L27: independent components analysis

The “cocktail party” problem

Definition of ICA

Independence and uncorrelatedness

Independence and non-Gaussianity

Preprocessing for ICA

The FastICA algorithm

Non-linear ICA

The cocktail party problem

Imagine that you are at a large party where several conversations are being held at the same time

- Despite the strong background, you are able to focus your attention on a specific conversation (of your choice), and ignore all others
- At the same time, if someone were to call our name from the other name of the room, we would immediately be able to respond to it
- How is it that we can separate different flows of information that occur at the same time and share the very same frequency bands?

Material in this lecture was obtained from [Hyvarinen and Oja, 2000]

Let's formalize this scenario

- Two people are speaking simultaneously
  - We will denote their sound pressure waveforms by $s_1(t)$ and $s_2(t)$
- Two microphones are placed at different locations
  - We will denote their recorded signals by $x_1(t)$ and $x_2(t)$
- We will assume that the recorded signals $x_i(t)$ are a linear combination of the sources $s_i(t)$

$$\begin{cases} x_1(t) = a_{11}s_1(t) + a_{12}s_2(t) \\ x_2(t) = a_{21}s_1(t) + a_{22}s_2(t) \end{cases}$$

  - where the coefficients aij would depend on the relative distance between the microphones and the speakers
- Note that this is a very oversimplified model, since we are ignoring very basic phenomena such as propagation delays and reverberances in the room

Our goal is to find the sources $s_i(t)$ from mixed signals $x_j(t)$

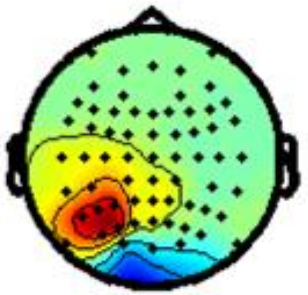
- Obviously, if we knew the mixing coefficients a_{ij}, the problem could be trivially solved through matrix inversion
- But how about when a_{ij} are unknown?

To solve for both a_{ij} (actually, its inverse) and $s_i(t)$, we need to make further assumptions

- One such assumption would be that the speech waveforms of the two speakers are statistically independent, which is not that unrealistic
- Interestingly, this simple assumption is sufficient to solve the problem and, in some cases, the assumption need not be strictly true

The same principles can be (and have been) used for a variety of problems

- Separating sources of activity in the brain from electrical (EEG) and magnetic (MEG, fMRI) recordings
- Denoising and detrending of sensor signals
- Finding "interesting" projections in high-dimensional data (projection pursuit)



Definition of ICA

Assume that we observe n linear mixtures $x_1, x_2, \ldots x_n$, from n independent observers

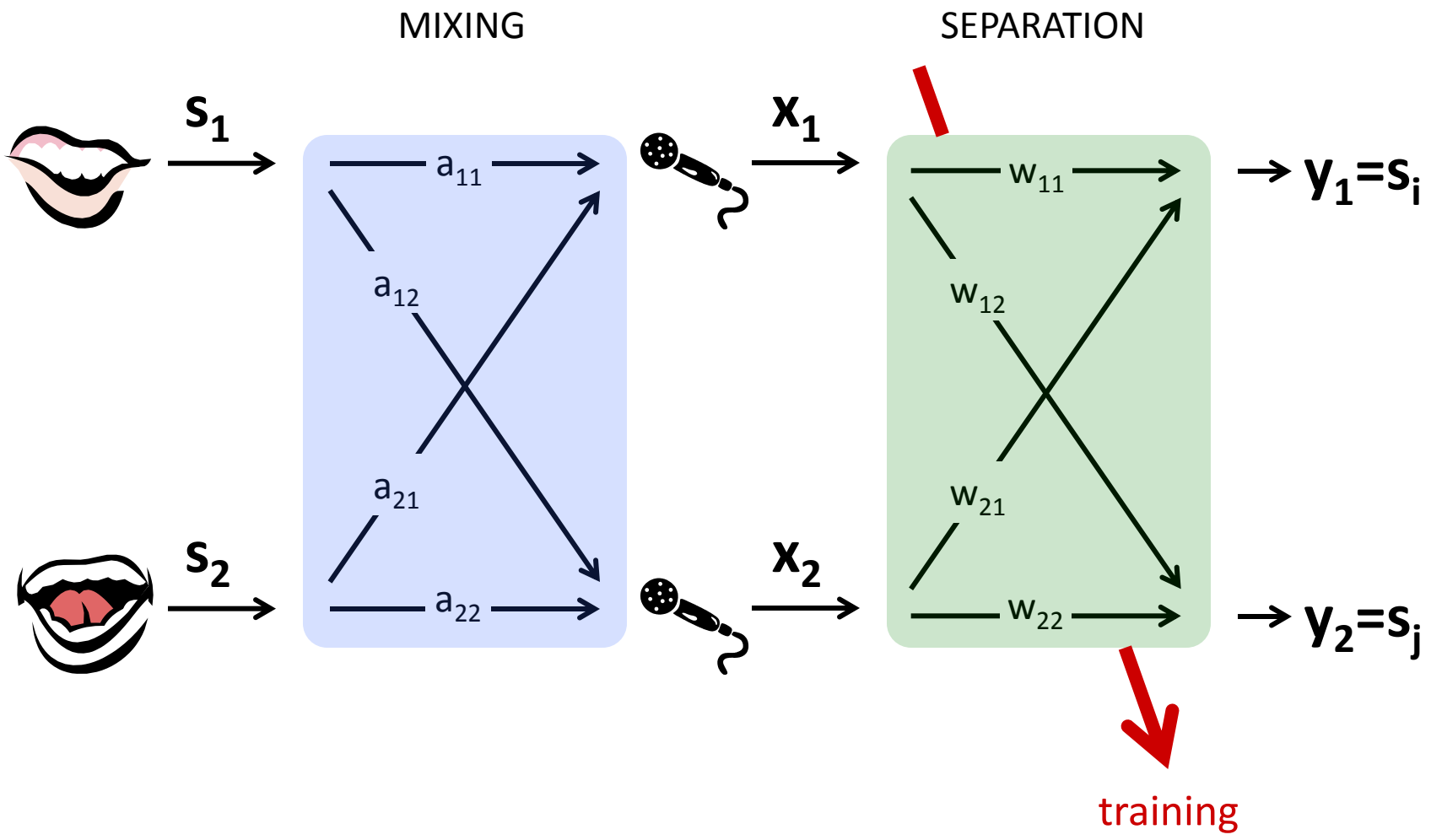
$$x_j(t) = a_{j1}s_1(t) + a_{j2}s_2(t) + \cdots + a_{jn}s_n(t)$$

- Or, using matrix notation, $x = As$
- Our goal is to find a de-mixing matrix W such that $s = Wx$

Assumptions

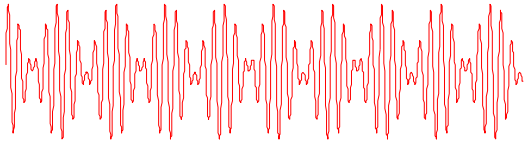
- Both mixture signals and source signals are zero-mean (i.e. $E[x_i] = E[s_j] = 0, \forall i, j$)
  - If not, we simply subtract their means
- The sources have non-Gaussian distributions
  - More on this in a minute
- The mixing matrix is square, i.e., there are as many sources as mixing signals
  - This assumption, however, can sometimes be relaxed

Blind source separation

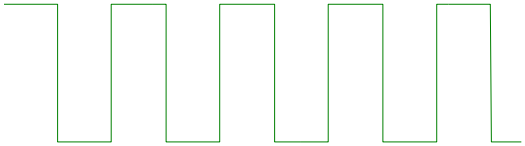


An example

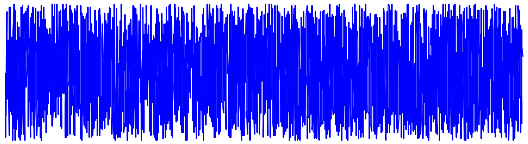
$s_1(n)=\sin(100n)\cos(10n)$



$s_2=\text{sign}(\sin(10n))$

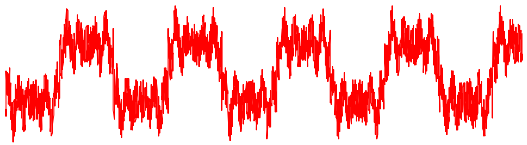


$s_3=\text{rand}(n)$

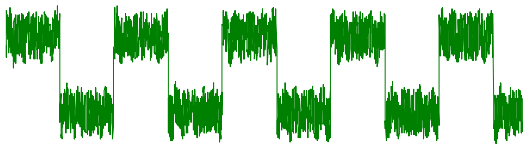


$x=As$

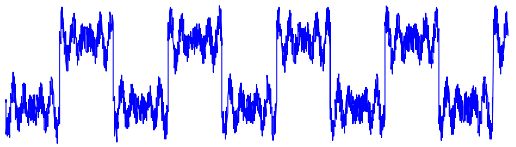
x_1



x_2

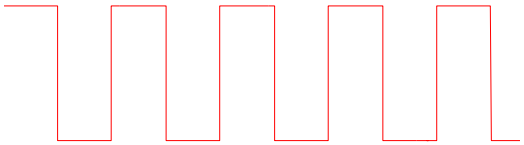


x_3

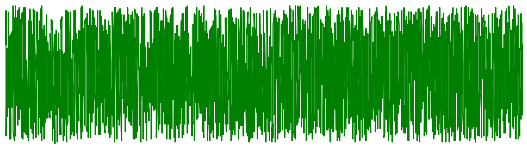


FastICA

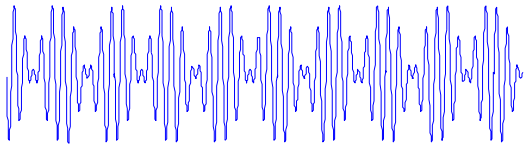
y_1



y_2



y_3



Ambiguities of ICA

The variance of the ICs cannot be determined

- Since both s and A are undetermined, any multiplicative factor in s, including a change of sign, could be absorbed by the coefficients of A

$$x_j(t) = (ka_{j1})s_1(t) + (ka_{j2})s_2(t)$$
$$= a_{j1}(ks_1(t)) + a_{j2}(ks_2(t))$$

- To resolve this ambiguity, source signals are assumed to have unit variance

$$E[s_i^2] = 1$$

The order of ICs cannot be determined

- Since both s and A are unknown, any permutation of the mixing terms would yield the same result
- Compare this with PCA, where the order of the components can be determined by their eigenvalues (their variance)

Independence vs. uncorrelatedness

What is independence?

- Two random variables y_1 and y_2 are said to be independent if knowledge of the value of y_1 does not provide any information about the value of y_2, and viceversa

$$p(y_1|y_2) = p(y_1) \Leftrightarrow p(y_1, y_2) = p(y_1)p(y_2)$$

What is uncorrelatedness?

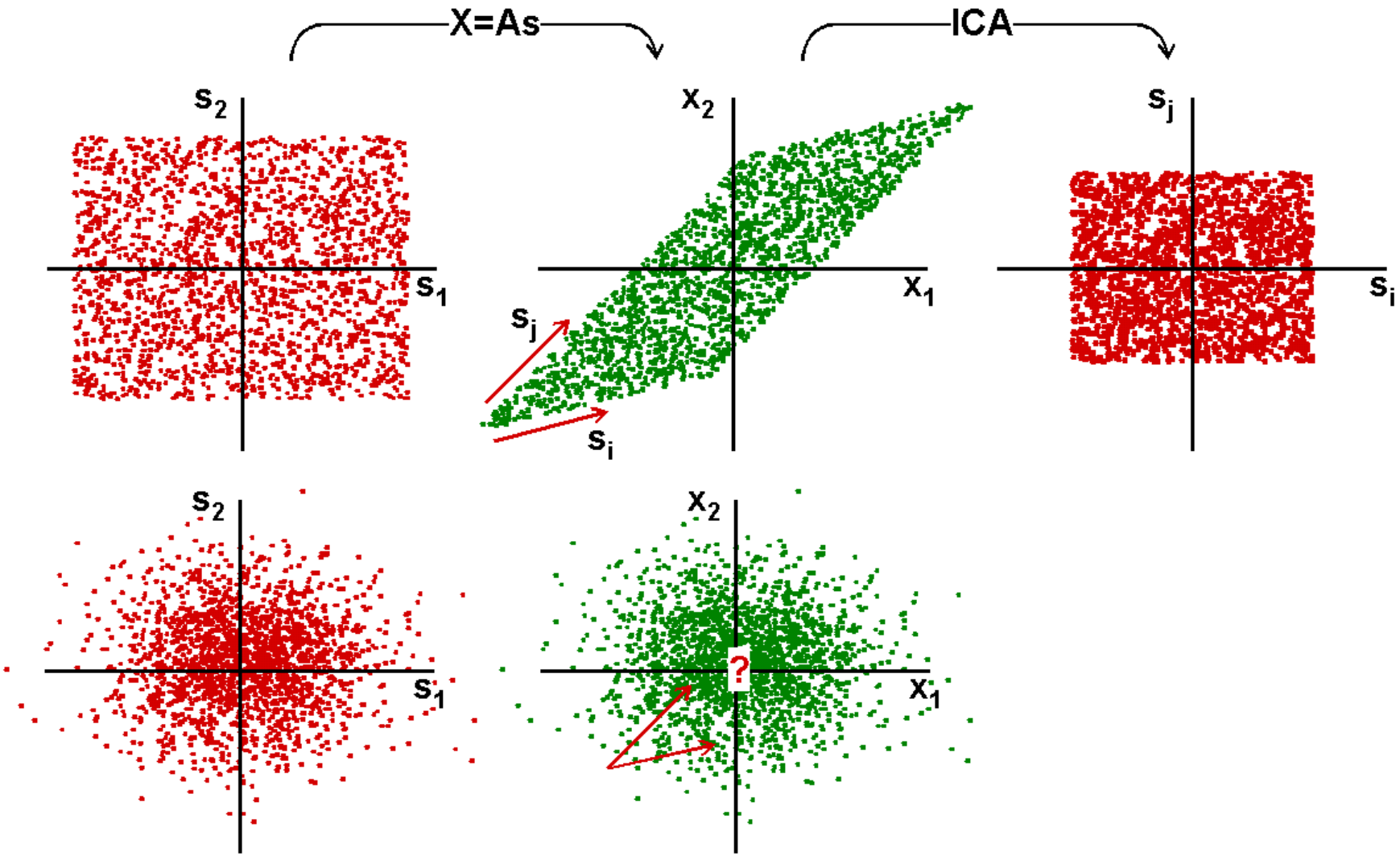
- Two random variables y_1 and y_2 are said to be uncorrelated if their covariance is zero

$$E[y_1^2 y_2^2] = 0$$

Equivalences

- Independence implies uncorrelatedness
- Uncorrelatedness DOES NOT imply independence…
  - Unless the random variables y_1 and y_2 are Gaussian, in which case uncorrelatedness and independence are equivalent
  - Note that, in this case, the covariance matrix is diagonal, and $p(x_1, x_2)$ can be trivially factorized as the product of the two univariate densities $p(x_1)$ and $p(x_2)$

Why can't Gaussian variables be used with ICA?



Independence and non-Gaussianity

As we have just seen, a necessary condition for ICA to work is that the signals be non-Gaussian

- Otherwise, ICA cannot resolve the independent directions due to symmetries
- Besides, if signals are Gaussian, one may just use PCA to solve the problem (!)

We will now show that finding the independent components is equivalent to finding the directions of largest non-Gaussianity

- For simplicity, let us assume that all the sources have identical distributions
- Our goal is to find the vector w such that $y = w^T x$ is equal to one of the sources s
- We make the change of variables $z = A^T w$,
  - This leads to $y = w^T x = w^T A s = z^T s$
  - Thus, y is a linear combination of the sources s
- According to the CLT, the signal y is more Gaussian than the sources s since it is a linear combination of them, and becomes the least Gaussian when it is equal to one of the sources
- Therefore, the optimal w is the vector that maximizes the non-Gaussianity of $w^T x$, since this will make y equal to one of the sources

- The trick is now how to measure "non-Gaussianity"…

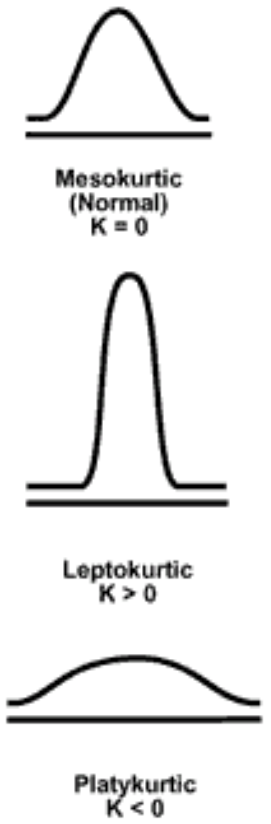
Measures of non-Gaussianity

Kurtosis

- The classical measure of non-Gaussianity is kurtosis, which is defined as the fourth order cummulant

$$kurt(y) = E[y^4] - 3(E[y^2])^2$$

- Kurtosis can be both positive or negative
  - When kurtosis is zero, the variable is Gaussian
  - When kurtusis is positive, the variable is said to be supergaussian or leptokurtic
    - Supergaussians are characterized by a "spiky" pdf with heavy tails, i.e., the Laplace pdf
  - When kurtosis is negative, the variable is said to be subgaussian or platykurtic
    - Subgaussians are characterized by a rather "flat" pdf
- Thus, the absolute value of the kurtosis can be used as a measure of non-Gaussianity
  - Kurtosis has the advantage of being computationally cheap
  - Unfortunately, kurtosis is rather sensitive to outliers



Negentropy

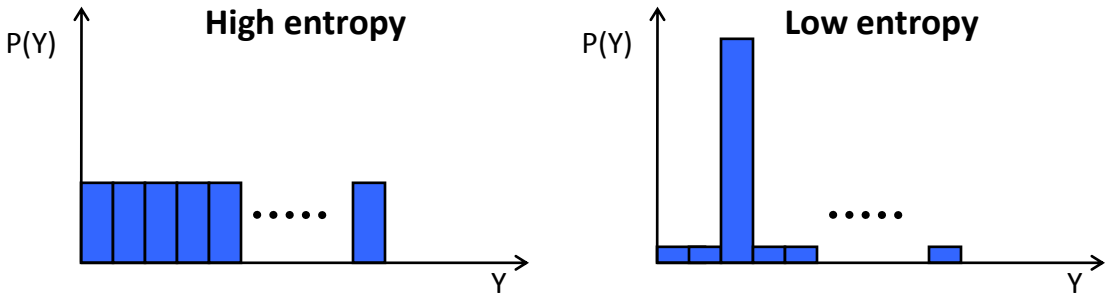
- An information-theoretic quantity of differential entropy
- The entropy of a variable can be thought of as a measure of randomness
  - For a discrete-valued variable, the entropy $H(Y)$ is defined as

$$H(Y) = -\sum_i P(Y = a_i) \log P(Y = a_i)$$

  - whereas for a continuous-valued variable, the (differential) entropy is

$$H(Y) = -\int p(y) \log p(y) dy$$

  - A uniform variable has the largest entropy among discrete-valued variables, whereas a Gaussian has the largest entropy among continuous valued variables



- To obtain a measure of non-Gaussianity, one may then take a differential measurement of entropy relative to a Gaussian; this is known as negentropy

$$J(y) = H(y_G) - H(y)$$

  - where y_G is a Gaussian variable with the same variance as y
- Note that $J(y)$ is always non-negative, and only equal to zero for a Gaussian
- Properties
  - Negentropy is statistically robust
  - Unfortunately, it is also computationally intensive, since it requires density estimation, possibly non-parametric

Approximations of negentropy

- Since the estimation of negentropy is difficult, one typically uses approximations proposed by Hyvarinen, which have the form

$$J(y) \propto [E\{G(y)\} - E\{G(v)\}]^2$$

  - where v is a Gaussian variable N(0,1), y is assumed to be zero-mean, and G is a nonquadratic function
  - Several choices of G have been shown to work well, including

$$G_1(u) = \frac{1}{a_1} \log \cosh(a_1 u) \quad 1 \leq a_1 \leq 2$$

$$G_2(u) = -\exp(-u^2/2)$$

- These approximations have several advantages
  - Even in cases when they are not accurate, they are consistent (always non-negative and zero if y is Gaussian)
  - They provide a tradeoff between the properties of the two classical measures (kurtosis and negentropy)
  - They are computationally simple, fast to compute, and have good statistical properties (robustness)

Preprocessing for ICA

ICA can be made simpler and better conditioned it the data is preprocessed prior to the analysis

- **Centering**
  - This step consists of subtracting the mean of the observation vector

$$x' = x - E[x]$$

  - The mean vector can be added to the estimates of the sources afterwards

$$s = s' + A^{-1}E[x]$$

- **Whitening**
  - Whitening consists of applying a linear transform to the observations so that its components are uncorrelated and have unit variance

$$\tilde{x} = Wx \Rightarrow E[\tilde{x}\tilde{x}^T] = I$$

  - This can be achieved through principal components

$$\tilde{x} = ED^{-1/2}E^T x$$

    - where (the columns of) E and (the diagonal of) D are the are eigenvector and eigenvalues of $E[xx^T]$, respectively

$$E[xx^T] = EDE^T$$

- Whitening (continued)
  - Note that whitening makes the mixing matrix orthogonal

$$\tilde{x} = ED^{-1/2}E^T x \Rightarrow$$
$$\tilde{x} = ED^{-1/2}E^T As = \tilde{A}s \Rightarrow$$
$$\underbrace{E[\tilde{x}\tilde{x}^T]}_{I} = \tilde{A}\,\underbrace{E[ss^T]}_{I}\,\tilde{A} = \tilde{A}\tilde{A}^T = I$$

  - Which has the advantage of halving the number of parameters that need to be estimated, since an orthogonal matrix only has $n(n-1)/2$ free parameters
    - For a 2 source problem, there will only be one parameter (an angle) to be estimated!
  - Since computing PCA is straightforward, it is then worthwhile to reduce the complexity of the ICA problem by whitening the data

The FastICA algorithm for one unit

FastICA is a very efficient method of maximizing the measures of non-Gaussianity mentioned earlier

- In what follows, we will assume that the data has been centered and whitened
- We will first start with a single-unit problem, then generalize to multiple units

FastICA for one unit

- The goal is to find a weight vector w that maximizes the negentropy estimate

$$J(w^T x) \propto (E[G(w^T x)] - E[G(v)])^2$$

- Note that the maxima of $J(w^T x)$ occurs at a certain optima of $E\{G(w^T x)\}$, since the second part of the estimate is independent of w
- According to the Kuhn-Tucker conditions, the optima of $E\{G(w^T x)\}$ unde the constraint $E\{(w^T x)^2\} = \|w\|^2 = 1$ occurs at points where

$$F(w) = E[x g(w^T x)] - \beta w = 0$$

  - where $g(u) = dG(u)/du$
  - The constraint $E\{(w^T x)^2\} = \|w\|^2 = 1$ occurs because the variance of $w^T x$ must be equal to unity (by design): if the data is pre-whitened, then the norm of w must be equal to one
- The problem can be solved as an approximation of Newton's method
  - To find a zero of $f(x)$, apply the iteration $x_n = x_n - f(x_n)/f'(x_n)$

- Computing the Jacobian of $F(w)$ yields

$$JF(X) = E\{xx^T g'(w^T x)\} - \beta I$$

- To simplify inversion of this matrix, we approximate the first term of the expression by noting that the data is sphered

$$E[xx^T g'(w^T x)] \approx E[xx^T]E[g'(w^T x)] = \underbrace{E[g'(w^T x)]}_{a\ scalar} I$$

  - So the Jacobian is diagonal, which simplifies the inversion

- Thus, the (approximate) Newton's iteration becomes

$$w^+ = w - (E[xg(w^T x)] - \beta w)/(E[g'(w^T x)] - \beta)$$

- This algorithm can be further simplified by multiplying both sides by $\beta - E[g'(w^T x)]$, which yields the FastICA iteration

(1) Choose an initial (e.g., random) weight vector w
(2) Let $w^+ = E\{xg(w^T x)\} - E\{g'(w^T x)\}w$
(3) Let $w = w^+/\|w^+\|$
(4) If not converged, go back to (2)

The FastICA algorithm for several units

To estimate several independent components, we run the one-unit FastICA with several units $w_1, w_2, \dots, w_n$

- To prevent several of these vectors from converging to the same solution, we decorrelate outputs $w_1^T x, w_2^T x, \dots, w_n^T x$ at each iteration
- This can be done using a deflation scheme based on Gram-Schmidt
  - We estimate each independent component one by one
  - With p estimated components $w_1, w_2, \dots, w_p$, we run a 1-unit ICA iteration for w_{p+1}
  - After each iteration, we subtract from w_{p+1} its projections $\left(w_{p+1}^T w_j\right) w_j$ on the previous vectors w_j
  - Then, we renormalize w_{p+1}

$$(1)\ Let\ w_{p+1} = w_{p+1} - \sum_{j=1}^{P} w_{p+1}^T w_j w_j$$

$$(2)\ Let\ w_{p+1} = w_{p+1} / \sqrt{w_{p+1}^T w_{p+1}}$$

- Or, if all components must be computed simultaneously (to avoid asymmetries), the following iteration proposed by Hyvarinen can be used

$$(1)\ Let\ W = W / \sqrt{\|WW^T\|}$$

$$(2)\ Repeat\ until\ convergence\quad W = \frac{3}{2}W - \frac{1}{2}WW^TW$$