WICA: nonlinear weighted ICA

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Abstract. Independent Component Analysis (ICA) aims to find a coordinate system in which the components of the data are independent. In this paper we construct a new nonlinear ICA model, called WICA, which obtains better and more stable results than other algorithms. A crucial tool is given by a new efficient method of verifying nonlinear dependence with the use of computation of correlation coefficients for normally weighted data. Our code for WICA is available on Github.

1 Introduction

Linear Independent Components Analysis (ICA) is an important data analysis technique, which aims to identify a linear function such that the components of the dataset obtained after the transformation are independent. Commonly, the independence is approximated using some measure of nongaussianity, e.g. kurtosis (Hyvärinen 1999; Bell & Sejnowski 1995), skewness (Spurek et al. 2017). Clearly, the obvious limitation of ICA is the restriction to linear transformations, as the real world data usually contains complex, nonlinear dependencies, see for instance (Larson 1998; Ziehe et al. 2000). Designing an efficient and easily implementable nonlinear analogue of ICA is a much more complex problem than its linear counterpart. A fundamental problem is that the solution of nonlinear ICA is in principle non-identifiable, as without any constraints on the space of the mixing functions, there exists an infinite number of valid solutions (Hyvärinen & Pajunen 1999). However, the key challenge in developing nonlinear variant of ICA lies in devising an efficient measure of independence.

One of the most common nonlinear method is MISEP (Almeida 2003) which, similar to the popular INFOMAX algorithm (Bell & Sejnowski 1995), uses the mutual information criterion. In consequence, the procedure involves the calculation of the Jacobian of the modeled nonlinear transformation, which often causes a computational overhead when both the input and output dimensions are large. Another approach is applied in NICE (Dinh et al. 2014). Authors propose a fully invertible neural network architecture where the Jacobian is trivially obtained. The independent components are then estimated using the maximum likelihood criterion. The drawback of both MISEP and NICE is that they require choosing the prior distribution family of the unknown independent components. An alternative approach is given by ANICA (Adversarial Non-linear ICA) (Brakel & Bengio 2017), where the independence measure is directly learned from the data. However, the key challenge in developing a nonlinear variant of ICA lies in devising an efficient measure of independence. ANICA comes at the cost of added instability, which was also noted by the authors.

In this paper we present a competitive approach to nonlinear independent components analysis – WICA (nonlinear weighted ICA). Crucial role in our approach is played by the conclusion from (Bedychaj et al. 2019), which proves that to verify nonlinear independence it is sufficient to check the linear independence of the normally weighted dataset, see Fig. Based on this result we introduce weighted independence index (wii) which is based on computing weighted covariance and can be applied to the verification of the nonlinear independence, see Section Consequently, the con-
structured WICA algorithm is based on simple operations on matrices, and therefore is ideal for GPU calculation and parallel processing. We construct it by incorporating the introduced cost function in a commonly used in ICA problems auto-encoder framework (Brakel & Bengio 2017), where the role of the decoder is to limit the unmixing function so that the learned by the encoder independent components contain the information needed to reconstruct the inputs, see Section 3.

We verified our algorithm in the case of a source signal separation problem. We present the results of WICA for nonlinear mixes of images and for the decomposition of electroencephalogram signals. It occurs that WICA outperforms other methods of nonlinear ICA, both with respect to unmixing quality and the stability of the results, see Fig 1.

To fairly evaluate various nonlinear ICA methods in the case of higher dimensional datasets, we introduce a new index called OTS based on Spearman’s rank correlation coefficient. In the definition of OTS, similarly to clustering accuracy (ACC) (Hassibi 2003), we use optimal transport to obtain the minimal mismatch cost. This approach has its merit here, since the correspondence between the input coordinates and the reconstructed components in a higher dimensional space is nontrivial.

Another important ingredient of the paper is the introduction of a new, fully invertible nonlinear mixing function. In the case of linear ICA there exists many experiments settings that can be used in order to evaluate and compare different methods. Such standards are unfortunately not present in the case of nonlinear ICA. Therefore it is not clear what kind of nonlinear mixing should be used in the benchmark experiments. In most cases the authors usually use mixing functions, which correspond with the models architecture (Almeida 2003, Brakel & Bengio 2017). In the paper we propose a new nonlinear mixing function based on the flow models (Dinh et al. 2014, Kingma & Dhariwal 2018), which can be used for verification of nonlinear methods.

2 Weighted independence index

Let us consider a random vector $X$ in $\mathbb{R}^d$ with density $f$. Then $X$ has independent components iff $f$ factors as

$$f(x_1, \ldots, x_d) = f_1(x_1) \cdot \ldots \cdot f_d(x_d),$$

for some densities $f_i$, where $i \in \{1, 2, \ldots, d\}$. This functions are called marginal densities of $f$. A related, but much weaker notion, is the linear independence. We say that $X$ has uncorrelated (linearly independent) components, if the covariance of $X$ is diagonal. Contrary to the independence, correlation (linear independence) has fast and easy to compute estimators. Clearly independence implies linear independence, but the opposite is not valid, see Fig. 2.

Let us mention that there exist other measures which verify the independence. One of the most well-known measures of independence of random vectors is the distance correlation (dCor) (Székely et al. 2007), which is applied in (Matteson & Tsay 2017) to solve the linear ICA problem. Unfortunately, to verify the independence of components of the samples, dCor needs $2^d N^4$ comparisons, where $d$ is the dimension of the sample and $N$ is the sample size. Moreover, even a simplified version of dCor which checks only pairwise independence has high complexity and does not obtain very good results (which can be seen in experiments from Section 3). This motivates the research into fast, stable and efficient measures of independence, which are adapted to GPU processing.

In this section we fill this gap and introduce a method of verifying independence which is based on the covariance of the weighted data. The covariance scales well with respect to the sample size and data dimension, therefore the proposed covariance-based index inherits similar properties.

To proceed further, let us introduce weighted random vectors.

**Definition 2.1.** Let $w : \mathbb{R}^d \rightarrow \mathbb{R}_+$ be a bounded weighting function. By $X_w$ we denote a weighted random vector with a density

$$f_w(x) = \frac{w(x) f(x)}{\int w(z) f(z) dz}.$$

**Observation 2.1.** Let $X$ be a random vector which has independent components, and let $w$ be an arbitrary weighting function. Then $X_w$ has independent components as well.

One of the main results of (Bedychaj et al. 2019) is that the strong version of the inverse of the above theorem holds. Given $m \in \mathbb{R}^d$, we consider the weighting of $X$ by the standard normal gaussian with center at $m (N(m, I))$:

$$X_{[m]} = X_{N(m, I)}.$$

We quote the following result which follows directly from the proof of Theorem 2 from (Bedychaj et al. 2019):

**Theorem 2.1.** Let $X$ be a random vector, let $p \in \mathbb{R}^d$ and $r > 0$ be arbitrary.

If $X_{[q]}$ has linearly independent components for every $q \in B(p, r)$, where $B(p, r)$ is a ball with center in $p$ and radius $r$, then $X$ has independent components.

Given sample $X = (x_i) \subset \mathbb{R}^d$, vector $p \in \mathbb{R}^d$, and weights $w_i = N(p, I)(x_i)$, we define the weighted sample as:

$$X_{[p]} = (x_i, w_i).$$

Then the mean and covariance for the weighted sample $X_{[p]} = (x_i, w_i)$ is given by:

$$\text{mean}_W = \frac{1}{\sum_i w_i} \sum_i w_i x_i$$

and

$$\text{cov}_W = \frac{1}{\sum_i w_i} \sum_i w_i (x_i - \text{mean}_W)(x_i - \text{mean}_W)^T.$$

This is just the normalization of $w(x) f(x)$.
The informal conclusion from the above theorem can be stated as follows: if \( \text{cov} X[p] \) is approximately diagonal for a sufficiently large set of \( p \), then the sample \( X \) was generated from a distribution with independent components.

Let us now define an index which will measure the distance from being independent. We define the weighted independence index - \( \text{wii}(X,p) \) - as

\[
\text{wii}(X,p) = \frac{2}{d(d-1)} \sum_{i<j} c_{ij},
\]

where \( d \) is the dimension of \( X \) and

\[ c_{ij} = \frac{2z_{ij}^2}{z_{ii}^2 + z_{jj}^2}, \]

for \( Z = [z_{ij}] = \text{cov} X[p] \).

**Observation 2.2.** Let us first observe that \( c_{ij} \) is a close measure to the correlation \( \rho_{ij} \), namely:

\[ c_{ij} \leq \rho_{ij}^2, \]

where the equality holds iff the \( i \)-th and \( j \)-th components in \( X[p] \) have equal standard deviations.

**Proof.** Obviously

\[ \rho_{ij}^2 = \frac{z_{ij}^2}{z_{ii} \cdot z_{jj}}, \]

Since \( ab \leq \frac{1}{4}(a^2 + b^2) \) (where the equality holds iff \( a = b \)), we obtain the assertion of the observation. \( \square \)

Consequently, \( \text{wii}(X,p) = 1 \) iff all components of \( X[p] \) are linearly dependent and have equal standard deviations. Thus, the minimization of \( \text{wii} \) simultaneously aims at maximizing the independence and increasing the difference between the standard deviations.

We extend the index for a sequence of points \( \{p_1, \ldots, p_n\} \) , as the mean of the indexes for each \( p_i \):

\[ \text{wii}(X; \{p_1, \ldots, p_n\}) = \frac{1}{n} \sum_{i=1}^{n} \text{wii}(X, p_i). \]

### 3 Description of the WICA algorithm

To implement the weighted independence index in practice, we need to find the optimal choice of weighting centers \( (p_i) \). First, we assume that the dataset in question is normalized componentwise (in particular, variance of each coordinate is one). We argue that the right choice of \( (p_i) \) should satisfy the following two conditions:

- selected weights do not concentrate on a small percentage of the data.
- for different centers selected from the dataset, weights diversify the data points.

At first glance, it would seem that the natural choice for points \( (p_i) \) is to sample them from the standard normal distribution. However, the conducted by us preliminary experiments (see Fig. [3]) demonstrate that sampling from \( N(0, 1/d) \) would be a better choice.

![Figure 3.](image)

In the experiment, we sampled twenty points from \( N(0, 1) \) (x-axis). Then, we calculate weights of the points respectively to \( N(0, 1) \) and \( N(0, 1/d) \). We present values of those weights (sorted decreasingly) in the case when the center is chosen according to \( N(0, 1) \) vs. \( N(0, 1/d) \). One can see that weights derived from \( N(0, 1/d) \) actually balance more data points, in contrary to \( N(0, 1) \) which focus on smaller amount of data.

**Theoretical analysis.** Let us now discuss the theoretical foundations behind the results from Fig [3]. Consider the case when the data come from the standard normal distribution. For given weights \( w \) and density \( f \) we define measure \( P(w, f) \) as:

\[
P(w, f) = \frac{\int w(x)f(x)dx}{\int w^2(x)f(x)dx}.
\]

Observe that if \( w \) is constant on a subset \( U \) of some space \( S \) (for which functions \( w \) and \( f \) are well-defined) and zero otherwise, then the above reduces to \( \mu(U) \), where \( \mu \) is counting measure. Intuitively, \( P(w, f) \) returns percentage of the population which has nontrivial weights.

Let us consider the case when \( \mu \) is given by the standard normal density

\[ u(x) = N(p, 1)(x) \]

and our dataset is normalized as stated above. Then, directly from [1], one obtains:

\[
P(w, f) = \frac{\int N(p, 1)(x)N(0, 1)(x)dx}{\int N(p, 1)^2(x)N(0, 1)(x)dx}.
\]

Applying the formula for the product of two normal densities:

\[
N(m_1, \Sigma_1)(x) \cdot N(m_2, \Sigma_2)(x) = c_e N(m_e, \Sigma_e)(x),
\]

where

\[
c_e = N(m_1 - m_2, \Sigma_1 + \Sigma_2)(0),
\]

\[
\Sigma_e = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1},
\]

and

\[
m_e = \Sigma_e^{-1}m_1 + \Sigma_2^{-1}m_2,
\]

we get:

\[
\int N(p, 1)(x)N(0, 1)(x)dx = N(p, 2\mu)(0),
\]

for the numerator, and

\[
\int N(p, 1)^2(x)N(0, 1)(x)dx = N(0, 2\mu)(0)N(p, 2\mu)(0).
\]

for the denominator. The equation for the denominator follows from the simple fact that:

\[
N(p, 1)^2(x) = N(0, 2\mu)(0) \cdot N(p, 2\mu)(0).
\]
Summarizing, we obtain that
\[ P(N(p, I), N(0, I)) = \frac{N(p, 2I)^2(0)}{N(0, 2I)(0)N(p, \frac{1}{2}I)(0)} = \left(\frac{1}{2}\right)^D/2 \exp(-\frac{1}{2}\|p\|^2). \] (2)

Normalizing (2) by its maximum obtained at 0, we get
\[ \exp(-\frac{1}{2}\|p\|^2). \]

Clearly if \( p \) would be chosen from the standard normal distribution, the value of \( \|p\|^2 \) for large dimensions equals approximately \( d \), and consequently the weights for the randomly chosen points will become concentrated at single point (see Fig 3). To obtain the quotient approximately constant, we should choose \( p \) so that its norm is approximately one. Hence, it leads to the choice of \( p \) from the distribution \( N(0, \frac{1}{d}I) \).

One can observe, that if \( X \sim N(0, I) \), then we can sample from \( N(0, I/d) \) by taking the mean of \( d \) randomly chosen vectors from \( X \). This leads to the following definition:

**Definition 3.1.** For the dataset \( X \subset \mathbb{R}^d \), we define
\[ \text{wii}(X) = \mathbb{E}\{\text{wii}(Y,p) : p \text{ a mean of random } d \text{ elements of } Y\}, \]
where \( Y \) is a componentwise normalization of \( X \) and \( \mathbb{E} \) stands for expected value.

Let us summarize why centering the weights at the mean of \( d \) elements from the dataset has good properties:
- if the data is restricted to some subspace \( S \) of the space, then mean also belongs to \( S \);
- if the data comes from normal distribution \( N(m, \Sigma) \), then mean of \( d \) elements comes from \( N(m, \Sigma/d) \);
- if the data has heavy tails (i.e. comes from Cauchy distribution), then the distribution of mean for \( d \) elements set can be close to the original dataset mean.

The realisation of this idea in practice is provided by our algorithm – WICA – a nonlinear ICA model based on the wii index. Following the ANICA (Brakel & Bengio 2017), we used an Auto-Encoder (AE) architecture.

**Auto-Encoder model.** Let \( X \subset \mathbb{R}^d \) denote the input data. An Auto-Encoder is a model consisting of an encoder function \( \mathcal{E} : \mathbb{R}^d \to \mathcal{Z} \) and a complementary decoder function \( \mathcal{D} : \mathcal{Z} \to \mathbb{R}^d \), aiming to enforce coding of the input variables that minimizes the reconstruction error:
\[ \text{rec}_\text{error}(X; \mathcal{E}, \mathcal{D}) = \sum_{i=1}^d \|x_i - \mathcal{D}(\mathcal{E}x_i)\|^2. \]

**WICA cost function.** In this paragraph we describe the actual cost function used in the WICA model.

To obtain independence in the latent space, we add to the standard Auto-Encoder cost function the weighted independence index wii computed in the latent. Thus our final cost function is given by
\[ \text{cost}(X; \mathcal{E}, \mathcal{D}) = \text{rec}_\text{error}(X; \mathcal{E}, \mathcal{D}) + \beta \text{wii}(\mathcal{E}X). \] (3)

where \( \beta \) is a hyperparameter which aims to weight the role of reconstruction with that of independence (analogous to \( \beta\)-VAE (Higgins et al. 2017)). The training procedure follows the steps:

**Algorithm 1 WICA**
1. Take mini-batch \( X' \) from the dataset \( X \).
2. Normalize componentwise \( \mathcal{E}X' \), to obtain \( Y \).
3. Compute \( p_1, \ldots, p_d \), where \( p_i \) is the mean of randomly chosen \( d \) elements from \( Y \).
4. Minimize:
\[ \text{rec}_\text{error}(X', \mathcal{E}, \mathcal{D}) + \beta \text{wii}(Y, p_1, \ldots, p_d). \]

![Figure 4. Results of the proposed mixing over synthetic lattice data. One may observe that after multiple iterations of the proposed mixing, results become highly nonlinear.](image)

4 Setting up the experiments

**Nonlinear mixing.** We start this section with a discussion of possible definitions of the nonlinear mixing function used for benchmarking the ICA methods. In the beginning we shortly explain some approaches used in the linear ICA, and then move forward to propose a mixing which benefits from properties desired in the comparison of the results obtained by nonlinear ICA algorithms.

In the case of linear ICA the experiments are usually conveyed on an artificial dataset, which is obtained by mixing two or more of independent source signals. This allows for the comparison of the results returned by the analyzed methods with the original independent components. In real-world applications such a procedure is of course infeasible, but in experimental setting it provides a good basis for benchmarking different models. In classical ICA setup, creating an artificial mixing function is equivalent to selecting a random invertible matrix \( A \), such that \( X = A \cdot S \), where \( S \) are the true sources and \( X \) are the observations, which are then passed to the evaluated
methods. Such mixing is used by [Bedychaj et al. 2019][Hyvärinen 1999][Spurek et al. 2017]. Unfortunately, there do not exist any mixing standards for the nonlinear ICA problem. A common setup of the comparable environments needed to test the nonlinear models of ICA is to interface linear mixes of signals with nonlinear functions [Almeida 2003][Brakel & Bengio 2017]. During our experiments we found that the proposed methods of nonlinear mixes are ineffective in large dimensions. The aforementioned approaches usually apply only a shallow stack of linear projections followed by a non-linearity. In consequence, the obtained observations are either close to the linear mixing (and therefore not hard enough to be properly challenging for the linear models) or become degenerate (i.e. all points cluster towards zero). Because of these disadvantages we propose our own mixing, inspired by [Kingma & Dhariwal 2018][Dinh et al. 2014] network architecture.

Let S be a sample of vectors with independent components. We apply a random isometry on S, by taking $X = (UV^T)S$, where $UV^T$ comes from the Singular Value Decomposition on a random matrix $A_{ij} \sim N(0, 1)$. Next we split $X \in \mathbb{R}^d$ into half $(x_i, x_j) \rightarrow (x_i, x_j + \phi(x_i))$, similarly as it was done in [Kingma & Dhariwal 2018]. Function $\phi$ is a randomly initialized neural network with two hidden layers and tanh activations after each of them. This approach can be iterated over multiple times to achieve the desired level of nonlinear mixing.

The proposed mixing procedure scales well in higher dimensions by iterating over the splits in $\mathbb{R}^d$. Additionally, it is also easily invertible, therefore there is a guarantee that the source components may be retrieved. The effects of applying the proposed mixing to two-dimensional data are presented in Fig. 4.

| Measure | Dim | Mixes | WICA | FastICA | ANICA | dCor | PNLMISEP |
|---------|-----|-------|------|---------|-------|------|---------|
| I(\cdot) | 2   | 50    | 0.828 ± 0.105 | 0.672 ± 0.001 | 0.842 ± 0.136 | 0.794 ± 0.071 | 0.824 ± 0.115 |
|         | 4   | 50    | 0.735 ± 0.053 | 0.468 ± 0.001 | 0.676 ± 0.003 | 0.736 ± 0.076 | 0.799 ± 0.123 |
|         | 6   | 50    | 0.735 ± 0.031 | 0.425 ± 0.001 | 0.503 ± 0.052 | 0.661 ± 0.065 | 0.697 ± 0.103 |
|         | 8   | 50    | 0.766 ± 0.028 | 0.453 ± 0.018 | 0.427 ± 0.048 | 0.595 ± 0.052 | 0.627 ± 0.022 |
|         | 10  | 50    | 0.766 ± 0.025 | 0.341 ± 0.036 | 0.405 ± 0.032 | 0.563 ± 0.040 | 0.667 ± 0.084 |
|         | 2   | 10    | 0.798 ± 0.048 | 0.652 ± 0.001 | 0.938 ± 0.088 | 0.899 ± 0.076 | 0.948 ± 0.041 |
|         | 4   | 10    | 0.890 ± 0.065 | 0.582 ± 0.001 | 0.784 ± 0.062 | 0.554 ± 0.264 | 0.652 ± 0.360 |
|         | 6   | 10    | 0.807 ± 0.043 | 0.419 ± 0.001 | 0.571 ± 0.056 | 0.666 ± 0.064 | 0.779 ± 0.046 |
|         | 8   | 10    | 0.784 ± 0.025 | 0.457 ± 0.058 | 0.431 ± 0.054 | 0.594 ± 0.051 | 0.769 ± 0.097 |
|         | 10  | 10    | 0.742 ± 0.030 | 0.405 ± 0.077 | 0.405 ± 0.032 | 0.536 ± 0.041 | 0.758 ± 0.103 |

Table 1. Comparison between nonlinear ICA methods (PNLMISEP, dCor, ANICA, WICA) and the classical linear ICA approach (FastICA) on images separation problem (with different dimensions) by using max correlation and OTS measures. In the experiment we tuned and trained four models (excluding FastICA, which is a linear model) and present mean and standard deviation in the tabular form.

5 Experiments

Image separation One of the most figurative application of ICA is the separation of images. The experiment environment in such a

we introduce a new measure based on the nonlinear Spearman’s rank correlation coefficient and optimal transport.

Let Z denote the signal retrieved by an ICA algorithm and let $r_{ij}(z^j, s^k)$ be the Spearman’s rank correlation coefficient between the $j$-th component of Z and $k$-th component of S. We define the Spearman’s distance matrix $M(Z, S)$ as

$$M(Z, S) = \{1 - |r_{ij}(z^j, s^k)|\}_{j,k=1...d},$$

where the zero entries indicate a monotonic relationship between the corresponding features.

This matrix is then used as the transportation cost of the components. Formally, we compute the value of the optimal transport problem formulated in terms of integer linear programming:

$$OTS = 1 - I_s(Z, S),$$

$$I_s(Z, S) = \min \frac{1}{d} \sum_{j,k} \gamma_{j,k} M(Z, S)_{j,k}$$

subject to:

$$\sum_{k} \gamma_{j,k} = A_j \text{ for all } j \in \{1, \ldots, d\},$$

$$\sum_{j} \gamma_{j,k} = A_k \text{ for all } k \in \{1, \ldots, d\},$$

$$\gamma_{j,k} \in \{0, 1\} \text{ for all } j, k \in \{1, \ldots, d\}$$

where $A_j = A_k = 1$.

In consequence of the last constraint, the obtained transport plan $\gamma$ defines a one-to-one map from the retrieved signals to the original sources. In addition, the proposed Spearman-based measure (OTS) is sensitive to monotonic nonlinear dependencies and also relatively easy to compute with the use of existing tools for integer programming.
Figure 5. Two dimensional example of unmixing natural images. One can easily spot that WICA has the smallest amount of artifacts persisted after the process of retrieving the signals. All of the scatter plots were normalized and are presented in the same scale. It is valuable to look also on connected marginal histograms, where some of the similarities between original signal and its retrieved counterpart also resembles.

An original EEG mixture taken for this experiment, consisted of 40 scalp electrode signals. Experiment showed that WICA is able to handle multidimensional data highly above tested on other nonlinear models. Moreover, WICA results for this task works well enough to be used as a preliminary step of cleaning the data. Results of WICA decomposition are presented on Fig 6.

6 Conclusion

In this paper we presented a new approach to the nonlinear ICA task. In addition to the investigation of WICA method, which proves to be...
Figure 6. Results of analysis done on EEG signals. After deletion of suspicious signals selected by an expert from decomposition, one can easily spot that the reconstructed signal is more homogeneous, and does not have as much artifacts as the original EEG data. In both methods the same amount of signals was cleared. The results of both methods are satisfying, although it seems that WICA persist scale of the retrieved signals.

7 Acknowledgements

The work of P. Spurek was supported by the National Centre of Science (Poland) Grant No. 2019/33/B/ST6/00894. The work of J. Tabor was supported by the National Centre of Science (Poland) Grant No. 2017/25/B/ST6/01271. A. Nowak carried out this work within the research project “Bio-inspired artificial neural networks” (grant no. POIR.04.04.00-00-14DE/18-00) within the Team-Net program of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund.

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