Independent Component Analysis
Theoretical Foundation

Marijo Simunovic

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1 Introduction

Independent Component Analysis (ICA) is an umbrella term for a set of mathematical and computational methods where the goal is to separate a multivariate signal (a mixture) into additive components (original signals). These signals are often referred to as independent components (IC). A detailed overview of different approaches can be found in [6]. ICA is often motivated as a method for solving *cocktail-party problem* [3] where we want to reconstruct the voices signals of n speakers based on the audio recordings of n microphones. Other possible uses include reconstruction of neural activity from EEG recordings [10], image sharpening [8] or face recognition [2].

We can think of ICA as an estimation of generative model [5]. The observables are n random variables x_1, x_2, ..., x_n. The assumption is that these random variables are formed as linear combination of n unknown (latent) variables s_1, s_2, ..., s_n. The $i-th$ component is formed as a mixture:

$$x_i = a_{i1} * s_1 + a_{i2} * s_2 + ... + a_{in} * s_n; \quad i = 1, 2, ..., n. \tag{1}$$

The mixture coefficients are also unknown. We can write down the same formulation in matrix notation:

$$\mathbf{x} = \mathbf{A} * \mathbf{s} \tag{2}$$

where $\mathbf{x}$ and $\mathbf{s}$ are n-vectors and $\mathbf{A}$ is a mixture matrix where i-th row contains the mixture coefficients of the x_i-th variable.

2 Restrictions of ICA

The basic requirement for ICA methods to work is *independence*. It is assumed that the independent components are statistically independent. We say that the the random variables are independent if their joint probability distribution function (pdf) is equal to the product of their marginal distributions, i.e.

$$p(s_1, s_2, ..., s_n) = p_1(s_1) * p_2(s_2) * ... * p_3(s_n). \tag{3}$$

Two vectors s_1 and s_2 are linearly independent if there is no non-zero scalar a such that

$$a * s_1 + s_2 = 0 \tag{4}$$

Geometrically, vectors s_1 and s_2 do not lie on the same line. If two vectors are *statistically* independent their covariance is:

$$cov(s_1, s_2) = 0 \tag{5}$$

For two *linearly* dependent vectors

$$cov(s_1, s_2) = cov(\frac{1}{a} * s_1, s_2) = \frac{1}{a} var(s_2) \neq 0. \tag{6}$$

Therefore, two *linearly* dependent vectors cannot be statistically independent (linear independence of vectors, however, is not guarantee of their statistical independence). Furthermore, the distributions of independent components need to be *nongaussian*. ICA methods often rely on higher-order cumulants for the estimation of mixture coefficients. These higher-order cumulants are zero for gaussian distribution making the application impossible of ICA in this case.

We typically assume that the mixing matrix A is square, i.e. we model the problem in such way that the number of independent components is equal to the number of observed mixtures. Once the mixture matrix is known we can determine the original signals as

$$\mathbf{s} = \mathbf{A}^{-1} * \mathbf{x} \tag{7}$$

under assumption that the $\mathbf{A}$ is invertible.

Once these requirements are satisfied we can determine the original components up to trivial indeterminacies. Firstly, we cannot determine the variances of independent components. Both the ICs and mixture coefficients are unknown. Therefore, any scalar multiplier in sources can be canceled by dividing the corresponding entries in mixture matrix:

$$x_i = (\frac{1}{k_1} * a_{i1}) * (s_1 * k_1) + ... + (\frac{1}{k_n} * a_{in}) * (s_n * k_n)s; \quad i = 1, 2, ..., n. \tag{8}$$

Due to this fact, we typically fix the magnitudes of mixture components to have unit variance: $E\left[s^2\right] = 1$. This still leaves us with a sign ambiguity. In addition, we cannot determine order of independent components as we can arbitrarily permute the independent components:

$$\mathbf{x} = \mathbf{A} * \mathbf{P}^{-1} * \mathbf{P} * \mathbf{s} \tag{9}$$

Here $\mathbf{P}$ is permutation matrix (entries are 1s and 0s) and $\mathbf{P} * \mathbf{s}$ is the original vector $\mathbf{s}$ with changed order of entries s_i. Matrix $\mathbf{A} * \mathbf{P}^{-1}$ is a new mixture matrix $\mathbf{M}$ to be determined by ICA methods.

2.1 Independent components with time structure

If independent components are time signals the ICA model is:

$$x(t) = A * s(t) \tag{10}$$

If the data has time-dependencies the autocovariance values are often different from zero:

$$cov(x_i(t), x_i(t-\tau)) \neq 0, \quad \tau = 1, 2, 3, ... \tag{11}$$

When source signals have time structure (colored statistics) they are even allowed to be Gaussian. There are enough equations to solve the blind source separation problem without high-order statistics. In addition to the autocovariances, we are also interested into covariance values between different signals, i.e $cov(x_i(t), x_j(t-\tau))$, where $i \neq j$. We can write down all these statistics using time-lagged covariance matrix of mixed signals:

$$C_\tau^{\mathbf{X}} = E\left[\mathbf{x}(t) * \mathbf{x}(t-\tau)^T\right] \tag{12}$$

and independent components

$$C_\tau^{\mathbf{S}} = E\left[\mathbf{s}(t) * \mathbf{s}(t-\tau)^T\right]. \tag{13}$$

The matrix $C_\tau^{\mathbf{S}}$ is diagonal due to the independence of the sources.

Typically, when we are doing the reconstruction we first whiten the mixture data (see 4 in this document for the introduction to whitening) and we are working on whitened data $z(t)$. We aim to find an unmixing orthogonal matrix W which will reconstruct original signals

$$W * \mathbf{z}(t-\tau) = \mathbf{s}(t-\tau), \quad \tau = 0, 1, 2, 3... \tag{14}$$

From (13) and using (14) it follows:

$$C_\tau^{\mathbf{Z}} = W^T * E\left[\mathbf{s}(t) * \mathbf{s}(t-\tau)^T\right] * W = W^T * C_\tau^{\mathbf{S}} * W \tag{15}$$

This means that the matrix W is part of the eigenvalue decomposition of $C_\tau^{\mathbf{Z}}$ We can therefore have a simple algorithm [11] to compute matrix W:
1. whiten the centered data $\mathbf{x}(t)$ to obtain $\mathbf{z}(t)$.
2. Compute eigenvalue decomposition of time-lagged covariance matrix $C_\tau^{\mathbf{Z}}$ for some time lag τ.
3. The rows of the separating matrix W are given by eigenvectors of decomposition in step 2.

The algorithm works as long as the eigenvalues are uniquely defined - this is true if and only if the lagged covariances are different for all the ICs. One can search for a suitable time lag where this condition is satisfied. However, if the ICs have identical power spectra (identical autocovariances) they cannot be estimated using this method.

3 ICA and Gaussian Distributions

. In case of Gaussian distribution first two moments are enough to sufficiently characterize the random variable. First moment is mean:

$$\mu_x = E[x] = \int_{-\infty}^{\infty} x * p_x(x) dx \tag{16}$$

and second is variance, defined as:

$$\sigma_x^2 = E\left[(x - \mu_x)^2\right] = \int_{-\infty}^{\infty} (x - \mu_x)^2 * p_x(x) dx \tag{17}$$

. By extension we define n-th order moment as:

$$v^n = E\left[(x - \mu_x)^n\right] = \int_{-\infty}^{\infty} (x - \mu_x)^n * p_x(x) dx. \tag{18}$$

From the Central Limit Theorem it follows that the distribution of the of the sum of centralized independent and identically distributed random variables converges against the standard normal distribution. The task of ICA is to reconstruct the original signals from a mixture. Therefore, when we are trying to reconstruct the mixing matrix we would like to check that the resulting signals are less Gaussian than the observed mixture. Another aspect worth considering is that the linear mixture of two Gaussian random variables results in new Gaussian distribution. This makes it impossible to infer if the original signals contained a single or multiple Gaussian distributed sources. Therefore, ICA methods are useful if only at most one source signal was Gaussian distributed (with already mentioned exception to the methods that use time structure of signals).

One measure of gaussianity is *kurtosis*. Kurtosis is fourth order momenth statistics:

$$\kappa = v_4 = \frac{E\left[(x - \mu_x)^4\right]}{\sigma^4} \tag{19}$$

The kurtosis of a Gaussian is equal to 3. A distribution with a positive kurtosis (> 3) is called super-Gaussian (or leptokurtic) and distribution with negative kurtosis (< 3) is sub-Gaussian (or platykurtic).

In practice, we use approximations of the above equations, with mean as

$$\mu_x = \frac{1}{M} \sum_{i=1}^{M} x_i \tag{20}$$

variance as

$$\sigma^2(x) = \frac{1}{M} \sum_{i=1}^{M} (x_i - \mu_x)^2 \tag{21}$$

and finally kurtosis as:

$$\kappa(x) = \frac{1}{M} \sum_{i=1}^{M} \left(\frac{x_i - \mu_x}{\sigma} \right)^4 \tag{22}$$

It is visible from the equation that the kurtosis is quite sensitive to the outliers. Entries far away from mean will dominate the summation due to the exponent. Instead of using kurtosis, it is common to measure the non-gaussianity using *negentropy*. Negentropy J is defined as:

$$J = H(y_{gauss}) - H(y) \tag{23}$$

where y_{gauss} is a Gaussian random variable of same covariance matrix as y. H denotes entropy of random variable. In discrete case it is defined as:

$$H(Y) = -\sum_i P(Y = a_i) log P(Y = a_i) \tag{24}$$

where a_i are all possible realizations of Y. Among all distributions of the same variance, Gaussian has the highest entropy [4]. Therefore, negentropy is always greater or equal to zero (in case y is also Gaussian). The more the distribution is concentrated on a specific set of values the lower is the entropy. This motivates the usage of negentropy as a measure of distance from the Gaussian distribution. There are problems with using negentropy directly in practice. Estimating negentropy would required an estimate of *pdf* which is often computationaly difficult problem. Classicaly, negentropy can be approximated as:

$$J(y) \approx \frac{1}{12} E\left[y^3\right] - \frac{1}{48} kurt(y)^2 \tag{25}$$

This approximation still suffers from the sensitivity of kurtosis to outliers. The researchers have therefore come up with more robust approximations based on the maximization of entropy [9], of the form:

$$J(y) \approx \left(E\left[G(y)\right] - E\left[G(\nu)\right]\right)^2 \tag{26}$$

Choosing G wisely, i.e. using a slowly growing function one obtains robust estimators:

$$G(u) = \frac{1}{a_1} logcosh(a_1 * u) \tag{27}$$

where $1 \leq a_1 \leq 2$, or

$$G(u) = -exp(-\frac{u^2}{2}) \tag{28}$$

4 Whitening

Given some random variables, it is straightforward to linearly transform them into uncorrelated variables. Two random variables are uncorrelated if their covariance is zero:

$$cov(y_1, y_2) = E\left[y_1 * y_2\right] - E\left[y_1\right] * E\left[*y_2\right] = 0 \tag{29}$$

When working with ICA methods we typically centralize the data so we can safely assume that the mean of random variables are equal to 0. In that case,

covariance is equal to correlation and uncorelatedness is the same thing as zero correlation. A slightly stronger property, *whiteness*, of a zero mean random vector y means that the components of the vector are uncorrelated and that their variance is equal unity. Therefore, the covariance (and correlation) matrix is identity matrix I. We can use various methods to whiten a vector. Commonly, this is done using the SVD decomposition of covariance matrix or eigenvalue decomposition of covariance matrix. Whitening operation transform the original mixing matrix into a new, orthogonal mixing matrix V':

$$y = V * z = V * A * s = V' * s \tag{30}$$

This constraints the search space of a mixing matrix to a space of orthogonal matrices. An orthogonal matrix contains $\frac{n*(n-1)}{2}$ degrees of freedom. In higher dimensional spaces, orthogonal matrices have half a number of parameters in comparison to the arbitrary mixing matrix that we would like to estimate.

5 FastICA

Fast ICA [7] uses a fixed-point iteration scheme for finding maximum of non-gaussianity of $\mathbf{w}^T * x$ [7]. The input data x is assumed to be centered and whitened. We set the random weight vector w and normalize it such that $||w|| = 1$. Then we calculate the new weight vector as

$$w_{new} = E\left[x * G(w^T * x)\right] - E\left[G_{prim}(w^T * x)\right] * w \tag{31}$$

A detailed derivation of the vector update rule is given in [5]. The new weight vector is normalized and compared to the old value. The convergence is defined as a dot-product which is equal to 1 (within a given tolerance) ignoring the sign of the dot product as we can define the ICs only up to a multiplicative constant. Geometrical interpretation is that the angle between two consecutive vector updates stays under some predefined value.

This algorithm estimates only a single independent component. If we want to extend the algorithm for multiple components we also need to ensure that the weight vectors are decorrelated in order to prevent convergence to the same vector. A simple way to achieve this is Gramm-Schmidt method. If we have estimated up to w_{p-1} weight vectors, we can orthogonalize the vector w_p as follows:

$$w_p = w_p - \sum_{i=i}^{p-1}(w_p^T * w_i) * w_i \tag{32}$$

The alternative is to perform symmetric decorrelation of all vectors at the same time using following update rule:

$$W = (W * W^T)^{-\frac{1}{2}} * W \tag{33}$$

where W is unmixing matrix we are trying to estimate.

We tested the implementation with mixture of the images from recently published synthetic dataset [1] and two randomly generated signals with Gaussian and Poisson distribution, respectively. The notebook with the example is available under:
https://github.com/m5imunovic/studious-engine/notebooks/ICAApplication.ipynb

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