A Conceptual Explicit Expression of the Separation Matrix in Independent Component Analysis

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ABSTRACT

Shown here is a relation between the separation matrix in ICA and the pseudo-inverse of the mixing matrix. Derived here is a relation between the separation matrix

\[
W_{ICA} = PAR\Sigma^{-1/2}\Phi^T
\]

and

\[
R^{-1}a(t) = \sigma^{-1/2}p(t) \implies \Phi^{-1}R^{-1}a(t) = \sigma^{-1/2}p(t)
\]

where

\[
\sigma(t) = [\sigma_1(t), \sigma_2(t), \ldots, \sigma_n(t)]^T
\]

and \(\Phi(t) = [\Phi_1(t), \Phi_2(t), \ldots, \Phi_n(t)]^T\) are matrices consisting of the element-wise Fourier inverse transforms of \(\Sigma(t)\) and \(\Phi(\omega)\), respectively, and \(\otimes\) denotes matrix convolution.

INTRODUCTION

Independent Component Analysis (ICA) is usually regarded as a basic tool for blind source signal separation [1] assuming that source signals are mutually independent. ICA realizes source separation by maximizing independence among resultant signals into which the observed signals are to be separated even in case no field information is available.

Although ICA has been frequently explained to have close connection to Principal Component Analysis (PCA) [1, 2, 3], little has been explained about the concrete relation between them. As the basic notion of PCA is the minimum mean-square error, and the least-squares solution of an over-determined set of linear equations is obtained using the pseudo-inverse of the coefficient matrix. Derived here is a relation between the separation matrix in ICA and the pseudo-inverse of the mixing matrix, based on a semi closed-form expression of the separation matrix.

The separation matrix in ICA is obtained by maximizing a measure of independence among separated signals employing one of iterative algorithms, such as relative gradient method, deflation algorithm, FastICA algorithm and so forth. As maximizing mutual independence cannot determine the magnitude balance between source signals and the mixing paths nor identification of individual sources, there remain ambiguities in amplitude and identification among sources. The former inevitably causes the so-called “scaling problem”, while the latter, “permutation problem”. Fortunately, these problems are usually not serious in case of instantaneous mixtures as we will be enough satisfied so far as separation is realized regardless of mutual amplitude and identification or labeling of individual sources.

Independence among separated signals requires uncorrelatedness among them as a necessary condition, thus diagonality is required on the covariance matrix of separated signals. The fact that “we don’t care mutual amplitude among source signals” allows us to neglect mutual amplitude among separated signals. Considering in that way, we can introduce equi-variance requirement on the covariance matrix of the signals to be obtained as estimates for source signals. That means we can forcibly make the covariance matrix of the observed signals be a unit matrix employing an arbitrary scaling matrix.

A cascade processing of

1. sphering the covariance matrix of the observed signals
2. applying matrices representing
   • free axis rotation of the sphered covariance matrix
   • amplitude ambiguity
   • permutation ambiguity

yields a conceptual closed-form expression of the separation matrix in ICA.

MIXING MODELS

We can express an observation model of an instantaneous mixing process as

\[
x(t) = HS(t).
\]

where \(x(t)\) denotes an \(m\) dimensional time-varying vector representing observed signals, \(s(t)\) denotes an \(n \leq m\) dimensional time-varying vector representing source signals, both having the discrete time variable \(t\), and \(H\) is an \(m \times n\) matrix representing a scalar mixture from a set of \(n\) sources to a set of \(m\) sensors without any time delay. Here, \(H\) is assumed to be

\[
s(t) = \begin{bmatrix} s_1(t) \\ s_2(t) \\ \vdots \\ s_n(t) \end{bmatrix},
\]

\[
x(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ \vdots \\ x_m(t) \end{bmatrix},
\]

\[
H = \begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1n} \\ h_{21} & h_{22} & \cdots & h_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ h_{m1} & h_{m2} & \cdots & h_{mn} \end{bmatrix}.
\]
time-invariant with element $h_{ij}$ representing a scalar mixing amplitude from sources $S_j$ to receiving sensor $R_i$ in case of an instantaneous mixture. Each element in both $x(t)$ and $s(t)$ is assumed to be zero-mean without losing generality.

In case of convolutive mixture, the model should be modified as follows:

$$x(t) = h(t) \otimes s(t),$$

where $\otimes$ represents matrix convolution [4], signifying that

$$x_i(t) = \sum_{j=1}^{n} h_{ij}(t) s_j(t),$$

where $h_{ij}(t)$ denotes impulse response of propagation path from source $S_j$ to receiving sensor $R_i$, and * symbolizes convolution. This model allows any types of propagation including reflection, refraction, diffraction, absorption and so forth. Eq.(2) includes Eq.(1) as its special case where each element of $h(t)$ is a single complex value representing delay and decay but not a time function.

**ASSUMPTION ON SOURCE SIGNALS**

In case $H$ or $h(t)$ is known, it is straightforward to obtain the least-squares estimate for $s(t)$. However in case $H$ or $h(t)$ is not known, at least an appropriate restriction should be introduced to obtain a meaningful estimate for $s(t)$. The assumption employed in ICA is the statistical independence among source signals, expressed as

$$\Pr(s_1(t), s_2(t), \cdots, s_n(t)) = \prod_{j=1}^{n} \Pr(s_j(t)).$$

It requires uncorrelatedness among source signals as a necessary condition expressed as diagonality of the covariance matrix as

$$C_s \overset{\text{def}}{=} \mathbb{E}[s(t)s^H(t)]: \text{diagonal},$$

where $H$ denotes an adjoint matrix (vector in this case).

**SOURCE SIGNALS ESTIMATION**

Source signal estimation is formulated as to obtain $\hat{s}(t)$, the estimate for $s(t)$ in Eq.(1) in case of instantaneous mixing, or in Eq.(2) in case of convolutive mixing.

**In case of instantaneous mixture**

We can assume that $\hat{s}(t)$ is expressed by the following form:

$$\hat{s}(t) = \mathbf{W} x(t),$$

where $\mathbf{W}$ is called the “separation matrix”, whose size is $n \times m$. The situation to obtain $\mathbf{W}$ is divided into two cases: one where $H$ is measurable, and the other where it is not measurable.

**I) In case $H$ is measurable**

In case $H$ is measurable,

$$\hat{s}(t) = H^+ x(t)$$

gives the least-squares solution for $s(t)$, where $^+$ signifies the “Moore-Penrose pseudo-inverse” of matrices [5] of the least-squares type, expressed as follows:

$$H^+ \overset{\text{def}}{=} (H^T H)^{-1} H^T$$

So, the separation matrix in this case is given as

$$\mathbf{W}_G = H^+ = (H^T H)^{-1} H^T$$

based on conceptual pseudo-inversion of the mixing process.

Needless to say,

$$H^+ = H^{-1} \quad \text{in case } m = n \text{ and } |H| \neq 0.$$  

**II) In case $H$ is not measurable**

In case $H$ is not measurable, it is impossible to obtain $\mathbf{W}$ from $H$. So, some constraints are required in order to determine $\mathbf{W}$. To estimate $\mathbf{W}$ and $s(t)$ without knowing $H$ is called “Blind Source Separation (BSS)”.

(a) Basic Requirements on $\mathbf{W}$ for BSS

As mentioned above, introduced in ICA for BSS is independence among source signals. Independence among source signals requires uncorrelatedness among them, or diagonality of the covariance matrix of $s(t)$ as a necessary condition. Then,

$$C_s \overset{\text{def}}{=} \mathbb{E}[s(t)s^H(t)]$$

$$= \text{diag}[\sigma_1^2, \sigma_2^2, \cdots, \sigma_n^2] \overset{\text{def}}{=} \Sigma,$$

where $\sigma_j^2$ corresponds to the power of source $S_j$.

Equations (6) and (11) leads

$$C_t = C_w \overset{\text{def}}{=} \mathbb{E}[\mathbf{W} x(t) [\mathbf{W} x(t)]^T]$$

$$= \mathbf{W} [\mathbb{E}[x(t)x(t)^T] \mathbf{W}^T$$

$$= \mathbf{W} C_s \mathbf{W}^T = \Sigma$$

The equation noted above tells that the separation matrix $\mathbf{W}$ is required to be an $n \times m$ matrix which diagonalize the covariance matrix $C_s$ of the $m$-dimensional observation vector $x(t)$.

Although the size of $C_s$ is $m \times m$, the size of the diagonal matrix $\Sigma$ is $n(\leq m) \times n$, as the size of $\mathbf{W}$ is $n \times m$, and only $n$, out of $m$, eigenvalues are supposed to be significantly large and the others are presumed to be small, since the rank of the covariance matrix $C_s$ is thought to be $n$ under an ideal condition. Then, in case the number of sources is known as $n$, diagonalization should be carried out so as to obtain the largest $n$ eigenvalues as the diagonal elements in order to obtain source signals.

So, a “possible” separation matrix $\mathbf{W}$ of size $n \times m$ is required to be a matrix $\mathbf{W}_d$ consisting of $n$ row vectors corresponding to the largest $n$ eigenvalues of the covariance matrix $C_s$ as follows:

$$\mathbf{W}_d = \Phi^e$$

where

$$\Phi^T C_s \Phi = \Sigma$$

in which $\Sigma$ denotes a diagonal matrix having largest $n$ eigenvalues of $C_s$ on the diagonal, and $\Phi$ is an $n \times n$ matrix consisting of the corresponding $n$ eigenvectors of size $m$. Although $\mathbf{W}_d$ fulfills the requirement for diagonalizing the covariance matrix, or producing uncorrelated signals as separated source signals, it does not necessarily yield statistical independence. Thus, $\mathbf{W}_d$ is not the separation matrix yet.

(b) On Mutual Amplitude among $\hat{s}_j(t)$’s

As expressed in Eq.(1), BSS can be regarded as decomposition of $x(t)$ into a product of matrix $H$ and vector $s(t)$, there arises ambiguity of amplitude assignment between $H$ and $s(t)$, because the product $H s(t)$ can be rewritten as

$$H s(t) = H A^{-1} A s(t)$$

where

$$A \overset{\text{def}}{=} \text{diag}[^a_1, ^a_2, \cdots, ^a_n]$$

is an $n \times n$ diagonal “amplitude matrix” having $n$ non-zero values as its diagonal elements and zeros in all other places.
Considering the possible structure of the product $\mathbf{H}\mathbf{s}(t)$ as described above, we can understand that $\mathbf{x}(t)$ in Eq.(1) can be decomposed into any combination of product between a matrix $\mathbf{H}\mathbf{A}^{-1}$ and a vector $\mathbf{a}(t)$ with an arbitrary amplitude matrix $\mathbf{A}$, but not the fixed form of the product $\mathbf{H}\mathbf{s}(t)$. This is called the “Amplitude Ambiguity” or “Scaling Problem” of ICA.

However the Amplitude Ambiguity is not serious in BSS for instantaneous mixture, as the amplitude of each separated signals is thought to be not so important once the waveform of each target source is obtained.

So, it is feasible to estimate a matrix that whiten or sphere $\mathbf{C}$, assuming that actual solution is $\mathbf{a}(t)$ including arbitrary amplitude matrix $\mathbf{A}$ that shares amplitude between $\mathbf{H}\mathbf{A}^{-1}$ and $\mathbf{a}(t)$. Under this model, $\mathbf{C}$, the covariance matrix of source signal vector $\mathbf{s}(t)$, can be assumed to be a unit matrix of size $n$.

$$
\mathbf{C} = \mathbf{E}[\mathbf{s}(t)\mathbf{s}'(t)] = \mathbf{I}_n \tag{17}
$$

(c) Whitening or Sphering

We presume that separation matrix $\mathbf{W}$ should be able to whiten $\mathbf{C}$, or transform $\mathbf{C}$ into a unit matrix as

$$
\mathbf{C} = \mathbf{\Sigma}^{-\frac{1}{2}}\mathbf{\Phi}'\mathbf{C}\mathbf{\Phi}\mathbf{\Sigma}^{-\frac{1}{2}} = \mathbf{I}_n, \tag{18}
$$

where $\mathbf{I}_n$ denotes the unit matrix of size $n$, and

$$
\mathbf{W}_w = \mathbf{\Sigma}^{-\frac{1}{2}}\mathbf{\Phi}' \tag{19}
$$

is thought to express a candidate for the separation matrix $\mathbf{W}$ under condition of uncorrelatedness among signals in $\hat{\mathbf{x}}(t)$.

$\mathbf{W}_w$ is only a possible example of matrices that transform $\mathbf{C}$ into a unit matrix, or make $\hat{s}_j(t)$’s mutually uncorrelated and normalized to have unit variances.

(d) Ambiguities

Multiplying any ortho-normal matrix from the left side does not affect the sphereness of the covariance matrix. So, the separation matrix $\mathbf{W}$ should contain an ortho-normal matrix representing arbitrariness of axis rotation in the $n$-dimensional source space.

Considering the ambiguity in amplitude, the separation matrix $\mathbf{W}$ should contain a diagonal matrix representing arbitrariness of sharing amplitudes between source sides and path sides.

As ICA tries to just divide a set of received signals into source signals assuming independence among sources, it cannot identify individual sources. That means the separation is made without regard to source ID. This requires the separation matrix $\mathbf{W}$ to contain a matrix that has a single one in each row and column, and zeros at all other positions, representing the permutation among sources.

So, the separation matrix by ICA is to be expressed as follows:

$$
\mathbf{W}_{\text{ICA}} = \mathbf{PAR}\mathbf{W}_w = \mathbf{PAR}\mathbf{\Sigma}^{-\frac{1}{2}}\mathbf{\Phi}', \tag{20}
$$

where $\mathbf{R}$, $\mathbf{A}$ and $\mathbf{P}$ are matrices for representing ambiguities in axis rotation, amplitude sharing and labeling source ID’s, respectively. Though $\mathbf{R}$ has no special name other than an “orthonormal matrix for Axis Rotation”, $\mathbf{A}$ is called “Amplitude Matrix” or “Scaling Matrix”, while $\mathbf{P}$ is called “Permutation Matrix”.

Each element in the joint indeterminacy $\mathbf{PAR}$ is thought to be determined as specific one by the measure, such as kurtosis, negentropy or mutual information, employed to express the degree of independency among $\hat{s}_j(t)$’s and the algorithm adopted to maximize the measure together with the initial values for iterative procedures employed.

In case of convolutive mixture

Sound fields are usually produced in environments enclosed by reflective surfaces, or at least environments that contain some items like floors, walls, furniture or other objects with sound reflecting surfaces. In such sound fields, received sounds inevitably consist of reflective waves and diffraactive waves having longer path lengths besides the shortest direct wave. So, sound received by a microphone is actually a sum of sounds including reflected ones that can be expressed as a sum of convolutions of source signals and the impulse responses from sources to the microphone. That leads Eq.(2), or

$$
\mathbf{x}(t) = \mathbf{h}(t) \otimes \mathbf{s}(t), \tag{21}
$$

where $\otimes$ represents matrix convolution [4]. The separation or deconvolution is required to be expressed as

$$
\hat{\mathbf{s}}(t) = \mathbf{w}(t) \circlearrowleft \mathbf{x}(t). \tag{22}
$$

Like the instantaneous cases, situation to obtain $\mathbf{w}(t)$ is divided into two cases: one where $\mathbf{h}(t)$ is measurable, and the other where it is not measurable.

(I) In case $\mathbf{h}(t)$ is measurable

In case $\mathbf{h}(t)$ is measurable, $\mathbf{w}(t)$ is conceptually required to be the convolutive inverse of $\mathbf{h}(t)$.

Taking Fourier transform of Eq. (21), we have

$$
\mathbf{X}(j\omega) = \mathbf{H}(j\omega) \mathbf{S}(j\omega), \tag{23}
$$

where

$$
\mathbf{X}_i(j\omega) = \mathcal{F}\{x_i(t)\} \quad \text{for} \quad i = 1, 2, \ldots, m \tag{24}
$$

$$
\mathbf{S}_j(j\omega) = \mathcal{F}\{s_j(t)\} \quad \text{for} \quad j = 1, 2, \ldots, n \tag{25}
$$

$$
\mathcal{H}_j(j\omega) = \mathcal{F}\{h_j(t)\} \tag{26}
$$

with $\mathcal{F}$ representing Fourier transform. As the least-squares solution for $\mathbf{S}(j\omega)$ is obtained as

$$
\hat{\mathbf{s}}(j\omega) = \mathbf{W}_c(j\omega) \mathbf{X}(j\omega) = \mathbf{H}^+(j\omega) \mathbf{X}(j\omega), \tag{27}
$$

$\mathbf{H}^+(j\omega)$ should be determined so as to satisfy the following relation

$$
\mathbf{H}^+(j\omega) \mathbf{H}(j\omega) = \mathbf{I}_n \tag{28}
$$

As its time-domain expression, we have

$$
\mathbf{h}^{\oplus}(t) \otimes \mathbf{h}(t) = \mathbf{\delta}^{(n)}(t), \tag{29}
$$

where $\mathbf{h}^{\oplus}(t)$, defined as “Generalized Convolutive Inverse of $\mathbf{h}(t)$”, is a matrix having element-wise Fourier inverse transform of $\mathbf{H}^+(j\omega)$.

Element-wise description yields

$$
\sum_{k=1}^{m} \hat{h}_k^{\oplus}(t) * h_k(t) = \{ \begin{array}{c} \delta(t) \\ 0 \end{array} \} \quad \text{for} \quad i = j (\leq n) \quad \text{otherwise} \tag{30}
$$

Employing $\hat{h}_j^{\oplus}(t)$, the least-squares estimate for $s_j(t)$ is obtained as

$$
\hat{s}_j(t) = \sum_{i=1}^{m} \hat{h}_j^{\oplus}(t) * x_i(t), \tag{31}
$$

We have a convolutive matrix expression as

$$
\hat{\mathbf{s}}(t) = \mathbf{h}^{\oplus}(t) \otimes \mathbf{x}(t), \tag{32}
$$
Comparing Eqs.(22) and (32), we have the time-domain least-squares separation matrix as the "generalized convolutive inverse matrix" as follows:

$$w_G(t) = h^\omega(t).$$  (33)

From Eq.(27), we have a frequency-domain expression of the least-squares separation matrix for frequency $\omega$ as

$$W_G(j\omega) = H^+(j\omega).$$  (34)

The equation above can be obtained also by taking element-wise Fourier transform of Eq.(33).

(II) In case $h(t)$ is not measurable

Frequency-domain ICA is most frequently used for blind separation of mixed convolved signals. The frequency-domain expression of receiving sounds from $n$ sources by $m$ microphones is formulated as Eq.(23).

Let’s assume that separation by ICA in the frequency domain based on independence among source signals is expressed as follows using separation matrix $W_{ICA}(j\omega)$

$$\hat{S}(j\omega) = W_{ICA}(j\omega)X(j\omega).$$  (35)

As the separation matrix $W_{ICA}(j\omega)$ is obtained for each frequency bin so as to maximize independence among $\hat{S}(j\omega)$’s of the frequency bin, the basic framework is the same as the case of unknown $H$ in the instantaneous mixture. So, ambiguities in both amplitude and permutation, or order among elements in $\hat{S}(j\omega)$, arise also in this case. Since $\hat{s}(t)$, the estimate for individual source waves, is obtained as element-wise Fourier inverse transform of $\hat{S}(j\omega)$, the ambiguities cause serious problems in this case if the ambiguities are not removed.

This difficulty, however, is not the subject of this paper, so we assume that these ambiguities are formulated by introducing a permutation matrix $P$, an amplitude matrix $A$ and an arbitrary orthonormal matrix $R$ into $W_{ICA}(j\omega)$.

Like the instantaneous case, we have the frequency-domain expression of $W_{ICA}(j\omega)$ in Eq.(35) as

$$W_{ICA}(j\omega) = P(j\omega)A(j\omega)R(j\omega)\Sigma^{-1}(j\omega)\Phi^T(j\omega).$$  (36)

Taking Fourier inverse transform of both sides of the equation above, we have a time-domain expression as follows:

$$w_{ICA}(t) = p(t) \odot a(t) \odot r(t) \odot \sigma^{-1}(t) \odot \Phi^T(t),$$  (37)

where $\sigma(t)$ and $\Phi(t)$ are matrices of size $n \times n$ having element-wise Fourier inverse transforms of $\Sigma^{-1}(j\omega)$ and $\Phi(j\omega)$, respectively, and $p(t), a(t)$ and $r(t)$ are element-wise Fourier inverse transforms of $P(j\omega), A(j\omega)$ and $R(j\omega)$, respectively, while $\odot$ denotes matrix convolution.

RELATION BETWEEN THE SEPARATION MATRIX BY ICA AND THE PSEUDO-INVERSE OF THE MIXING MATRIX

Assuming that matrices for representing appropriate amplitude, permutation and rotation of the orthogonal axes as $A, P$ and $R$, respectively, we can admit that the orthogonal basis in ICA and that in least-squares estimation are common. So, we will calculate the basis for in least-squares estimation to equate it to that in ICA.
(IV) Relation between $W_{ICA}$ and $W_G$ by equalizing $\Phi$

Comparing Eq.(43) and Eq.(7) under Eq.(9), we can presume $\Phi^{-1}_n T$ to be $W$ in Eq.(6). So,

$$W_G = V \Phi^{-1}_n T.$$  \hspace{1cm} \text{(43)}

Substituting $\Phi^{-1}_n T$ of Eq.(43) into Eq.(20), we have

$$W_{ICA} = PAR \Sigma^{-\frac{1}{2}} \Gamma_n V^{-1} W_G$$  \hspace{1cm} \text{(44)}

which gives the relation between $W_{ICA}$, the separation matrix in ICA, and $W_G$, the pseudo-inverse of the mixing matrix, in instantaneous mixture case.

In case of convolutive mixture

Comparing Eq.(27) and Eq.(35) under Eq.(36), the frequency-domain relation between $W_{ICA}(j\omega)$, the separation matrix by ICA, and $W_G(j\omega)$, the matrix that gives the least-squares solution for convolutive case is obtained as

$$W_{ICA}(j\omega) = P(j\omega)A(j\omega)R(j\omega) \Sigma^{-\frac{1}{2}}(j\omega) \Gamma_n(j\omega) V(j\omega)^{-1} W_G(j\omega).$$  \hspace{1cm} \text{(45)}

The time-domain relation between $w_{ICA}(t)$ and $w_G(t)$ is formally obtained by taking the Fourier inverse transform of Eq.(45) introducing inverse Fourier transform of each term as follows:

$$w_{ICA}(t) = p(t) \otimes a(t) \otimes r(t) \otimes \sigma^{-\frac{1}{2}}(t) \otimes \gamma_n(t) \otimes v(t)^{-1} \otimes w_G(t),$$  \hspace{1cm} \text{(46)}

where $w_G(t)$ is identical to $h_\otimes(t)$, the convolutive generalized inverse [4] of $h(t)$, $p(t)$, $a(t)$, $r(t)$, $\sigma(t)$ and $\gamma_n(t)$ are element-wise Fourier inverse transforms of $P(j\omega)$, $A(j\omega)$, $R(j\omega)$, $\Sigma(j\omega)$, $\Gamma_n(j\omega)$ and $V(j\omega)$, respectively.

As $h(t)$ is not measurable in blind separation, we cannot calculate $\gamma_n(t)$, $v(t)^{-1}$ nor $h_\otimes(t)$, so the equation noted above expresses only conceptual relation between $w_{ICA}(t)$ and $w_G(t)$, but not indicating any procedure to obtain $w_{ICA}(t)$ from $w_G(t)$.

CONCLUSIONS

A conceptual expression for the separation matrix in ICA is shown for both instantaneous case and convolutive case. Presented as a by-product is a relation between the separation matrix in ICA for blind separation and the pseudo-inverse of the mixing matrix under condition of transfer function being measurable for both instantaneous mixture and convolutive mixture. Though validity of the results is not strictly verified nor confirmed by any means, the obtained result looks reasonable. Strict mathematical verification or confirmation by simulation is desirable in the future.

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