Exact Minimax Optimality of Spectral Methods in Phase Synchronization and Orthogonal Group Synchronization



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#### Phase Synchronization

Problem Setup:

- $\bullet$  *n* unit complex numbers  $z_1^*, \ldots, z_n^* \in \mathbb{C}$ , each one corresponds to a phase / angle in (0*,* 2*π*]
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- *•* We want to estimate them from their incomplete and noisy pairwise comparisons



If not missing,  $X_{jk} =$  noisy version of  $z_j^* \overline{z_k^*}$ 

# Motivation: Single Particle Cryo-EM

Schematic drawing of the imaging process:



The standard cryo-EM reconstruction problem:



#### Model



For 
$$
1 \le j < k \le n
$$
,  
\n
$$
X_{jk} := \begin{cases} z_j^* \overline{z_k^*} + \sigma W_{jk}, & \text{if } A_{jk} = 1, \\ 0, & \text{if } A_{jk} = 0, \end{cases}
$$

where  $A_{jk}$  ∼ Bernoulli $(p)$  and  $W_{jk}$  ∼  $CN(0, 1)$ .

Matrix Form: Let 
$$
z^* = (z_1^*, \dots, z_n^*)^T
$$
. Then  
\n $X = A \circ (z^* z^{*H} + \sigma W) = A \circ (z^* z^{*H}) + \sigma A \circ W$ 

# Spectral Method (aka Eigenvector Method [Singer, A. (2011)])

Motivation:  $\mathbb{E}X = pz^*z^{*H} - pI_n$ . Its leading eigenvector is  $z^*/\sqrt{n}$ .

Step 1: Let *u* be the leading eigenvector of *X*. Step 2: The spectral estimator  $\hat{z}$  is defined as

$$
\hat{z}_j = \begin{cases} \frac{u_j}{|u_j|}, \text{ if } u_j \neq 0, \\ 1, \quad \text{if } u_j = 0. \end{cases}
$$

Eigendecomposition + Normalization

To measure its performance:

$$
\ell(\hat{z},z^*):=\frac{1}{n}\min_{a\in\mathbb{C}_1}\sum_{j=1}^n\big|\hat{z}_j-z_j^*a\big|^2
$$

# Existing Results

With high probability, if  $\frac{np}{\log n} \to \infty$ , then

$$
\ell(\hat{z},z^*) \leq C\left(\frac{\sigma^2}{np} + \frac{1}{np}\right).
$$

Two sources of errors:

- 1.  $\frac{\sigma^2}{n r}$  $\frac{\sigma^2}{np}$ : from additive Gaussian noises
- 2.  $\frac{1}{np}$ : from missing data

However, the minimax risk is

$$
\inf_{z \in \mathbb{C}^n} \sup_{z^* \in \mathbb{C}^n_1} \mathbb{E}\ell(z, z^*) \ge (1 - o(1)) \frac{1}{2} \frac{\sigma^2}{np}.
$$

(If we consider all possible methods, how small the error can be?)

### New Result 1: Exact Recovery for No-additive-noise Case

When  $\sigma = 0$ :  $Z_i$  $\operatorname{z}_k^*$ 

$$
X_{jk} = \begin{cases} z_j^* \overline{z_k^*}, & \text{if } A_{jk} = 1, \\ 0, & \text{if } A_{jk} = 0. \end{cases}
$$

Matrix form: 
$$
X = A \circ (z^* z^{*H})
$$

#### Lemma

*If*  $\sigma = 0$  and  $\frac{np}{\log n} \to \infty$ . With high probability,  $\ell(\hat{z}, z^*) = 0$ , i.e., *the spectral method achieves the exact recovery.*

# New Result 2: Exact Minimax Optimality

#### Theorem (**Z.**. 2024)

 $\textit{Assume}\ \frac{np}{\sigma^2}\rightarrow\infty$  and  $\frac{np}{\text{log}\,n}\rightarrow\infty.$  With high probability

$$
\ell(\hat{z}, z^*) \le (1 + o(1)) \frac{1}{2} \frac{\sigma^2}{np}.
$$

Remarks:

- *•* Achieves the exact minimax risk
- **•**  $\frac{np}{σ^2}$  → ∞ is for consistency
- *• np* log *<sup>n</sup>* ≳ 1 is for the comparison graph *A ∼* Erdös-Rényi(*n, p*) to be connected



### New Result 2: Exact Minimax Optimality

Theorem (**Z.**. 2024)

 $\textit{Assume}\ \frac{np}{\sigma^2}\rightarrow\infty$  and  $\frac{np}{\text{log}\,n}\rightarrow\infty$ . With high probability

$$
\ell(\hat{z}, z^*) \le (1 + o(1)) \frac{1}{2} \frac{\sigma^2}{np}.
$$

Remarks:

*•* As good as more sophisticated procedures including maximum likelihood estimation (MLE), generalized power method (GPM), and semidefinite programming (SDP), under this parameter regime.

Novelty 1: Choice of the "population matrix"

*•* In literature, *X* is viewed as a perturbation of E*X*



- *•* Consequently, *u* is viewed as a perturbation of *z ∗*/ *√ n*, the leading eigenvector of E*X*.
- *•* The distance between *u* and *z ∗*/ *√ n* can be upper bounded by the Davis-Kahan Theorem, which leads to the existing loose bound.

Novelty 1: Choice of the "population matrix"

• In our analysis, recall  $X = A \circ (z^* z^{*H}) + \sigma A \circ W$ . We view  $X$ as a perturbation of  $A \circ (z^*z^{*\mathsf{H}})$ .



- *•* Consequently, we view *u* as a perturbation of *u ∗* , the leading eigenvector of  $A \circ (z^*z^{*\mathsf{H}})$ .
- *u* is closer to  $u^*$  than to  $z^*/\sqrt{n}$ .

Novelty 2: Approximating eigenvectors by their first-order approximations

- *•* Classical matrix perturbation theory such as Davis-Kahan Theorem focuses on analyzing inf $_{b \in \mathbb{C}_1} ||u - u^*b||$ .
- *•* We show *u* can be well-approximated by its first-order approximation  $\tilde{u}$  defined as

$$
\tilde{u}:=\frac{Xu^*}{\|Xu^*\|},
$$

- $\inf_{b \in \mathbb{C}_1} ||u \tilde{u}b||$  is much smaller than  $\inf_{b \in \mathbb{C}_1} ||u u^*b||$ , meaning  $u$  is closer to  $\tilde{u}$  than to  $u^*$ .
- We study  $\tilde{u}$  to understand behavior of  $u$  and the performance of the spectral method.

Novelty 2: Approximating eigenvectors by their first-order approximations

A general perturbation result:

#### Lemma (**Z.**. 2024)

*Consider two Hermitian matrices*  $Y, Y^* \in \mathbb{C}^{n \times n}$ . Let  $\mu_1^* \ge \mu_2^* \ge \ldots \ge \mu_n^*$  be the eigenvalues of  $Y^*$ . Let  $v^*$  (resp.  $v$ ) be *the eigenvector of Y ∗ (resp. Y ) corresponding to its largest eigenvalue. If*  $||Y - Y^*|| \le \min\{\mu_1^* - \mu_2^*, \mu_1^*\}/4$ *, we have* 

$$
\inf_{b \in \mathbb{C}_1} \left\| v - \frac{Yv^*}{\|Yv^*\|}b \right\| \le \frac{40\sqrt{2}}{9(\mu_1^* - \mu_2^*)} \Bigg( \left( \frac{4}{\mu_1^* - \mu_2^*} + \frac{2}{\mu_1^*} \right) \|Y - Y^*\|^2 + \frac{\max\{|\mu_2^*|, |\mu_n^*|\}}{\mu_1^*} \|Y - Y^*\| \Bigg).
$$

*If Y*<sup>∗</sup> is rank-one, it gives  $\|Y-Y^*\|^2/(\mu_1^*)^2$  vs.  $\|Y-Y^*\|/\mu_1^*$ from Davis-Kahan.

#### Generalization to Orthogonal Group Synchronization

 $Z_1^*, \ldots, Z_n^* \in \mathcal{O}(d)$  are  $d \times d$  orthogonal matrices



For  $1 \leq i \leq k \leq n$ ,

$$
X_{jk}:=\begin{cases} Z_j^*(Z_k^*)^T+\sigma W_{jk}, \text{ if } A_{jk}=1,\\ 0, \text{ if } A_{jk}=0, \end{cases}
$$

where  $A_{jk}$  ∼ Bernoulli $(p)$  and  $W_{jk}$  ∼  $\mathcal{MN}(0, I_d, I_d)$ .

Generalization to Orthogonal Group Synchronization

Spectral Method:

Step 1:  $U = (u_1, \ldots, u_d) \in \mathbb{R}^{nd \times d}$  to include the leading  $d$ eigenvectors of *X*. Write

$$
U = \begin{pmatrix} U_1 \\ U_2 \\ \dots \\ U_n \end{pmatrix}
$$

such that  $U_j \in \mathbb{R}^{d \times d}$  is its *j*th block. Step 2:

$$
\hat{Z}_j := \begin{cases} \mathcal{P}(U_j), & \text{if } \det(U_j) \neq 0, \\ I_d, & \text{if } \det(U_j) = 0, \end{cases}
$$

Here the mapping  $\mathcal{P}:\mathbb{R}^{d\times d}\to\mathcal{O}(d)$  is from the polar decomposition.

# Exact Minimax Optimality in Orthogonal Group **Synchronization**

#### Theorem (**Z.**. 2024)

 $\textit{Assume}\ d = O(1).$  Assume  $\frac{np}{\sigma^2}\to\infty$  and  $\frac{np}{\log n}\to\infty.$  With high *probability*

$$
\ell^{od}(\hat{Z}, Z^*) \le (1 + o(1)) \frac{d(d-1)\sigma^2}{2np}.
$$

The minimax risk is

$$
\inf_{Z \in \mathbb{R}^{nd \times d}} \sup_{Z^* \in \mathcal{O}(d)^n} \mathbb{E} \ell^{\text{od}}(Z, Z^*) \ge (1 - o(1)) \, \frac{d(d-1)\sigma^2}{2np}.
$$

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