Independent Component Analysis via Energy-based and Kernel-based Mutual Dependence Measures

Ze Jin
Department of Statistical Science
Cornell University
Ithaca, NY 14850

David S. Matteson†
Department of Statistical Science
Cornell University
Ithaca, NY 14850

Abstract

We apply both distance-based (Jin and Matteson, 2017) and kernel-based (Pfister et al., 2016) mutual dependence measures to independent component analysis (ICA), and generalize dCovICA (Matteson and Tsay, 2017) to MDMICA, minimizing empirical dependence measures as an objective function in both deflation and parallel manners. Solving this minimization problem, we introduce Latin hypercube sampling (LHS) (McKay et al., 2000), and a global optimization method, Bayesian optimization (BO) (Mockus, 1994) to improve the initialization of the Newton-type local optimization method. The performance of MDMICA is evaluated in various simulation studies and an image data example. When the ICA model is correct, MDMICA achieves competitive results compared to existing approaches. When the ICA model is misspecified, the estimated independent components are less mutually dependent than the observed components using MDMICA, while they are prone to be even more mutually dependent than the observed components using other approaches.

1 INTRODUCTION

Since most natural processes have multiple components, multivariate analysis is more compelling than univariate analysis. Nevertheless, multivariate analysis is considerably more complicated than univariate analysis, because it accounts for the mutual dependence between all variables. Due to the curse of dimensionality, it becomes essential to interpret multivariate data through a simplified representation via dimension reduction.

Independent component analysis (ICA) represents multivariate data by mutually independent components (ICs). Thus, linear combinations of ICs capture the structure of multivariate data even when other linear projection methods, such as principal component analysis (PCA), are not sufficient. As a classical unsupervised learning method, ICA has been developed for applications including blind source separation, feature extraction, brain imaging, etc. Hyvärinen et al. (2004) provide a comprehensive overview of ICA approaches to estimate ICs.

Let $Y = (Y_1, \ldots, Y_d) \in \mathbb{R}^d$ be a random vector as observations. Assume that $Y$ has a nonsingular, continuous distribution $F_Y$, with $E(Y_j) = 0$ and $\text{Var}(Y_j) < \infty$, $j = 1, \ldots, d$. Let $X = (X_1, \ldots, X_d) \in \mathbb{R}^d$ be a random vector as ICs. In particular, the univariate components $X_1, \ldots, X_d$ are mutually independent, and at most one component $X_j$ is Gaussian. Without loss of generality, $X$ is assumed to be standardized such that $E(X_j) = 0$ and $\text{Var}(X_j) = 1$, $j = 1, \ldots, d$. A linear latent factor model to estimate $X$ from $Y$ is given by

$Y = MX,$

where $M \in \mathbb{R}^{d \times d}$ is a nonsingular mixing matrix.

Prewhitened random variables are uncorrelated and thus more convenient to work with from both practical and theoretical perspectives. Let $\Sigma_Y = \text{Cov}(Y)$ be the covariance matrix of $Y$, and $H = \Sigma_Y^{-1/2}$ be an uncorrelating matrix. Let $Z = HY = (Z_1, \ldots, Z_d) \in \mathbb{R}^d$ be a random vector as uncorrelated observations, such that $\Sigma_Z = \text{Cov}(Z) = I_d$, the $d \times d$ identity matrix. Then the relation between $Z$ and $X$ is

$X = M^{-1}Y = M^{-1}H^{-1}Z \triangleq WZ,$  \hspace{1cm} (1)

where $W = M^{-1}H^{-1} \in \mathbb{R}^{d \times d}$ is a nonsingular unmixing matrix. Given that $Z$ are uncorrelated, $W$ is an
orthogonal matrix, with \(d(d - 1)/2\) free elements rather than \(d^2\). We aim to simultaneously estimate \(W\) and \(X\), such that the components of \(X\) satisfy the assumption of mutual independence.

Many popular ICA approaches minimize the mutual information or maximize the non-Gaussianity of the estimated components under the constraint that they are uncorrelated. Examples include the fourth-moment matrix diagonalization of FOBI (Cardoso [1989] and JADE (Cardoso and Souloumiac [1993]), the information criterion of Infomax (Bell and Sejnowski [1995]), the maximum negentropy of FastICA (Hyvärinen and Oja [1997]), and the maximum likelihood principle of ProDenICA (Hastie and Tibshirani [2003]) and Spline-LCA (Risk et al. [2017]; Jin et al., 2017).

Some other ICA approaches minimize the mutual dependence between the estimated components using a specific dependence measure. While dependence measures have been extensively studied, two classes have attracted a great deal of attention. One is the distance-based energy statistics (Székely and Rizzo [2013]), Székely et al. [2007] proposed distance covariance (dCov) to measure pairwise dependence, and Jin and Matteson [2017] extended it to mutual dependence measures (MDMs). Another is the kernel-based maximum mean discrepancies (MMDs) (Gretton et al., 2007), Gretton et al. [2005] proposed Hilbert–Schmidt independence criterion (HSIC) to measure pairwise dependence, and Pfister et al. [2016] generalized it to \(d\)-variable Hilbert–Schmidt independence criterion (dHSIC) measuring mutual dependence. Sejdinovic et al. [2013] showed that these two classes of measures are equivalent in the sense that MMDs can be interpreted as energy statistics with a distance kernel, and energy statistics can be interpreted as MMDs with a negative-type semimetric.

Meanwhile, Chen and Bickel [2005] and Eriksson and Koivunen [2003] applied a characteristic function-based dependence measure to ICA, for which Jin and Matteson [2017] provided a closed-form expression as an MDM and studied its asymptotic properties. Bach and Jordan [2002] applied a kernel-based dependence measure to ICA, which was formulated as an HSIC in Gretton et al. [2005]. Motivated by the properties of HSIC, Shen et al. [2007] proposed FastKICA based on a mutual dependence measure extension, which is the sum of all pairwise HSIC while its 0 value does not imply mutual independence. Inspired by the properties of dCov, Matteson and Tsay [2017] proposed dCovICA based on another mutual dependence measure extension, which is a sum of squared dCov and equals 0 if and only if mutual independence holds.

However, Matteson and Tsay [2017] only demonstrated the results of a single measure from the class of energy-statistics, using multiple values to initialize the local optimization without any comparison. Thus, in this paper, we generalize dCovICA to a new approach, MD-MICA, by applying the mutual dependence measures proposed in Jin and Matteson [2017] and Pfister et al. [2016], and make two contributions as follows. First, we extend its ICA framework to accommodate mutual dependence measures from both classes of energy statistics and MMDs, and compare the performance of these measures in numerical studies. Second, we study the non-convex optimization problem when estimating ICs under this ICA framework, and investigate the improvement of using multiple values over a single value for initialization through Latin hypercube sampling, a random sampling method. In addition, we introduce a global optimization method, Bayesian optimization, to further improve the initialization of local optimization.

The rest of this paper is organized as follows. We generalize the ICA framework of dCovICA in Section 2. In Section 3 we give a brief overview of dCov and MDMs, propose the new ICA approach, MD-MICA, based on MDMs, and derive its asymptotic properties. In Section 4 we introduce Latin hypercube sampling and Bayesian optimization to aid the initialization of subsequent local optimization method when estimating ICs. We present the simulation results in Section 5 and a real data example in Section 6. Finally, Section 7 summarizes our work.

## 2 ICA FRAMEWORK

For \(d \geq 2\), the group of \(d \times d\) orthogonal matrices is denoted by \(O(d)\), and its subgroup with determinant 1 is denoted by \(SO(d)\). For \(i \neq j\), we start with the identity matrix \(I_d\), and substitute \(\cos(\psi)\) for the \((i, i)\) and \((j, j)\) elements, \(-\sin(\psi)\) for the \((i, j)\) element, and \(\sin(\psi)\) for the \((j, i)\) element, then we obtain a Givens rotation matrix denoted by \(G_{i,j}(\psi)\).

Let \(\theta = \{\theta_{i,j} : 1 \leq i < j \leq d\}\) denote a vector of rotation angles with length \(p = d(d - 1)/2\), and let \(\theta_1 = \{\theta_{i,j} : i + 1 \leq j \leq d\}\) such that \(\theta = \{\theta_1 : 1 \leq i \leq d - 1\}\). Then any rotation matrix \(W \in SO(d)\) can be parameterized via \(\theta\) as \(W(\theta)\), or equivalently a product of \(p\) Givens rotation matrices determined by \(\theta\) as

\[
W(\theta) = G(\theta_1)(\theta_{d-1}) \ldots G(1)(\theta_1),
\]

where \(G^{(k)}(\theta_k) = G_{k,d}(\theta_{k,d}) \ldots G_{k,k+1}(\theta_{k,k+1})\) represents the rotations of the \(k\)th row with respect to all the \(\ell\)th rows, \(\ell > k\).

See CRAN for an accompanying R package **EDMeasure**.
Although this decomposition is not unique, the $k$th row of $W(\theta)$ is the same as the $k$th row of the partial product $G^{(k)}(\theta_k) \ldots G^{(1)}(\theta_1)$. As a result, let $X(\theta) = W(\theta)Z$, we observe that the subset of angles in $\{\theta_{i,j} : 1 \leq i \leq k, i < j \leq d\} = \{\theta_i : 1 \leq i \leq k\}$ fully determines the $k$th element of $X$. We define a support of $\theta$ as

$$\Theta = \left\{ \theta_{i,j} : \begin{array}{l} 0 \leq \theta_{1,j} \leq 2\pi, \\ 0 \leq \theta_{i,j} < \pi, \\ i \neq 1. \end{array} \right\},$$

and its subset with respect to $\theta_i$ as $\Theta_i$. Matteson and Tsay (2011) proved that there is a unique inverse mapping of $\hat{W} \in SO(d)$ into $\theta \in \Theta$, which is continuous if either all elements on the main-diagonal of $W$ are positive, or all elements of $W$ are nonzero.

Unfortunately, the non-identification issue regarding $W$ and $X$ still exists because the sign and order of the components are not identifiable. Given any signed permutation matrix $P_{\pm}$, (1) is equivalent to

$$(P_{\pm} X) = P_{\pm} X = P_{\pm} W Z = (P_{\pm} W) Z,$$

where $P_{\pm} X$ and $P_{\pm} W$ become an alternative to $X$ and $W$, as the new ICs and unmixing matrix. However, the identification up to a signed permutation is adequate in terms of modeling multivariate data by linear combinations of ICs. To make a fair comparison between different estimates, a metric invariant to the three ambiguities, scale, sign, and order of the ICs will be presented in Section 5.

Let $Y \in \mathbb{R}^{n \times d}$ be an i.i.d. sample of observations from $F_Y$, where $Y_j \in \mathbb{R}^n$ is an i.i.d. sample of observations from $F_{Y_j}$, $j = 1, \ldots, d$. Let $\Sigma_Y$ be the sample covariance matrix of $Y$, and $\hat{H} = \Sigma_Y^{1/2}$ be the estimated uncorrelated matrix. Although $\Sigma_Y$ is unknown in practice, the sample covariance is a consistent estimate under the finite second-moment assumption, i.e., $\Sigma_Y \overset{a.s.}{\rightarrow} \Sigma_Y$ as $n \rightarrow \infty$. Let $Z = Y \hat{H}' \in \mathbb{R}^{n \times d}$ be the estimated uncorrelated observations, such that $\Sigma_{Z_{i,i}} = I_d$, and $\Sigma_{Z_{j,k}} \overset{a.s.}{\rightarrow} I_d$ as $n \rightarrow \infty$.

To simplify notation, we assume that $Z$, an uncorrelated i.i.d. sample is given, with mean zero and unit variance. Let $X(\theta) = ZW(\theta)' \in \mathbb{R}^{n \times d}$ be a sample of $X$. Then we estimate $W(\theta)$ through $\hat{\theta}$, and define an ICA estimator as

$$\hat{\theta} = \arg \min_{\theta \in \Theta} f(X(\theta)) = \arg \min_{\theta \in \Theta} f(ZW(\theta)').$$

where $f$ is an objective function measuring the mutual dependence among $X(\theta)$. Given the estimate $\hat{\theta}$, the estimated unmixing matrix is $\hat{W} = W(\hat{\theta})$, and the estimated ICs are $\hat{X} = X(\hat{\theta}) = Z\hat{W}' = ZW(\hat{\theta})'$.

### 3 APPLYING MDM TO ICA

We reduce the estimation of ICs to the problem of choosing the function $f$ in (3), which is expected to be a measure of mutual dependence. Following Matteson and Tsay (2017), we primarily focus on distance-based energy statistics because of their compact representations as expectations of pairwise Euclidean distances, while all the results can be easily extended to kernel-based MMDs according to the equivalence between these two classes in Sejdinovic et al. (2013).

We use $(\cdot, \ldots, \cdot)$ to concatenate (vector) components into a vector. Let $t = (t_1, \ldots, t_d), X = (X_1, \ldots, X_d) \in \mathbb{R}^p$ where $t_j, X_j \in \mathbb{R}^p$, $p_j$ is a dimensional margin, $j = 1, \ldots, d$, and $p = \sum_{j=1}^d p_j$ is the total dimension. The subset of components to the right of $X_c$ is denoted by $X_{c+} = (X_{c+1}, \ldots, X_d)$, $c = 0, \ldots, d-1$. The subset of components excluding $X_c$ is denoted by $X_{c-} = (X_1, \ldots, X_{c-1}, X_{c+}), c = 1, \ldots, d-1$. The “$X$” under the assumption that $X_1, \ldots, X_d$ are mutually independent is denoted by $\tilde{X} = (\tilde{X}_1, \ldots, \tilde{X}_d)$, where $\tilde{X}_j \overset{d}{=} X_j$, $j = 1, \ldots, d$, $\tilde{X}_1, \ldots, \tilde{X}_d$ are mutually independent, while $X, \tilde{X}$ are independent. Let $X', X''$ be independent copies of $X$ such that $X', X''$ have the same distribution as $X$, while they are all independent, i.e., $X, X', X'' \overset{i.i.d.}{\rightarrow} F_X$, and $\tilde{X}$ be an independent copy of $\tilde{X}$. The Euclidean norm of $X$ is denoted by $|X|$. The weighted $L_2$ norm $\| \cdot \|_w$ of any complex-valued function $\eta(t)$ is defined by $\| \eta(t) \|_w^2 = \int_{\mathbb{R}^p} |\eta(t)|^2 w(t) dt$ where $|\eta(t)|^2 = \eta(t)\eta(t)'$, $\eta(t)'$ is the complex conjugate of $\eta(t)$, and $w(t)$ is any positive weight function for which the integral exists.

Let $X = \{X^k = (X_1^k, \ldots, X_d^k) : k = 1, \ldots, n\}$ be an i.i.d. sample from $F_X$, the joint distribution of $X$, and let $X_j = \{X_j^k : k = 1, \ldots, n\}$ be the corresponding i.i.d. sample from $F_{X_j}$, the marginal distribution of $X_j$, $j = 1, \ldots, d$, such that $X = \{X_1, \ldots, X_d\}$. Denote the joint characteristic function of $X$ as $\phi_X(t) = E[e^{i(t,X)}]$ and its empirical version as $\hat{\phi}_X(t) = \frac{1}{n} \sum_{k=1}^n e^{i(t,X^k)}$, and the joint characteristic function of $\tilde{X}$ as $\phi_{\tilde{X}}(t) = \prod_{j=1}^d E[e^{i(t,X_j^j)}]$, and its empirical version as $\hat{\phi}_{\tilde{X}}(t) = \prod_{j=1}^d \frac{1}{n} \sum_{k=1}^n e^{i(t,X_j^j)}$. In addition, a simplified empirical version of $\hat{\phi}_{\tilde{X}}(t)$ is defined by $\hat{\phi}_{\tilde{X}}(t) = \frac{1}{n} \sum_{k=1}^n e^{i(t,X_1^k, \ldots, X_{d-1}^k)}$ to substitute $\hat{\phi}_{\tilde{X}}(t)$ as a simplification, where $X_j^{k+1}$ is interpreted as $X_j^k$ for $k > 0$.

### 3.1 DISTANCE COVARIANCE ($d = 2$)

Székely et al. (2007) proposed distance covariance to capture non-linear and non-monotone pairwise depen-
The nonnegative distance covariance $V(X)$ is defined by

$$V(X) = \left\| \phi_X(t) - \phi_{\tilde{X}}(t) \right\|^2_{w_1},$$

$$= \int_{R^p} |\phi_X(t) - \phi_{\tilde{X}}(t)|^2 w_1(t) \, dt,$$

where the weight $w_1(t) = (K_{p_1} K_{p_2}|t_1|^{p_1+1} |t_2|^{p_2+1})^{-1}$, $K_q = \frac{2\pi^{q/2}(1/2)}{2\Gamma((q+1)/2)}$, and $\Gamma$ is the gamma function.

An equivalence to pairwise independence is implied by the definition of $V(X)$. If $E|X| < \infty$, then $V(X) \in [0, \infty)$, and $V(X) = 0$ if and only if $X_1, X_2$ are pairwise independent. In addition, if $E|X_1 X_2| < \infty$, $V^2(X)$ can be interpreted as expectations

$$V^2(X) = E|X_1 - X_1'| |X_2 - X_2'| + E|X_1 - X_2'| E|X_2 - X_2'| - 2E|X_1 - X_1'| E|X_2 - X_2'|.$$

An equivalence to mutual independence is implied by $V(X)$.

### 3.2 Asymmetric and Symmetric Measures ($d \geq 2$)

The asymmetric and symmetric measures of mutual dependence $R(X), S(X)$ are defined by

$$R(X) = \sum_{c=1}^{d-1} V^2((X_c, X_{c+})), \quad (4)$$

$$S(X) = \sum_{c=1}^{d} V^2((X_c, X_{-c})). \quad (5)$$

Analogous to $V(X)$, if $E|X| < \infty$, then $R(X), S(X) \in [0, \infty)$, and $R(X), S(X) = 0$ if and only if $X_1, \ldots, X_d$ are mutually independent.

Correspondingly, the empirical asymmetric and symmetric measures of mutual dependence $\hat{R}_n(X), \hat{S}_n(X)$ are defined by $\hat{R}_n(X) = \sum_{c=1}^{d-1} \hat{V}_n^2((X_c, X_{c+})), \hat{S}_n(X) = \sum_{c=1}^{d} \hat{V}_n^2((X_c, X_{-c})),$ which can be implemented with the time complexity $O(n^2)$. If $E|X| < \infty$, then we have $\hat{R}_n(X) \xrightarrow{a.s.} R(X)$ and $\hat{S}_n(X) \xrightarrow{a.s.} S(X)$ as $n \to \infty$.

### 3.3 Complete Measure ($d \geq 2$)

The complete measure of mutual dependence $Q(X)$ is defined by

$$Q(X) = \left\| \phi_X(t) - \phi_{\tilde{X}}(t) \right\|^2_{w_2},$$

$$= \int_{R^p} |\phi_X(t) - \phi_{\tilde{X}}(t)|^2 w_2(t) \, dt,$$

where $w_2(t) = (K_{q_1} K_{q_2}|t_1|^{q_1+1} |t_2|^{q_2+1})^{-1}$, $K_q = \frac{2\pi^{q/2}(1/2)}{2\Gamma((q+1)/2)}$, and $\Gamma$ is the gamma function.

An equivalence to mutual independence is implied by the definition of $Q(X)$ as well. If $E|X| < \infty$, then $Q(X) \in [0, \infty)$, and $Q(X) = 0$ if and only if $X_1, \ldots, X_d$ are mutually independent. In addition, $Q(X)$ can be interpreted as expectations

$$Q(X) = E|X - \tilde{X}| + E|X' - \tilde{X}'| - E|X - X'| - E|\tilde{X} - \tilde{X}'|.$$

We estimate $Q(X)$ by two empirical versions. One is the empirical complete measure of mutual dependence $Q_n(X)$, defined by $Q_n(X) = \left\| \phi_X(t) - \phi^*_X(t) \right\|^2_{w_2} = \int_{R^p} |\phi_X(t) - \phi^*_X(t)|^2 w_2(t) \, dt,$ which can be interpreted as complete V-statistics. We skip the details of $Q_n$ and will not apply it to ICA, since it is computationally prohibitive with the time complexity $O(n^{2d})$. Another one is the simplified empirical complete measure of mutual dependence $Q^*_n(X)$, defined by $Q^*_n(X) = \left\| \phi_X(t) - \phi^*_X(t) \right\|^2_{w_2} = \int_{R^p} |\phi_X(t) - \phi^*_X(t)|^2 w_2(t) \, dt,$
which can be interpreted as incomplete V-statistics

\[ Q^s_n(X) = \frac{2}{n^2} \sum_{k,l=1}^{n} |X^k - (X^k_{1}, \ldots, X^k_{d} + d - 1)| \]
\[ + \frac{1}{n^2} \sum_{k,l=1}^{n} |X^k - X^l| \]
\[ - \frac{1}{n^2} \sum_{k,l=1}^{n} |(X^k_{1}, \ldots, X^k_{d} + d - 1) - (X^k_{1}, \ldots, X^l_{d} + d - 1)|. \]

The naive implementation of \( Q^s_n(X) \) has the time complexity \( O(n^2) \). If \( E|X| < \infty \), then \( Q_n(X), Q^s_n(X) \) converge a.s. to \( Q(X) \) as \( n \to \infty \).

3.4 MDMICA APPROACH AND ITS ASYMPTOTIC PROPERTIES

Inspired by the nice statistical properties of MDMs, we propose an ICA approach, MDMICA based on MDMs. To be specific, we define three MDMICA estimators, i.e., MDMICA (asy), MDMICA (sym), and MDMICA (com) by applying \( f(X) = R_n(X), S_n(X), Q^s_n(X) \) in (3) respectively as

\[ \hat{\theta}^{asy}_n = \min_{\theta \in \Theta} R_n(X(\theta)) = \min_{\theta \in \Theta} R_n(ZW(\theta)'), \]

and similar expressions follow for \( \hat{\theta}^{sym}_n, \hat{\theta}^{com}_n \). Further, we define another estimator, MDMICA (hsic), by applying dHSIC in the same way.

Since the ICA model only allows scalar components, we apply a special case of MDM to ICA where the marginal dimension \( p_j = 1, j = 1, \ldots, d \), and the total dimension \( p = d \). Without loss of generality, we assume that \( E(Y) = 0 \) and \( \text{Cov}(Y) = I_d \), and therefore \( Z = Y \) and \( Z = Y \) throughout this section. Let \( \mathcal{G} \) denote a large enough compact subset of the space \( \Theta \) defined by (2). The asymptotic properties of the MDMICA estimators are derived as follows.

**Theorem 1.** If \( Y \) has a nonsingular, continuous distribution \( F_Y \) with \( E|Y|^2 < \infty \), if there exists a unique minimizer \( \theta_0 \in \mathcal{G} \) of (2), and if \( W(\theta_0) \) satisfies the conditions for a unique continuous inverse to exist, then \( \hat{\theta}^{asy}_n \overset{a.s.}{\longrightarrow} \theta_0 \) as \( n \to \infty \).

When the ICA model is misspecified, convergence to the pseudo-true value \( \theta_0 \) is obtained. Under similar conditions, \( \hat{\theta}^{sym}_n, \hat{\theta}^{com}_n \) also converge a.s. as \( n \to \infty \) due to similar arguments.

We then establish the root-\( n \) consistency of the MDMICA estimators under some regularity conditions no matter whether the ICA model holds or it is misspecified.

**Theorem 2.** If the assumptions of Theorem[1] hold, and if the ICA model assumptions hold, then \( |\hat{\theta}^{asy}_n - \theta_0| = O_P(n^{-1/2}) \).

**Theorem 3.** If the ICA model is misspecified but the remaining assumptions stated in Theorem [2] hold, and if \( E[|\hat{\omega}_n R_n(X(\theta))|_{\theta=\theta_0}] = O_P(n^{-1/2}) \), where \( \theta_0 \) denotes the pseudo-true value, then \( |\hat{\theta}^{asy}_n - \theta_0| = O_P(n^{-1/2}) \).

Under similar conditions, \( \hat{\theta}^{sym}_n, \hat{\theta}^{com}_n \) are also consistent as \( n \to \infty \) due to similar arguments.

The proofs of Theorem 1, 2, and 3 are similar to those of Theorem 2.1, 2.2, and Corollary 2.1 in [Matteson and Tsay (2017)] respectively, considering the same nature of \( R_n(X), S_n(X), Q^s_n(X) \) as energy statistics, and replacing the empirical cumulative distribution function (ECDF) with the identity function in derivations.

4 IMPROVING INITIALIZATION OF LOCAL METHODS

In the literature, there are two primary schemes to estimate ICs with regard to how the optimization is implemented. For one, the components are extracted one at a time, known as the deflation scheme. For another, the components are extracted simultaneously, known as the parallel scheme. The deflation scheme has the advantage of lower computational cost over the parallel scheme. While the parallel scheme enjoys greater statistical efficiency, since the deflation scheme accumulates estimation uncertainty at each step in its sequential procedure.

For our ICA framework, the objective function \( f \) in (3) has \( d(d - 1)/2 \) parameters \( \theta_{i,j} \in \theta \), which can be estimated in both deflation (sequential) and parallel (joint) manners. Specifically, the deflation scheme estimates all \( \theta_{i,j} \in \theta \) for each \( i \) at a time, while the parallel scheme estimates all \( \theta_{i,j} \in \theta \) together at once.

In view of the special structures of associated measures, both deflation and parallel schemes are appropriate for MDMICA (asy), which only fits MDMICA (asy, def) and MDMICA (asy, par), while MDMICA (sym), MDMICA (com), and MDMICA (hsic) only fit the parallel scheme. The MDMICA algorithms for both deflation and parallel schemes are described in Alg. 1 below.

Estimating \( \theta \) through (3) involves minimization of a non-convex but locally convex objective function \( f \), which requires initialization and iterative algorithms. The default method for MDMICA is a Newton-type local optimization method, for which we explore two ways of finding a good initialization.

The first way is to perform a random sampling method, Latin hypercube sampling (LHS) [McKay et al. (2000)]
Algorithm 1 MDMICA (Z, f)

1. Initialize \( \theta \) and \( W(\theta) \) via \( \hat{\theta} \).
2. (deflation scheme)
   \[ \text{for } i = 1, \ldots, d - 1 \text{ do} \]
   a. Solve \( \hat{\theta}_i = \arg\min_{\theta \in \Theta} f(ZW(\theta)) \) using newton-type local optimization.
   b. Update \( \theta_i \leftarrow \hat{\theta}_i \).
   end \text{for}

2. (parallel scheme)
   Solve \( \hat{\theta} = \arg\min_{\theta \in \Theta} f(ZW(\theta)) \) using newton-type local optimization.

3. Output \( \hat{\theta} = \{ \hat{\theta}_i : 1 \leq i \leq d - 1 \} \), \( \hat{W} = W(\hat{\theta}) \), and \( \hat{X} = ZW(\hat{\theta})' \).

uniformly over the space \( \Theta \) to obtain a number of parameter values. Then we evaluate the objective function at each value and record the value minimizing it, which is used to initialize the subsequent local optimization algorithm. Based on our experience, the number of parameter values sampled should grow with the dimension.

The second way is to take advantage of a global optimization method, Bayesian optimization (BO) (Mockus 1994), where the objective function \( f \) is treated as a black box. It is applicable when the function is expensive to evaluate, the derivative is unavailable, or the optimization problem is non-convex. Bayesian optimization is one of the most efficient approaches in terms of the number of function evaluations consumed, as Jones (2001), Brochu et al. (2010), Snoek et al. (2012) illustrated that it outperforms other state-of-the-art global optimization algorithms on a number of challenging problems.

Bayesian optimization models the objective with respect to the parameter values as a Gaussian process, for which we adopt two popular kernels, squared exponential (exp) and Matérn 5/2 (Matérn). A prior is set over the objective function and then updated with actual evaluations to get a posterior using the Bayesian technique. The utility-based selection of the next evaluation point on the objective function trades off between exploration and exploitation.

5 SIMULATION STUDIES

In this section, we evaluate the performance of our MDMICA estimators by performing simulations similar to Matteson and Tsay (2017), and compare them with the FastICA estimator, the Infomax estimator, and the JADE estimator. MDMICA (asy) is omitted because it is the same as dCovICA. Moreover, we elaborate on the implementation and error metric of ICA.

Furthermore, we try various options for each estimator. For FastICA, we evaluate three functions used to approximate negentropy in both deflation and parallel schemes, logarithm of hyperbolic cosine (logcosh), kurtosis (kur), and exponential (exp). For Infomax, we evaluate three nonlinear (squashing) functions, hyperbolic tangent (tanh), logistic (log), and extended Infomax (ext). For MDMICA (hsic), we investigate the Gaussian (gau) kernel. However, FastICA (kur) and FastICA (exp) are omitted since their performance is quite similar to that of FastICA (logcosh). Similarly, Infomax (log) and Infomax (ext) are omitted.

We simulate the ICs \( X \in \mathbb{R}^{n \times d} \) from eighteen distributions using \texttt{rjordan} in the R package ProDenICA (Hastie and Tibshirani 2010) with sample size \( n \) and dimension \( d \). See Figure 1 for the density functions of the eighteen distributions. Then we generate a mixing matrix \( M \in \mathbb{R}^{d \times d} \) with condition number between 1 and 2 using \texttt{mixmat} in the R package ProDenICA (Hastie and Tibshirani 2010), and obtain the observations \( \hat{Y} = \hat{X}M' \), which are centered by their sample mean and then prewhitened by their sample covariance to obtain uncorrelated observations \( Z = \hat{Y}H' \). Finally, we obtain the estimate \( W \) based on \( Z \) via [3], and evaluate the estimation accuracy by comparing the estimate \( \hat{W} \) to the ground truth \( W_0 = (HM)^{-1} \). Moreover, the Newton-type local optimization is implemented by \texttt{nlm} in the R package \texttt{stats} (R Core Team 2014), and Bayesian optimization is implemented by \texttt{BayesianOptimization} in the R package \texttt{rBayesianOptimization} (Yan 2016).

![Figure 1: Density plots of the 18 distributions.](image_url)

To take the uncertainty in both prewhitening the observations and estimating the ICs into account when comparing the estimates from different approaches, we use the metric MD proposed by Ilmonen et al. (2010) to measure the error between an estimate \( \hat{W} \) and the corresponding truth \( W_0 \), which is defined as

\[
\text{MD}(\hat{M}, M) = \frac{1}{\sqrt{d-1}} \inf_{P,D} \|PD\hat{W}W_0^{-1}I_d\|_F,
\]

where \( \| \cdot \|_F \) denotes the Frobenius norm, \( P \) is a \( d \times d \)
permutation matrix, and $D$ is a $d \times d$ diagonal matrix with nonzero diagonal elements. MD is invariant to the three ambiguities associated with ICA as a result of taking the infimum, for which the optimal $P, D$ are solved by the Hungarian method \cite{Papadimitriou and Steiglitz, 1998}.

**Model 1.** [Different distributions of ICs] We sample $X$ from one distribution in the eighteen distributions, with $d = 3, n = 1000$. We obtain $10d$ points using LHS, and select the best initial point. See Figure 2 for the error metrics of all eighteen distributions with 100 trials.

MDMICA achieves competitive results with JADE and dCovICA, and also outperforms FastICA and Infomax in most cases. MDMICA (sym) is equal and often better than dCovICA, while they have similar performance due to their similar structures. MDMICA (hsic) is equal and often better than MDMICA (com), while they have similar performance due to their similar structures. Further, MDMICA (com) and MDMICA (hsic) are less sensitive to different distributions than dCovICA and MDMICA (sym) in general. Lastly, there is no remarkable difference between the deflation and parallel schemes.

**Model 2.** [Different dimensions of ICs] We sample $X$ from one distribution in the eighteen distributions, with $d \in \{2, 3, 4\}, n = 1000$. We pick $10d$ points using LHS, and select the best initial point. See Figure 3 for the error metrics of the 1st distribution with 100 trials.

The errors of all estimators increase as the dimension $d$ grows. As in the previous model, JADE, dCovICA, and MDMICA have similar performance, and significantly outperform FastICA and Infomax.

**Model 3.** [Different initializations of local optimization] We sample $X$ from $d$ randomly selected distributions of the eighteen distributions, with $d = 4, n = 1000$. We implement three ways to select the initial point for the Newton-type local optimization method. The first way is to sample one point using LHS, and then proceed. The second way is to sample $10d$ points using LHS, and then select the point out of $10d$ with the lowest objective. The third way is to run $10d$ iterations using BO, with its initial points from $10d$ sampled points using LHS, and then select the point out of $20d$ with the lowest objective. See Table 1 for the error metrics, objective values, and computational times of the tuple as the (4th, 11th, 12th, 18th) distributions with 50 trials.

The performance of dCovICA and MDMICA is greatly improved by selecting the best point from multiple initial points, as LHS and LHS + BO produce smaller objective values and more accurate estimates than a single point with lower mean and standard error. The reason is two-fold. First, LHS and BO offer the subsequent local optimization method better initial points in terms of lower objective, which leads to a better estimate in terms of lower objective as well. Second, a better estimate with lower objective is likely to be a better solution with lower MD, since the objective is a truly mutual dependence measure. Moreover, LHS + BO has noticeable advantage over LHS alone for MDMICA (com) and MDMICA (hsic), but only marginal advantage over LHS alone for dCovICA (def), dCovICA (par), and MDMICA (sym).

dCovICA and MDMICA take remarkably longer computational time than the others, which makes sense because the optimization problem of dCovICA and MDMICA is especially difficult to solve, as it has $d(d-1)/2$ parameters and becomes high-dimensional quickly. This obstacle in turn motivates us to improve the local optimization by choosing a better initialization point.

**Model 4.** [Misspecified ICA model] We sample $X = (X_1, X_2)$ from one distribution in the eighteen distributions, with $n = 1000$. Let $Y_1 = X_1, Y_2 = (X_2)^2$. We pick $10d$ points using LHS, and select the best initial point. See Table 2 for the results of the 1st distribution with 1 trial.

We use $R_n, S_n, Q_n$ to measure the mutual dependence between the components before (w.r.t. $Z$) and after (w.r.t. $X$) the optimization. dCovICA and MDMICA successfully decreases the mutual dependence between the components through optimization, while FastICA, Infomax, and JADE are unable to and even increase it. Therefore, ICA methods based on mutual dependence measures outperform others in reducing the mutual dependence given that the ICA model is misspecified.

### 6 IMAGE DATA

Fulfilling the task of unmixing vectorized images similar to \cite{Virta et al., 2016}, we consider the three gray-scale images in the R package ICS \cite{Nordhausen et al., 2008}, depicting a cat, a forest road, and a sheep respectively. Each image is represented by a $130 \times 130$ matrix, where each element indicates the intensity value of a pixel. We standardize the three images such that the intensity values across all the pixels in each image have mean zero and unit variance. Then we vectorize each image into a vector of length $130^2$, and combine the vectors from all three images as a matrix $X$, with $d = 3, n = 130^2$.

We use mixmat in the R package ProDenICA \cite{Hastie and Tibshirani, 2010} again to generate a mixing matrix $A \in \mathbb{R}^{ppp}$, and mix the three images to obtain the observations $Y = XA^T$, which are centered by their sample mean, then prewhitened by their sample covariance to obtain uncorrelated observations $Z = YH^T$.

We estimate the intensity values $\hat{S}$ initialized from $10d$ points using LHS. See Figures 4 for the recovered im-
ages, where the Euclidean norm of vectorized errors is computed to evaluate the estimation accuracy. Indicated by the estimated images and errors, dCovICA and MDMICA outperforms JADE. Moreover, MDMICA (com) achieves the best overall performance.
Table 2: Mutual dependence measures of observed components (before optimization, $Z$) and estimated independent components (after optimization, $\hat{X}$) with 1 trial for Model 4 (misspecified ICA model).

| Estimator          | $R_n(Z)$ ($10^{-3}$) | $R_n(\hat{X})$ | $S_n(Z)$ ($10^{-3}$) | $S_n(\hat{X})$ | $Q^*_n(Z)$ ($10^{-3}$) | $Q^*_n(\hat{X})$ |
|--------------------|----------------------|-----------------|----------------------|-----------------|-----------------------|-----------------|
| FastICA (logcosh, def) | 0.531               | 0.606           | 1.062                | 2.062           | 3.088                 | 3.330           |
| FastICA (logcosh, par) | 0.588               | 1.031           | 1.176                | 2.062           | 2.786                 | 3.330           |
| Infomax (tanh)      | 0.606               | 0.441           | 1.212                | 0.882           | 2.797                 | 2.677           |
| JADE                | 1.031               | 0.441           | 2.062                | 0.882           | 2.797                 | 2.677           |
| dCovICA (def)       | 0.548               | 0.441           | 1.097                | 0.882           | 2.797                 | 2.677           |
| dCovICA (par)       | 0.441               | 0.441           | 2.797                | 2.677           | 2.677                 | 2.677           |
| MDMICA (sym)        | 0.441               | 0.441           | 2.797                | 2.677           | 2.677                 | 2.677           |
| MDMICA (com)        | 0.446               | 0.443           | 2.677                | 2.677           | 2.677                 | 2.677           |
| MDMICA (hsic)       | 0.443               | 0.443           | 2.677                | 2.677           | 2.677                 | 2.677           |

7 CONCLUSION

Resorting to recently proposed mutual dependence measures including MDMs in Jin and Matteson (2017) and dHSIC in Pfister et al. (2016), we generalize dCovICA in Matteson and Tsay (2017) to a new ICA approach, MDMICA, taking empirical dependence measures as an objective function for the estimation of ICs. In addition, we study the asymptotic properties of MDMICA.

When solving the non-convex minimization problem to estimate ICs, we apply LHS and BO to select a better initial point for the Newton-type local optimization method.

MDMICA achieves competitive results with JADE and dCovICA, and outperforms FastICA and Infomax in numerical studies, under different distributions and dimensions of ICs. When the ICA model is misspecified, MDMICA decreases the mutual dependence between components via optimization, while other approaches cannot and even increase it. We illustrate the advantage of using multiple initial points from LHS and BO over a single initial point.

During the image recovery task from mixed image data, MDMICA not only nicely recovers the true images, but also achieves lower overall errors than other approaches, which demonstrates the value of MDMICA in real data applications.
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