

MACHINE LEARNING

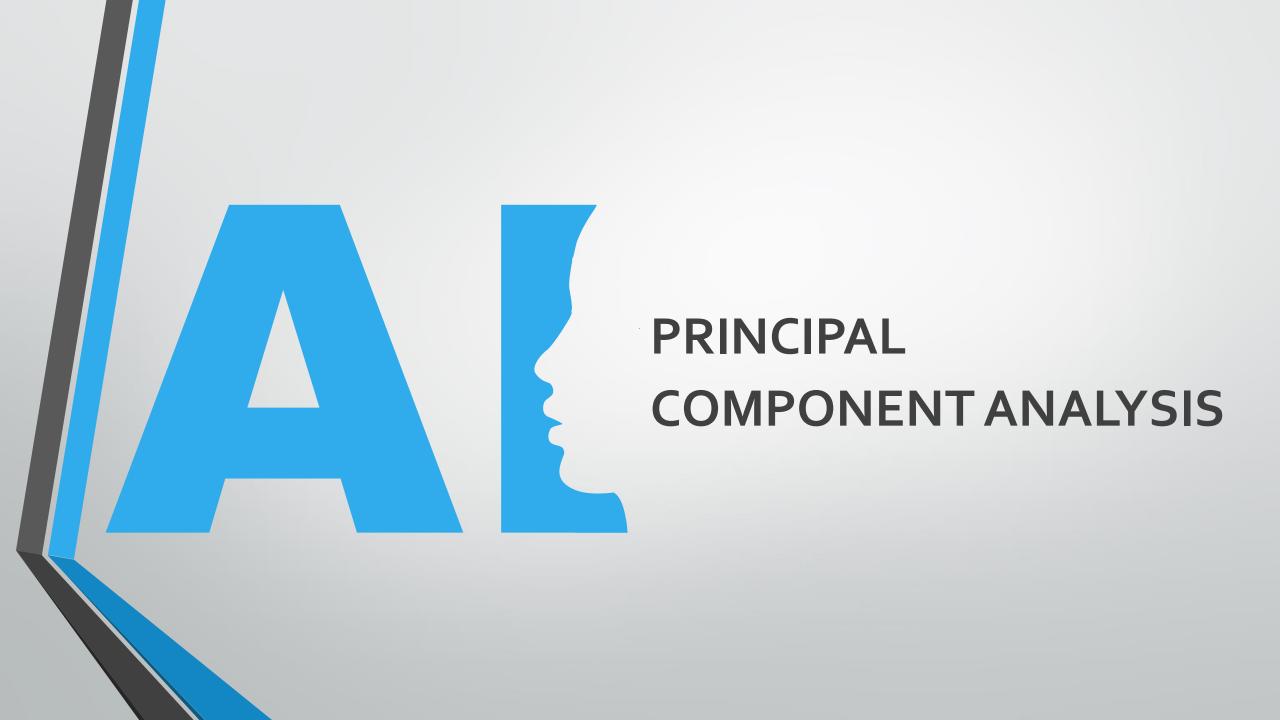
UNSUPERVISED LEARNING II

AGENDA

O1 Principal Component Analysis

O2 Independent Component Analysis





INTRODUCTION



The algorithm has a similar motivation as factor analysis, where it tries to identify the subspace in which the data approximately lies. However, PCA will only require an eigenvector calculation and doesn't make use of the EM algorithm.

Given a dataset $\{x^{(i)}; i = 1,...,m\}$ where $x^{(i)} \in \mathbb{R}^n$, $(n \ll m)$ we want to reduce it to a low-dimensional dataset of k dimensions (k < n).

The motivation is that there may be two different attributes, unknown to us that are almost linearly dependent (redundancy - correlation).

Thus, the **data** really **lies** approximately on an n-1 **dimensional subspace**.



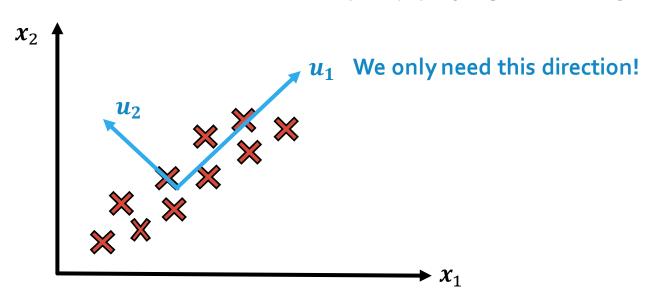


EXAMPLE:

Consider a dataset resulting from a survey of pilots for radio-controlled helicopters:

- $x_1^{(i)}$: measure of the piloting skill of pilot i.
- $x_2^{(i)}$: captures how much he/she enjoys flying.

Only the most committed students, the ones that truly enjoy flying, become good pilots.





NORMALIZATION

Prior to running the PCA algorithm, we will normalize the data to have mean 0 and variance 1:

$$x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{\sigma_j}$$

$$\mu_j = \frac{1}{m} \sum_{i=1}^m x_j^{(i)}$$

$$\sigma_j^2 = \frac{1}{m} \sum_{i=1}^m \left(x_j^{(i)} - \mu_j \right)^2$$

Dividing by the standard deviation σ_j rescales each coordinate to have unit variance, which ensures that different attributes are all treated on the same "scale."

PRINCIPAL COMPONENT ANALYSIS SETTING THE PROBLEM



The **main question** to be addressed is the following:

How do we compute the "major axis of variation" u, the direction on which the data approximately lies?

We can **set** this **problem** as **finding** the **unit vector** u, so that **when** the **data is projected** onto the **direction** of u, the **variance of** the **projected data** is **maximized**.

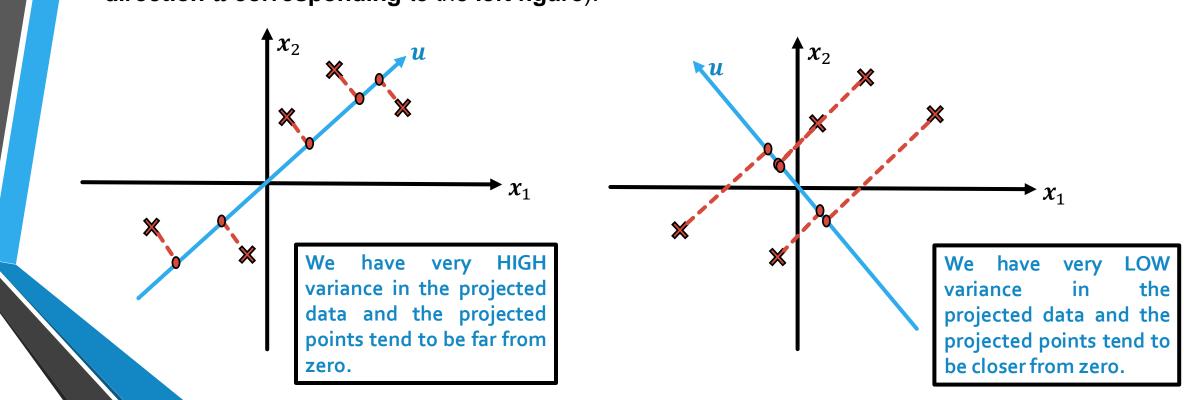
In other words, if we were to approximate the data as lying in the direction/subspace corresponding to u, as much as possible of this variance is still retained.

PRINCIPAL COMPONENT ANALYSIS SETTING THE PROBLEM



EXAMPLE:

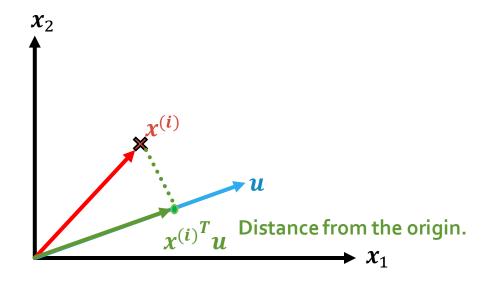
Consider the following dataset already normalized: (we would like to automatically select the direction u corresponding to the left figure).



THE ALGORITHM



To formalize the algorithm, note that given unit vector u and a point x, the length of the projection of x onto u is given by x^Tu .



To maximize the variance of the projections, we would like to choose a unit-length u to maximize:

$$\frac{1}{m} \sum_{i=1}^{m} (x^{(i)}^{T} u)^{2} = \frac{1}{m} \sum_{i=1}^{m} u^{T} x^{(i)} x^{(i)}^{T} u$$

THE ALGORITHM



Therefore, we want to maximize the following expression with respect to unit vector u, where we have the constraint $||u||_2 = 1$:

$$\frac{1}{m} \sum_{i=1}^{m} u^{T} x^{(i)} x^{(i)}^{T} u = u^{T} \left(\frac{1}{m} \sum_{i=1}^{m} x^{(i)} x^{(i)}^{T} \right) u$$

$$\max_{u:\|u\|_{2}=1} u^{T} \left(\frac{1}{m} \sum_{i=1}^{m} x^{(i)} x^{(i)^{T}}\right) u$$

The **covariance matrix** will be **substituted** as follows:

$$\max_{u:||u||_2=1}u^T(\Sigma)u$$

THE ALGORITHM



We construct the Lagrangian constraint:

$$||u||_2 = 1$$

$$||u||_2 - 1 = 0$$

Substituting in the **Lagrangian**, where λ is the **Lagrange multiplier**:

$$L(u,\lambda) = u^{T}(\Sigma)u - \lambda(||u||_{2} - 1)$$

$$L(u,\lambda) = u^{T}(\Sigma)u - \lambda(u^{T}u - 1)$$

Taking the gradient with respect to u and applying the property $\nabla_u u^T A u = 2Au$ (symmetric covariance):

$$\nabla_{u}L(u,\lambda)=2\Sigma u-2\lambda u$$





Setting the **gradient** to **0**:

$$2\Sigma u - 2\lambda u = 0$$

$$\Sigma u = \lambda u$$

This is the problem of finding the eigen vectors and eigen values of Σ

$$\lambda u - \Sigma u = 0$$

$$(\lambda I - \Sigma)u = 0$$

$$det(\lambda I - \Sigma)u = 0$$

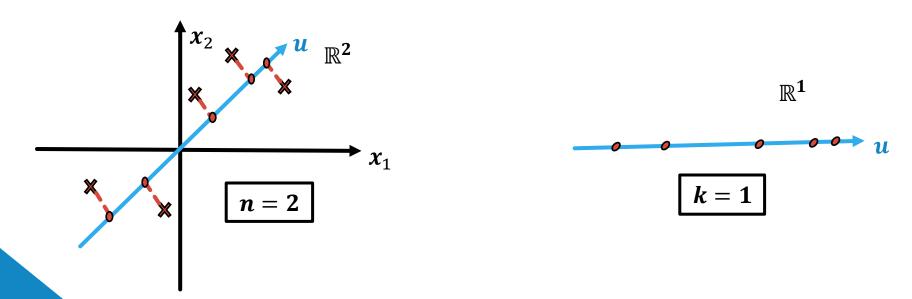
THE ALGORITHM



If we want to find a 1-dimensional subspace to approximate the data, we should choose u to be the principal eigenvector of the covariance matrix Σ .

More generally, if we wish to project our data into a k-dimensional subspace (k < n), we should choose u_1, \ldots, u_k to be the top k eigenvectors of the covariance matrix Σ .

The $u_i's$ will now form a new, orthogonal basis for the data.



THE ALGORITHM



If we want to represent our original input vector $x^{(i)}$ in this new basis, we compute the following vector $x'^{(i)}$:

$$x^{\prime(i)} = \begin{bmatrix} u_1^T x^{(i)} \\ u_2^T x^{(i)} \\ \vdots \\ u_k^T x^{(i)} \end{bmatrix} \in \mathbb{R}^k$$

Therefore, our original vector $x^{(i)}$ that was in an d-dimensional space is now represented in a lower k-dimensional space.

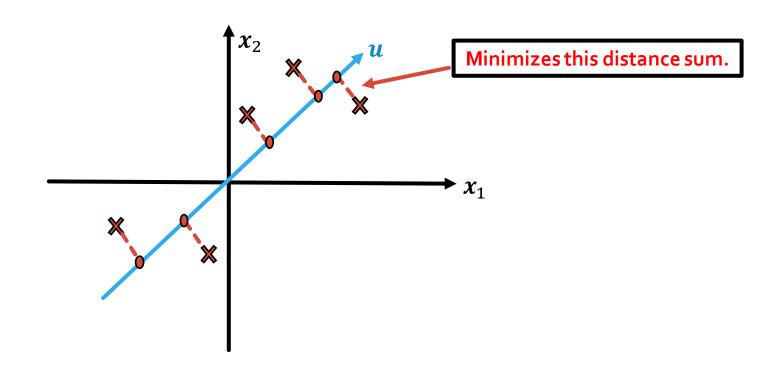
This is the reason why the PCA algorithm is also called the dimensionality reduction algorithm.

The vectors u_1, \ldots, u_k are called the first k principal components of the data.





You can also think about PCA as an algorithm that tries to choose a subspace that minimizes the squared mean error sum of the differences between the projected data and the original data.







SUMMARY:

- 1. Normalize the data to 0 mean and unit variance.
- 2. Compute the covariance matrix:

$$\Sigma = \frac{1}{m} \sum_{i=1}^{m} x^{(i)} x^{(i)^T}$$

3. Find the k eigen vectors of Σ .

PRINCIPAL COMPONENT ANALYSIS SINGULAR VALUE DECOMPOSITION



One of the main problems resides in computing the covariance matrix Σ , which can be very large in many cases (high dimensional data).

We are going to use Singular Value Decomposition (SVD) from linear algebra which stated that any matrix $A \in \mathbb{R}^{m \times n}$ can be decomposed as follows:

$$A = UDV^T$$

Where $U \in \mathbb{R}^{m \times n}$, $D \in \mathbb{R}^{n \times n}$ and $V^T \in \mathbb{R}^{n \times n}$. Matrix D is diagonal:

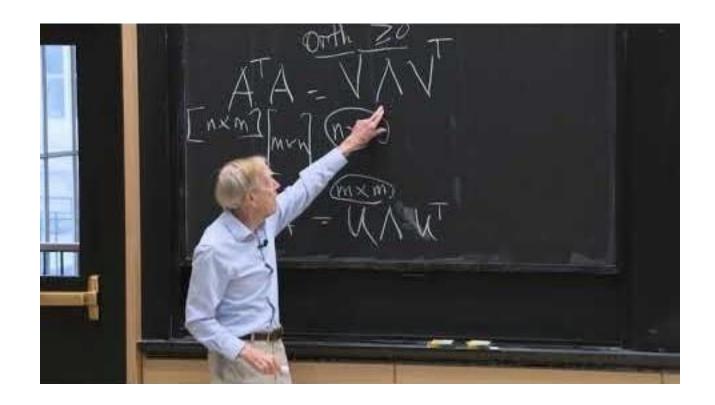
$$D = egin{bmatrix} \sigma_1 & 0 & 0 & 0 \ 0 & \sigma_2 & 0 & 0 \ dots & \cdots & \ddots & dots \ 0 & \cdots & 0 & \sigma_n \end{bmatrix}$$

Where σ_i are called the **singular values** of **matrix** A.

PRINCIPAL COMPONENT ANALYSIS SINGULAR VALUE DECOMPOSITION



For a detailed description on Singular Value Decomposition check this video from MIT:



https://www.youtube.com/watch?v=rYz83XPxiZo

PRINCIPAL COMPONENT ANALYSIS SINGULAR VALUE DECOMPOSITION



In this **decomposition** we have the **following**:

- U's columns: eigen vectors of AA^T .
- V's columns: eigen vectors of A^TA .

You can compute it in Python using "numpy.linalg.svd(A)".

This mathematical technique can be used in PCA to compute eigen vectors much more efficiently.

THE ALGORITHM



Let us start by **representing** the **covariance matrix** Σ as follows:

$$\Sigma = \frac{1}{m} \sum_{i=1}^{m} x^{(i)} x^{(i)^T} = X^T X$$

Where we have that *X* is:

$$X = \begin{bmatrix} -x^{(1)} - \\ -x^{(2)} - \\ \vdots \\ -x^{(m)} - \end{bmatrix}$$

Therefore:

$$X^{T}X = \begin{bmatrix} | & | & | \\ x^{(1)} & x^{(2)} & \dots & x^{(m)} \\ | & | & | \end{bmatrix} \begin{bmatrix} -x^{(1)} - \\ -x^{(2)} - \\ \vdots \\ -x^{(m)} \end{bmatrix}$$

THE ALGORITHM



To get the k eigen vectors of X we apply SVD to it:

$$X = UDV^T$$

The top k columns of V will be the top k eigen vectors of $X^TX = \Sigma$.

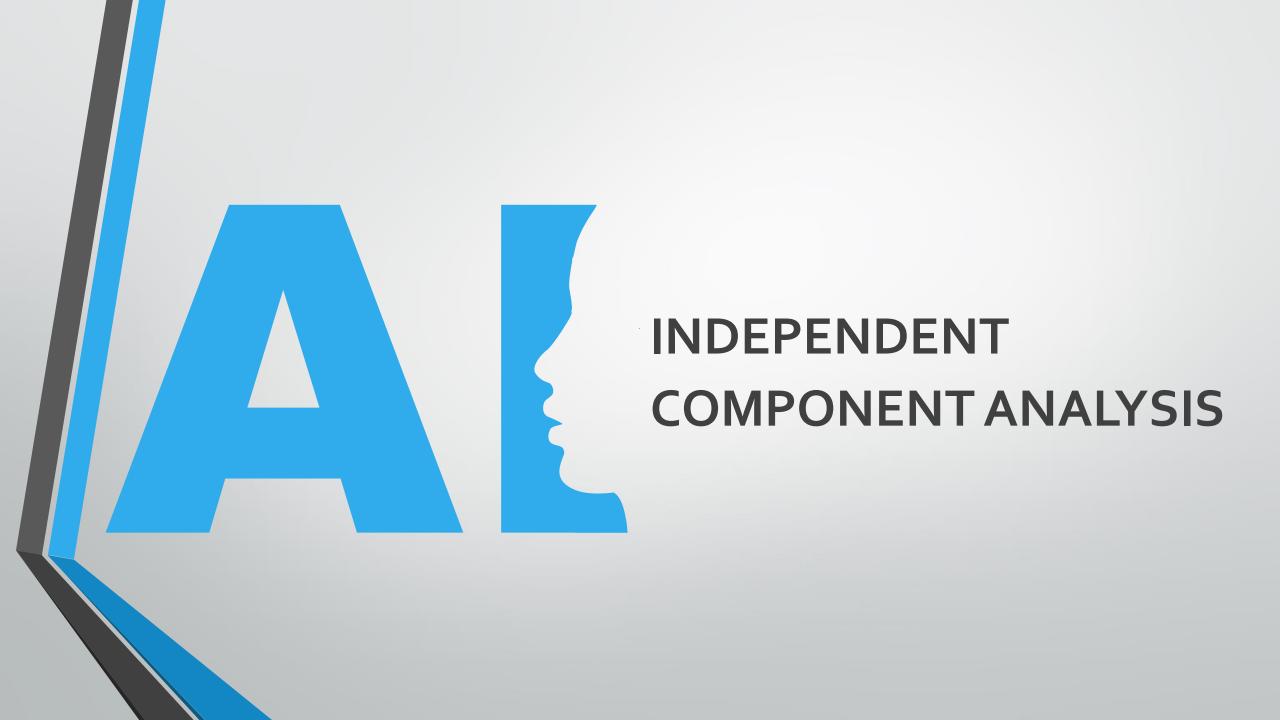
Thus, now we have a method to compute eigen vectors with highly dimensional data.

THE ALGORITHM



Some of the **applications** of the **algorithm include**:

- Compression of data.
- Visualizing high dimensional data to see clusters (anomaly detection).
- Pre-processing the data before it is fed to a supervised learning algorithm allowing less computational expense and reducing the complexity of the learnt hypothesis (reduce overfitting).
- Noise reduction (only consider the most important features and remove slight variations that do not contribute).
- Matching (distance calculations).



THE ALGORITHM



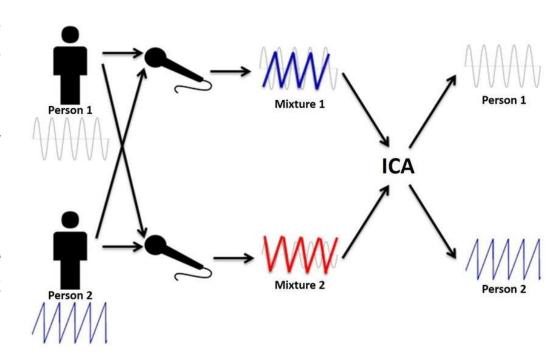
INTRODUCTION

The **new objective** will reside in **finding** the **independent components** that **capture** the **greatest variation** of the **data**.

The motivating example is the cocktail party problem: let us define n different microphones and n speakers placed in a room.

Because each microphone is a different distance from each speaker, it captures a different combination of the speakers' voices.

Using the microphone recordings, can we separate out the original n speakers' speech signals?



THE ALGORITHM



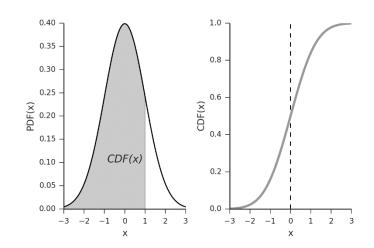
INTRODUCTION

First, we are going to remember **cumulative distribution functions** (**CDFs**). Let us suppose that you have a **random variable** s and has a **probability density function** $p_s(s)$.

Therefore its **cumulative distribution function** will be:

$$F(s) = P(S \le s) = \int_{-\infty}^{s} p_s(t) dt$$

Example Gaussian:



THE ALGORITHM



FORMALIZATION

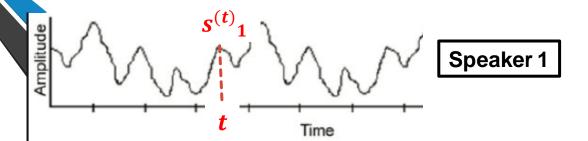
Let us assume that some data $s \in \mathbb{R}^n$ is generated via n independent sources. What we observe is: x = As

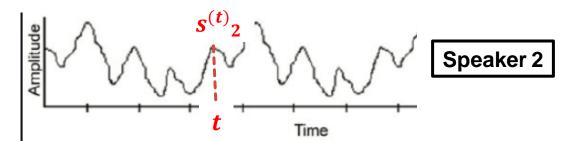
where A is an unknown square matrix called the mixing matrix (linear combination of n sources).

Making repeated observations gives us a dataset: $\{x^{(i)}; i = 1, ..., m\}$ and the objective is to recover the sources $s^{(i)}$ that had generated our data $(x^{(i)} = As^{(i)})$.

In the **cocktail party problem** we have:

- $s^{(i)} \in \mathbb{R}^n$, where each $s^{(i)}_{j}$ is the sound that speaker j was producing at time i.
- $x^{(i)} \in \mathbb{R}^n$, where each $x^{(i)}_j$ is the acoustic reading that microphone j recorded at time i.









FORMALIZATION

Let us define $W = A^{-1}$ as the unmixing matrix. Therefore, the objective is to find W, such that the sources $s^{(i)}$ can be recovered from the recordings $x^{(i)}$ by computing:

$$s^{(i)} = Wx^{(i)}$$

where the entries of W are computed as follows, where $w_i \in \mathbb{R}^n$:

$$W = \begin{bmatrix} -w_1^T - \\ \vdots \\ -w_n^T - \end{bmatrix}$$

THE ALGORITHM



AMBIGUITIES: PERMUTATION

The following question arises:

To what degree can $W = A^{-1}$ be recovered?

Given only the recordings $x^{(i)}$ and no prior information of both, the sources $s^{(i)}$ and the mixing matrix A, many inherent ambiguities arise that makes impossible to recover some information of W from A.

Concretely, let us define P as $n \times n$ permutation matrix (each row and column has exactly one "1").

If z is a vector, then Pz is another vector that contains a permuted version of z's coordinates.

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

THE ALGORITHM



AMBIGUITIES: PERMUTATIONS

Given only the recordings $x^{(i)}$, there is no way to distinguish between W and PW (permutated version of unmixing matrix) because you obtain the same sources but in different order.

The **permutation** of the **original sources** is **ambiguous**, but this **doesn't matter** for **most applications**.

The only drawback is that you will not know which source corresponds to each speaker.

THE ALGORITHM



AMBIGUITIES: SCALING

There is no way to recover the correct scaling of the w_i 's.

If a single column of A were scaled by a factor of α , and the corresponding source were scaled by a factor of $1/\alpha$, then there is again no way to determine that this had happened given only the $x^{(i)}$'s.

Example:

$$x^{(i)} = As^{(i)}$$

$$x^{(i)} = (2A)(0.5s^{(i)})$$

Again, for the applications that we are concerned with, this ambiguity does not matter (scaling a speaker's speech signal $s_j^{(i)}$ by some positive factor α , affects only the volume of that speaker's speech).

THE ALGORITHM



AMBIGUITIES:

Both, **permutations** and **scaling**, will be the **only sources** of **ambiguity** so long as the **sources** s_i are **non-Gaussian**.

Example:

We have n = 2, and $s \sim N(0, I)$. Here, I is the **2x2 identity matrix**. Note that the contours of the **density** are **rotationally symmetric**.

If we observe some x = As, the distribution of x will be Gaussian, $x \sim N(0, AA^T)$.

$$E_{s\sim N(0,I)}[x] = E[As] = AE[s] = 0$$

$$Cov[x] = E_{s \sim N(0,I)}[xx^T] = E[Ass^TA^T] = AE[ss^T]A^T = ACov[s]A^T = A(I)A^T$$

THE ALGORITHM



AMBIGUITIES:

Now, let R be an arbitrary orthogonal (rotation/reflection) matrix, so that $RR^T = R^TR = I$, and let A' = AR.

If the **data** had been **mixed according** to A' instead of A, we would have instead observed x' = A's.

The distribution of x' is also Gaussian, $x' \sim N(0, AA^T)$, since

$$E_{s\sim N(0,I)}[x'(x')^T] = E[A'ss^T(A')^T]$$

$$E_{s\sim N(0,I)}[x'(x')^T] = E[ARss^T(AR)^T]$$

$$E_{s\sim N(0,I)}[x'(x')^T] = AR(I)R^TA^T$$

$$E_{s \sim N(0,I)}[x'(x')^T] = ARR^TA^T$$

THE ALGORITHM



AMBIGUITIES:

Therefore, whether the mixing matrix is A or A', we would observe data from a $N(0, AA^T)$ distribution.

Thus, there is **no way** to **tell** if the **sources** were **mixed** using A and A'. There is an **arbitrary** rotational component in the **mixing matrix** that **cannot** be **determined from** the **data**.

This was defined by the **assumption** that **sources** had a **multivariate standard normal distribution**, which is **rotationally symmetric**.

So long as the data is NOT Gaussian, it is possible, given enough data, to recover the d independent sources.

THE ALGORITHM

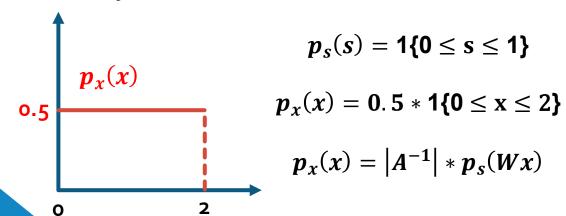
LINEAR TRANSFORMATIONS:

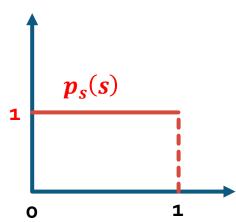
Suppose a random variable s is drawn according to some density $p_s(s)$, where $s \in \mathbb{R}$. Thus, our random variable x will be defined as follows ($A \in \mathbb{R}$):

$$x = As$$

What will be the density of x, $p_x(x)$?

If we assume that $p_s(s) = Uniform[0, 1]$ and A = 2, then x is distributed uniformly in the interval [0, 2]. More concretely, we have:





THE ALGORITHM



LINEAR TRANSFORMATIONS:

More generally, if s is a vector-valued distribution with density p_s , and x = As for a square, invertible matrix A, then the density of x is given by $(W = A^{-1})$.

$$p_x(x) = p_s(Wx) \cdot |W|$$

THE ALGORITHM



DERIVATION:

We suppose that the distribution of each source s_j is given by a density p_s , and that the joint distribution of the sources s is given by:

$$p(s) = \prod_{j=1}^{n} p_s(s_j)$$

Therefore, we **assume** that the **sources** are **independent**.

Substituting the derivation of linear transformations $p_x(x) = p_s(Wx) \cdot |W|$, we obtain the distribution of x (microphones):

$$p(x) = \prod_{j=1}^{n} p_s(w^T_j x) \cdot |W|$$

THE ALGORITHM

DERIVATION:

Given a real-valued random variable z, its cumulative distribution function (cdf) F is defined by:

$$F(z_0) = P(z \leq z_0) = \int_{-\infty}^{z_0} p_z(z) dz$$

and the **density** is the **derivative** of the **cdf**: $p_z(z) = F'(z)$.

Thus, to **specify** a **density** for the s_i 's, we need to **define** a **cdf** for it. **Recalling** that a **cdf** has to be a **monotonic function** that **increases** from **zero** to **one**.

A good choice (we cannot pick a Gaussian) is the sigmoid function:

$$g(z) = \frac{1}{1 + e^{-z}}$$



THE ALGORITHM

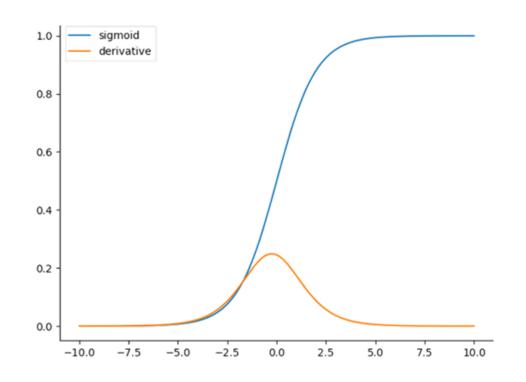
DERIVATION:

Therefore, we have that the **density** of the **sources** $p_s(s)$ is **defined** as follows:

$$p_s(s) = g'(z) = g(z)(1 - g(z))$$

An important note is that if you have prior knowledge that the sources' densities take a certain form, then it is a good idea to substitute that in here.

In the absence of such knowledge, the sigmoid function can be thought of as a reasonable default that seems to work well for many problems.







DERIVATION:

The log-likelihood can be represented as follows:

$$p(x^{(i)}) = \log \prod_{j=1}^{n} p_s(w^T_j x^{(i)}) \cdot |W|$$

$$l(W) = \log \prod_{i=1}^{m} \prod_{j=1}^{n} p_s(w^T_j x^{(i)}) \cdot |W|$$

$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} log g'(w^{T}_{j}x^{(i)}) + log|W| \right)$$





DERIVATION:

The objective is to compute the unmixing matrix W that maximizes the likelihood:

$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} log g'(w^{T}_{j}x^{(i)}) + log|W| \right)$$

$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} log g(w^{T}_{j} x^{(i)}) (1 - g(w^{T}_{j} x^{(i)})) + log |W| \right)$$

$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} log \ g(w^{T}_{j} x^{(i)}) + log \left(1 - g(w^{T}_{j} x^{(i)}) \right) \right) + mn \log |W|$$

IDEPENDENT COMPONENT ANALYSIS T H E A L G O R I T H M



$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} log \frac{1}{1 + e^{-w^{T}_{j}x^{(i)}}} + \log \left(1 - \frac{1}{1 + e^{-w^{T}_{j}x^{(i)}}} \right) \right) + mn \log |W|$$

$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} log \, 1 - \log \left(1 + e^{-w^{T}_{j} x^{(i)}} \right) + \log \left(\frac{1 + e^{-w^{T}_{j} x^{(i)}} - 1}{1 + e^{-w^{T}_{j} x^{(i)}}} \right) \right) + mn \log |W|$$

$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} -\log\left(1 + e^{-w^{T}_{j}x^{(i)}}\right) + \log\left(e^{-w^{T}_{j}x^{(i)}}\right) - \log\left(1 + e^{-w^{T}_{j}x^{(i)}}\right) \right) + mn\log|W|$$

$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} -2 \log \left(1 + e^{-w^{T}_{j} x^{(i)}} \right) + \log \left(e^{-w^{T}_{j} x^{(i)}} \right) \right) + mn \log |W|$$

INDEPENDENT COMPONENT ANALYSIS T H E A L G O R I T H M



DERIVATION:

$$l(W) = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} -2 \log \left(1 + e^{-w^{T}_{j} x^{(i)}} \right) + \log \left(e^{-w^{T}_{j} x^{(i)}} \right) \right) + mn \log |W|$$

$$l(W) = \left(\sum_{i=1}^{m} \left(\sum_{j=1}^{n} -2 \log \left(1 + e^{-w^{T}_{j}x^{(i)}}\right) - w^{T}_{j}x^{(i)}\right)\right) + mn \log|W|$$

Taking the gradient with respect to W and applying the following property $\nabla_W |W| = |W| (W^{-1})^T$:

$$\nabla_{W} l(W) = \left(\sum_{i=1}^{m} \left(\sum_{j=1}^{n} -2 \frac{-x^{(i)} e^{-w^{T} j x^{(i)}}}{1 + e^{-w^{T} j x^{(i)}}} - x^{(i)} \right) \right) + mn \left(\frac{1}{|W|} \right) |W| (W^{-1})^{T}$$

$$\nabla_{W} l(W) = \left(\sum_{i=1}^{m} \left(\sum_{j=1}^{n} 2 \frac{e^{-w^{T}_{j} x^{(i)}}}{1 + e^{-w^{T}_{j} x^{(i)}}} x^{(i)} - x^{(i)} \right) \right) + mn(W^{-1})^{T}$$

T H E A L G O R I T H M



DERIVATION:

$$\nabla_{W} l(W) = \left(\sum_{i=1}^{m} \left(\sum_{j=1}^{n} 2 \frac{e^{-w^{T}_{j} x^{(i)}}}{1 + e^{-w^{T}_{j} x^{(i)}}} x^{(i)} - x^{(i)} \right) \right) + mn(W^{-1})^{T}$$

$$\nabla_{W} l(W) = \left(\sum_{i=1}^{m} \left(\sum_{j=1}^{n} 2 \frac{e^{-w^{T}_{j} x^{(i)}}}{1 + e^{-w^{T}_{j} x^{(i)}}} - 1 \right) x^{(i)} \right) + mn(W^{-1})^{T}$$

Substituting back the sigmoid function $g(w^T_j x^{(i)}) = \frac{e^{-w^T_j x^{(i)}}}{1 + e^{-w^T_j x^{(i)}}}$:

$$\nabla_{W}l(W) = \left(\sum_{i=1}^{m} \left(\sum_{j=1}^{n} 2g(w^{T}_{j}x^{(i)}) - 1\right)x^{(i)}\right) + mn(W^{-1})^{T}$$

THE ALGORITHM



DERIVATION:

$$\nabla_{W}l(W) = \left(\sum_{i=1}^{m} \left(\sum_{j=1}^{n} 2g(w^{T}_{j}x^{(i)}) - 1\right)x^{(i)}\right) + mn(W^{-1})^{T}$$

We know that this can be expressed as a dot product:

$$abla_W l(W) = \sum_{i=1}^m egin{bmatrix} 2g(w^T_1 x^{(i)}) - 1 \ 2g(w^T_2 x^{(i)}) - 1 \ dots \ 2g(w^T_n x^{(i)}) - 1 \end{bmatrix} x^{(i)^T} + mn(W^{-1})^T$$

THE ALGORITHM



DERIVATION:

Now, we can compute W for a single training example using stochastic gradient descent:

$$W \coloneqq W - \alpha \nabla_W l(W)$$

$$W := W - \alpha \begin{bmatrix} 2g(w^{T}_{1}x^{(i)}) - 1 \\ 2g(w^{T}_{2}x^{(i)}) - 1 \\ \vdots \\ 2g(w^{T}_{n}x^{(i)}) - 1 \end{bmatrix} x^{(i)^{T}} + n(W^{-1})^{T}$$

$$W \coloneqq W + \alpha \begin{pmatrix} \begin{bmatrix} 1 - 2g(w^T_1 x^{(i)}) \\ 1 - 2g(w^T_2 x^{(i)}) \\ \vdots \\ 1 - 2g(w^T_n x^{(i)}) \end{bmatrix} x^{(i)^T} + (W^{-1})^T \end{pmatrix}$$

THE ALGORITHM



SUMMARY:

- 1. Initialize an unmixing matrix W.
- 2. Compute W using stochastic gradient descent until convergence.

$$W \coloneqq W - \alpha \nabla_W l(W)$$

3. Compute $s^{(i)} = Wx^{(i)}$ to recover the original sources.