Abstract

The performance of standard algorithms for Independent Component Analysis quickly deteriorates under the addition of Gaussian noise. This is partially due to a common first step that typically consists of whitening, i.e., applying Principal Component Analysis (PCA) and rescaling the components to have identity covariance, which is not invariant under Gaussian noise.

In our paper we develop the first practical algorithm for Independent Component Analysis that is provably invariant under Gaussian noise. The two main contributions of this work are as follows:

1. We develop and implement an efficient, Gaussian noise invariant decorrelation (quasi-orthogonalization) algorithm using Hessians of the cumulant functions.
2. We propose a very simple and efficient fixed-point GI-ICA (Gradient Iteration ICA) algorithm, which is compatible with quasi-orthogonalization, as well as with the usual PCA-based whitening in the noiseless case. The algorithm is based on a special form of gradient iteration (different from gradient descent). We provide an analysis of our algorithm demonstrating fast convergence following from the basic properties of cumulants. We also present a number of experimental comparisons with the existing methods, showing superior results on noisy data and very competitive performance in the noiseless case.
of $s$. For simplicity, we assume $A \in \mathbb{R}^{d \times d}$ is square and of full rank. The latent components of $s$ are viewed as containing the information describing the makeup of the observed signal (voices of individual speakers in the cocktail party setting). The goal of Independent Component Analysis is to approximate the matrix $A$ in order to recover the latent signal $s$. In practice, most methods ignore the noise term, leaving the simpler problem of recovering the mixing matrix $A$ when $x = As$ is observed.

Arguably the two most widely used ICA algorithms are FastICA [13] and JADE [6]. Both of these algorithms are based on a two step process:

1. The data is centered and whitened, that is, made to have identity covariance matrix. This is typically done using principal component analysis (PCA) and rescaling the appropriate components. In the noiseless case this procedure orthogonalizes and rescales the independent components and thus recovers $A$ up to an unknown orthogonal matrix $R$.

2. Recover the orthogonal matrix $R$.

Most practical ICA algorithms differ only in the second step. In FastICA, various objective functions are used to perform a projection pursuit style algorithm which recovers the columns of $R$ one at a time. JADE uses a fourth-cumulant based technique to simultaneously recover all columns of $R$.

Step 1 of ICA is affected by the addition of a Gaussian noise. Even if the noise is white (has a scalar times identity covariance matrix) the PCA-based whitening procedure can no longer guarantee the whitening of the underlying independent components. Hence, the second step of the process is no longer justified. This failure may be even more significant if the noise is not white, which is likely to be the case in many practical situations. Recent theoretical developments (see, [2] and [3]) consider the case where the noise $\eta$ is an arbitrary (not necessarily white) additive Gaussian variable drawn independently from $s$.

In [2], it was observed that certain cumulant-based techniques for ICA can still be applied for the second step if the underlying signals can be orthogonalized. Orthogonalization of the latent signals (quasi-orthogonalization) is a significantly less restrictive condition as it does not force the underlying signal to have identity covariance (as in whitening in the noiseless case). In the noisy setting, the usual PCA cannot achieve quasi-orthogonalization as it will whiten the mixed signal, but not the underlying components. In [3], we show how quasi-orthogonalization can be achieved in a noise-invariant way through a method based on the fourth-order cumulant tensor. However, a direct implementation of that method requires estimating the full fourth-order cumulant tensor, which is computationally challenging even in relatively low dimensions. In this paper we derive a practical version of that algorithm based on directional Hessians of the fourth univariate cumulant, thus reducing the complexity dependence on the data dimensionality from $d^4$ to $d^3$, and also allowing for a fully vectorized implementation.

We also develop a fast and very simple gradient iteration (not to be confused with gradient descent) algorithm, GI-ICA, which is compatible with the quasi-orthogonalization step and can be shown to have convergence of order $r - 1$, when implemented using a univariate cumulant of order $r$. For the cumulant of order four, commonly used in practical applications, we obtain cubic convergence. We show how these convergence rates follow directly from the properties of the cumulants, which sheds some light on the somewhat surprising cubic convergence seen in fourth-order based ICA methods [13][18][22]. The update step has complexity $O(N d \bar{d})$ where $N$ is the number of samples, giving a total algorithmic complexity of $O(N d^3)$ for step 1 and $O(N d^2 t)$ for step 2, where $t$ is the number of iterations for convergence in the gradient iteration.

Interestingly, while the techniques are quite different, our gradient iteration algorithm turns out to be closely related to Fast ICA in the noiseless setting, in the case when the data is whitened and the cumulants of order three or four are used. Thus, GI-ICA can be viewed as a generalization (and a conceptual simplification) of Fast ICA for more general quasi-orthogonalized data.

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1This process of orthogonalizing the latent signals was called quasi-whitening in [2] and later in [3]. However, this conflicts with the definition of quasi-whitening given in [12] which requires the latent signals to be whitened. To avoid the confusion we will use the term quasi-orthogonalization for the process of orthogonalizing the latent signals.
We present experimental results showing superior performance in the case of data contaminated by Gaussian noise and very competitive performance for clean data. We also note that the GI-ICA algorithms are fast in practice, allowing us to process (decorrelate and detect the independent components) 100 000 points in dimension 5 in well under a second on a standard desktop computer. Our Matlab implementation of GI-ICA is available for download at [http://sourceforge.net/projects/giica/].

Finally, we observe that our method is partially compatible with the robust cumulants introduced in [20]. We briefly discuss how GI-ICA can be extended using these noise-robust techniques for ICA to reduce the impact of sparse noise.

The paper is organized as follows. In section 2 we discuss the relevant properties of cumulants, and discuss results from prior work which allows for the quasi-orthogonalization of signals with non-zero fourth cumulant. In section 3 we discuss the connection between the fourth-order cumulant tensor method for quasi-orthogonalization discussed in section 2 with Hessian-based techniques seen in [2] and [11]. We use this connection to create a more computationally efficient and practically implementable version of the quasi-orthogonalization algorithm discussed in section 2. In section 4 we discuss new, fast, projection-pursuit style algorithms for the second step of ICA which are compatible with quasi-orthogonalization. In order to simplify the presentation, all algorithms are stated in an abstract form as if we have exact knowledge of required distribution parameters. Section 5 discusses the estimators of required distribution parameters to be used in practice. Section 6 discusses numerical experiments demonstrating the applicability of our techniques. Finally, in section 7 we briefly summarize our results and possible future work.

Related Work. The name Independent Component Analysis refers to a broad range of algorithms addressing the blind signal separation problem as well as its variants and extensions. There is an extensive literature on ICA in the signal processing and machine learning communities due to its applicability to a variety of important practical situations. For a comprehensive introduction see the books [8, 14]. In this paper we develop techniques for dealing with noisy data by introducing new and more efficient techniques for quasi-orthogonalization and subsequent component recovery. The quasi-orthogonalization step was introduced in [2], where the authors proposed an algorithm for the case when the fourth cumulants of all independent components are of the same sign. A general algorithm with complete theoretical analysis was provided in [3]. That algorithm required estimating the full fourth-order cumulant tensor.

We note that Hessian based techniques for ICA were used in [21, 2, 11], with [11] and [2] using the Hessian of the fourth-order cumulant. The papers [21] and [11] proposed interesting randomized one step noise-robust ICA algorithms based on the cumulant generating function and the fourth cumulant respectively in primarily theoretical settings. The gradient iteration algorithm proposed is closely related to the work [18], which provides a gradient-based algorithm derived from the fourth moment with cubic convergence to learn an unknown parallelepiped in a cryptographic setting. For the special case of the fourth cumulant, the idea of gradient iteration has appeared in the context of FastICA with a different justification, see e.g. [16, Equation 11 and Theorem 2]. We also note the work [12], which develops methods for Gaussian noise-invariant ICA under the assumption that the noise parameters are known. Finally, there are several papers that considered the problem of performing PCA in a noisy framework. [5] gives a provably robust algorithm for PCA under a sparse noise model. Using a Bayesian framework, [4] performs PCA robust to white Gaussian noise, and [9] extends the Bayesian techniques to be robust to sparse noise when there are sufficiently more dimensions than underlying source signals, and when the additive noise in ICA does not include non-white Gaussian noise, these techniques can be viewed as alternatives for step 1 of ICA.

2 Using Cumulants to Orthogonalize the Independent Components

Properties of Cumulants: Cumulants are similar to moments and can be expressed in terms of certain polynomials of the moments. However, cumulants have additional properties which allow independent random variables to be algebraically separated. We will be interested in the fourth order multi-variate cumulants, and univariate cumulants of arbitrary order. Denote by $Q_x$ the fourth order cumulant tensor for the random vector $x$. So, $Q_x^{ijkl}$ is the cross-cumulant between the random variables $x_i$, $x_j$, $x_k$, and $x_l$, which we alternatively denote as $\text{Cum}(x_i, x_j, x_k, x_l)$. Cumulant tensors
are symmetric, i.e. \((Q_x)_{ijkl}\) is invariant under permutations of indices. Multivariate cumulants have the following properties (written in the case of fourth order cumulants):

1. (Multilinearity) If \(x\) is a random vector, and \(\alpha\) is a scalar, then
   \[
   \text{Cum}(\alpha x_i, x_j, x_k, x_l) = \alpha \text{Cum}(x_i, x_j, x_k, x_l).
   \]
   If \(y\) is a random variable, then
   \[
   \text{Cum}(x_i + y, x_j, x_k, x_l) = \text{Cum}(x_i, x_j, x_k, x_l) + \text{Cum}(y, x_j, x_k, x_l).
   \]

2. (Independence) If \(x_i\) and \(x_j\) are independent random variables, then
   \[
   \text{Cum}(x_i, x_j, x_k, x_l) = 0.
   \]
   When \(x\) and \(y\) are independent, \(Q_{x+y} = Q_x + Q_y\).

3. (Vanishing Gaussian) Cumulants of order 3 and above are zero for Gaussian random variables.

The first order cumulant is the mean, and the second order multivariate cumulant is the covariance matrix. We will denote by \(\kappa_r(x)\) the order-\(r\) univariate cumulant, which is equivalent to the cross-cumulant of \(x\) with itself \(r\) times: \(\kappa_r(x) := \text{Cum}(x, x, \ldots, x)\) (where \(x\) appears \(r\) times). In the univariate case, these properties become:

1. (Additivity) If \(x\) and \(y\) are independent random variables, then \(\kappa_r(x + y) = \kappa_r(x) + \kappa_r(y)\).
2. (Homogeneity) If \(\alpha\) is a scalar and \(x\) a random variable, then \(\kappa_r(\alpha x) = \alpha^r \kappa_r(x)\).
3. (Vanishing Gaussians) The first-order mean and second-order variance are the only non-zero cumulants of Gaussian random variables.

**Quasi-Orthogonalization Using Cumulant Tensors.** Recalling our original notation, \(x = As + b + \eta\) gives the generative ICA model. We define an operation of fourth-order tensors on matrices:

For \(Q \in \mathbb{R}^{d \times d \times d \times d}\) and \(M \in \mathbb{R}^{d \times d}\), \(Q(M)\) is the matrix such that

\[
Q(M)_{ij} := \sum_{k=1}^{d} \sum_{l=1}^{d} Q_{ijkl} m_{lk}.
\]

We can use this operation to orthogonalize the latent random signals.

**Definition 2.1.** A matrix \(W\) is called a quasi-orthogonalization matrix if there exists an orthogonal matrix \(R\) and a nonsingular diagonal matrix \(D\) such that \(WA = RD\).

We will need the following results from [3]. Here we use \(A_q\) to denote the \(q^{th}\) column of \(A\).

**Lemma 2.2.** Let \(M \in \mathbb{R}^{d \times d}\) be an arbitrary matrix. Then, \(Q_x(M) = ADAT^T\) where \(D\) is a diagonal matrix with entries \(d_{qq} = \kappa_4(s_q)A_q^T A_q\).

**Theorem 2.3.** Suppose that each component of \(s\) has non-zero fourth cumulant. Let \(M = Q_x(I)\), and let \(C = Q_x(M^{-1})\). Then \(C = ADAT^T\) where \(D\) is a diagonal matrix with entries \(d_{qq} = 1/\|A_q\|_2^2\). In particular, \(C\) is positive definite, and for any factorization \(BB^T\) of \(C\), \(B^{-1}\) is a quasi-orthogonalization matrix.

It is worth noting that if each component of \(s\) has fourth cumulant of the same sign, then \(M = Q_x(I)\) will be either positive or negative definite, and (negating \(M\) if it is negative-definite) a factorization of \(M\) could be used instead for quasi-orthogonalization. However, the inversion trick in Theorem 2.3 is necessary to cancel out the fourth-cumulant signs in the general case.

### 3 Quasi-Orthogonalization using Cumulant Hessians

We have seen in Theorem 2.3 a tensor-based method which can be used to quasi-orthogonalize observed data. However, this method naively requires the estimation of \(O(d^4)\) terms from data. There is a connection between the cumulant Hessian-based techniques used in ICA [2, 11] and the tensor-based technique for quasi-orthogonalization described in Theorem 2.3 that allows the tensor-method to be rewritten using a series of Hessian operations. We make this connection precise.
Algorithm 1: Hessian-based algorithm to generate a quasi-orthogonalization matrix.

1: function FINDQUASIORTHOGONALIZATIONMATRIX(x)
2: \begin{align*}
&\text{Let } M = \frac{1}{12} \sum_{i=1}^{d} H_{uu}(u^T x)_{|u|=0}. \text{ See Equation (6) for the estimator.} \\
&\text{Let } U \Lambda U^T \text{ give the eigendecomposition of } M^{-1} \\
&\text{Let } C = \sum_{i=1}^{d} \lambda_i H_{uu}(u^T x)_{|u|=U_i}. \text{ See Equation (6) for the estimator.} \\
&\text{Factorize } C \text{ as } B B^T. \\
&\text{return } B^{-1} \\
\end{align*}
3: end function

below. The Hessian version requires only $O(d^3)$ terms to be estimated from data and simplifies the computation to consist of matrix and vector operations.

Let $H_u$ denote the Hessian operator with respect to a vector $u \in \mathbb{R}^d$. The following lemma connects Hessian methods with our tensor-matrix operation (a special case is discussed in \cite[Section 2.1]{2}).

**Lemma 3.1.** $H_u(\kappa_4(u^T x)) = ADA^T$ where $d_{qq} = 12(u^T A_q)^2 \kappa_4(s_q)$.

**Proof.** By the properties of cumulants: $\kappa_4(u^T A s) = \sum_q (u^T A q)^4 \kappa_4(s_q)$. Taking derivatives yields

$$
\partial_{u_i u_j} \kappa_4(u^T A s) = 12 \sum_q (u^T A q)^2 \kappa_4(s_q) a_{iq} a_{jq}.
$$

In matrix form, this reads $H_u f(u) = ADA^T$ where $D$ is a diagonal matrix with entries $d_{qq} = 12 \kappa_4(s_q)(u^T A q)^2$.

In Lemma \[3.1\], the diagonal entries can be rewritten as $d_{qq} = 12 \kappa_4(s_q)(A_q^T uu^T A_q)$. By comparing with Lemma \[2.2\] we see that applying $Q_x$ against a symmetric, rank one matrix $uu^T$ can be rewritten in terms of the Hessian operations:

$$
Q_x(uu^T) = \frac{1}{12} H_u(\kappa_4(u^T x)).
$$

This formula extends to arbitrary symmetric matrices by the following Lemma.

**Lemma 3.2.** Let $M$ be a symmetric matrix with eigen decomposition $U \Lambda U^T$ such that $U = (u_1, u_2, \ldots, u_d)$ and $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d)$. Then,

$$
Q_x(M) = \frac{1}{12} \sum_{i=1}^{d} \lambda_i H_{uu}(u_i^T x).
$$

**Proof.** Use the linearity of summations and \[1\] to see:

$$
Q_x(M) = Q_x \left( \sum_{i=1}^{d} \lambda_i u_i u_i^T \right) = \sum_{i=1}^{d} \lambda_i Q_x(u_i u_i^T) = \frac{1}{12} \sum_{i=1}^{d} \lambda_i H_{uu}(u_i u_i^T). \quad \square
$$

The matrices $I$ and $M^{-1}$ in Theorem \[2.3\] are symmetric. As such, the tensor-based method for quasi-orthogonalization can be rewritten using Hessian operations. This is done in Algorithm \[1\].

4 \quad Gradient Iteration ICA

In the preceding sections, we discussed techniques to quasi-orthogonalize data. For this section, we will assume that quasi-orthogonalization is accomplished, and discuss deflationary approaches that can quickly recover the directions of the independent components. Let $W$ be a quasi-orthogonalization matrix. Then, define $y := W x = W A s + W \eta$. Note that since $\eta$ is Gaussian noise, so is $W \eta$. There exists a rotation matrix $R$ and a diagonal matrix $D$ such that $W A = RD$.

Let $\hat{s} := D s$. The coordinates of $\hat{s}$ are still independent random variables. Gaussian noise makes recovering the scaling matrix $D$ impossible. We aim to recover the rotation matrix $R$. 


To see why recovery of \( D \) is impossible, we note that a white Gaussian random variable \( \eta_1 \) has independent components. It is impossible to distinguish between the case where \( \eta_1 \) is part of the signal, i.e. \( W(A(s + \eta_1) + W\eta) \), and the case where \( A\eta_1 \) is part of the additive Gaussian noise, i.e. \( WAs + W(A\eta_1 + \eta) \), when \( s, \eta_1, \) and \( \eta \) are drawn independently. In the noise-free ICA setting, the latent signal is typically assumed to have identity covariance, placing the scaling information in the columns of \( A \). The presence of additive Gaussian noise makes recovery of the scaling information impossible since the latent signals become ill-defined. Following the idea popularized in FastICA, we will discuss a deflationary technique to recover the columns of \( R \) one at a time.

**Fast Recovery of a Single Independent Component.** In the deflationary approach, a function \( f \) is fixed that acts upon a directional vector \( u \in \mathbb{R}^d \). Based on some criterion (typically maximization or minimization of \( f \)), an iterative optimization step is performed until convergence. This technique was popularized in FastICA, which is considered fast for the following reasons:

1. As an approximate Newton method, FastICA requires computation of \( \nabla u f \) and a quick-to-compute estimate of \( (H_u(f))^{-1} \) at each iterative step. Due to the estimate, the computation runs in \( O(Nd) \) time, where \( N \) is the number of samples.
2. The iterative step in FastICA has local quadratic order convergence using arbitrary functions, and global cubic-order convergence when using the fourth cumulant \[13\].

We note that cubic convergence rates are not unique to FastICA and have been seen using gradient descent (with the correct step-size) when choosing \( f \) as the fourth moment \[18\]. Our proposed deflationary algorithm will be comparable with FastICA in terms of computational complexity, and the iterative step will take on a conceptually simpler form as it only relies on \( \nabla u \kappa_r \). We provide a derivation of fast convergence rates that relies entirely on the properties of cumulants. As cumulants are invariant with respect to the additive Gaussian noise, the proposed methods will be admissible for both standard and noisy ICA.

While cumulants are essentially unique with the additivity and homogeneity properties \[17\] when no restrictions are made on the probability space, the preprocessing step of ICA gives additional structure (like orthogonality and centering), providing additional admissible functions. In particular, \[20\] designs “robust cumulants” which are only minimally effected by sparse noise. Welling’s robust cumulants have versions of the additivity and homogeneity properties (as is discussed in Appendix \[A\]), and are consistent with our update step. For this reason, we will state our results in greater generality.

Let \( G \) be a function of univariate random variables that satisfies the additivity, degree-\( r \) (\( r \geq 3 \)), and homogeneity, and (for the noisy case) the vanishing Gaussians properties of cumulants. Then for a generic choice of input vector \( v \), Algorithm \[2\] will demonstrate order \( r - 1 \) convergence. In particular, if \( G \) is \( \kappa_3 \), then we obtain quadratic convergence; and if \( G \) is \( \kappa_4 \), we obtain cubic convergence. Lemma \[4\] helps explain why this is true.

**Lemma 4.1.** \( \nabla v G(v \cdot y) = r \sum_{i=1}^{d} (v \cdot R_i)^{r-1} G(\tilde{s}_i)R_i \).

**Proof.** This follows almost directly from the assumptions on \( G \):

\[
\nabla v G(v \cdot y) = \nabla v G(v \cdot (R\tilde{s} + W\eta)) = \nabla v G(v \cdot R\tilde{s}) = \nabla v \sum_{i=1}^{d} (v \cdot R_i)^{r-2} G(\tilde{s}_i)R_i = r \sum_{i=1}^{d} (v \cdot R_i)^{r-1} G(\tilde{s}_i)R_i \tag*{\square}
\]

If we consider what is happening in the basis of the columns of \( R \), then up to some multiplicative constant, each coordinate is raised to the \( r - 1 \) power and then renormalized during each step of Algorithm \[2\] This ultimately leads to the order \( r - 1 \) convergence.

**Theorem 4.2.** If for a unit vector input \( v \) to Algorithm \[2\] \( h = \arg \max_i |(v \cdot R_i)^{r-2} G(\tilde{s}_i)| \) has a unique answer, then \( v \) has order \( r - 1 \) convergence to \( R_h \) up to sign. In particular, if the following conditions are met:

1. There exists a coordinate random variable \( s_i \) of \( s \) such that \( G(s_i) \neq 0 \).
2. \( v \) inputted into Algorithm \[2\] is chosen uniformly at random from the unit sphere \( S^{d-1} \).

Then Algorithm \[2\] converges to a column of \( R \) (up to sign) almost surely, and convergence is of order \( r - 1 \).
By convergence up to sign, we include the possibility that $v$ oscillates between $R_h$ and $-R_h$ on alternating steps. This can occur if $G(s_i) < 0$ and $r$ is odd.

**Proof of Theorem 4.2.** Since $G$ is 0 for Gaussian random variables, and since the noise separates by additivity, we can drop $W\eta$ from all calculations. For simplicity, we will consider the change of coordinates $u := R^{-1}v$. As a special case of Lemma 4.1 where $R$ is the identity, we get:

$$\nabla_u G(u \cdot \tilde{s}) = r \sum_{i=1}^{d} u_i^{r-1} G(\tilde{s}_i) e_i.$$  \hfill (2)

**Claim 4.2.1.** $\nabla_u G(u \cdot \tilde{s}) = R^{-1} \nabla_v G(v \cdot y)$.

**Proof of Claim.** Using Lemma 4.1:

$$\nabla_v G(v \cdot y) = r \sum_{i=1}^{n} (v \cdot R_i)^{r-1} G(\tilde{s}_i) R_i$$

$$= r \sum_{i=1}^{n} (R^{-1}v)_i^{r-1} G(\tilde{s}_i) R e_i$$

$$= R \left( r \sum_{i=1}^{n} (u_i)^{r-1} G(\tilde{s}_i) e_i \right) = R \nabla_u G(u \cdot \tilde{s}).$$

Multiplying both sides by $R^{-1}$ gives the Claim. \hfill $\blacksquare$

$R^{-1}$ is the change of coordinates from the observed coordinate system to the coordinate system of the independent components. Hence, the update rule $v \leftarrow \nabla_v G(v \cdot y)$ in the observed coordinate system has the same effect as the update rule $u \leftarrow \nabla_u G(u \cdot \tilde{s})$ in the coordinates of $\tilde{s}$. $v$ converges to a column of $R$ (up to sign) precisely if $u$ converges to some canonical vector $\pm e_j$ (up to sign). It suffices to consider what happens in the coordinate system of $\tilde{s}$.

Without loss of generality, suppose that the coordinates of $u$ are ordered such that:

$$|u_1^{r-2}G(\tilde{s}_1)| > |u_2^{r-2}G(\tilde{s}_2)| \geq \cdots \geq |u_d^{r-2}G(\tilde{s}_d)|$$  \hfill (3)

Since there exists $i$ such that $G(s_i) \neq 0$, and since $u$ is drawn uniformly at random from the unit sphere along with $v$, such an ordering can be achieved almost surely by reindexing $u$. If any $u_i^{r-2}G(\tilde{s}_i) = 0$, the resulting value of $u_i$ after any update will always be 0, ensuring that $u$ does not converge to $e_i$.

Let $m$ denote the largest index $i$ such that $|u_i^{r-2}G(\tilde{s}_i)| > 0$. If $m = 1$, then convergence will be achieved after one update, leaving nothing to prove. So, assume $m > 1$. Let $u(k)$ denote $u$ after the $k^{th}$ update, with $u(0)$ denoting the input value of $u$. Define for $i, j \in \{1, 2, \ldots, m\}$:

$$\rho(i, j; k) := \begin{vmatrix} u_i(k) \\ u_j(k) \end{vmatrix}$$

$$g_{ij} := \begin{vmatrix} G(\tilde{s}_i) \\ G(\tilde{s}_j) \end{vmatrix}$$

$$c_{ij} := \begin{vmatrix} u_i(0)^{r-2}G(\tilde{s}_i) \\ u_j(0)^{r-2}G(\tilde{s}_j) \end{vmatrix} = \rho(i, j; 0)^{r-2}g_{ij}$$

where by assumption, $c_{ij} > 1$ for any $j > 1$. We will see that $\rho(i, j; k)$ has order $r - 1$ growth with respect to $k$:

$$\rho(i, j; k) = \begin{vmatrix} u_i(k) \\ u_j(k) \end{vmatrix} = \begin{vmatrix} u_i(k-1)^{r-1}G(\tilde{s}_i) \\ u_j(k-1)^{r-1}G(\tilde{s}_j) \end{vmatrix}$$

$$= \cdots = \rho(i, j; 0)^{(r-1)^k}g_{ij}^{\sum_{m=0}^{k-1}(r-1)^m}$$

$$= \left(c_{ij}g_{ij}^{-1}\right)^{1/(r-2)(r-1)^k}g_{ij}^{\sum_{m=0}^{k-1}(r-1)^m}$$
Algorithm 2 A fast algorithm to recover a single column of $R$ when $\nu$ is drawn generically from the unit sphere. Equations (4) and (5) provide $k$-statistic based estimates of $\nabla_{\nu} \kappa_3$ and $\nabla_{\nu} \kappa_4$, which can be used as practical choices of $\nabla_{\nu} G$ on real data.

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<thead>
<tr>
<th>Line</th>
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<tbody>
<tr>
<td>1: <strong>function</strong> G1-ICA($\nu$, $y$)</td>
</tr>
<tr>
<td>2: <strong>repeat</strong></td>
</tr>
<tr>
<td>3: $\nu \leftarrow \nabla_{\nu} G(\nu^T y)$</td>
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<tr>
<td>4: $\nu \leftarrow \nu / | \nu |_2$</td>
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<tr>
<td>5: <strong>until</strong> Convergence <strong>return</strong> $\nu$</td>
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<td>6: <strong>end function</strong></td>
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where $\frac{1}{r-2} (r-1)^k = \sum_{m=0}^{k-1} (r-1)^m + 1$ since $r-2$ can be written as $(r-1) - 1$. We get:

$$\rho(i, j; k) = c_{ij}^{1/(r-2)} |(r-1)^k - 1| g_{ij}^{1/(r-2)}$$

In particular, $\rho(1, j; k) = c_{1j}^{1/(r-2)} |(r-1)^k - 1| g_{1j}^{1/(r-2)} > c_{1j}^{(r-1)^{k-1}} g_{1j}^{1/(r-2)}$.

Assume without loss of generality that $\nu$ is symmetric. However, since $\nu$ is almost surely.

As a Corollary to Theorem 4.2 we get:

Recovering all Independent Components. As a Corollary to Theorem 4.2 we get:

**Corollary 4.3.** Suppose $R_1, R_2, \ldots, R_k$ are known for some $k < d$. Suppose there exists $i > k$ such that $G(s_i) \neq 0$. If $\nu$ is drawn uniformly at random from $S^{d-1} \cap \text{span}(R_1, \ldots, R_k)$, where $S^{d-1}$ denotes the unit sphere in $\mathbb{R}^d$, then Algorithm 2 with input $\nu$ converges to a new column of $R$ almost surely.

Since the indexing of $R$ is arbitrary, Corollary 4.3 gives a solution to noisy ICA, in Algorithm 3. In practice (not required by the theory), it may be better to enforce orthogonality between the columns of $R$ by orthogonalizing $\nu$ against previously found columns of $R$ at the end of each step in Algorithm 2. We expect the fourth or third cumulant function will typically be chosen for $G$.

### 5 Time Complexity Analysis and Estimation of Cumulants

To implement Algorithms 1 and 2 requires the estimation of functions from data. We will limit our discussion to estimation of the third and fourth cumulants, as lower order cumulants are more statistically stable to estimate than higher order cumulants. $\kappa_3$ is useful in Algorithm 2 for non-symmetric distributions. However, since $\kappa_3(s_i) = 0$ whenever $s_i$ is a symmetric distribution, it is plausible that $\kappa_3$ would not recover all columns of $R$. When $s$ is suspected of being symmetric, it
Algorithm 3 Algorithm for ICA in the presence of Gaussian noise. \( \hat{A} \) recovers \( A \) up to column order and scaling. \( R^T W \) is the demixing matrix for the observed random vector \( x \).

For simplicity of the theoretical arguments, these algorithms have been discussed as if we know the distributions of the observed random variables and can make all required computations exactly. So, matrix multiplication against a random vector should be read as defining a new distribution. In practice, the random vectors would be replaced by data matrices, and function computations would be approximated as described in Section 5.

```
function GAUSSIANROBUSTICA(G, x)
    \( \hat{W} = \text{FINDQUASIORTHOGRAMMA}(x) \)
    \( y = Wx \)
    \( R, \text{colmns} = \emptyset \)
    for \( i = 1 \) to \( d \) do
        Draw \( v \) from \( S^{d-1} \cap \text{span}(R, \text{colmns})^\perp \) uniformly at random.
        \( R, \text{colmns} = R, \text{colmns} \cup \{\text{GI-ICA}(v, y)\} \)
    end for
    Construct a matrix \( R \) using the elements of \( R, \text{colmns} \) as columns.
    \( \hat{s} = R^T y \)
    \( \hat{A} = (R^T W)^{-1} \)
return \( \hat{A}, \hat{s} \)
end function
```

is prudent to use \( \kappa_4 \) for \( G \). Alternatively, one can fall back to \( \kappa_3 \) when \( \kappa_3 \) is detected to be near 0.

Denote by \( z^{(1)}, z^{(2)}, \ldots, z^{(N)} \) the observed samples of a random variable \( z \). Given a sample, each cumulant can be estimated in an unbiased fashion by its \( k \)-statistic. Denote by \( k_r(z^{(i)}) \) the \( k \)-statistic sample estimate of \( \kappa_r(z) \). Letting \( m_r(z^{(i)}) := \frac{1}{N} \sum_{i=1}^{N} (z^{(i)} - \bar{z})^r \) give the \( r \)th sample central moment, then

\[
\kappa_3(z^{(i)}) := \frac{N^2 m_3(z^{(i)})}{(N - 1)(N - 2)}, \quad \kappa_4(z^{(i)}) := \frac{N^2 (N + 1) m_4(z^{(i)}) - 3(N - 1) m_2(z^{(i)})^2}{(N - 1)(N - 2)(N - 3)}
\]

gives the third and fourth \( k \)-statistics \([13]\). However, we are interested in estimating the gradients (for Algorithm \([2]\)) and Hessians (for Algorithm \([1]\)) of the cumulants rather than the cumulants themselves. The following Lemma shows how to obtain unbiased estimates:

**Lemma 5.1.** Let \( z \) be a \( d \)-dimensional random vector with finite moments up to order \( r \). Let \( z^{(i)} \) be an iid sample of \( z \). Let \( \alpha \in \mathbb{N}^d \) be a multi-index. Then \( \partial^{\alpha} \kappa_r(u \cdot z^{(i)}) \) is an unbiased estimate for \( \partial^{\alpha} \kappa_r(u \cdot z^{(i)}) \).

**Proof.** Let the derivatives below be with respect to \( u \). Since \( k_r \) is unbiased, we have

\[
\partial^{\alpha} \kappa_r(u \cdot z) = \partial^{\alpha} \mathbb{E}_{z^{(i)}} [k_r(u \cdot z^{(i)})] = \mathbb{E}_{z^{(i)}} [\partial^{\alpha} k_r(u \cdot z^{(i)})].
\]

To justify the second equality, we need to verify the conditions for differentiation under the integral sign. We have \( (z^{(i)}, u) \mapsto k_r(u \cdot z^{(i)}) \) is a multivariate polynomial. It is enough to expand it as a sum of monomials and justify the step for every monomial. Each monomial is of the form \( f(u) g(z^{(i)}) \) where \( g \) is of degree \( r \). Thus, under our assumptions it is integrable over \( z^{(i)} \) for every fixed \( u \).

Moreover,

\[
\partial^{\alpha} \mathbb{E}_{z^{(i)}} [f(u) g(z^{(i)})] = \partial^{\alpha} f(u) \mathbb{E}_{z^{(i)}} [g(z^{(i)})] = \mathbb{E}_{z^{(i)}} [\partial^{\alpha} f(u) g(z^{(i)})].
\]
If we mean-subtract (via the sample mean) all observed random variables, then the resulting estimates are:

\[ \nabla_u k_3(u \cdot y) = \frac{3N^2 \sum_{i=1}^{N} ((u \cdot y^{(i)})^2 y^{(i)})}{N(N-1)(N-2)} \]  

\[ \nabla_u k_4(u \cdot y) = \frac{N^2}{(N-1)(N-2)(N-3)} \left\{ 4N + 1 - \frac{12(N-1)}{N^2} \sum_{i=1}^{N} (u \cdot y^{(i)})^3 y^{(i)} \right\} \]  

\[ \mathcal{H}_u k_4(u \cdot x) = \frac{N^2}{(N-1)(N-2)(N-3)} \left\{ 12N + 1 - \frac{12(N-1)}{N^2} \sum_{i=1}^{N} (u \cdot x^{(i)})^2 (xx^T)^{(i)} \right\} \]  

Using (6) to estimate \( \mathcal{H}_u k_4(u^T x) \) from data when implementing Algorithm 1, the resulting quasi-orthogonalization algorithm runs in \( O(Nd^2) \) time. Using (4) or (5) to estimate \( \nabla_u G(y^T y) \) (with \( G \) chosen to be \( k_3 \) or \( k_4 \) respectively) when implementing Algorithm 2 gives an update step that runs in \( O(Nd) \) time. If \( t \) bounds the number of iterations to convergence in Algorithm 2, then \( O(Nd^2t) \) steps are required to recover all columns of \( R \) once quasi-orthogonalization has been achieved.

6 Simulation Results

In Figure 1, we compare our algorithms to the baselines JADE \([7]\) and versions of FastICA \([10]\), using the code made available by the authors. Except for the choice of the contrast function for FastICA, the baselines were run using default settings. All tests were done using artificially generated data. In implementing our algorithms (available at \([19]\)), we opted to enforce orthogonality during the update step of Algorithm 2 with previously found columns of \( R \). In Figure 1, we compare our algorithms on five distributions: the Laplace distribution, the Bernoulli distribution with parameter 0.5, the t-distribution with 5 degrees of freedom, the exponential distribution, and the continuous uniform distribution. Most of these distributions are symmetric, making GI-\( \kappa_3 \) inadmissible. To demonstrate the potential advantage of \( \kappa_3 \) on skewed data, we also include one test on noise-free data drawn using 10 independent exponential distributions in Appendix B.

When generating data for the ICA algorithm, we generate a random mixing matrix \( A \) with condition number 10 (minimum singular value 1 and maximum singular value 10), and intermediate singular values chosen uniformly at random. \( A \) was generated via a reverse SVD, \( A = U \Sigma V^T \), where \( U \) and \( V \) were chosen randomly among all orthogonal matrices. The scales of all underlying source signals were set to have variance 1. Where a Gaussian noise was added, the noise was made white (i.e., a multiple of \( I \)). The noise magnitude indicates the strength of an additive white Gaussian noise. We define 100% noise magnitude to mean variance 10, with 25% noise and 50% noise indicating variances 2.5 and 5 respectively. Performance was measured using the Amari Index introduced in 1. Let \( \hat{B} \) denote the approximate demixing matrix returned by an ICA algorithm, and let \( M = \hat{B} A \). Then, the Amari index is given by:

\[ E := \sum_{i=1}^{n} \sum_{j=1}^{n} \left( \frac{|m_{ij}|}{\max_k |m_{ik}|} - 1 \right) + \sum_{j=1}^{n} \sum_{i=1}^{n} \left( \frac{|m_{ij}|}{\max_k |m_{kj}|} - 1 \right). \]

The Amari index takes on values between 0 and the dimensionality \( d \). It can be roughly viewed as the distance of \( M \) from the nearest scaled permutation matrix \( PD \) (where \( P \) is a permutation matrix and \( D \) is a diagonal matrix).
From the noiseless data, we see that quasi-orthogonalization requires more data than whitening in order to provide accurate results. Once sufficient data is provided, all fourth order methods (GI-$\kappa_4$, JADE, and $\kappa_4$-FastICA) perform comparably. The difference between GI-$\kappa_4$ and $\kappa_4$-FastICA is not statistically significant over 50 runs with 100 000 samples. We note that GI-$\kappa_4$ under whitening and $\kappa_4$-FastICA have the same update step (up to a slightly different choice of estimators), with GI-$\kappa_4$ differing to allow for quasi-orthogonalization. Where provided, the error bars give a 2$\sigma$ confidence interval on the mean Amari index. In all cases, error bars for our algorithms are provided, and error bars for the baseline algorithms are provided when they do not hinder readability.

It is clear that all algorithms degrade with the addition of Gaussian noise. However, GI-$\kappa_4$ under quasi-orthogonalization degrades far less when given sufficient samples. For this reason, the quasi-orthogonalized GI-$\kappa_4$ outperforms all other algorithms (given sufficient samples) including the $\log \cosh$-FastICA, which performs best in the noiseless case. Contrasting the performance of GI-$\kappa_4$ under whitening with itself under quasi-orthogonalization, it is clear that quasi-orthogonalization is necessary to be robust to Gaussian noise.

Run times were indeed reasonably fast. For 100 000 samples on the varied distributions ($d = 5$) with 50% Gaussian noise magnitude, GI-$\kappa_4$ (including the orthogonalization step) had an average running time\(^2\) of 0.19 seconds using PCA whitening, and 0.23 seconds under quasi-orthogonalization. The corresponding average number of iterations to convergence per independent component (at 0.0001 error) were 4.16 and 4.08. We report the mean number of steps to convergence (per independent component) over the 50 runs in Figure 2 for the 50% noise distribution ($d = 5$), and note that once sufficiently many samples were taken, the number of steps to convergence becomes remarkably small. Finally, we note that for sufficiently skewed distributions, GI-$\kappa_3$ under whitening outperforms all baseline algorithms on noiseless data (see Appendix B). GI-$\kappa_3$ is consistent with quasi-orthogonalization under Gaussian noise.

7 Discussion and Future Work

We have demonstrated a practical method for performing ICA under Gaussian noise. The first key point is using a relaxation of whitening which is invariant to additive Gaussian noise. We provide the first practical implementation of quasi-orthogonalization, which like whitening orthogonalizes the

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\(^2\) Using a standard desktop with an i7-2600 3.4 GHz CPU and 16 GB RAM.
latent independent signals. Quasi-orthogonalization is a relaxation since neither are the data scaled to have unit variance, nor are the columns of the quasi-orthogonalized mixing matrix \( W A \) scaled to have unit norm. We provide a novel analysis of cumulant-based ICA algorithms which extends fast convergence rates seen in ICA to the quasi-orthogonal setting, resulting in a class of fast, Gaussian noise invariant algorithms.

We note that our update step extends naturally to include cumulant-like objects which are robust to sparse noise such as those presented in [20]. As noted earlier, there are techniques in the literature [5, 9] to perform PCA in the presence of sparse noise which could conceivably be used for the first step of ICA. It would be interesting to combine these techniques and experiment with ICA which is more robust to sparse noise.

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References


respectively in the standard fashion. Under the orthogonality constraints of ICA, and noting that from the derivatives of $\psi$ have versions of the additivity and homogeneity properties (for $\alpha$-robust cumulants of order $r > 2$) required for admissibility into Algorithm 2 in the Gaussian noise-free case. Before proceeding, it should be noted that these cumulants are designed to be robust to extreme outliers rather than Gaussian noise. As such, Welling’s robust cumulants are not fully in-line with the quasi-orthogonalization technique of this paper, which is not designed with sparse noise in mind. However, there are versions of PCA designed to be robust against sparse noise which should be compatible with Welling’s robust cumulants.

In this Appendix, we argue that Welling’s robust cumulants are admissible in the Gaussian-noise free case to the ICA Algorithm 2 given a suitable whitening or quasi-orthogonalization step. While we outline many of the necessary definitions, we make no claim to completeness, and we refer the reader to sections 2 and 3 of [20] for additional explanation. Given quasi-orthogonal random vector $y = \tilde{R}\tilde{s}$, an $\alpha$-robust characteristic function can be defined for the random vector $y$ as:

$$\psi^{(\alpha)}(t) := \mathbb{E}[\exp(\text{i}\alpha y^T t)g(\alpha, \tilde{s})]$$

where $g(\alpha, \tilde{s})$ is defined via the multi-variate standard normal probability density function $\phi$ as $g(\alpha, \tilde{s}) := \frac{\phi(\alpha, \tilde{s})}{\phi(0, \tilde{s})} = \exp(-(1/2)(\alpha^2 - 1)||\tilde{s}||_2^2)$. Then, the moments and cumulants are defined from the derivatives of $\psi^{(\alpha)}(t)$ and the second characteristic function $\psi^{(2)}(t) := \log \psi^{(1)}(t)$ respectively in the standard fashion. Under the orthogonality constraints of ICA, and noting that $||\cdot||_2$ is invariant under rotations, then $g(\alpha, y) = g(\alpha, \tilde{s})$. We can write:

$$\psi^{(\alpha)}(t) = \mathbb{E}[\exp(\text{i}\alpha y^T t)g(\alpha, y)]$$

which gives the form required for producing sample estimates.

When defining the robust moments (and cumulants) in the direction of unit vector $u$, we use the following directional $\alpha$-robust first characteristic function:

$$\psi^{(\alpha)}(t) := \mathbb{E}[\exp(\text{i}\alpha (u \cdot y)t)g(\alpha, \tilde{s})]$$

The robust moments in direction $u$ take on the form:

$$\mu^{(\alpha)}_{r,\tilde{s},u}(y) := \alpha^r \mathbb{E}[(u \cdot y)^rg(\alpha, \tilde{s})] = \alpha^r \mathbb{E}[(u \cdot y)^r]g(\alpha, y).$$

where the last equality lends itself to sampling estimates.

The robust cumulants $\kappa^{(\alpha)}_{r,\tilde{s},u}$ are related to the robust moments using the typical moment expansions, except that $\mu^{(\alpha)}_{0,\tilde{s},u}$ cannot be assumed 1, and $\mu^{(\alpha)}_{1,\tilde{s},u}$ cannot be assumed 0 for centered data as is generally
done. We refer the reader to Appendix A of [20] for the expansions of the $\alpha$-robust cumulants in terms of $\alpha$-robust moments. The following Theorem gives a version of the additivity and homogeneity properties for robust cumulants. These versions are consistent with the proof of Lemma[4.1] and hence the proof of Theorem 4.2 in the noise-free case, giving that the $\alpha$-robust cumulants are admissible to Algorithm[2].

**Theorem A.1.** Let $r > 2$. Then the $\alpha$-robust cumulant $\kappa^{(\alpha)}_{r,\mathbf{s},\mathbf{u}}$ is additive in that

$$
\kappa^{(\alpha)}_{r,\mathbf{s},\mathbf{u}}(y) = \sum_{j=1}^{d} \kappa^{(\alpha)}_{r,\mathbf{s},\mathbf{u}}((\mathbf{u} \cdot R_i)\tilde{s}_i).
$$

$\kappa^{(\alpha)}_{r,\mathbf{s},\mathbf{u}}$ is homogeneous of order $r$ in that

$$
\kappa^{(\alpha)}_{r,\mathbf{s},\mathbf{u}}((\mathbf{u} \cdot R_i)\tilde{s}_i) = (\mathbf{u} \cdot R_i)^r \kappa^{(\alpha)}_{r,\mathbf{s},\mathbf{u}}(\tilde{s}_i).
$$

**Proof.** To see additivity, it suffices to show that the directional second characteristic function has the desired additivity property:

$$
\Psi^{(\alpha)}_{\mathbf{u},\tilde{s}}(t) = \log \mathbb{E}[\exp(i\alpha(\mathbf{u} \cdot \tilde{s})t)g(\alpha, \tilde{s})] \\
= \log \mathbb{E}\left[\exp\left(i\alpha(\mathbf{u} \cdot \sum_{i=1}^{d} R_i\tilde{s}_i) t\right) \exp\left(-\frac{1}{2}(\alpha^2 - 1)||\tilde{s}||^2\right)\right] \\
= \log \prod_{j=1}^{d} \mathbb{E}[\exp(i\alpha(\mathbf{u} \cdot R_j\tilde{s}_j)t)g(\alpha, \tilde{s}_j)] \\
= \sum_{j=1}^{d} \log \mathbb{E}[\exp(i\alpha((\mathbf{u} \cdot R_j)\tilde{s}_j) t)g(\alpha, \tilde{s}_j)].
$$

To see the homogeneity property, we note that the $r^{th}$ $\alpha$-robust cumulant has a moment expansion which consists of a sum of terms where each term has order $r$. Thus, it suffices to show that the $\alpha$-robust moments have the desired homogeneity property:

$$
\mu_{r,\tilde{s}_i}((\mathbf{u} \cdot R_i)\tilde{s}_i) = \alpha^r \mathbb{E}[(\mathbf{u} \cdot R_i\tilde{s}_i)^r g(\alpha, \tilde{s}_i)] = \alpha^r (\mathbf{u} \cdot R_i)^r \mathbb{E}[\tilde{s}_i^r g(\alpha, \tilde{s}_i)] = (\mathbf{u} \cdot R_i)^r \mu_{r,\tilde{s}_i}(\tilde{s}_i).
$$

Note that we have not explored the properties of Welling’s robust cumulants under additive Gaussian noise. While these robust cumulants are known to be zero for Gaussian random variables, we have only shown additivity for independent random variables which operate in orthogonal directions. As such, we do not claim that Welling’s robust cumulants are admissible under heavy Gaussian noise like the traditional cumulants.

**B Skew Data Plot**

Comparison of ICA algorithms on skewed data. All latent random variables are drawn independently from the Exponential distributions, and mixed similarly to the other experiments from Section 6. Notably, GI-$\kappa_3$ (white) compares favorably against all baselines. We do not compare against the skew-based implementation of FastICA because the update steps happen to be the same due to the moment expansion of $\kappa_3$. 