Chapter 3: Independent Component Analysis^a

As in the chapter on factor analysis (Chapter 2) we assume that the observations $\{x_i^0\}_{i=1}^n$ are n realizations of an \mathbb{R}^p -valued random variable X^0 , and we let $X = X^0 - \mathbb{E}[X]$.

Then, the independent component analysis (ICA) model assumes that

$$X = \mathbf{B}S, \quad \mathbf{B} \in \mathbb{R}^{p \times p}, \quad \mathbb{E}[S] = 0, \quad \text{Var}(S) = \mathbf{I}_p$$
 (3.1)

where the p components of the \mathbb{R}^p -valued random variable S are independent random variables and where \mathbf{B} is invertible.

Remark: The ICA model holds true if X is Gaussian and if Var(X) is full rank, in which case \boldsymbol{B} and S can be obtained using population PCA^b.

Unlike the factor analysis model, where the factor F has typically no physical existence, in ICA the variable S is a real signal that we want to recover from X. Remark that this is the reason why the matrix B is assumed to be invertible.

A typical (toy) application of ICA is to recover the p = 2 signals S_1 and S_2 emitted by two persons speaking simultaneously in a room from the signals X_1 and X_2 recorded by two microphones.

^aThe main reference for this chapter is [?].

^bTo see this recall that $X = \Gamma Y$ where $\Gamma \in O(p)$ and where $Y \sim \mathcal{N}_p(0, \mathbf{L})$, with \mathbf{L} a diagonal matrix having the eigenvalues of $\mathrm{Var}(X)$ as non-zero entries (see Chapter 1, page 24). If $\mathrm{Var}(X)$ is full rank the matrix \mathbf{L} is invertible, and thus $X = (\Gamma \mathbf{L}^{1/2})(\mathbf{L}^{-1/2}Y)$. This shows that the ICA model holds with $\mathbf{B} = \Gamma \mathbf{L}^{1/2}$ and with $S = \mathbf{L}^{-1/2}Y \sim \mathcal{N}_p(0, \mathbf{I}_p)$ (recall that $S \sim \mathcal{N}_p(0, \mathbf{I}_p)$ implies that $S_1, \ldots, S_p \stackrel{\mathrm{iid}}{\sim} \mathcal{N}_1(0, 1)$).

ICA model: Discussion of its assumptions and problem formulation

• In (3.1) there is no loss of generality to assume that $Var(S) = \mathbf{I}_p$. Indeed, if $X = \tilde{\mathbf{B}}\tilde{S}$ with $\mathbf{\Psi} := Var(\tilde{S}) \neq \mathbf{I}_p$ then, letting $\mathbf{B} = \tilde{\mathbf{B}}\mathbf{\Psi}^{1/2}$ and $S = \mathbf{\Psi}^{-1/2}\tilde{S}$, we have

$$X = \tilde{\boldsymbol{B}}\tilde{S} = (\tilde{\boldsymbol{B}}\boldsymbol{\Psi}^{1/2})(\boldsymbol{\Psi}^{-1/2}\tilde{S}) = \boldsymbol{B}S, \quad \text{Var}(S) = \boldsymbol{I}_p$$
 (3.2)

implying that (3.1) holds.

Remark: (3.2) shows that $Var(\tilde{S})$ cannot be recovered from X if we only know that $X = \tilde{\boldsymbol{B}}\tilde{S}$ for some matrix $\tilde{\boldsymbol{B}} \in \mathbb{R}^{p \times p}$.

• Recalling that S is a true signal that we want to recover, the assumption that the components of S are independent is necessary to make \mathbf{B} identifiable (the identifiability of \mathbf{B} will be discussed more precisely later). In particular, if we only assume that the components of S are uncorrelated then S can only be recovered up to an orthogonal transformation since, for all $\mathbf{G} \in O(p)$, $X = \mathbf{B}S = (\mathbf{B}\mathbf{G}^{\top})(\mathbf{G}S)$ where $\operatorname{Var}(\mathbf{G}S) = \operatorname{Var}(S)$.

We assume for now that $Var(X) = \mathbf{I}_p$. In this case, the ICA model (3.1) implies that

$$\operatorname{Var}(X) = \operatorname{Var}(\boldsymbol{B}S) = \boldsymbol{B}\boldsymbol{B}^{\top} = \boldsymbol{I}_{p}$$

showing that if (3.1) holds then B must be an orthogonal matrix^a

Therefore, under the assumption $Var(X) = \mathbf{I}_p$ we have $X = \mathbf{B}S$ if and only if $S = \mathbf{B}^{\top}X$, and thus under (3.1) and the assumption $Var(X) = \mathbf{I}_p$ the matrix $\mathbf{B} \in O(p)$ is such that the components of the random variable $\mathbf{B}^{\top}X$ are independent.

^aRecall that the ICA model assumes that \boldsymbol{B} is invertible

Defining B through an optimization problem

For a given random variable Z we denote by $g_Z(z)dz$ its probability distribution (w.r.t. some reference measure dz) and we let

$$H(Z) = -\int g_Z(z) \log (g_Z(z)) dz.$$

Remark: The quantity H(Z) is called the entropy of Z.

We also recall that the Kullback-Leibler (KL) divergence between the distributions p(z)dz and q(z)dz is given by

$$\mathrm{KL}(p||q) = \int \log \left(\frac{p(z)}{q(z)}\right) p(z) \mathrm{d}z$$

and we also recall the following result:

Lemma 3.1 For any distributions p(z)dz and q(z)dz we have $KL(p||q) \ge 0$, where the equality holds if and only if p = q.

Easy computations show that if $Z = (Z_1, ..., Z_p)$ is and \mathbb{R}^p -valued random variable then the KL divergence between the distributions $g_Z(z)$ dz and $\prod_{j=1}^p g_{Z_j}(z_j)$ dz can be written as follows:

$$KL(g_Z||\prod_{j=1}^p g_{Z_j}) = \sum_{j=1}^p H(Z_j) - H(Z) =: I(Z).$$

By Lemma 3.1, $I(Z) \ge 0$ and I(Z) = 0 if and only if all the components of Z are independent. Therefore, I(Z) can be interpreted as a measure of independence between the components of Z. (The quantity I(Z) is called the mutual information of Z.)

Under the assumption $Var(X) = \mathbf{I}_p$, it follows that the matrix \mathbf{B} in (3.2) verifies

$$\boldsymbol{B} \in \operatorname*{argmin}_{\boldsymbol{G} \in O(p)} I(\boldsymbol{G}^{\top} X). \tag{3.3}$$

Two key lemmas for finding an approximate solution to (3.3)

Lemma 3.2 Let Y be a continuous and real-valued random variable with $\mathbb{E}[Y] = 0$ and Var(Y) = 1, and let $Z \sim \mathcal{N}_1(0,1)$. Then, $H(Z) \geq H(Y)$, where the equality holds if and only if $Y \sim \mathcal{N}_1(0,1)$.

$$\begin{split} \mathrm{KL}(p_Y||p_Z) &= \int \log \left(\frac{p_Y(y)}{p_Z(y)}\right) p_Y(y) \mathrm{dy} = -H(Y) - \int \log(p_Z(y)) p_Y(y) \mathrm{dy} \\ &= -H(Y) - \int \left(-\frac{1}{2} \log(2\pi) - \frac{y^2}{2}\right) p_Y(y) \mathrm{dy} \\ &= -H(Y) - \int \left(-\frac{1}{2} \log(2\pi) - \frac{z^2}{2}\right) p_Z(z) \mathrm{dz} \\ &= -H(Y) - \int \log(p_Z(z)) p_Z(z) \mathrm{dz} \\ &= -H(Y) + H(Z) \end{split}$$

where the third equality uses the fact that $\mathbb{E}[Y^2] = \mathbb{E}[Z^2]$. Then, the result follows from Lemma 3.1.

To proceed further for any \mathbb{R} -valued random variable Y such that $\mathbb{E}[Y] = 0$ and $\operatorname{Var}(Y) = 1$ we let J(Y) = H(Z) - H(Y), with $Z \sim \mathcal{N}_1(0, 1)$.

Remark: By Lemma 3.2, for any \mathbb{R} -valued random variable Y such that $\mathbb{E}[Y] = 0$ and $\mathrm{Var}(Y) = 1$ we have $J(Y) \geq 0$, where the equality holds if and only if $Y \sim \mathcal{N}_1(0,1)$. Hence, the quantity J(Y), called the negentropy of Y, is a measure of distance to normality.

Lemma 3.3 Assume $Var(X) = \mathbf{I}_p$. Then, the matrix \mathbf{B} in (3.2) is such that $\mathbf{B} \in \operatorname{argmax}_{\mathbf{G} \in O(p)} \sum_{j=1}^p J(g_{(j)}^\top X)$.

Proof: Let $p_X(\cdot)$ be the density of X and let $Y = \mathbf{G}^\top X$. Then, using the change of variables formula and the fact that $|\det(\mathbf{G})| = 1$, the density $p_Y(\cdot)$ of Y is defined by $p_Y(y) = p_X(\mathbf{G}y)$ and thus

$$H(\mathbf{G}^{\top}X) = H(Y) = -\int p_{Y}(y) \log (p_{Y}(y)) dy = -\int p_{X}(\mathbf{G}y) \log (p_{X}(\mathbf{G}y)) dy = -\int |\det(\mathbf{G}^{-1})| p_{X}(x) \log (p_{X}(x)) dx$$
$$= -\int p_{X}(x) \log (p_{X}(x)) dx$$
$$= H(X)$$

where the third equality uses the change of variables formula for integrals. Then the result follows from (3.3) and from the definition of $I(\mathbf{G}^{\top}X)$.

Approximating the solution to (3.3)

Using Lemma 3.2 and Lemma 3.3, it follows if $Var(X) = \mathbf{I}_p$ then the matrix \mathbf{B} in (3.2) verifies

$$\boldsymbol{B} \in \operatorname{argmax}_{\boldsymbol{G} \in O(p)} \sum_{j=1}^{p} J(g_{(j)}^{\top} X)$$
(3.4)

$$= \operatorname{argmax}_{\boldsymbol{G} \in O(p)} \Bigl\{ \sum_{j=1}^{p} \text{ "departure from Gaussianitiy of } \boldsymbol{g}_{(j)}^{\top} \boldsymbol{X} " \Bigr\}.$$

The quantity $J(g_{(j)}^{\top}X)$ is usually intractable but its interpretation in term of distance to normality provides a simple way to compute an approximate solution to (3.4): replace $J(g_{(j)}^{\top}X)$ by another measure of distance to normality!

In ICA, the departure from Gaussianitiy of $g_{(j)}^{\top}X$ is often measured by

$$\left(\mathbb{E}[\varphi(g_{(j)}^{\top}X)] - \mathbb{E}[\varphi(Z)]\right)^{2}, \quad Z \sim \mathcal{N}_{1}(0,1)$$
(3.5)

for some function $\varphi : \mathbb{R} \to \mathbb{R}$.

Remark: Using (3.5) with the function $\varphi(u) = \frac{1}{a} \log \cosh(au)$ for some $a \in [1, 2]$, or with the function $\varphi(u) = -e^{-u^2/2}$, often works well in practice and provide a reasonable approximation of the negentropy $J(g_{(j)}^{\top}X)$ [?].

Then, for a given choice of $\varphi : \mathbb{R} \to \mathbb{R}$ and assuming $\operatorname{Var}(X) = \mathbf{I}_p$, the matrix \mathbf{B} in (3.2) can be approximated by the matrix $\tilde{\mathbf{B}}$ verifying

$$\tilde{\boldsymbol{B}} \in \operatorname{argmax}_{\boldsymbol{G} \in O(p)} \sum_{j=1}^{p} \left(\mathbb{E}[\varphi(g_{(j)}^{\top}X)] - \mathbb{E}[\varphi(Z)] \right)^{2}$$
 (3.6)

where $Z \sim \mathcal{N}_1(0, 1)$.

Estimation of the approximate solution \tilde{B}

A possible approach for estimating the matrix $\tilde{\boldsymbol{B}}$ defined in (3.6) from the observations $\{x_i\}_{i=1}^n$ is as follows. For all $\boldsymbol{G} \in O(p)$ let

$$L(\boldsymbol{G}) = \sum_{j=1}^{p} \left(\mathbb{E}[\varphi(g_{(j)}^{\top}X)] - \mathbb{E}[\varphi(Z)] \right)^{2}$$

and

$$\hat{L}_n(\mathbf{G}, \{x_i\}_{i=1}^n) = \sum_{j=1}^p \left(\frac{1}{n} \sum_{i=1}^n \varphi(g_{(j)}^\top x_i) - \mathbb{E}[\varphi(Z)]\right)^2$$

so that $\hat{L}_n(\mathbf{G}, \{x_i\}_{i=1}^n) \approx L(\mathbf{G})^a$.

Then, noting that $\tilde{\boldsymbol{B}} \in \operatorname{argmax}_{\boldsymbol{G} \in O(p)} L(\boldsymbol{G})$, we can estimate $\tilde{\boldsymbol{B}}$ using the matrix $\tilde{\boldsymbol{B}}_n$ defined by

$$\tilde{\boldsymbol{B}}_n \in \operatorname{argmax}_{\boldsymbol{G} \in O(p)} \hat{L}_n(\boldsymbol{G}, \{x_i\}_{i=1}^n).$$
 (3.7)

The definition of $\hat{L}_n(\mathbf{G}, \{x_i\}_{i=1}^n)$ requires to compute $\mathbb{E}[\varphi(Z)]$, a quantity which, depending on the choice of φ , may be intractable. However, being a one dimensional integral, we can easily (and efficiently) estimate $\mathbb{E}[\varphi(Z)]$ using numerical integration methods.

Letting $\hat{\varphi}$ be an estimate of $\mathbb{E}[\varphi(Z)]$, a computable estimate $\tilde{\mathbf{B}}'_n$ of $\tilde{\mathbf{B}}$ is therefore defined by

$$\tilde{\boldsymbol{B}}'_{n} \in \operatorname{argmax}_{\boldsymbol{G} \in O(p)} \sum_{j=1}^{p} \left(\frac{1}{n} \sum_{i=1}^{n} \varphi(g_{(j)}^{\top} x_{i}) - \hat{\varphi} \right)^{2}.$$
 (3.8)

The set O(p) being compact if follows that if $\{X_i\}_{i=1}^n$ are i.i.d. copies of X then, under some conditions on φ , we have $\sup_{\mathbf{G}\in O(p)}|\hat{L}_n(\mathbf{G},\{X_i\}_{i=1}^n)-L(\mathbf{G})|\to 0$ in probability. Note that, whatever the distribution of X is, this uniform convergence result holds if φ is continuous an bounded, as this is the case for the choice $\varphi(u)=-e^{-u^2/2}$ mentioned earlier.

end for

Estimation of the approximate solution \tilde{B} (end)

A simple way to solve the optimization problem (3.8) is to use a projected gradient descend algorithm:

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A projected gradient descend algorithm for solving (3.8) 

Input: Matrix \tilde{\boldsymbol{B}}^{(0)} \in O(p) and step-size \gamma > 0 

for s \geq 1 do 

(i) Let \boldsymbol{C}_s = \tilde{\boldsymbol{B}}^{(s-1)} + \gamma \nabla_{\boldsymbol{B}} \sum_{j=1}^p \left(\frac{1}{n} \sum_{i=1}^n \varphi(x_i^\top \tilde{\boldsymbol{b}}_{(j)}^{(s-1)}) - \hat{\varphi}\right)^2 

(ii) Let \tilde{\boldsymbol{B}}^{(s)} = (\boldsymbol{C}_s \boldsymbol{C}_s^\top)^{-1/2} \boldsymbol{C}_s \in O(p). 

if Convergence=TRUE then 

(iii) return \tilde{\boldsymbol{B}}^{(s)}. 

(iv) break 

end if
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Remark: In practice, more sophisticated (and more efficient) methods are used to estimate the matrix $\tilde{\boldsymbol{B}}$ defined in (3.6) [see ? , Section 6].

Remark: Estimating \boldsymbol{B} through the estimation of the matrix $\tilde{\boldsymbol{B}}$ is called the FastICA method.

Estimation of \boldsymbol{B} when $\operatorname{Var}(X) \neq \boldsymbol{I}_d$

We now consider the general case where $Var(X) = \Sigma$ for some $\Sigma \neq I_p$. We assume below that Σ is full rank and let L be a diagonal matrix containing the eigenvalues of Σ and $\Gamma \in O(p)$ be the corresponding matrix of orthonormal eigenvectors.

Let
$$K = L^{-1/2}\Gamma^{\top}$$
, $B_W = KB$ and $W = KX$, and note that

(i) Under the ICA model the random variable W is such that $W = (KB)S = B_WS$ and such that

$$Var(W) = \boldsymbol{L}^{-1/2} \boldsymbol{\Gamma}^{\top} \boldsymbol{\Sigma} \boldsymbol{\Gamma} \boldsymbol{L}^{-1/2} = \boldsymbol{L}^{-1/2} \boldsymbol{\Gamma}^{\top} (\boldsymbol{\Gamma} \boldsymbol{L} \boldsymbol{\Gamma}^{\top}) \boldsymbol{\Gamma} \boldsymbol{L}^{-1/2} = \boldsymbol{I}_{p}.$$

(ii) Since $\mathbf{B}_W = \mathbf{K}\mathbf{B}$ we have $\mathbf{B} = \mathbf{K}^{-1}\mathbf{B}_W = \Gamma \mathbf{L}^{1/2}\mathbf{B}_W$.

Let Λ be the diagonal matrix containing the eigenvalues of the matrix $S := \frac{1}{n} X^{\top} X$, $A \in O(p)$ be the corresponding matrix of orthonormal eigenvectors and Y = XA be the matrix of principal components.

Then, (i)-(ii) suggest the following three steps for estimating \boldsymbol{B} :

- 1. Compute $\mathbf{W} = \mathbf{Y} \mathbf{\Lambda}^{-1/2}$. Remark that $\frac{1}{n} \mathbf{W}^{\top} \mathbf{W} = \mathbf{I}_p$ and recall that (under some conditions) we can interpret $\{w_i\}_{i=1}^n$ as "approximate" realizations of W (see Chapter 1, pages 24–25). The transformation $\mathbf{X} \mapsto \mathbf{W}$ of the data is called whitening.
- 2. Use $\{w_i\}_{i=1}^n$ and the approach introduced in this chapter for estimating \boldsymbol{B} when $\operatorname{Var}(X) = \boldsymbol{I}_p$ to compute an estimate $\tilde{\boldsymbol{B}}'_{n,W}$ of \boldsymbol{B}_W .
- 3. Estimate \boldsymbol{B} by

$$\hat{\boldsymbol{B}}_n := \boldsymbol{A} \boldsymbol{\Lambda}^{1/2} \tilde{\boldsymbol{B}}'_{n,W}. \tag{3.9}$$

Recovering the signals from the data

Recall that under the ICA model the observations $\{x_i\}_{i=1}^n$ are realizations of a random variable X such that $X = \mathbf{B}S$ with \mathbf{B} and S as in (3.1).

Under the ICA model we therefore have $x_i = \mathbf{B}s_i$ for all i and thus, denoting by \mathbf{S}_{sig} the $n \times p$ matrix with rows $\{s_i\}_{i=1}^n$,

$$oldsymbol{X} = oldsymbol{S}_{ ext{sig}} oldsymbol{B}^{ op}.$$

Given the estimate $\hat{\boldsymbol{B}}_n$ of \boldsymbol{B} defined in (3.9) we can estimate the matrix signals $\boldsymbol{S}_{\text{sig}}$ using

$$\hat{oldsymbol{S}}_{ ext{sig}} := oldsymbol{X} ig(\hat{oldsymbol{B}}_n^ opig)^{-1}.$$

Recalling that $\tilde{\boldsymbol{B}}'_{n,W} \in O(p)$, we have

$$egin{aligned} \hat{m{S}}_{ ext{sig}} &= m{X}ig(\hat{m{B}}_n^ opig)^{-1} = m{X}ig(ig(ilde{m{B}}_{n,W}'ig)^ opm{\Lambda}^{1/2}m{A}^ opig)^{-1} \ &= m{X}m{A}m{\Lambda}^{-1/2} ilde{m{B}}_{n,W}' \ &= m{W} ilde{m{B}}_{n,W}' \end{aligned}$$

and therefore computing the estimate $\hat{\mathbf{S}}_{\text{sig}}$ does not require to compute the estimate $\hat{\mathbf{B}}_n$ of \mathbf{B} .

Remark: Estimating S_{sig} by $\hat{S}_{\text{sig}} = W \tilde{B}'_{n,W}$ is natural. Indeed, under the ICA model we have $W = B_W S$ and thus, as we are interpreting the w_i 's as realizations of W, this implies that $w_i = B_W s_i$ for all i, and thus that $W = S_{\text{sig}} B_W^{\top} \Leftrightarrow S_{\text{sig}} = W B_W$.

Identifiability of the ICA model

Assume that $Var(X) = I_p$ and that the ICA model is correct, so that for some $\mathbf{B} \in O(p)$ we have $\mathbf{X} = \mathbf{S}_{sig}\mathbf{B}^{\top}$ where the rows of \mathbf{S}_{sig} are n realizations of S.

Then,

• If all the components of S are $\mathcal{N}_1(0,1)$ random variables then $\mathbf{G}S \stackrel{\text{dist.}}{=} S$ for any matrix $\mathbf{G} \in O(p)^a$. Therefore, in this case we have

$$X = \boldsymbol{B}S \stackrel{\text{dist.}}{=} \boldsymbol{B}\boldsymbol{G}S = (\boldsymbol{B}\boldsymbol{G})S, \quad \boldsymbol{B}\boldsymbol{G} \in O(p), \quad \forall \boldsymbol{G} \in O(p)$$

showing that the matrix \boldsymbol{B} , and thus the signals $\boldsymbol{S}_{\text{sig}}$, can only be estimated up to an orthogonal transformation.

• The columns of **B**, and thus the rows of S_{sig} , can only be estimated up to a multiplicative sign. To see this let D be a $p \times p$ diagonal matrix with such that $d_{jj} \in \{-1, 1\}$ for all j and let $\tilde{S} = DS$. Then,

$$X = \mathbf{B}S = \mathbf{B}\mathbf{D}^{-1}\mathbf{D}S = (\mathbf{B}\mathbf{D})\tilde{S}$$

where $\boldsymbol{BD} \in O(p)$ and $\operatorname{Var}(\tilde{S}) = \boldsymbol{I}_d$.

Remark: It can be shown that if at most one component of S is Gaussian and rank(\mathbf{B}) = p then the columns of the matrix $\mathbf{B} \in \mathcal{O}(p)$ are unique up to a multiplicative sign (see [?]).

^aUse the change of variable formula to show this.

Illustration of ICA

We let p = 3, $n = 1\,000$ and simulate the true signals matrix $\mathbf{S}_{\text{sig}} = [s_{ij}] \in \mathbb{R}^{n \times p}$ using

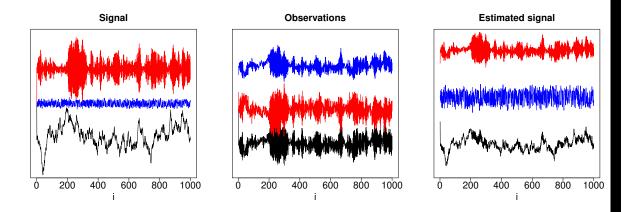
$$S_{ij} = \rho_j S_{(i-1)j} + \epsilon_{ij}, \quad \epsilon_{ij} \stackrel{\text{iid}}{\sim} \frac{1}{2} \mathcal{N}_1(-1, 0.25) + \frac{1}{2} \mathcal{N}_1(1, 0.25)$$

where $S_{(i-1)j} = 0$ for i = 1 and where $\rho_2 = -\rho_1 = 0.98$ and $\rho_3 = 0.2$. Remark that each row of the matrix S_{sig} is a trajectory of a Markov chain. The three Markov chains (i.e. the three signals) are mixed using the matrix

$$\boldsymbol{B} = \begin{pmatrix} 1 & -1 & -3 \\ 1 & 1 & 2 \\ -1 & 3 & -3 \end{pmatrix}.$$

Remark: In this example the distribution of S_i is not exactly the same for all i.

The true signals S_{sig} as well as the observations $X = S_{\text{sig}}B^{\top}$ and the ICA estimate \hat{S}_{sig} of S_{sig} (obtained with $\varphi(u) = \log \cosh(u)$) are shown in the following plots.



Remark: In the two plots the signals are shifted and coloured to facilitate the comparisons. In addition, the y-axis has been removed since, as shown above, we cannot estimate the variance of the components of S.