BIO-NICA: A BIOLOGICALLY INSPIRED SINGLE-LAYER NETWORK FOR NONNEGATIVE INDEPENDENT COMPONENT ANALYSIS

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ABSTRACT
Blind source separation, the problem of separating mixtures of unknown signals into their distinct sources, is an important problem for both biological and engineered signal processing systems. Nonnegative Independent Component Analysis (NICA) is a special case of blind source separation that assumes the mixture is a linear combination of independent, nonnegative sources. In this work, we derive a single-layer neural network implementation of NICA satisfying the following 3 constraints, which are relevant for biological systems and the design of neuromorphic hardware: (i) the network operates in the online setting, (ii) the synaptic learning rules are local, and (iii) the neural outputs are nonnegative.

Index Terms— Blind source separation, nonnegative independent component analysis, neural network, local learning rules

1. INTRODUCTION
Brains are well adapted to perform blind source separation [1, 2, 3, 4], the unsupervised signal processing problem of separating a mixture of unknown signals into their distinct sources. Understanding how brains solve blind source separation is an important problem in neuroscience, and is relevant in the design of neuromorphic hardware [5].

A special case of blind source separation is Nonnegative Independent Component Analysis (NICA), which assumes a generative model in which the mixture of stimuli is a linear combination of independent, nonnegative sources; i.e., \( x = As \), where \( s \) is a nonnegative vector of source intensities, \( A \) is a mixing matrix and \( x \) is the vector of mixed stimuli.

Plumbley [6] showed that when the sources are well-grounded (i.e., they have nonzero probability of taking infinitesimally small values), NICA can be solved in 2 steps (Fig. 1). In the first step, the mixture undergoes noncentered whitening; that is, the mixture is linearly transformed to have identity covariance matrix. The second step rotates the whitened mixture. Their network performs well experimentally and satisfies most of the biological constraints with the exception that the whitening layer can have negative neuronal outputs. However, there are advantages, for both biological and engineered systems, to a network that economizes the number of neurons, which take up valuable resources such as space [13] and energy [14].

In this work, we derive an algorithm named Bio-NICA (Alg. 1) that can be implemented by a single-layer network that satisfies all three biological constraints with the exception that the original sources can be expressed as the optimal solution of a single objective function that combines the two objectives from [12].

2. REVIEW OF THE 2-STEP METHOD
In this section, we review Plumbley’s analysis [6] and the objective functions introduced by Pehlevan et al. [12]. We use following notation. For an integer \( n \geq 1 \), let \( \mathbf{I}_n \) denote the \( n \times n \) identity matrix. Given \( T \) samples \( z_1, \ldots, z_T \) of a time series, we define the sample mean and covariance by

\[
\langle z \rangle := \frac{1}{T} \sum_{t=1}^{T} z_t, \quad C_{zz} := \frac{1}{T} \sum_{t=1}^{T} (z_t - \langle z \rangle)(z_t - \langle z \rangle)^T.
\]
Following Plumbley [6], we assume the following generative model. Let \( s_1, \ldots, s_T \) be \( T \) samples of \( d \)-dimensional source vectors whose components are uncorrelated and, without loss of generality, each have unit sample variance, i.e., \( C_{ss} = I_d \). Let \( k \geq d \) and \( A \) be a full rank \( k \times d \) mixing matrix, and define the \( k \)-dimensional mixture by \( x_t := As_t \).

### 2.1. Plumbley’s NICA method

We start by introducing the mathematics of the two steps: noncentered whitening followed by orthogonal transformation, Fig. 1 [6]. Noncentered whitening is a linear transformation \( h := Fx \) of the mixture, where \( h \in \mathbb{R}^d \) and \( F \) is a \( d \times k \) whitening matrix such that \( h \) has identity covariance matrix, i.e., \( C_{hh} = I_d \). The combined effect of source mixing and prewhitening steps, which is encoded in the matrix-matrix product \( FAs \), is an orthogonal transformation. To see this, use the facts that \( C_{ss} = I_d \), \( h = Fx \), and \( C_{hh} = I_d \) to write

\[
(FA)(FA)^\top = (FA)C_{ss}(FA)^\top = C_{hh} = I_d.
\]

In the second step, one looks for an orthogonal matrix \( R \) such that the transformation \( y := Rh \) is nonnegative. For the solution to be unique up to a permutation, the sources \( s \) must be well grounded, which means they have nonzero probability of taking infinitesimally small values, i.e., \( P(s_i < \delta) > 0 \) for all \( \delta > 0 \). In this case, the vector \( y \) is equal to a permutation of the sources \( s \); see [6] Theorem 1.

### 2.2. Similarity matching objectives

To obtain a 2-layer network that satisfies most of the biological constraints, Pehlevan et al. [12] proposed novel objective functions optimization of which leads to the noncentered whitening and rotation steps. Here we recall these objective functions as they are closely related to the single objective function we introduce. Let us define the \( k \times T \) concatenated data matrix \( X := [x_1, \ldots, x_T] \). In the first step, Pehlevan et al. [12] optimize, with respect to the \( d \times T \) matrix \( H := [h_1, \ldots, h_T] \), the following objective:

\[
\arg \max_{H \in \mathbb{R}^{d \times T}} \text{Tr}(\hat{X}^\top \hat{X}H^\top H) \quad \text{s.t.} \quad \hat{H}^\top \hat{H} \preceq TI_T, \quad (1)
\]

where \( \hat{Z} := [z_1 - \langle z \rangle, \ldots, z_T - \langle z \rangle] \) is the centered matrix, for \( Z \in \{X, H\} \). As shown in [15, 12], objective (1) is optimized when \( H \) is a noncentered whitened transformation of \( X \).

For the second step, Pehlevan et al. [12] introduce the following Nonnegative Similarity Matching (NSM) objective:

\[
\arg \min_{Y \in \mathbb{R}^d_+} \|Y^\top Y - H^\top H\|_{\text{Frob}}^2, \quad (2)
\]

where \( \mathbb{R}^{d \times T}_+ \) denotes the set of \( d \times T \) matrices with nonnegative entries. The objective minimizes the mismatch between similarities of the nonnegative outputs \( Y \) and the noncentered whitened mixtures \( H \) (as measured by inner products). As shown in [12], any orthogonal transformation of \( H \) to the nonnegative orthant, which corresponds to a permutation of the original sources, is a solution of the NSM objective (2).

From objectives (1) and (2), Pehlevan et al. [12] derive a 2-step algorithm for NICA that can be implemented in a 2-layer neural network, consisting of at least \( 2d \) neurons in the whitening layer and \( d \) neurons in the rotation layer, that operates in the online setting, uses local learning rules, and whose rotation layer has nonnegative neuronal outputs.

### 3. A COMBINED NSM OBJECTIVE

To derive a single-layer network for NICA, we propose a novel combined objective function for NICA. The key is to replace the Gram matrix \( H^\top H \) in the NSM objective (2) by terms depending only on \( X \), which will avoid the need for the noncentered whitening step derived from the objective (1).

Consider the eigendecomposition \( C_{zz} = U \Lambda U^\top \), where \( U \) is the \( d \times d \) diagonal matrix of positive eigenvalues and \( U \) is a \( k \times d \) matrix whose column vectors are the corresponding eigenvectors. Then the whitening matrix \( F \) must be of the form \( Q \Lambda^{-1/2} U^\top \), where \( Q \) is any \( d \times d \) orthogonal matrix. Thus, \( F^\top F = U \Lambda^{-1} U^\top \) is the Moore-Penrose inverse.
\( C_x^+ \). Since \( H = FX \), we can replace \( H^TH \) in Eq. \( \ref{eq:4} \) with \( X^TC_x^+X \), which results in the following NSM objective:

\[
\arg\min_{Y \in \mathbb{R}^{d_x \times T}} \|Y^TY - X^TC_x^+X\|^2_{\text{Frob}}.
\]

(3)

4. DERIVATION OF BIO-NICA

To derive our algorithm, we rewrite the minimization problem as a min-max problem which we solve by taking gradient descent-ascent steps that naturally correspond to neural activities and local synaptic updates.

4.1. A min-max formulation

Expanding the square in Eq. \( \ref{eq:3} \), normalizing by \( T^2 \), and dropping terms that do not depend on \( Y \) yields:

\[
\min_{Y \in \mathbb{R}^{d_x \times T}} \frac{1}{T^2} \text{Tr}(-2Y^TYX^TC_x^+X + Y^TYY^TY).
\]

(4)

We introduce auxiliary synaptic weight matrix variables \( W \) and \( M \), which results in the following min-max objective:

\[
\min_{W \in \mathbb{R}^{d \times k}} \min_{M \in \mathbb{S}_{++}^k} \max_{Y \in \mathbb{R}^{d_x \times T}} L(W, M, Y),
\]

(5)

where \( \mathbb{S}_{++}^k \) is the set of \( d \times d \) positive definite matrices and

\[
L(W, M, Y) := \text{Tr}\left( \frac{2}{T} Y^TMY - \frac{4}{T} Y^TWX \right) - \text{Tr}\left( M^2 - 2WC_x^+W^T \right).
\]

The equivalence between the minimization problem \( \ref{eq:3} \) and the min-max problem \( \ref{eq:5} \) can be verified by taking partial derivatives of \( L(W, M, Y) \) with respect to \( W \) (resp. \( M \)) and noting the minimum (resp. maximum) is achieved when \( W = \frac{1}{T} YX^T \) and \( \frac{1}{T} YY^T \) with their respective rank-1 approximations \( y_tX_t^+ \) and \( y_tY_t^+ \). Then, after interchange of the order of minimization with respect to \( Y \) with the optimization with respect to \( W \) and \( M \), we obtain:

\[
\min_{W \in \mathbb{R}^{d \times k}} \max_{M \in \mathbb{S}_{++}^k} \min_{Y \in \mathbb{R}^{d_x \times T}} L(W, M, Y),
\]

(6)

The interchange of the minimization with respect to \( Y \) and maximization with respect to \( M \) is justified by the fact that \( L(W, M, Y) \) satisfies the saddle point property with respect to \( Y \) and \( M \).

4.2. Offline algorithm

We first solve the min-max objective \( \ref{eq:6} \) in the offline setting by minimizing \( L(W, M, Y) \) over \( Y \) and then taking gradient descent-ascent steps in \( W \) and \( M \). The minimization over \( Y \) can be approximated by repeating the following projected gradient descent steps until convergence:

\[
Y \leftarrow [Y + \gamma(WX - MY)]^+,
\]

where \( \gamma > 0 \) is a small step size and \([.]^+\) denotes taking the positive part elementwise. Next, having minimized over \( Y \), we perform a gradient descent-ascent step of the objective function \( L(W, M, Y) \) with respect to \( W \) and \( M \):

\[
W \leftarrow W + 2\eta \left( \frac{1}{T} YX^T - WC_x^+ \right),
\]

(7)

\[
M \leftarrow M + \frac{\eta}{\tau} \left( \frac{1}{T} YY^T - M \right).
\]

(8)

Here \( \tau > 0 \) is the ratio between the learning rates for \( W \) and \( M \), and \( \eta \in (0, \tau) \) is the (possibly time-dependent) learning rate for \( W \). The upper bound \( \eta < \tau \) ensures that \( M \) remains positive definite given a positive definite initialization.

4.3. Online algorithm

To solve the min-max objective \( \ref{eq:6} \) in the online setting, we take stochastic gradient ascent-descent steps. At each time step \( t \), we first minimize over the output \( y_t \) by repeating the following projected gradient descent steps until convergence:

\[
y_t \leftarrow [y_t + \gamma(c_t - My_t)]^+,
\]

(9)

where \( c_t := WX_t \). We then take stochastic gradient descent-ascent steps in \( W \) and \( M \) by replacing the averages \( \frac{1}{T} YX^T \) and \( \frac{1}{T} YY^T \) in Eqs. \( \ref{eq:7} \)–\( \ref{eq:9} \) with their respective rank-1 approximations \( y_tX_t^+ \) and \( y_tY_t^+ \). While we could approximate the matrix \( WC_x^+ \) in Eq. \( \ref{eq:7} \) with \( W(x_t - x_t)(x_t - x_t)^T \), where \( x_t := \sum_{t' = 1}^{t} x_{t'} \), this approximation does not lead to local learning rules. Instead, since \( c_t := WX_t \), we note that

\[
WC_x^+ = \frac{1}{T} \sum_{t' = 1}^{t} (c_t - \langle c \rangle)(x_t - \langle x \rangle)^T,
\]

and replace \( WC_x^+ \) with the rank-1 approximation \( (c_t - \bar{c}_t)(x_t - \bar{x}_t)^T \), where \( \bar{c}_t := \sum_{t' = 1}^{t} c_{t'} \). This yields our online algorithm, which we call Bio-NICA.

Algorithm 1: Bio-NICA

input mixtures \( \{x_1, \ldots, x_T\} \); parameters \( \gamma, \eta, \tau \)
initialize \( W, M, x_0 = 0, \bar{c}_0 = 0 \)
for \( t = 1, 2, \ldots, T \) do
    \( c_t \leftarrow WX_t \)
    repeat
        \( y_t \leftarrow \left[ y_t + \gamma(c_t - My_t) \right]^+ \)
        until convergence
        \( x_t \leftarrow x_{t-1} + \frac{1}{T}(x_t - x_{t-1}) \)
        \( \bar{c}_t \leftarrow \bar{c}_{t-1} + \frac{1}{T}(c_t - \bar{c}_{t-1}) \)
        \( W \leftarrow W + 2\eta( y_t x_t^+ - c_t - \bar{c}_t)(x_t - x_t)^T \)
        \( M \leftarrow M + \frac{\eta}{\tau}( y_t Y_t^+ - M ) \)
    end for

Bio-NICA can be implemented in a single-layer neural network, Fig. \( \ref{fig:nn} \). The network consists of \( k \) input neurons and
At each time step $t$, the $k$-dimensional mixture $x_t$, which is represented in the input neurons, is multiplied by the weight matrix $W$, which is encoded by the feedforward synapses connecting the input neurons to the output neurons. This yields the $d$-dimensional projection $c_t = Wx_t$. This is followed by the fast recurrent neural dynamics in Eq. (9). Here the matrix $M$ is encoded by the lateral synapses connecting the neurons of the output layer. The equilibrium value of the dynamics (9) corresponds to the nonnegative output $y_t$ in Alg. 1. We assume the $k$ input neurons store the $k$-dimensional vectors $x_t, x_t'$, and the $d$ output neurons store the $d$-dimensional vectors $y_t, c_t, c_t'$, so the update for each synapse is local, i.e., it only depends on variables that are represented in the pre- and post-synaptic neurons.

5. NUMERICAL EXPERIMENTS

We evaluated Bio-NICA on synthetic and real datasets. The experimental details and the evaluation code are available at [github.com/flatironinstitute/bio-nica](https://github.com/flatironinstitute/bio-nica).

5.1. Mixture of sparse random uniform sources

We tested Bio-NICA on a synthetic dataset generated by i.i.d. samples, Fig. 1. Following [12], each source sample was set to zero with probability $1/2$ or sampled uniformly from the interval $(0, \sqrt{48/5})$ with probability $1/2$. We used random square mixing matrices with i.i.d. standard normal entries. We compared Bio-NICA to 2 online algorithms designed for NICA: Nonnegative PCA [8] and 2-layer NSM [12]. Nonnegative PCA requires noncentered pre-whitened inputs, which we implemented offline. To quantify the performance of the algorithms, we use the mean-squared error, \( \text{Error}(t) = \frac{1}{td} \sum_{t'=1}^{t} \|s_{t'} - Py_{t'}\|^2 \), where $P$ is the permutation matrix that minimizes the error at the final time point. In Fig. 3, we plot the performance of each of the algorithms on mixtures of 3- and 10-dimensional sources. We find that Bio-NICA is outperformed by the competing algorithms. Bio-NICA performs both the whitening and the rotation steps in a single layer which leads to a trade-off in performance. We view this as consistent with the fact that biological and engineered systems must make trade-offs between performance and resource efficiency.

5.2. Mixture of natural images

We applied Bio-NICA to the problem of recovering images from their mixtures. Three $252 \times 252$ image patches were chosen from a set of images of natural scenes previously used in [16, 8, 10, 12]. Each image is treated as one source, with the pixel intensities (shifted and scaled to be well-grounded and have unit variance) representing the $252^2 = 63,504$ samples. The source vectors were multiplied by a random $6 \times 3$ mixing matrix to generate 6-dimensional mixtures, which were presented to the algorithm 15 times, with randomly permuted order in each presentation. In Fig. 4, we show the sources, mixtures and recovered sources.

![Sources](image1.png) ![Mixtures](image2.png) ![Mixtures](image3.png) ![Recovered Sources](image4.png)

Fig. 4: Recovery of image sources by Bio-NICA.
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