Unsupervised data decompositions

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Objectives

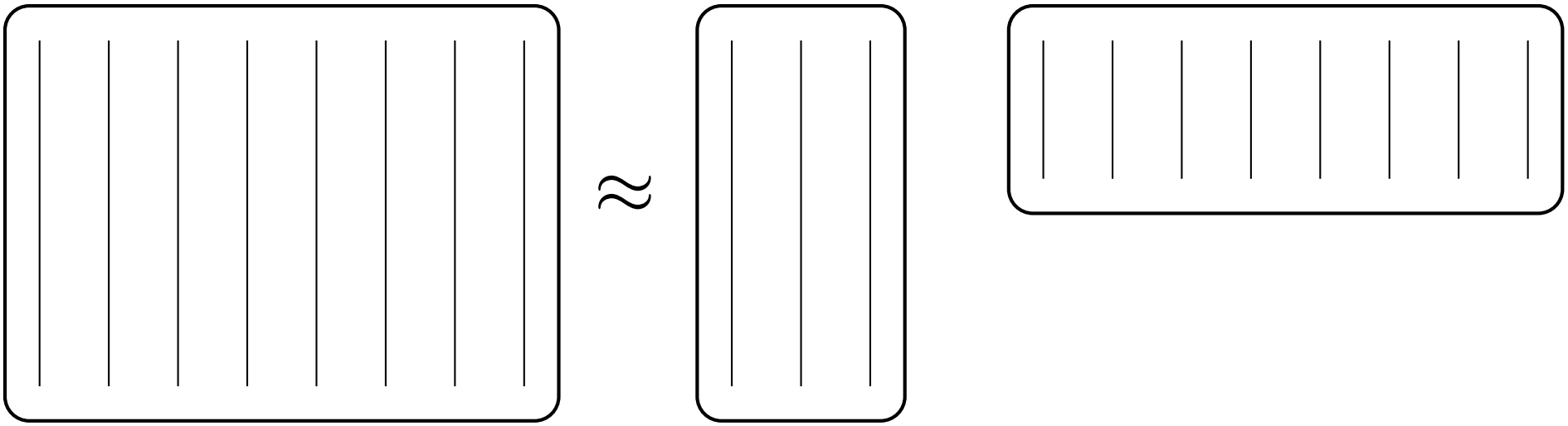
We search for **unsupervised decompositions** of data such that

$\mathbf{x}_n$	$\approx$	$\mathbf{A}$	$\mathbf{s}_n$
data vector		"explanatory variables"	"regressors"
		"basis", "dictionary"	"expansion coefficients"
		"patterns"	"activation coefficients"

and $\mathbf{A}$ is learnt from a set of data vectors $\mathbf{X} = [\mathbf{x}_1 \dots \mathbf{x}_N]$.

- $\mathbf{x}_n$ is a vector of size F
- $\mathbf{s}_n$ is a vector of size K
- $\mathbf{A}$ is a matrix of size $F \times K$, with usually $F \geq K$.

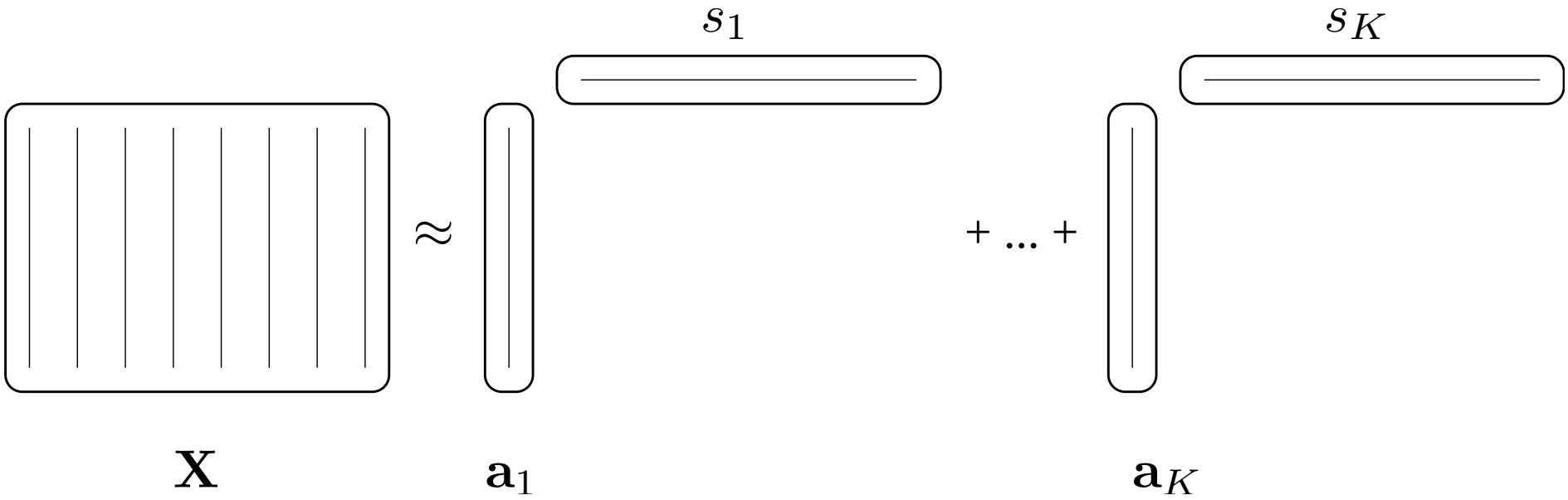
Example: dimensionality reduction



$\mathbf{X}$ $\mathbf{A}$ $\mathbf{S}$

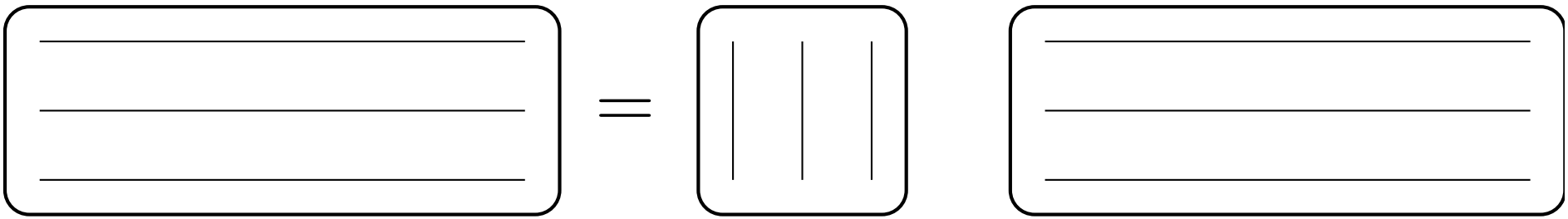
The $F \times N$ data matrix is approximated by $K(F + N)$ coefficients.

Example: dimensionality reduction (ctd)



The factorization is akin to a rank-K approximation.

Example: source separation



$\mathbf{X}$ $\mathbf{A}$ $\mathbf{S}$

The rows of **X** are mixed signals, **A** is a mixing matrix and the sources form the rows of **S**.

Questions

In matrix form, we search for the following factorization

$$\mathbf{X} \approx \mathbf{AS}$$

- What should the "$\approx$" entail ?
- What constraints should be imposed on $\mathbf{A}$ and/or $\mathbf{S}$?

Independent Component Analysis (ICA)

Sphering (aka whitening)

Besides decorrelation, the variance of the entries of $\mathbf{s}$ can be normalized to 1. This achieved for $\mathbf{S}_{SPH} = \mathbf{A}_{SPH}^T \mathbf{X}$ where

$$\mathbf{A}_{SPH} = \mathbf{E}_{1:K} \mathbf{D}_K^{-\frac{1}{2}}$$

Remark

The sphering matrix $\mathbf{A}_{SPH}$ is not unique. Indeed, for any unitary matrix $\mathbf{U}$ of size $K \times K$, the matrix $(\mathbf{A}_{SPH}\mathbf{U})$ is also a sphering matrix, as we may write

$$\begin{aligned} \mathrm{E}\{(\mathbf{A}_{SPH}\mathbf{U})^T \mathbf{x}\mathbf{x}^T (\mathbf{A}_{SPH}\mathbf{U})\} &= \mathbf{U}^T \mathbf{A}_{SPH}^T \mathbf{C}_{\mathbf{x}} \mathbf{A}_{SPH} \mathbf{U} \\ &= \mathbf{U}^T \mathbf{U} \\ &= \mathbf{I} \end{aligned}$$

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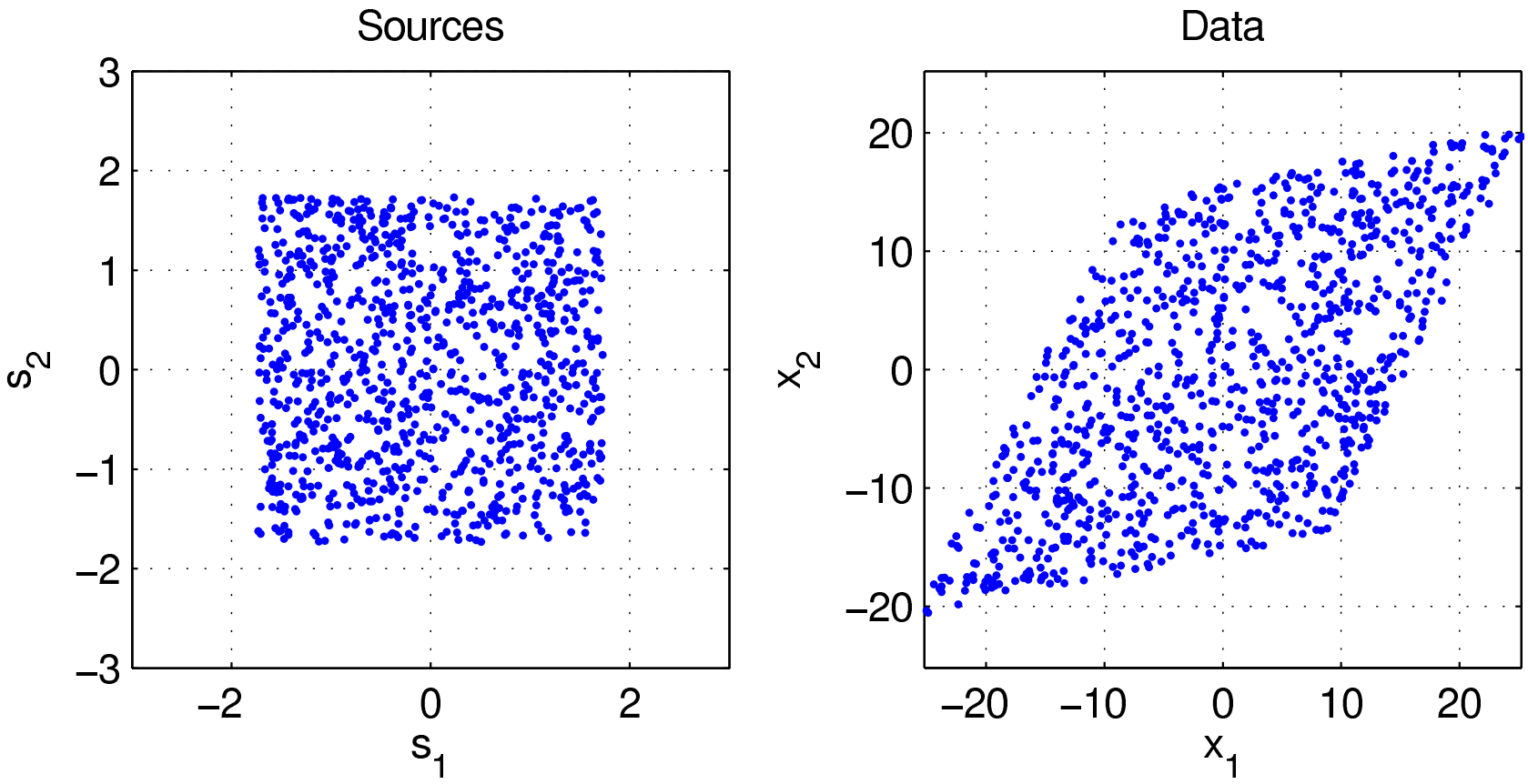
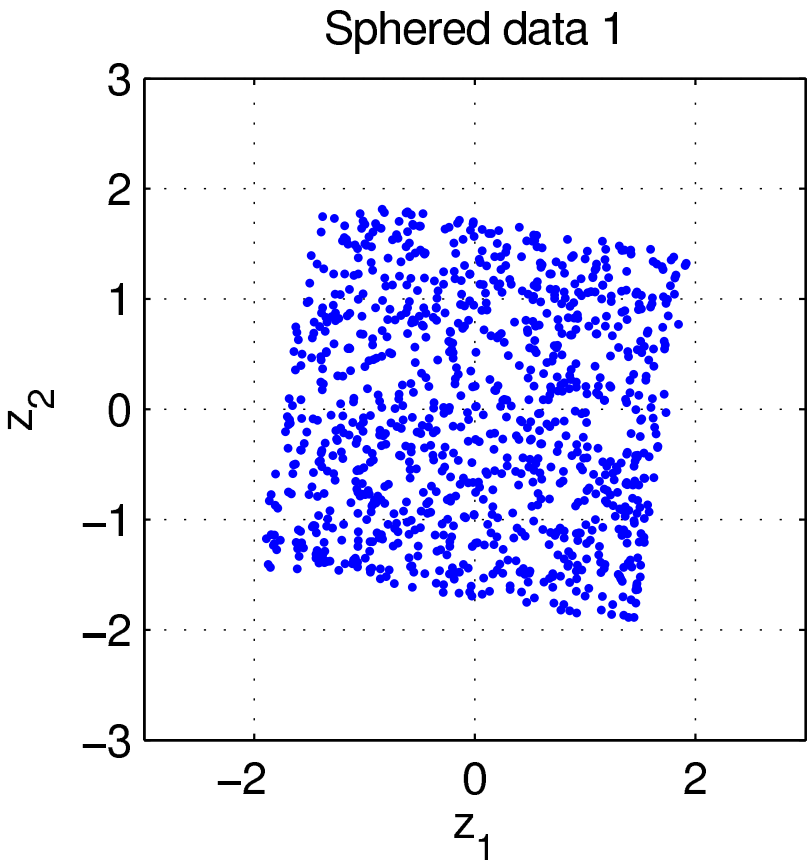
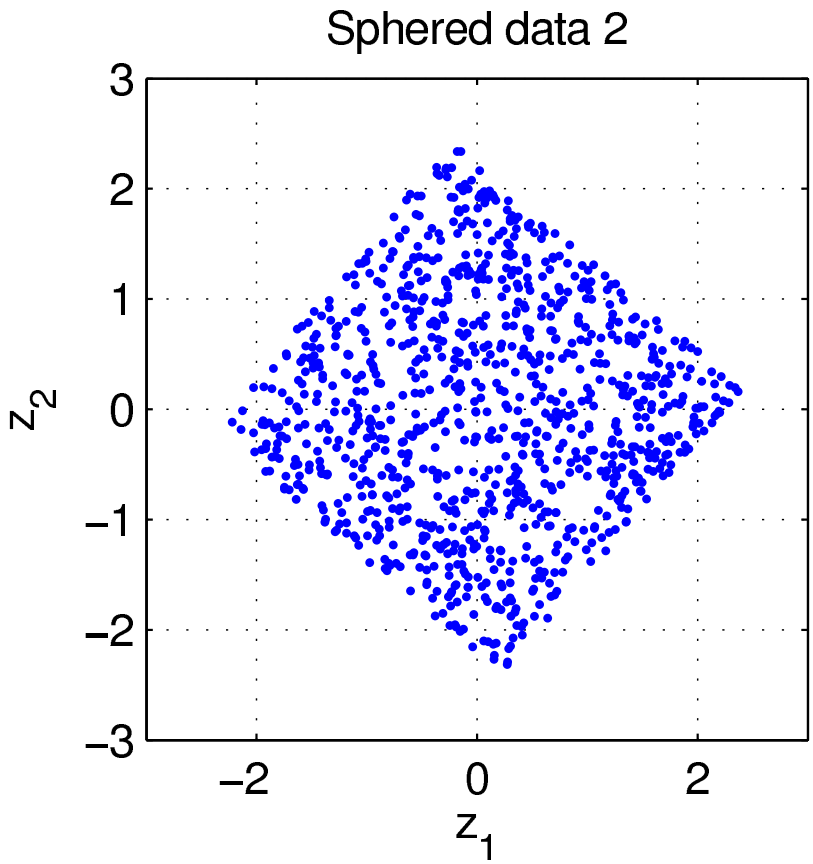
Example : uniform coefficients

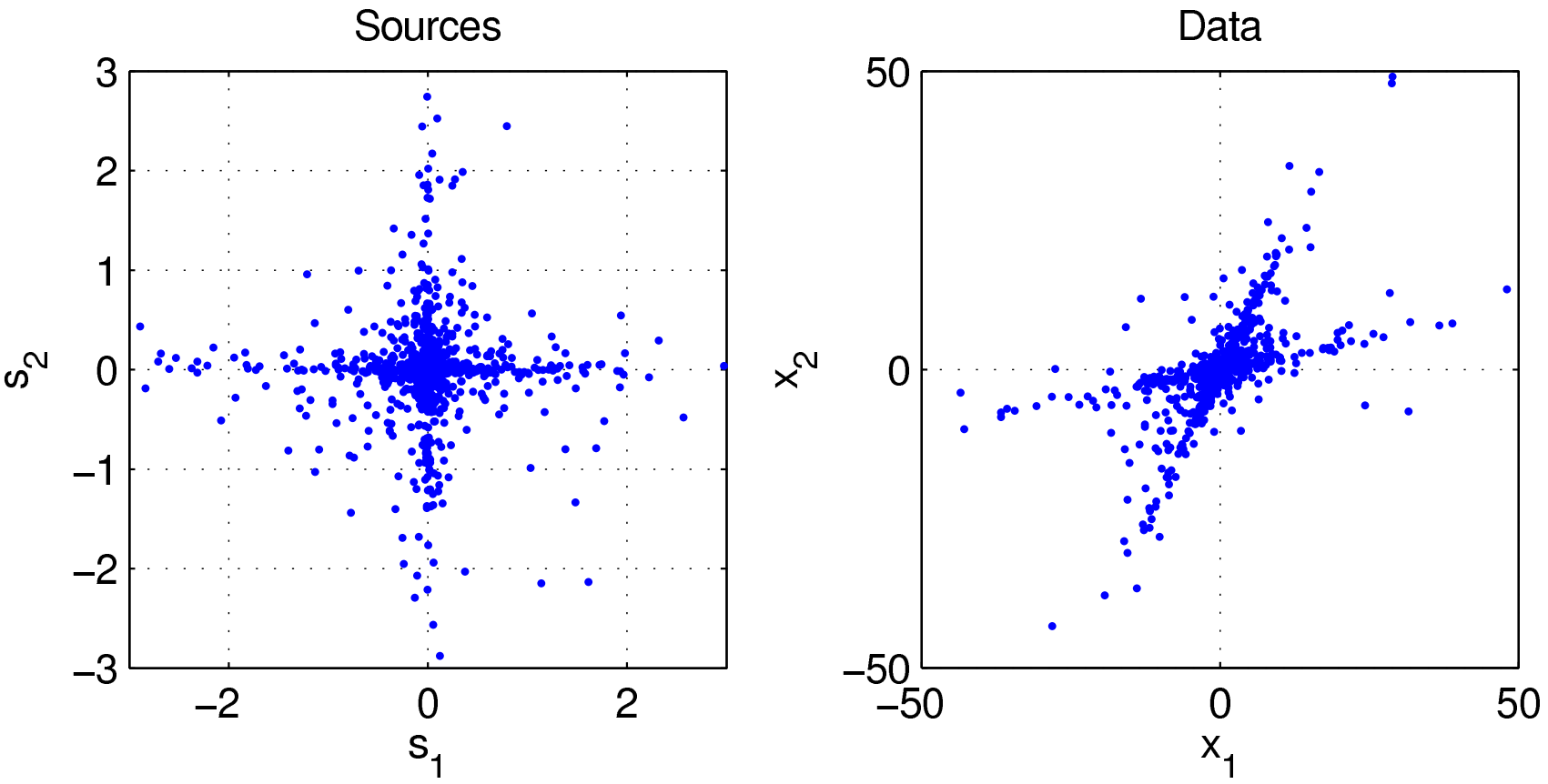


Example : uniform coefficients (ctd)

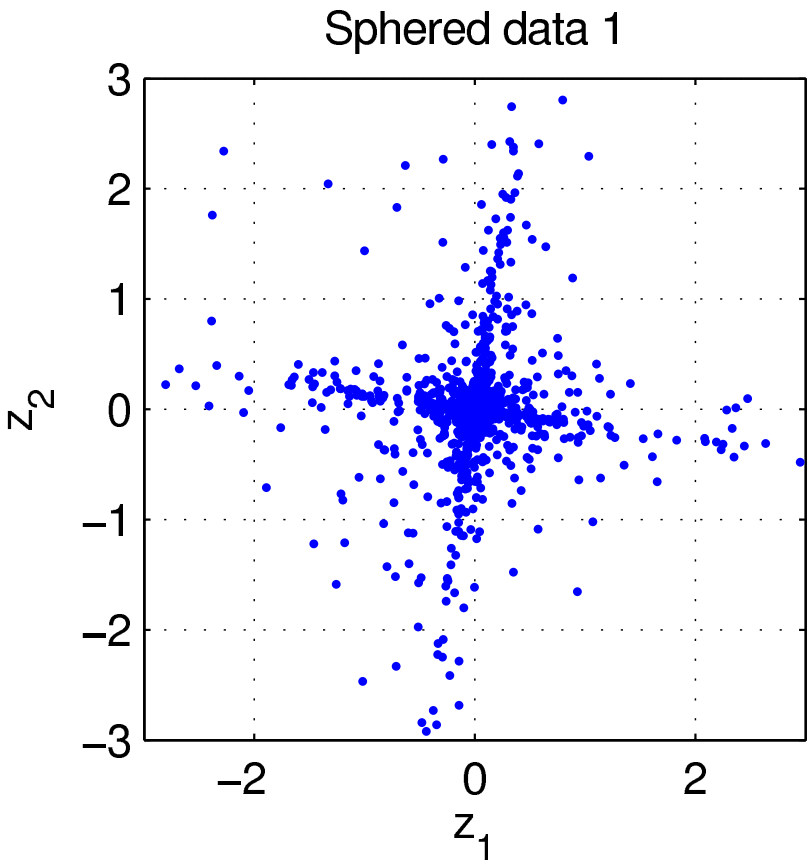


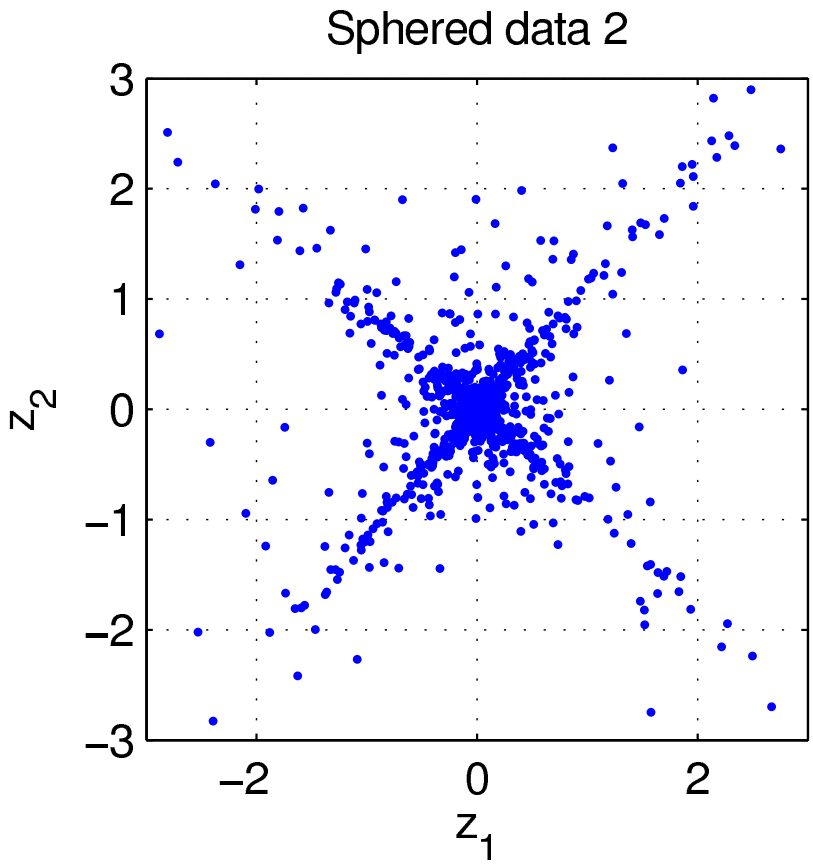


Example : sparse coefficients



Example : sparse coefficients (ctd)





Concept

Sphering returns coefficients $\mathbf{z} = \mathbf{A}_{SPH}^T \mathbf{x}$ that are uncorrelated and with unit variance, i.e., $\mathrm{E}\{\mathbf{z}\mathbf{z}^T\} = \mathbf{I}$.

Sphering is not unique as any rotation $\mathbf{U}\mathbf{z}$ is also white. Hence, one may choose the arbitrary rotation $\mathbf{U}$ so that $\mathbf{U}\mathbf{z}$ satisfies an additional criterion.

ICA aims at finding $\mathbf{U}_{ICA}$ so that the components of

$$\mathbf{s}_{ICA} = \mathbf{U}_{ICA}\mathbf{z} = \mathbf{U}_{ICA}\mathbf{A}_{SPH}^T \mathbf{x}$$

are sphered and **mutually independent**.

Concept (ctd)

Assume for simplicity that $F = K$. In other words, ICA decomposes the data as

$$\mathbf{x} = \mathbf{A}_{ICA}\,\mathbf{s}$$

such that the entries of $\mathbf{s}$ are mutually independent :

$$p(\mathbf{s}) = \prod_k p(s_k)$$

Given what precedes, ICA can be achieved in two steps :

1) Sphere the observations as $\mathbf{z} = \mathbf{A}_{SPH}^T\,\mathbf{x}$,
2) Find $\mathbf{U}_{ICA}$ such that the entries of $\mathbf{U}_{ICA}\,\mathbf{z}$ are mutually independent.

Concept (ctd)

Hence, in practice, given sphered data $\mathbf{z}_n = \mathbf{A}_{SPH}^T \mathbf{x}_n$ we need to

1) Construct a numerical criterion $C(\mathbf{Y})$ measuring the independence of the entries of the random vector $\mathbf{y}$ given realizations $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_N]$.
2) Solve the following optimization problem

$$\max_{\mathbf{U}} C(\mathbf{UZ})$$

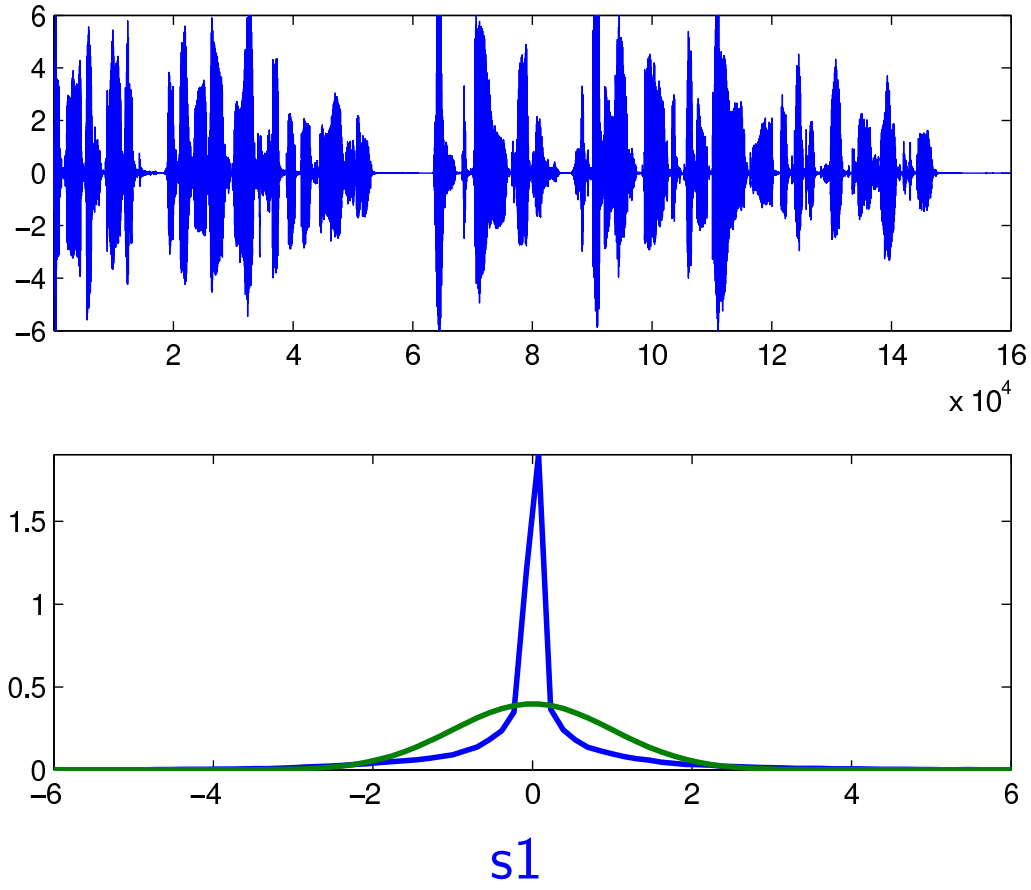
Nongaussian is independent

The Central Limit Theorem tells us that the distribution of the sum of independent random variables tends towards a gaussian distribution.

Basically, it implies that the sum of two random variables is "more gaussian" than the original random variables.

This suggests that the entries of $\mathbf{y} = \mathbf{Uz}$ should be searched as *nongaussian* as possible.

Nongaussian is independent (ctd)



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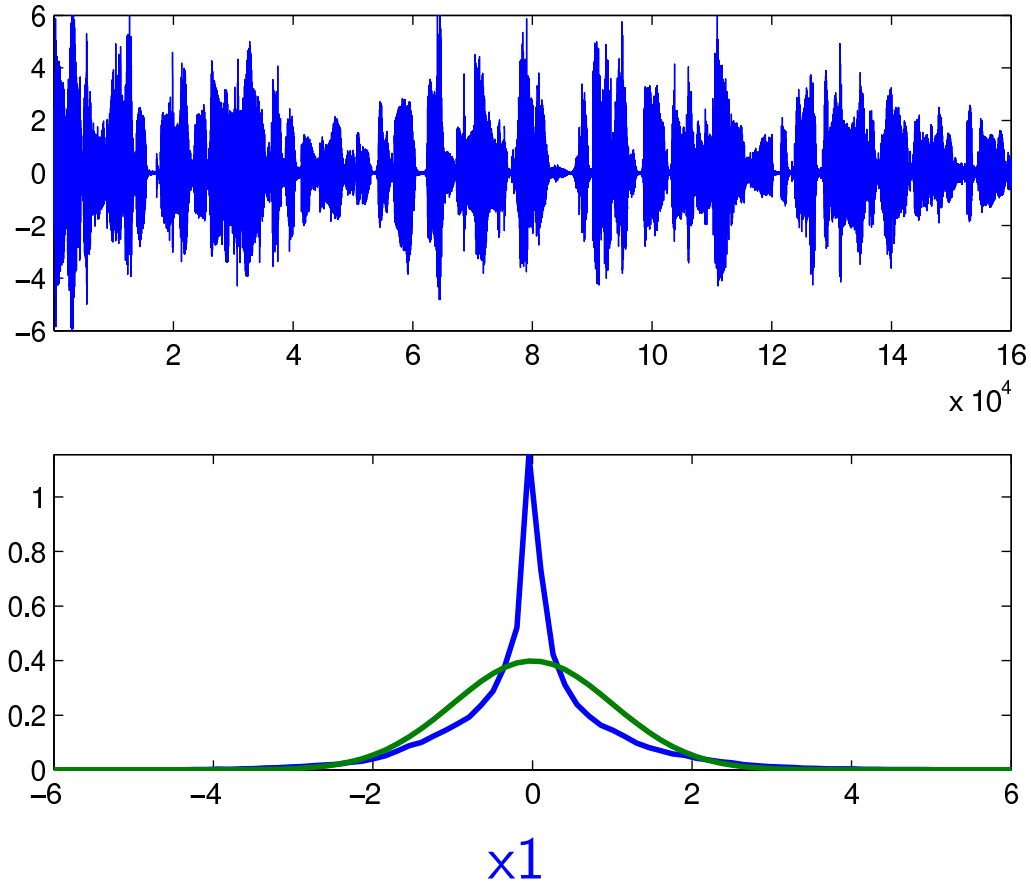

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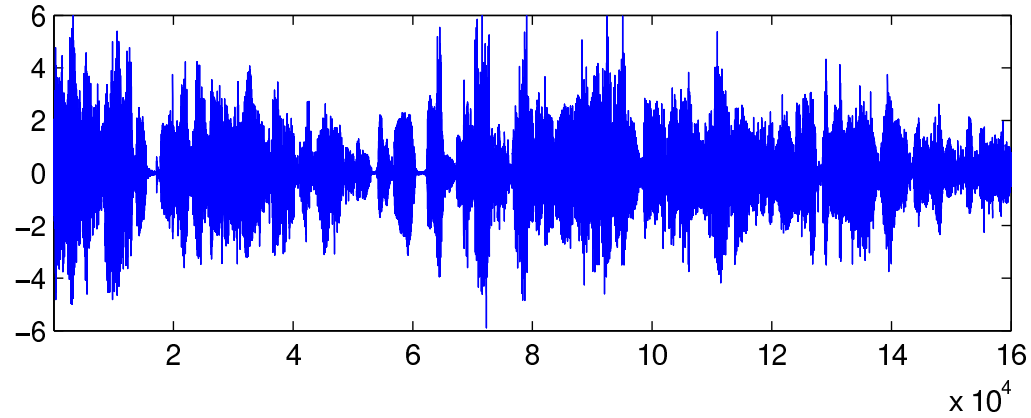
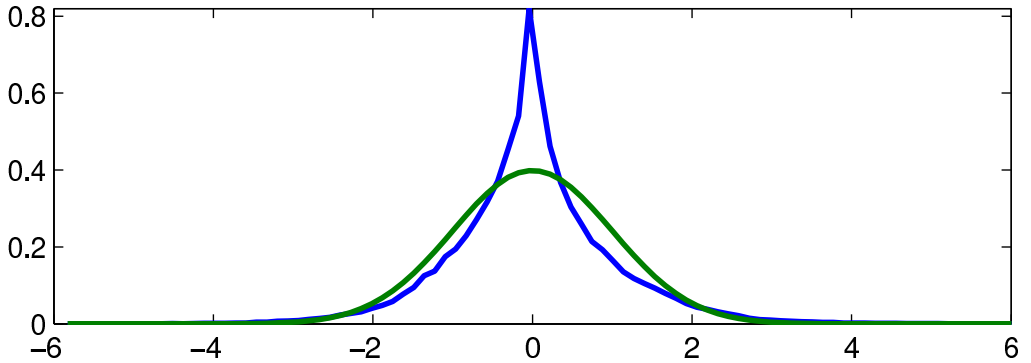
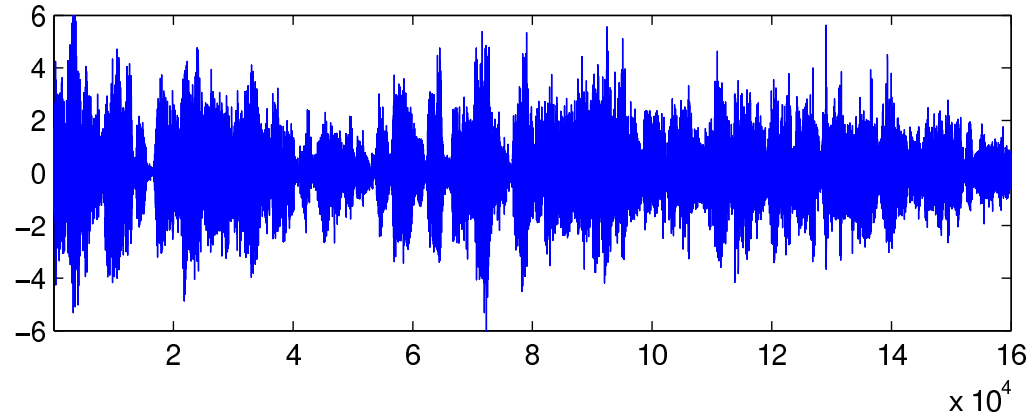
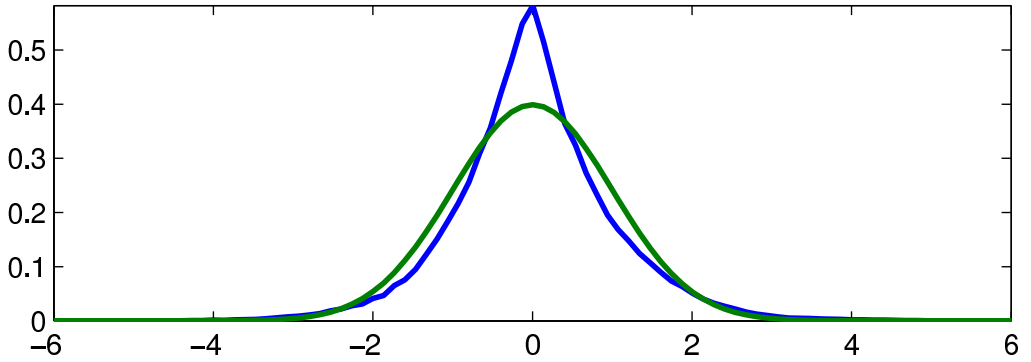




x2

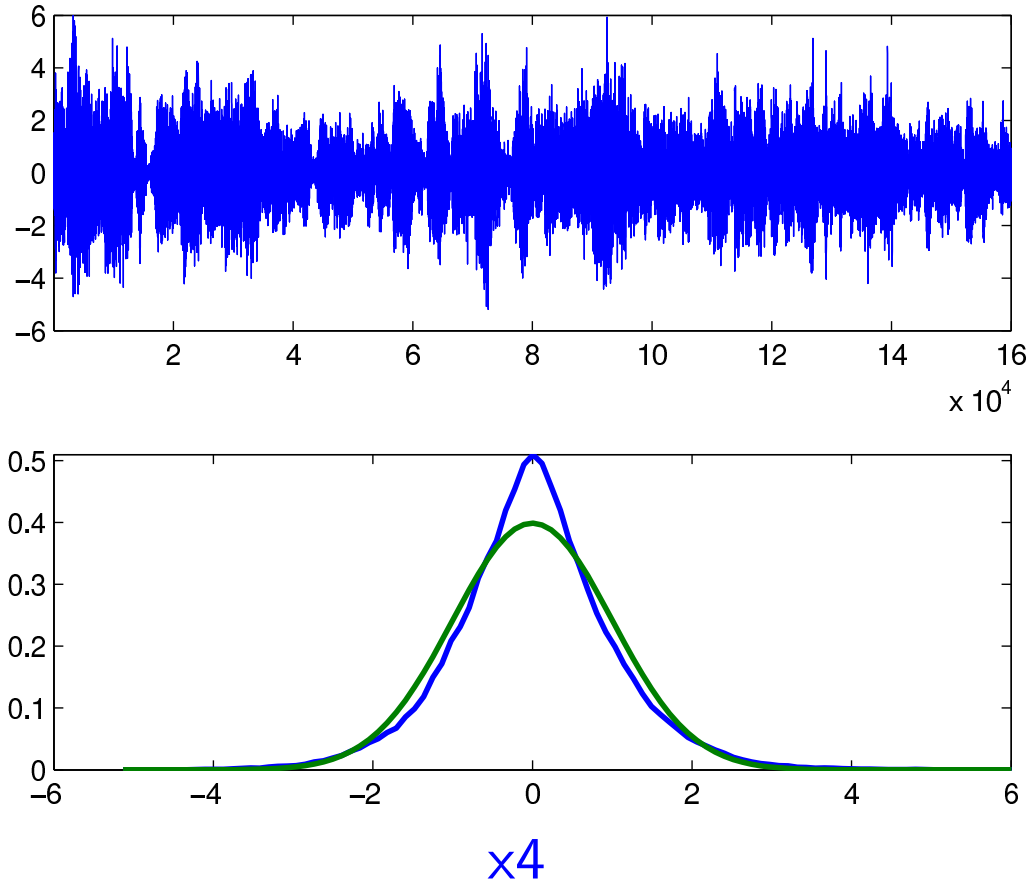
Nongaussian is independent (ctd)



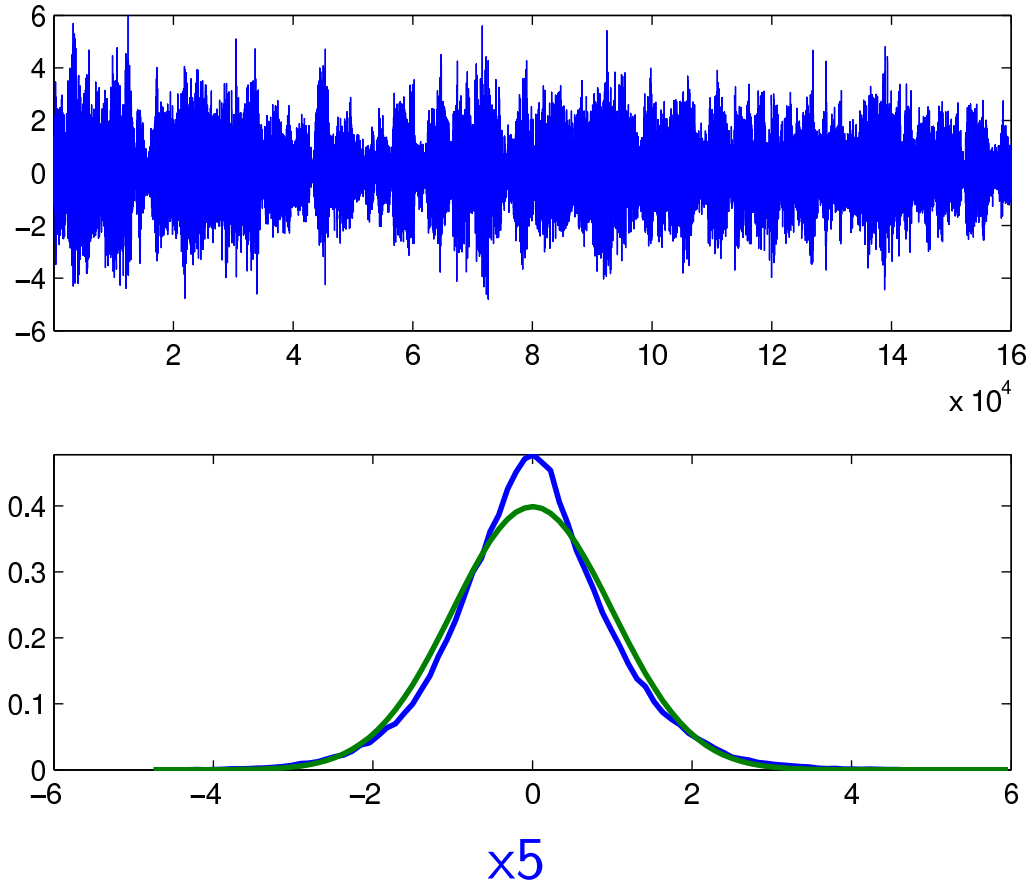


x3

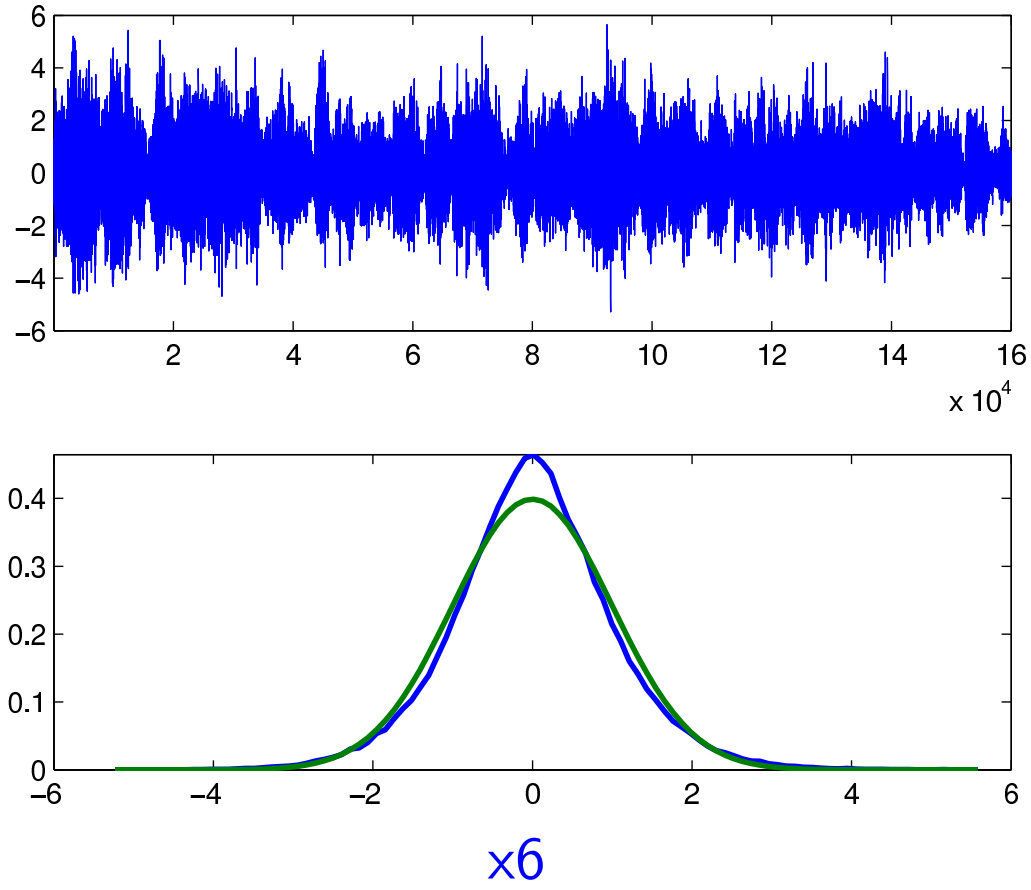
Nongaussian is independent (ctd)



Nongaussian is independent (ctd)



Nongaussian is independent (ctd)



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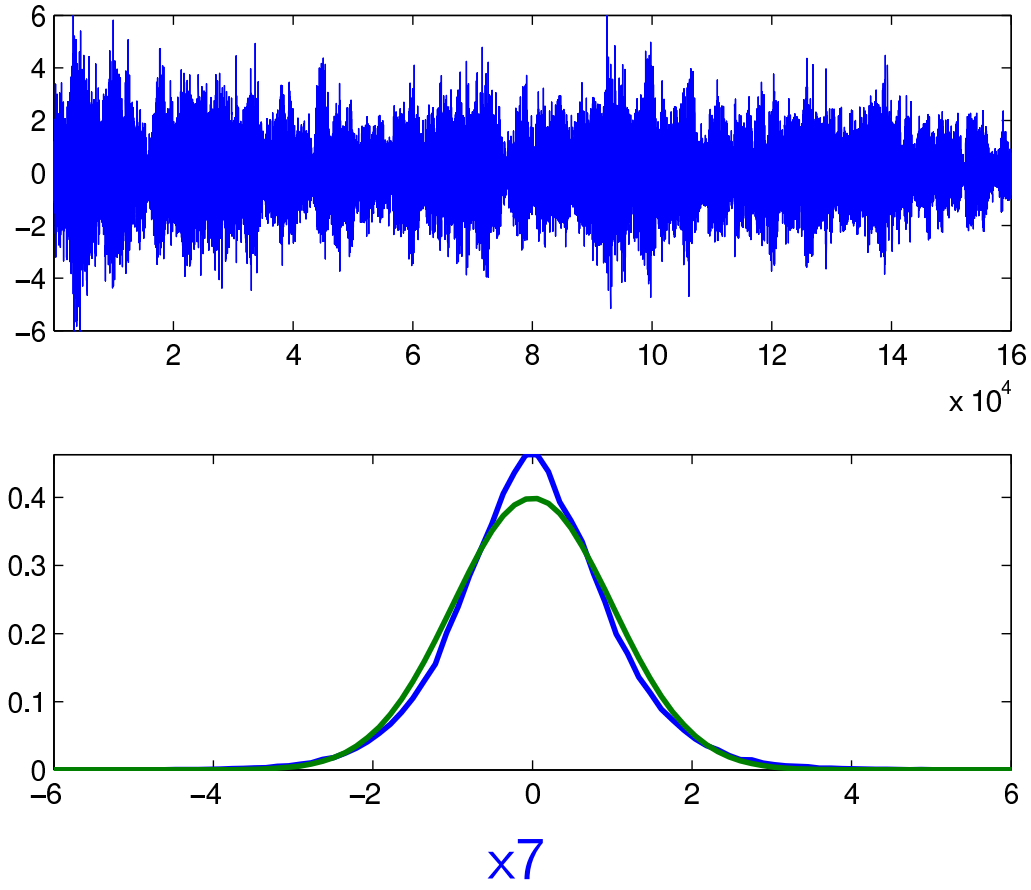

Nongaussian is independent (ctd)

This intuition can be made rigorous via the properties of *mutual information*, defined as

$$\begin{aligned} I\{\mathbf{y}\} &= KL[p(\mathbf{y})|\prod_f p(y_f)] \\ &= \int p(\mathbf{y}) \log \frac{p(\mathbf{y})}{\prod_f p(y_f)} d\mathbf{y} \\ &= \sum_f H\{y_f\} - H\{\mathbf{y}\} \end{aligned}$$

where $H\{\mathbf{y}\} = -\int p(\mathbf{y}) \log p(\mathbf{y}) d\mathbf{y}$ denotes *differential entropy*.

Nongaussian is independent (ctd)

The mutual information of $\mathbf{y} = \mathbf{U}\mathbf{z}$ can be written

$$\begin{aligned} I\{\mathbf{y}\} &= \sum_f H\{y_f\} - H\{\mathbf{z}\} - \log|\det \mathbf{U}| \\ &= \sum_f H\{y_f\} + cst \end{aligned}$$

Hence, because the Gaussian is the distribution with highest entropy (for given variance), minimizing $I\{\mathbf{y}\}$ (i.e., enforcing mutual independence) is equivalent to minimizing $\sum_f H\{y_f\}$ (i.e., enforcing nongaussianity).

Identifiability of ICA

This discussion implies that ICA cannot separate gaussian sources.

This is because the sum of gaussian random variables is itself gaussian.

The ICA model $\mathbf{X} = \mathbf{AS}$ (with $F = K$) is identifiable (up to scale and order ambiguities) when at most one source is gaussian.

Measures of nongaussianity

A quantitative measure of nongaussianity is the *kurtosis*, defined by

$$\text{kurt}\{y\} = \text{E}\{y^4\} - 3\text{E}\{y^2\}^2$$

- The Gaussian distribution has zero kurtosis
- Distributions "flatter" than the Gaussian are called *subgaussian* and have kurtosis < 0
- Distributions "peakier" than the Gaussian are called *supergaussian* and have kurtosis > 0.

Another common measure of nongaussianity is the *negentropy*, defined by

$$J\{y\} = H\{y_G\} - H\{y\}$$

where y_G denotes a Gaussian variable with same variance as y.

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FastICA algorithms

Using the kurtosis as a quantitative measure of nongaussianity, we are left with the following optimization problem

$$\max_{\mathbf{U}} \sum_{k} |\text{kurt}\{[\mathbf{U}^T\mathbf{z}]_k\}| \quad \text{subject to} \quad \mathbf{U}^T\mathbf{U} = \mathbf{I}$$

For simplicity, let's first consider the problem of finding only one maximally nongaussian component, i.e, solve

$$\max_{\mathbf{u}} \; C(\mathbf{u}) = |\text{kurt}\{\mathbf{u}^T\mathbf{z}\}| \quad \text{subject to} \quad \mathbf{u}^T\mathbf{u} = 1$$

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FastICA algorithms

For sphered, centered data $\mathbf{z}$, the criterion writes

$$C(\mathbf{u}) = |\mathrm{E}\{(\mathbf{u}^T\mathbf{z})^4\} - 3|$$

Its gradient thus writes

$$\nabla_{\mathbf{u}} C(\mathbf{u}) = 4\,\mathrm{sign}(\mathrm{E}\{(\mathbf{u}^T\mathbf{z})^4\} - 3)\,\mathrm{E}\{(\mathbf{u}^T\mathbf{z})^3\mathbf{z}\}$$

FastICA algorithms (ctd)

A suitable projected gradient ascent algorithm writes

Initialize $\mathbf{u}^{(0)}$
for $i = 1 : n_{iter}$ **do**
$\mathbf{u}^{(i)} \leftarrow \mathbf{u}^{(i-1)} + \alpha^{(i)} \nabla_{\mathbf{u}} C(\mathbf{u}^{(i-1)})$
$\mathbf{u}^{(i)} \leftarrow \frac{\mathbf{u}^{(i)}}{\|\mathbf{u}^{(i)}\|}$
end for

where $\alpha^{(i)}$ is a sequence of positive step sizes.

FastICA algorithms (ctd)

A faster algorithm, free of tuning parameters, may be obtained by observing that a stationary point of the criterion must point in the direction of the gradient.
Indeed the Lagrangian to the original problem

$$\max_{\mathbf{u}} \; C(\mathbf{u}) = |\text{kurt}\{\mathbf{u}^T\mathbf{z}\}| \quad \text{subject to} \quad \mathbf{u}^T\mathbf{u} = 1$$

writes

$$L(\mathbf{u}, \lambda) = C(\mathbf{u}) + \lambda(1 - \|\mathbf{u}\|^2)$$

so that a stationary point $\mathbf{u}^\star$ must satisfy $\nabla_{\mathbf{u}} C(\mathbf{u}^\star) = 2\lambda\mathbf{u}^\star$.

FastICA algorithms (ctd)

Hence, a fast fixed point algorithm can be obtained as

Initialize $\mathbf{u}^{(0)}$
for $i = 1 : n_{iter}$ **do**
$\mathbf{u}^{(i)} \leftarrow \frac{\nabla_{\mathbf{u}} C(\mathbf{u}^{(i-1)})}{\|\nabla_{\mathbf{u}} C(\mathbf{u}^{(i-1)})\|}$
end for

Though based on a heuristic, the convergence of this algorithm to a stationary point of the original constrained problem can be shown.

FastICA algorithms (ctd)

In practice, the expectation appearing in the gradient is replaced by sample averages, i.e,

$$\mathrm{E}\{(\mathbf{u}^T\mathbf{z})^3\mathbf{z}\} \approx \frac{1}{N}\sum_n (\mathbf{u}^T\mathbf{z}_n)^3\mathbf{z}_n$$

The estimation may however be quite sensitive to outliers so that other algorithms based on robust approximations of the negentropy should be used.

However, the optimization concepts hold, and lead to the family of FastICA algorithms.

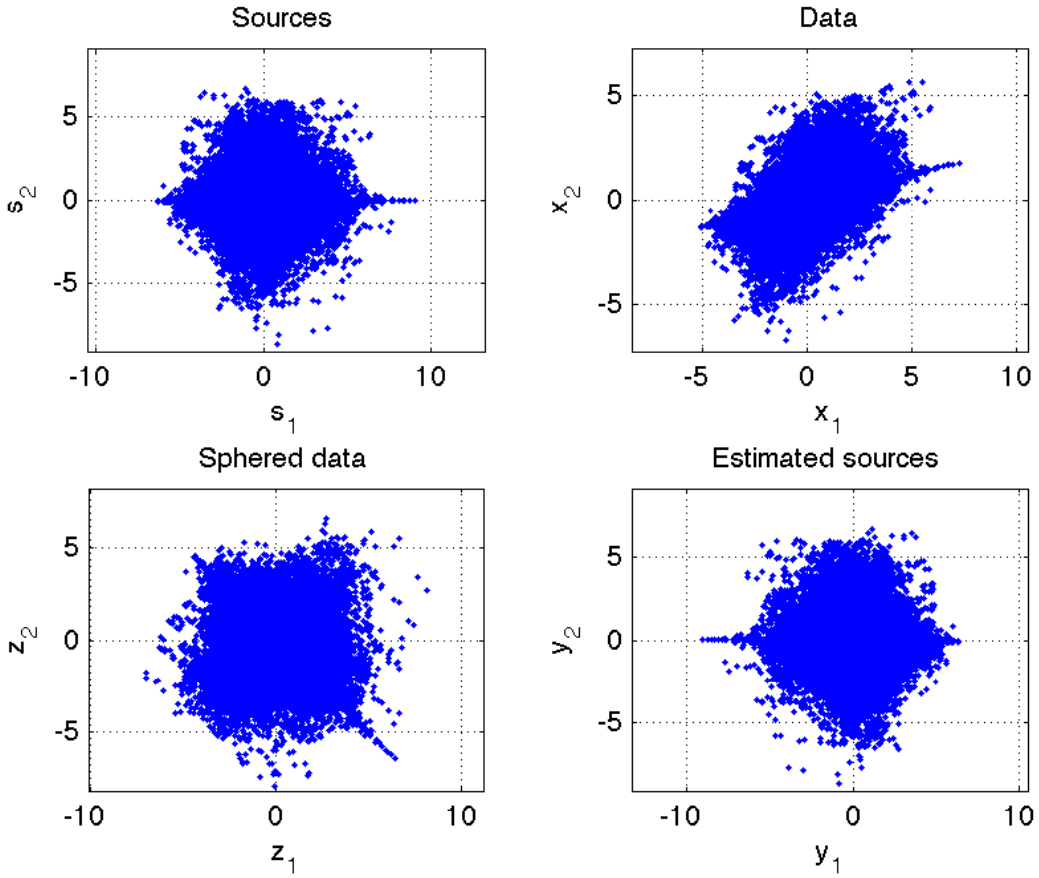
Fast ICA algorithms (ctd)

The "one-unit" optimization can be generalized to optimization of the whole matrix $\mathbf{U}$ through orthogonalization.

Initialize $\mathbf{u}_1^{(0)}, \ldots, \mathbf{u}_K^{(0)}$ (randomly)
for $i = 1 : n_{iter}$ **do**
  Do one iteration of a one-unit algorithm on every $\mathbf{u}_k$ in parallel
  Orthogonalize the set of vectors $\mathbf{u}_1^{(i)}, \ldots, \mathbf{u}_K^{(i)}$

end for

2 x 2 audio example



x_1 x_2 z_1 z_2 $\hat{s}_1$ $\hat{s}_2$

References

- A. Hyvärinen, J. Karhunen and E. Oja. *Independent Component Analysis*. Wiley, 2001.
- A. Hyvärinen and E. Oja. *Independent Component Analysis : Algorithms and Applications*. Neural Networks, 2000. [online]
- The FastICA package for MATLAB. `http://www.cis.hut.fi/projects/ica/fastica/`
- J.-F. Cardoso. *Blind Signal Separation: Statistical Principles*. Proceeding of the IEEE, 1998. [online]