



Output



In Reality



- Mixed signals are not instantaneous mixtures
  - The signals arrive with different delays at the two microphones

$$x_1 = a_{11}s_1(t - t_{11}) + a_{12}s_2(t - t_{12}),$$
$$x_2 = a_{21}s_1(t - t_{21}) + a_{22}s_2(t - t_{22})$$

  - The time-delay issue is hard for ICA to deal with

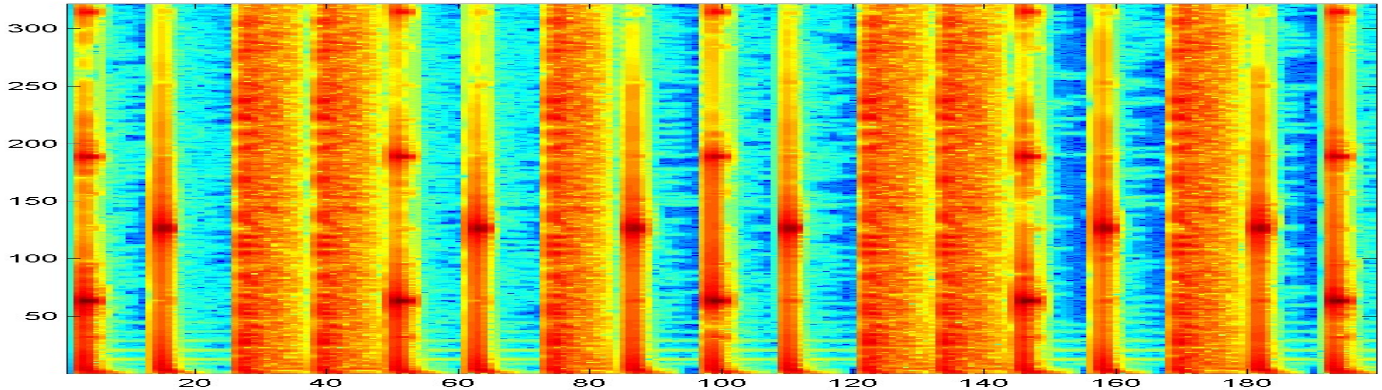
- You must do some clever things for it to work out

Some Explicit Limitations

- ICA is identifiable up to:
  - a sign change (plus or minus)
  - a scaling factor
  - This is just from the model: $\boldsymbol{x} = \boldsymbol{A}\boldsymbol{s}$

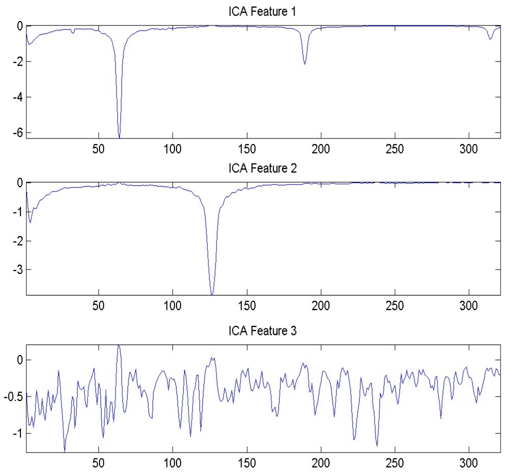
- ICA (unlike PCA) doesn't have a notion of importance
  - The order of the sources doesn't matter.
  - It's unique up to permutation as well.

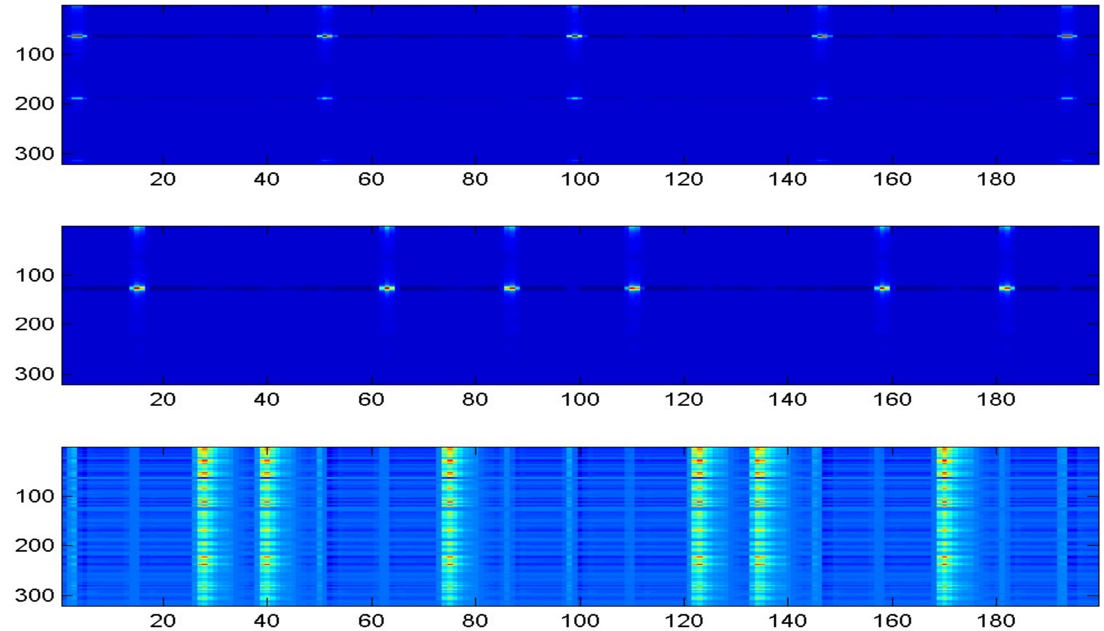
Another Example



- Three instruments..
  - $M = NS$,
  - $S = WM$ (through ICA)
  - $N = W^{+}$

The Notes

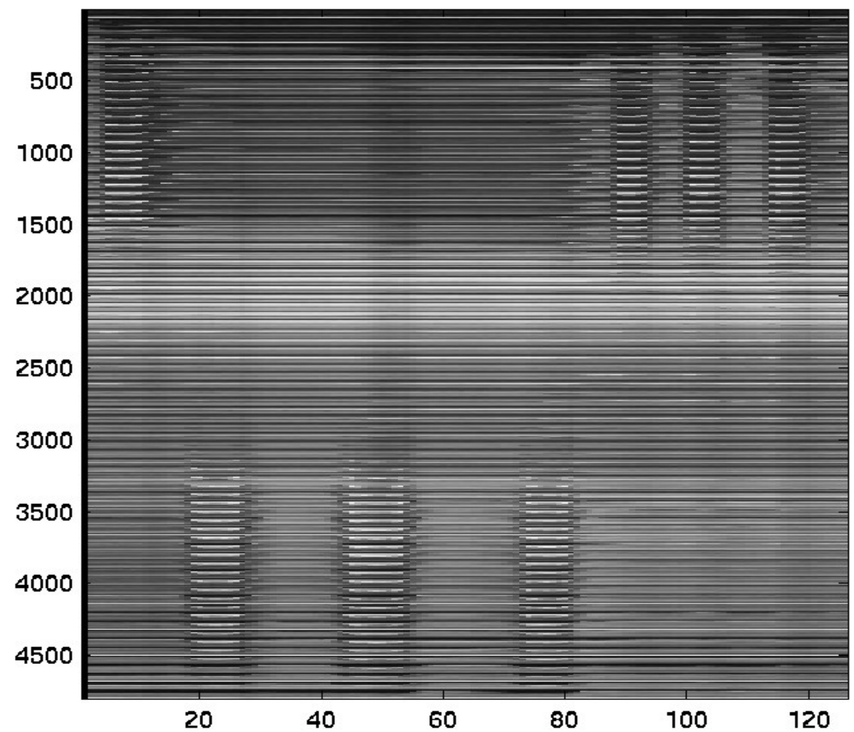




- Three instruments..

ICA for data exploration

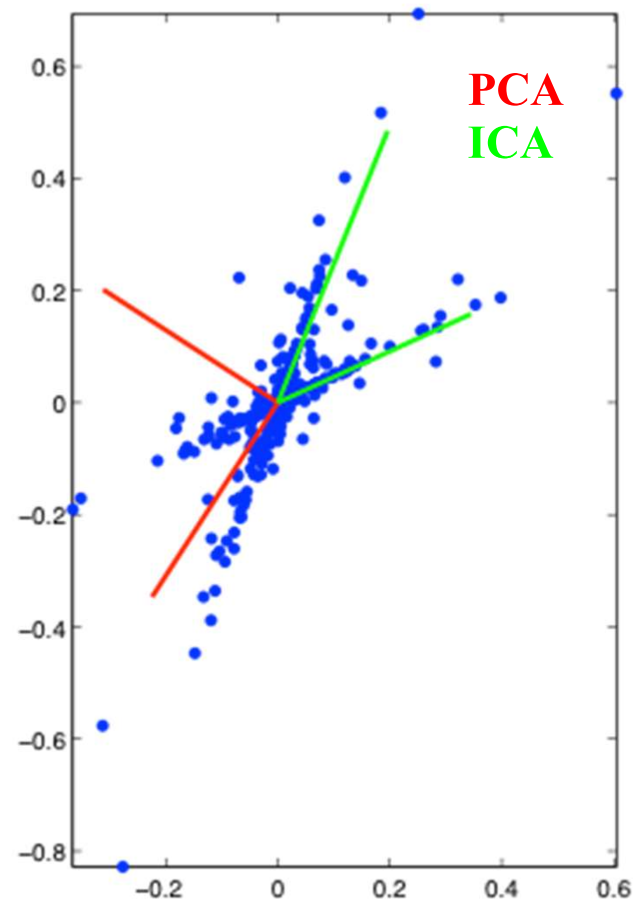
- The "bases" in PCA represent the "building blocks"
  - Ideally notes
- Very successfully used
- So can ICA be used to do the same?



ICA vs PCA bases

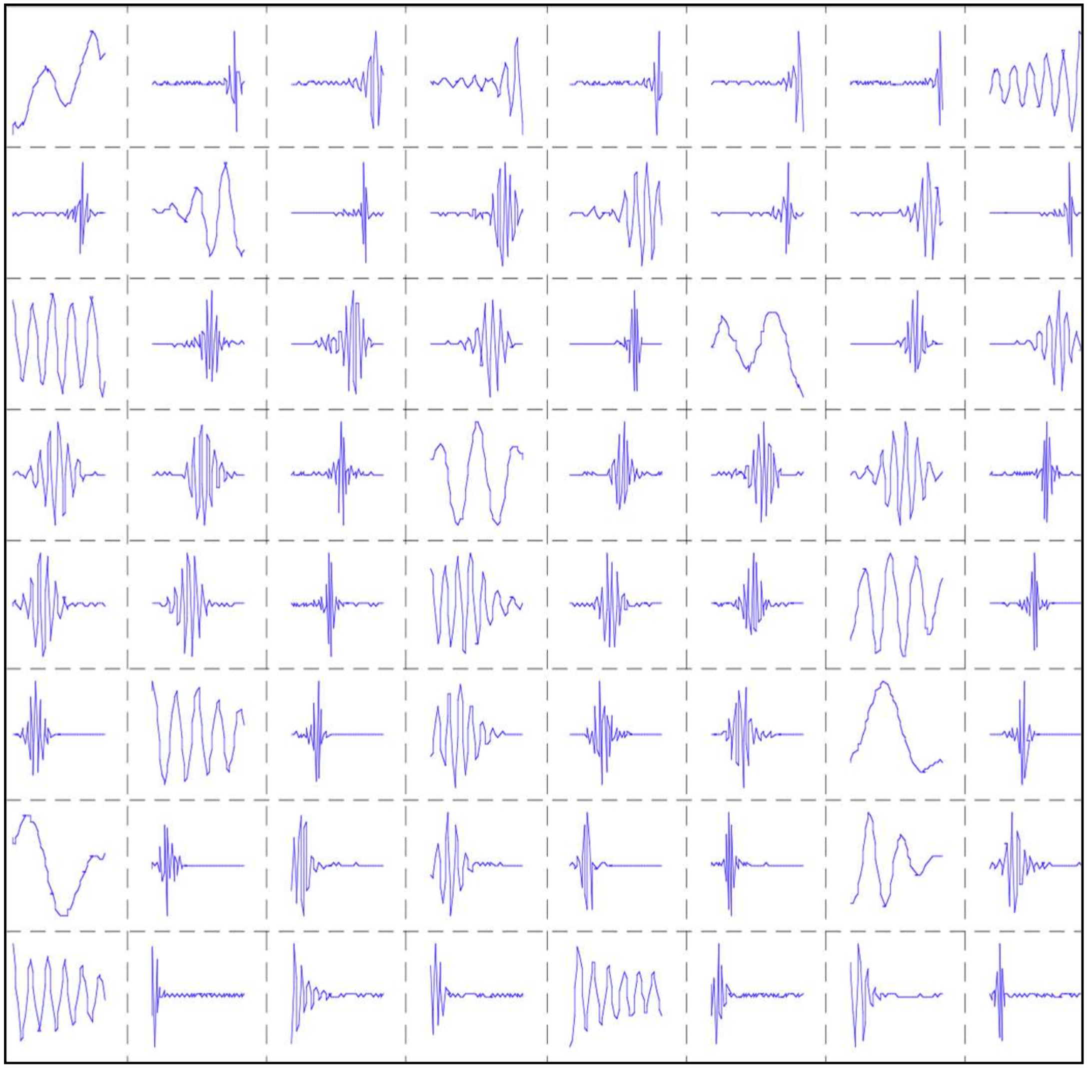
- Motivation for using ICA vs PCA
- PCA will indicate orthogonal directions of maximal variance
  - May not align with the data!
- ICA finds directions that are independent
  - More likely to "align" with the data

Non-Gaussian data

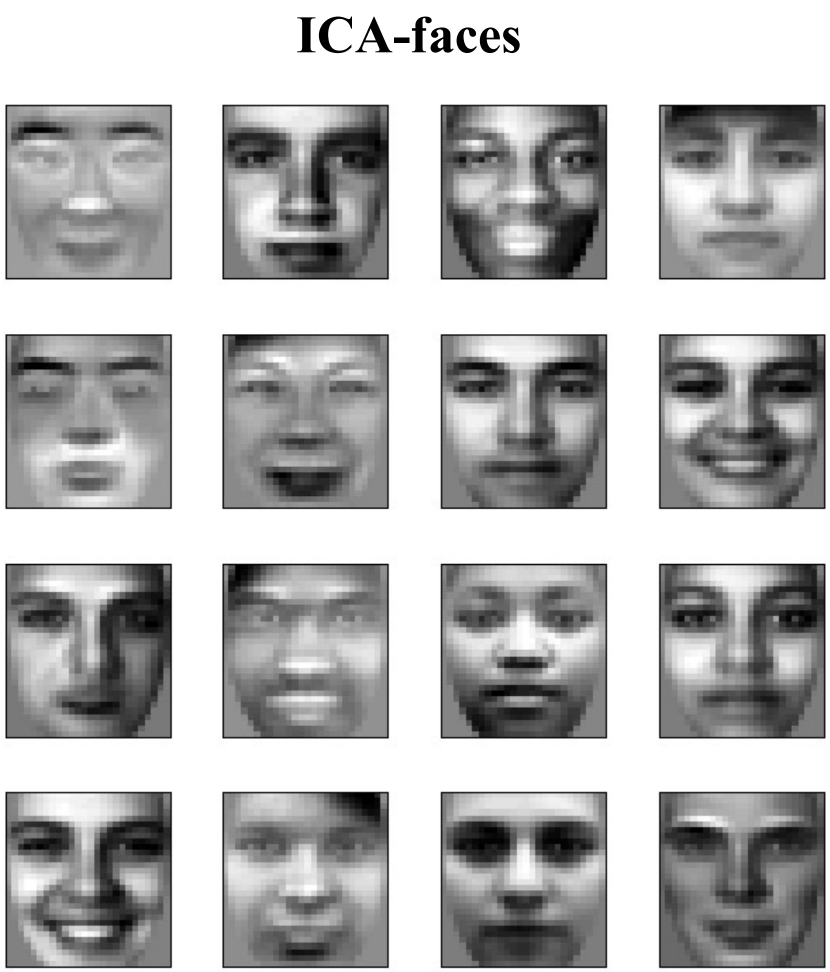


Finding useful transforms with ICA

- Audio preprocessing example
- Take a lot of audio snippets and concatenate them in a big matrix, do component analysis
- PCA results in the DCT bases
- ICA returns time/freq localized sinusoids which is a better way to analyze sounds
- Ditto for images
  - ICA returns localizes edge filters



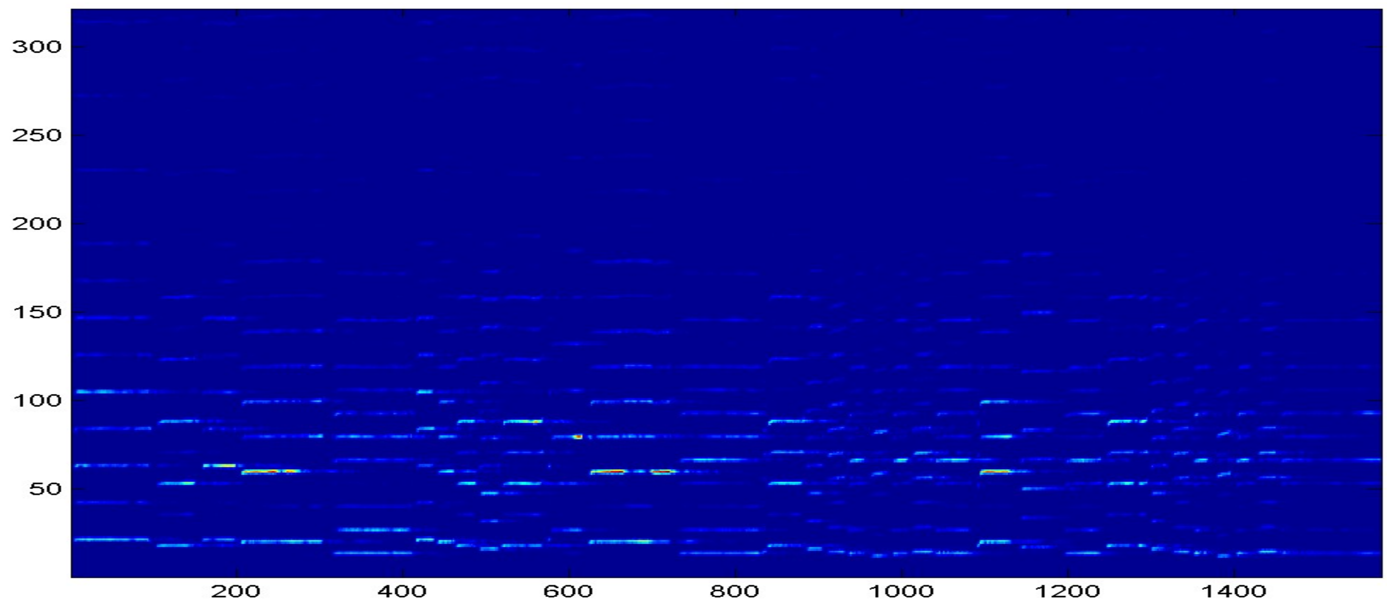
Example case: ICA-faces vs. Eigenfaces



ICA for Signal Enhncement

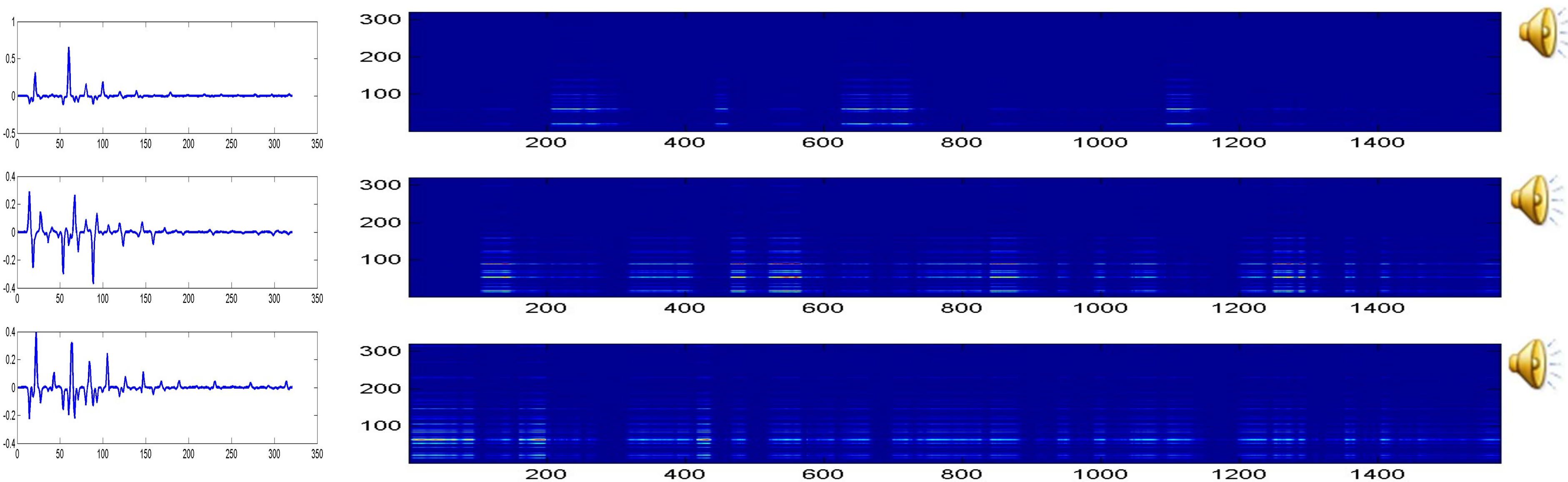
- Very commonly used to enhance EEG signals
- EEG signals are frequently corrupted by heartbeats and biorhythm signals
- ICA can be used to separate them out

So how does that work?



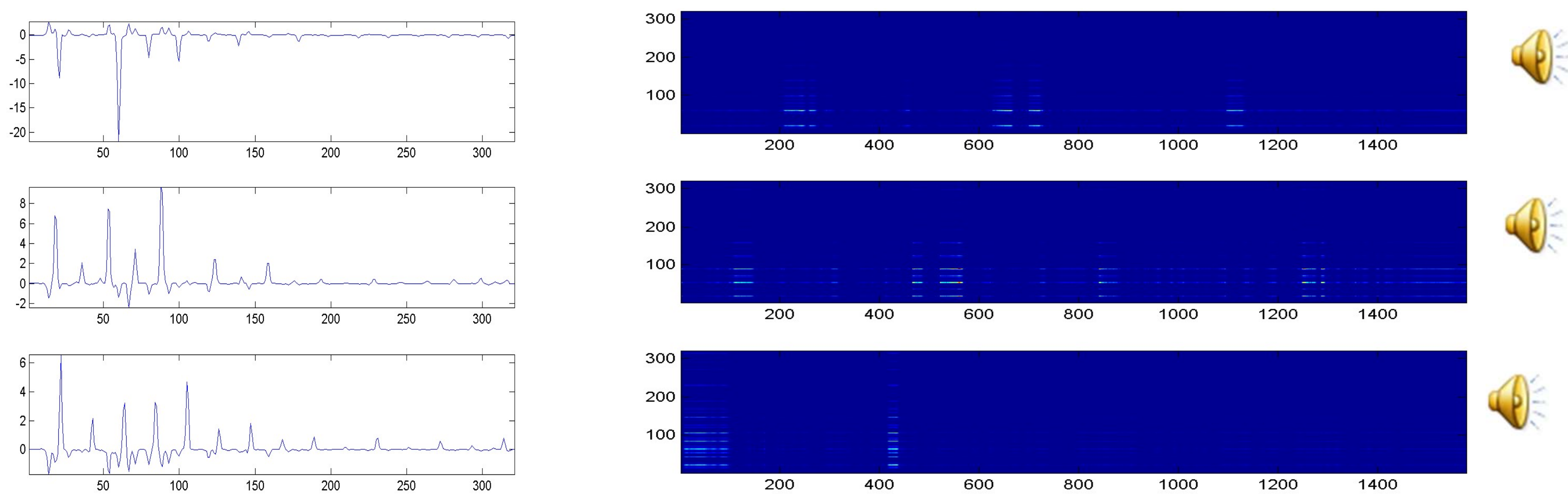
- There are 12 notes in the segment, hence we try to estimate 12 notes..

PCA solution



- There are 12 notes in the segment, hence we try to estimate 12 notes..

So how does this work: ICA solution



- Better..
  - But not much
- But the issues here?

ICA Issues

- No sense of *order*
  - Unlike PCA
- Get K independent directions, but does not have a notion of the “best” direction
  - So the sources can come in any order
  - *Permutation invariance*
- Does not have sense of *scaling*
  - Scaling the signal does not affect independence
- Outputs are scaled versions of desired signals in permuted order
  - In the best case
  - In worse case, output are not desired signals at all..

What else went wrong?

- *Notes are not independent*
  - Only one note plays at a time
  - If one note plays, other notes are *not* playing

- Will deal with these later in the course..