A Spectral Method for Stable Bispectrum Inversion with Application to Multireference Alignment

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Abstract—We focus on an alignment-free method to estimate the underlying signal from a large number of noisy randomly shifted observations. Specifically, we estimate the mean, power spectrum, and bispectrum of the signal from the observations. Since the bispectrum contains the phase information of the signal, reliable algorithms for bispectrum inversion are useful in many applications. We propose a new algorithm using spectral decomposition of the bispectrum phase matrix for this task. For clean signals, we show that the eigenvectors of the bispectrum phase matrix correspond to the true phases of the signal and its shifted copies. In addition, the spectral method is robust to noise. It can be used as a stable and efficient initialization technique for local non-convex optimization for bispectrum inversion.

I. INTRODUCTION

We consider the problem of estimating a discrete signal with the following observation model,

\[ \xi_j = R_s x + \varepsilon_j, \quad j \in \{1, 2, \ldots, M\} \tag{I.1} \]

where \( \xi_j \in \mathbb{R}^N \) and \( x \in \mathbb{R}^N \), correspond to the \( j \)-th observation and the underlying signal respectively. \( R_s : \mathbb{R}^N \rightarrow \mathbb{R}^N \) denotes a cyclic shift operator that shifts the underlying signal, i.e. \((R_s x)[n] = x[n + s \mod N]\). For the sake of brief notations, all indices are understood modulo \( N \), namely, in the range \( 0, \ldots, N-1 \). \( \varepsilon_j \) represents additive white Gaussian noise with zero mean and variance \( \sigma^2 \). In multi-reference alignment (MRA) [1], both \( x \) and the translations \( \{s_j\} \) are unknown and the primary goal is to recover \( x \) from noisy observations \( \{\xi_j\}_{j=1}^M \). The alignment-free approach in [2] uses the shift invariant features, such as mean, power spectrum, and bispectrum estimated from the data to recover the underlying signal \( x \). This type of invariant features are related to the method of moments [3].

Consider the case where the number of observations is much larger than the length of the signal, namely \( M \gg N \). In this regime, the invariant features approach has two important advantages over methods that rely on estimating the translations, 1) there will be no need to determine the translations in order to recover the signal hence reducing the computational complexity of the problem, and 2) with high level of noise, given enough samples, it does not suffer from the fundamental limit [4] for the pairwise alignment approach. Using invariant moments, the lower bound on the mean squared error (MSE) between the true and the recovered signal depends on the maximum order of the moments and the number of samples \( M \) as shown in [5] for classic MRA and in [6] for non-uniform distributions of translations. They were also extended to more general groups in [7]–[9]. These sample complexities provide the stability guarantee for signal recovery from the moment based invariant features.

Exploiting bispectrum as another invariant feature in addition to power spectrum adds the phase information for estimating the signal. The bispectrum also plays a central role in a variety of signal processing applications. For example, it is a key tool to separate Gaussian and non-Gaussian processes [10], [11]. It is also used in seismic signal processing [12], image deblurring [13], MIMO systems [14], feature extraction for radar [15], analysis of EEG signals [16], cryo-EM image classification [17] and cosmic background radiation analysis [18], [19]. A more general setting of bispectrum over compact groups was considered in [20]–[23]. Many of those applications require reliable algorithms to invert the bispectrum.

A variety of algorithms have been proposed to invert bispectrum [2], [12], [24]–[26]. In particular, two non-convex optimization algorithms on the manifold of phases in [2] are able to recover phases exactly (up to global time shift) with random initialization in the absence of noise. Several initialization algorithms were also proposed in [2], such as semidefinite programming (SDP), phase unwrapping by integer programming (IP), frequency marching (FM). The SDP and IP methods are computationally expensive, and therefore do not scale well with the signal length. Although FM is efficient with \( O(N^2) \) computational complexity, it is not robust to noise. In [5], Jennrich’s algorithm [27] was used to decompose the third-order moment tensor to recover the underlying signal.

In this letter, we propose a new initialization algorithm using spectral decomposition of the bispectrum phase matrix. For clean signals, we show that the eigenvectors of the bispectrum phase matrix correspond to the true phases of the signal and its shifted copies. With bispectrum estimated from the noisy observations, we propose a rule to select the eigenvector for robust estimation of the phase. The computational complexity of the spectral initialization given the invariant features is \( O(N^3) \), which is dominated by the eigendecomposition of an \( N \times N \) bispectrum phase matrix. We compare our spectral method with different bispectral inversion techniques through the relative error of reconstruction and computation time. In addition, we demonstrate that with the spectral initialization, the local non-convex approach converges much faster than the random initialization, thus reducing the overall computation time.

Throughout the letter we use the following notation. Vectors

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\( x \in \mathbb{R}^N \) and \( y \in \mathbb{C}^N \) denote the underlying signal and its discrete Fourier transform (DFT) respectively. We use \( \hat{a} = \text{phase}(a) \) for the phase of a complex number and \( \pi \) for its complex conjugate. When \( a = 0 \), we assume its phase \( \hat{a} = 1 \). We denote by \( z^* \) the conjugate-transpose of \( z \) and denote by \( \odot \) the Hadamard (entry-wise) product. \( C(z) \) denotes circulant matrices determined by their first row \( z \), i.e., \( C(z)[k_1, k_2] = z[k_2 - k_1] \).

Reproducible research: our code is available in https://github.com/ARKEYTECT/Bispectrum_Inversion.

II. INvariant Features for Multireference Alignment

We solve the MRA problem directly using features that are invariant under translations, namely, the DC component, power spectrum, and bispectrum of the signal. The DFT of a signal is defined as, \( \text{DFT}(x)[k] = \sum_{n=0}^{N-1} x[n] e^{-2\pi i nk/N} \). Shifting the signal in time domain introduces a phase shift in the Fourier coefficients, \( \text{DFT}(R_x x)[k] = y[k] e^{2\pi ikx/N} \). The DC component of the signal \( y[0] = N \mu_x = \sum_{n=0}^{N-1} x[n] \), where \( \mu_x \) is the mean of the signal, is clearly invariant to translation. The distribution of the mean of the observations \( \xi_j \) is then given by \( \mu_{\xi_j} \sim \mathcal{N} \left( \mu_x, \frac{\sigma^2}{NM} \right) \) and the unbiased estimate of \( \mu_x \) is defined as

\[
\hat{\mu} = \frac{1}{M} \sum_{j=1}^{M} \left( \frac{1}{N} \sum_{n=0}^{N-1} \xi_j[n] \right) \sim \mathcal{N} \left( \mu_x, \frac{\sigma^2}{NM} \right) . \tag{II.1}
\]

Therefore, the estimated DC component is \( \hat{y}[0] = N \hat{\mu} \).

In addition to the DC term, power spectrum, which is defined as \( P_x[k] = |y[k]|^2 \) for all \( k \in \{0, 1, \ldots, N-1\} \) provides the information of the Fourier magnitudes. The power spectrum only affects the phase of the Fourier coefficients, power spectrum is invariant to the translations. An estimator for the power spectrum from noisy samples is

\[
\hat{P}[k] = \frac{1}{M} \sum_{j=1}^{M} P_{\xi_j}[k] - N \sigma^2 \rightarrow P_x[k], \text{ as } M \rightarrow \infty, \tag{II.2}
\]

where its variance is dominated by \( \frac{N^2 \sigma^4}{M} \) for large \( \sigma \). An unbiased estimator of \( \sigma \) is derived from \( \hat{\sigma}^2 = \frac{1}{N} \text{Var} \left( \sum_{n=0}^{N-1} \xi_j[n] \right) \). In the letter, we assume that \( \sigma \) is known.

The bispectrum is a function of two frequencies \( k_1, k_2 = \{0, \ldots, N-1\} \) and is defined as,

\[
B_x[k_1, k_2] = y[k_1] y[k_2] y[k_2 - k_1] . \tag{II.3}
\]

For any shift \( s \), \( B_{R_x x}[k_1, k_2] \) is

\[
B_{R_x x}[k_1, k_2] = \left( y[k_1] e^{2\pi ik_1 s/N} \right) \left( y[k_2] e^{-2\pi ik_2 s/N} \right) \left( y[k_2 - k_1] e^{2\pi i(k_2-k_1) s/N} \right) = B_x[k_1, k_2] , \tag{II.3}
\]

Hence, the bispectrum is shift invariant and it contains the phase information of the signal \( x \). In matrix notation, we express \( B_x \) as

\[
B_x = yy^* \circ C(y) = Y \circ C(y) , \tag{II.4}
\]

where \( Y = yy^* \) is a rank-one matrix. For the bispectrum phase \( \hat{B}_x[k_1, k_2] = \text{phase}(B_x[k_1, k_2]) \), \( \hat{B}_x[k_1, k_2] = \hat{y}[k_1] \hat{y}[k_2] \hat{y}[k_2 - k_1] \). In matrix notation, it takes the form

\[
\hat{B}_x = \hat{Y} \circ C(\hat{y}) , \quad \text{where } \hat{Y} = \hat{y} \hat{y}^* . \tag{II.5}
\]

The expectation of the bispectrum built from noisy observation is

\[
\mathbb{E} \left\{ B_{\xi_j}[k_1, k_2] \right\} = B_x[k_1, k_2] + N \sigma^2 y[0] \left( \delta(k_1, k_2) + \delta(k_1, 0) + \delta(k_2, 0) \right) . \tag{II.6}
\]

Therefore, by removing the DC component for each \( \xi_j \), we get an unbiased estimator

\[
\hat{B} = \frac{1}{M} \sum_{j=1}^{M} B_{\xi_j} - \mu_{\xi_j} \rightarrow B_x - \mu_x, \text{ as } M \rightarrow \infty \tag{II.7}
\]

where \( \mu_{\xi_j} \) is the mean of signal \( \xi_j \), the variance of \( \hat{B} \) is controlled by \( \frac{N^2 \sigma^4}{M} \) for large \( \sigma \) and the estimator in (II.7) is asymptotically unbiased. Note that to ensure stable estimations of \( \mu_x \), \( P_x \) and \( B_x \), \( M \) is required to scale \( O(\sigma^2) \), \( O(\sigma^4) \) and \( O(\sigma^6) \) respectively.

The computational complexity of deriving estimations of the invariants is \( O(MN^2) \) and the storage requirement is \( O(N^2) \) [2]. Additionally, it requires only one pass over the data which is important in high-throughput experiments, when the number of observations is large. The invariant features can be computed in parallel.

III. Spectral Method for Phase Recovery in Bispectral Inversion

The signal reconstruction process could be split into three parts, namely, the DC component estimation, Fourier magnitude estimation, and phase estimation. Then an estimate of \( y \) denoted by \( \hat{y} \) is achieved. The estimated real signal \( \hat{x} \) is the inverse DFT of \( \hat{y} \).

Since \( x \) is real, \( y[k] = \overline{y[-k]} \) and \( C(y) \) and \( B_x \) in (II.4) are Hermitian matrices. The circulant matrix \( C(\hat{y}) \) can be diagonalized by the normalized DFT matrix \( F \) with \( F_{ij} = \frac{1}{\sqrt{N}} e^{-i \frac{2\pi ij}{N}} \), that is,

\[
C(\hat{y}) = F \text{diag}(F\hat{y}) F^* . \tag{III.1}
\]

Following Eq. (II.5) for a clean signal,

\[
\hat{B} = \hat{y} \hat{y}^* \circ C(\hat{y}) = \text{diag}(\hat{y}) F \text{diag}(F\hat{y}) F^* \text{diag}(\hat{y})^* \tag{III.2}
\]

Since \( y[k] \) are phases, the matrix \( V = \text{diag}(\hat{y}) F \) is a unitary matrix, i.e. \( VV^* = V^* V = I \). Therefore, columns of \( V \) are the eigenvectors of \( \hat{B} \) and \( F\hat{y} \) contains the corresponding eigenvalues. We use \( S \) to denote the permutation matrix that sorts \( F\hat{y} \) in descending order. \( S \) is an orthogonal matrix \( S^T = S^T S = I \). Therefore, we can rewrite Eq. (III.2) and,

\[
\hat{B} = VS^T \text{diag}(F\hat{y}) V^* S \tag{III.3}
\]

\[
= VS^T \text{diag}(SF\hat{y}) (VS^T)^* = UAU^*, \tag{III.3}
\]
where the diagonal matrix $\Lambda$ contains the eigenvalues of $\tilde{B}$ sorted in descending order, $\lambda_1 \geq \lambda_2 \cdots \geq \lambda_N$ with the corresponding eigenvectors $U = [u_1, u_2, \ldots, u_N]$. Eq. (III.3) reveals that $\tilde{y}$ is encoded in both $\Lambda$ and $U$. If the order of the eigenvalues in $\Lambda$ happen to be exactly the same as $F\tilde{y}$, i.e. $S = I$, then the phases can be computed from the inverse DFT of the sorted eigenvalues.

However, in general, the sorted eigenvalues correspond to an unknown permutation of $F\tilde{y}$. Recovering $\tilde{y}$ from $\Lambda$ involves searching through all possible permutations of the eigenvalues, which is computationally expensive. Thus, we exploit $U$ in order to derive $\tilde{y}$. Each column of $U$ with distinct eigenvalues contains the phases of the original signal and its shifted versions, since $u_i[k] = \frac{1}{\sqrt{N}} \tilde{y}[k] e^{-i \frac{2\pi}{N} i k} = \frac{1}{\sqrt{N}} \text{phase(DFT}(R_{s_i} x) [k])$, where $s_i \in [0, 1, \ldots, N - 1]$ and $k = 0, \ldots, N - 1$. Therefore, in the clean case, we can recover $\tilde{y}$ up to a phase shift from any column of $U$ with distinct eigenvalues. However, in the noisy case, some of the columns of $U$ are deeply contaminated by noise that they contain very little information about $\tilde{y}$, thus we can not choose any random column of $U$.

We propose to select the eigenvector of the bispectrum phase matrix with the largest minimum spectral gap. With $\{\lambda_i\}_{i=1}^N$ sorted in descending order, the minimum spectral gap $\Delta_i$ for $\lambda_i$ is defined as,

$$\Delta_i = \min(\lambda_{i-1} - \lambda_i, \lambda_i - \lambda_{i+1}), \quad \text{for } 1 < i < N$$

$$\Delta_1 = \lambda_1 - \lambda_2, \quad \text{and } \Delta_N = \lambda_N - \lambda_{N-1} - \lambda_N.$$  \hspace{1cm} (III.4)

Let us denote by $v$ the selected eigenvector. We assume the DC component phase is 1, i.e. $\hat{v}[0] = 1$ therefore we normalize by $\hat{v}[k] = v[k]/|v[0]|$. Since each enter of $\tilde{y}$ should have unit norm, therefore, the phase estimate $\tilde{y}[k] = \text{phase}(\hat{v}[k])$. The steps for our algorithm are illustrated in Algorithm 1. If there are multiple eigenvectors with the same spectral gap, we then consider the one with largest absolute eigenvalue.

Proposition II.2, proposition II.3 along with the corresponding proofs provided in Appendix A in [2] guarantee the stable estimation of the signal from the invariant features when enough number of samples are provided ($M \sim O(\sigma^9)$). The spectral method for phase estimation is more robust to noise than the sequential recovery approach used in the proof in [2, Appendix A]. Therefore, the stability results can be applied to our framework as well. Empirically, we find that the spectral method is more robust to noise than existing initialization algorithms (see Figures IV.1 and IV.3).

The computational complexity of the spectral method is $O(N^3)$. Combining with the complexity for feature generation in Section II, this leads to an overall complexity of $O(MN^2 + N^3) \rightarrow O(MN^2)$, when $M \gg N$.

IV. NUMERICAL EXPERIMENTS

In this section, we present the numerical results for the algorithm described in Algorithm 1. We use a random signal $x$ of length $N = 41$, each entry of the signal is an i.i.d. Gaussian random variable with mean zero and variance 1. $M$ randomly shifted and noisy observations of $x$ are generated following (I.1). We assess our method through relative reconstruction error defined as,

$$\text{relative error}(x, \hat{x}) = \min_{s \in \{0, \ldots, N-1\}} \frac{\|R_s \hat{x} - x\|_2}{\|x\|_2},$$

We compare our spectral method with several algorithms described in [2] such as iterative phase synchronization, optimization on phase manifold, frequency marching, phase unwrapping, SDP relaxation and known-shifts oracle. In addition, we include homogeneous MRA with Jennrich algorithm [5], which decomposes the invariant third-order moment tensor to extract the original signal. The known-shifts oracle aligns the underlying signals perfectly, therefore the estimation error is only due to the noise and not misalignment. This oracle is regarded as the best possible performance for MRA. We use Manopt toolbox [28] for the optimization on phase manifold to estimate phase. The tool box is also applied for the iterative phase synchronization for 15 iterations with warm-start. The estimation error are averaged over 50 trials. The experiments are conducted in MATLAB on a computer with Intel i7 7th generation quad core CPU.

Figure IV.1 shows the relative estimation error of all approaches mentioned above for fixed number of samples $M$ = $10^4$ and varying noise variance $\sigma^2$. The known-shifts oracle provides the most accurate estimation of the signal, followed by the iterative phase synchronization, and the optimization.

![Figure IV.1: Relative estimation error for the signal $x$ as a function of the noise variance $\sigma^2$ with $M$ = $10^4$ copies of observations. Note that the curves for the optim. on phase manifold and the iterative phase synch. overlap.](image)
on phase manifold. For $\sigma^2 \leq 0.32$, the spectral method is comparable to the optimization on phase manifold and the iterative phase synchronization in terms of relative recovery error. The homogeneous MRA with Jennrich’s algorithm works well at low noise level ($\sigma^2 < 0.025$). However, when noise variance increases, the estimation error becomes much larger than the new spectral method. Figure IV.2 shows the median computation times for estimating the signal from the invariant features over 50 trials. The new spectral approach is the second most efficient method, following the frequency marching method. Jennrich’s algorithm is also very efficient compared to the iterative methods. However, since it requires two eigendecompositions [5], it is less efficient than the spectral method proposed here.

We then fix the noise level at $\sigma = 1$ and vary the number of observations from $10$ to $10^5$. Figure IV.3 compares the estimation error of the spectral method against the baselines mentioned in the previous experiment. The known-shifts oracle indicates the lower bound for the recovery. The performance of two non-convex optimization methods are almost identical and they outperform the spectral method in terms of relative error (see Figure IV.3). Since the runtimes for the signal recovery from invariant features does not depend on the number of samples, they are the same as the runtimes shown in Figure IV.2 for $\sigma = 1$. The invariant features used here are computed from the Fourier coefficients of the signals, whereas the invariant features are computed directly from the signals in [5]. We find that for $N = 41$, our feature generation is two times faster than the implementation in [5] for all $M$.

Figure IV.2: Median computation times (in seconds) over 50 trials regarding to Fig. IV.1

![Figure IV.2](image)

Figure IV.3: Relative estimation error for the signal $x$ as a function of numbers of observations $M$. Note that curves regarding the optim. phase manifold and the iter. phase synch. overlap.

![Figure IV.3](image)

Figure IV.4: Median computation times (blue lines) and number of iterations (orange lines) for estimating phases using the optim. on phase manifold with random initialization (solid lines) and spectral initialization (dashed lines). The time for generating the initial guess using Algorithm 1 is included.

Figure IV.4 shows that spectral initialization reduces the number of iterations for the optimization on phase manifold to converge and reduces the total computation time. The results are computed over 500 trials. As $\sigma^2$ increases, the number of iterations after spectral initialization rises, because the initial guess deviates more from the ground truth.

V. Conclusion

In this letter, we introduced a new spectral initialization approach for recovering a signal from its noisy randomly shifted copies. The random shifts are unknown. We use shift invariant features to estimate the underlying signal. The invariant features approach has low computational complexity for large sample size compared to alternative methods, such as maximum marginalized likelihood [2]. Previously, two non-convex optimization approaches were proposed along with several initialization algorithms. The new spectral method for bispectral inversion achieves exact recovery when the observations are clean and is more robust to noise compared to previous initialization algorithms. It also reduces the number of iterations required for convergence of non-convex optimization methods compared to random initialization. We plan to rigorously analyze the noise-robustness of the spectral method in the future work.

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