Multi-Representation Manifold Learning on Fibre Bundles

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Outline

Motivation

Class Averaging and Phase Synchronization

Multi-Frequency Phase Synchronization

- A Multi-Frequency Formulation
- A Proof by Picture

Multi-Frequency Class Averaging

Some Representation Theoretic Patterns

From a Fibre Bundle Point of View

Joint work with Yifeng Fan (UIUC) & Zhizhen Zhao (UIUC)

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Representation?



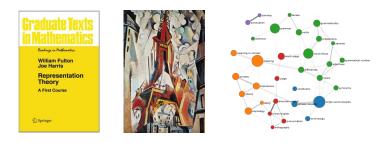


GTM129

Robert Delaunay (1885–1941)

Word2Vec

Representation?



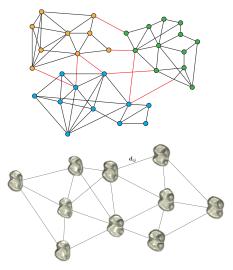
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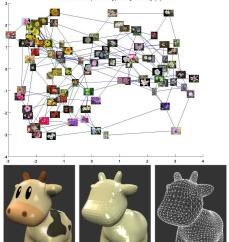
Word2Vec



Graph: A Flexible Data Representation



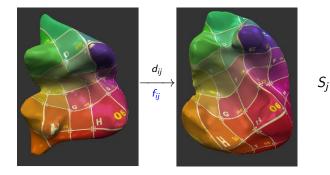
Two-dimensional Isomap embedding (with neighborhood graph).



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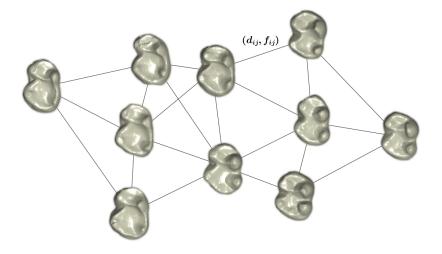
Non-Scalar Edge Weights

$$d_{\mathrm{cP}}\left(S_{i},S_{j}\right) = \inf_{\mathcal{C}\in\mathcal{A}\left(S_{i},S_{j}\right)} \inf_{R\in\mathbb{E}(3)} \left(\int_{S_{i}} \|R\left(x\right)-\mathcal{C}\left(x\right)\|^{2} d\mathrm{vol}_{S_{i}}\left(x\right)\right)^{\frac{1}{2}}$$



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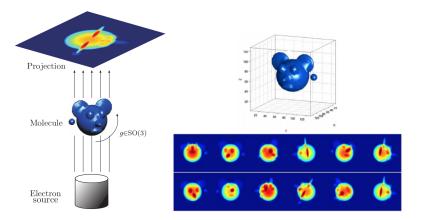
Do Graph Representations Have Enough Expressive Power?



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Cryo-Electron Microscopy



• Singer et al. "Viewing Angle Classification of Cryo-Electron Microscopy Images using Eigenvectors", SIAM Journal on Imaging Sciences, 4 (2), pp. 543–572 (2011).

Cryo-Electron Microscopy: Real Challenge is Low SNR

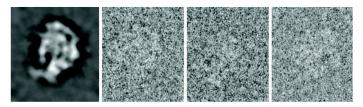


Fig. 3 The left most image is a clean simulated projection image of the E.coli 50S ribosomal subunit. The other three images are real electron microscope images of the same subunit

Apply Class Averaging to improve SNR!

- For each image, identify nearest neighbors in terms of similar viewing directions
- Average out the image with the identified neighbor images (with respect to the correct pairwise rotations)

[•] Hadani & Singer. "Representation Theoretic Patterns in Three-Dimensional Cryo-Electron Microscopy II – The Class Averaging Problem," Foundations of Computational Mathematics, 11 (5), pp. 589–616 (2011).

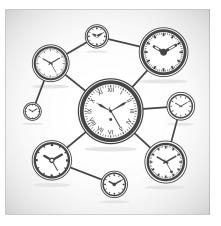
Phase Synchronization

▶ **Problem:** Recover rotation angles $\theta_1, \ldots, \theta_n \in [0, 2\pi]$ from noisy measurements of their pairwise offsets

 $\theta_{ij} \equiv \theta_i - \theta_j + \text{noise}$

for some or all pairs of (i, j)

 Examples: Class averaging in cryo-EM image analysis, shape registration and community detection



Phase Synchronization (Notation: $\mathbb{C}_1^n := [\mathrm{U}(1)]^n$)

Setup: Phase vector z = (e^{ιθ1},..., e^{ιθn})^T ∈ Cⁿ₁, noisy pairwise measurements in *n*-by-*n* Hermitian matrix

$$H_{ij} = egin{cases} e^{\iotaig(heta_i- heta_jig)} = z_iar{z}_j & ext{with prob. } r\in[0,1] \ ext{Uniform}\left(ext{U}(1)
ight) & ext{with prob. } 1-r \end{cases}$$

and $H_{ij} = \overline{H_{ji}}$. This is known as a random corruption model.

- Goal: Recover the true phase vector z (up to a global multiplicative factor)
- Existing method: Rank-1 recovery (e.g. convex relaxations)

$$\hat{x} := \operatorname*{arg\,min}_{x \in \mathbb{C}_1^n} \|xx^* - H\|_{\mathrm{F}}^2 \quad \Leftrightarrow \quad \hat{x} := \operatorname*{arg\,max}_{x \in \mathbb{C}_1^n} x^* Hx$$

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- Goal: Recover the true phase vector z (up to a global multiplicative factor)
- Spectral Relaxation: solve for the top eigenvector of H, denoted as x̃ (scaled to ||x̃||₂ = √n), then define x̂ ∈ C₁ⁿ by

$$\hat{x}_i := \tilde{x}_i / |\tilde{x}_i|$$

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► The rank-1 recovery formulation $\hat{x} := \underset{x \in \mathbb{C}_1^n}{\arg \min} \|xx^* - H\|_{\mathrm{F}}^2 \iff \hat{x} := \underset{x \in \mathbb{C}_1^n}{\arg \max} x^* Hx$ does not fully exploit that entries of x and H are **phases**!

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- ► Solve a family of coupled matrix factorization problems jointly $\hat{x}^{(k)} := \underset{x \in \mathbb{C}_{1}^{n}}{\arg \max} (x^{k})^{*} H^{(k)} x^{k}, \quad k = 1, 2, ..., k_{\max}$ where $x^{k} := (x_{1}^{k}, ..., x_{n}^{k})^{\top} \in \mathbb{C}_{1}^{n}$, and $H^{(k)}$ is the *n*-by-*n* Hermitian matrix with $H_{ij}^{(k)} := H_{ij}^{k}$, and then "stitch up" the individual estimates $\hat{x}^{(1)}, ..., \hat{x}^{(k_{\max})}$ to recover \hat{x}

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- ► The "stitching" step strives to recover e^{iθ} from noisy measurements of e^{iθ},..., e^{ikmaxθ}, which is a version of harmonic retrieval

Multi-Frequency Phase Synchronization

Multi-Frequency Formulation:

$$\max_{x\in\mathbb{C}_1^n}\sum_{k=1}^{k_{\max}}(x^k)^*H^{(k)}x^k$$

where $x^k := (x_1^k, \dots, x_n^k)^\top \in \mathbb{C}_1^n$, and $H^{(k)}$ is the *n*-by-*n* Hermitian matrix with $H_{ij}^{(k)} := H_{ij}^k$

- Intuition: Matching higher trigonometric moments
- Two-stage Algorithm: (i) Good initialization (ii) Local methods e.g. gradient descent or (generalized) power iteration

▶ Fix k_{max} ≥ 1, build H⁽²⁾,..., H^(k_{max}) out of H = H⁽¹⁾ by taking entrywise powers of H

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- ► For each k = 1,..., k_{max}, find a reasonably good symmetric rank-1 approximation

$$W^{(k)} := \underset{\substack{Y=Y^{\top}\\ \operatorname{rank}(Y)=1}}{\operatorname{arg\,max}} \left\| H^{(k)} - Y \right\|_{F}^{2}$$

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using e.g. spectral method

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For all 1 ≤ i, j ≤ n, find the "peak location" of the spectrogram

$$\hat{ heta}_{ij} := rgmax_{\phi \in [0,2\pi]} \left| rac{1}{2} \sum_{k=-k_{\max}}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k \phi}
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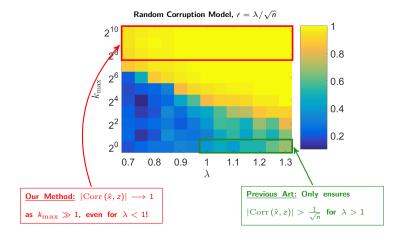
using e.g. spectral method

For all 1 ≤ i, j ≤ n, find the "peak location" of the spectrogram

$$\hat{ heta}_{ij} := rgmax_{\phi \in [0,2\pi]} \left| rac{1}{2} \sum_{k=-k_{ ext{max}}}^{k_{ ext{max}}} W_{ij}^{(k)} e^{-\iota k \phi}
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• Apply the spectral method yet again to the Hermitian matrix \widehat{H} to get $\widehat{x} \in \mathbb{C}_1^n$, where $\widehat{H}_{ij} = e^{\iota \widehat{\theta}_{ij}}$

How well does it work? Evaluate correlation $|Corr(\hat{x}, z)|$



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New Theory: Strong Recovery

Theorem (G.–Zhao 2019). Under (mild) assumptions, with high probability, the multi-frequency phase synchronization algorithm produces an estimate \hat{x} satisfying

$$|\operatorname{Corr}(\hat{x},z)| \geq 1 - rac{C'}{k_{\max}^2}$$

provided that

$$k_{\max} > \max\left\{5, \frac{1}{\sqrt{2}\pi - 2 - 4\sqrt{2}\pi C_2 \sigma \sqrt{\log n/n}}\right\}$$

In particular, $|\operatorname{Corr}(\hat{x}, z)| \to 1$ as $k_{\max} \to \infty$.

Why does it work?

By a perturbation analysis, after solving each subproblem

$$W^{(k)} := \underset{\substack{Y=Y^{\top}\\ \operatorname{rank}(Y)=1}}{\operatorname{arg\,max}} \left\| H^{(k)} - Y \right\|_{F}^{2}$$

we expect $W^{(k)} = z^k (z^k)^* + E^{(k)} \approx z^k (z^k)^*$, where $z_i = e^{\iota \theta_i}$

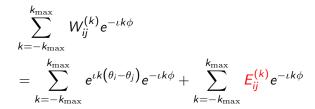
The peak finding step is expected to ensure

$$\hat{\theta}_{ij} = \underset{\phi \in [0,2\pi]}{\arg \max} \left| \frac{1}{2} \sum_{k=1}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k\phi} \right|$$
$$\approx \underset{\phi \in [0,2\pi]}{\arg \max} \left| \frac{1}{2} \sum_{k=1}^{k_{\max}} e^{\iota k \left(\theta_i - \theta_j\right)} e^{-\iota k\phi} \right| = \theta_i - \theta_j$$

provided that $E^{(k)}$ does not "perturb away" the maximum!

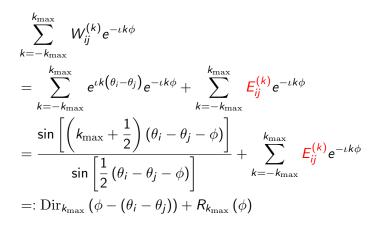
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Landscape Analysis of the Dirichlet Kernel



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Landscape Analysis of the Dirichlet Kernel

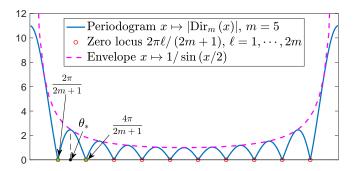


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A Proof by Picture (Notation: $\Delta \theta_{ij} := \hat{\theta}_{ij} - (\theta_i - \theta_j)$)

Key Observation: $|\Delta heta_{ij}| \le heta_* < rac{4\pi}{2k_{\max}+1}$ whenever

$$2k_{\max} + 1 - ||R_{k_{\max}}||_{\infty} > \frac{1}{\sin(\theta_*/2)} + ||R_{k_{\max}}||_{\infty}$$

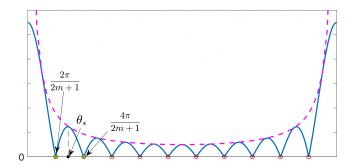


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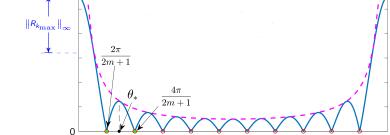
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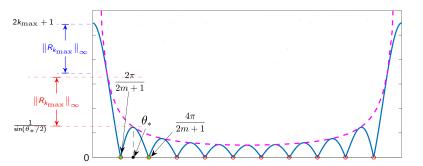


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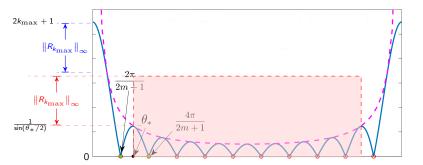
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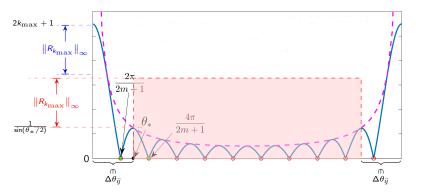
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 $\Leftrightarrow 2k_{\max} - ||R_{k_{\max}}||_{\infty} > \frac{1}{\sin\left(\frac{\pi}{2k_{\max}+1}\right)} + ||R_{k_{\max}}||_{\infty}$

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 $\Leftrightarrow 1 - \frac{1}{2k_{\max}\sin\left(\frac{\pi}{2k_{\max}+1}\right)} > \frac{1}{k_{\max}}\|R_{k_{\max}}\|_{\infty} \sim \left\|\boldsymbol{E}_{ij}^{(k)}\right\|_{\infty}$

What are the odds? Can be estimated with a uniform upper bound for the $E_{ii}^{(k)}$,s!

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Eigenvector perturbation analysis in ℓ_{∞} -norm!

- Standard perturbation bounds use ℓ₂-norm (e.g. Davis–Kahan), but most application scenarios of spectral methods require bounding the ℓ_∞-norm
- Active research area in recent years, e.g. [Eldridge et al. (2017)]; [Abbe et al. (2017)]; [Fan et al. (2018)]; [Zhong & Boumal (2018)]
- Sharpest results to date use a "leave-one-out" trick popularized by statisticians

Lemma (G.–Zhao 2019). For any $0 < \epsilon \le 2$, with probability at least $1 - O(n^{-(2+\epsilon)})$, there exists absolute constant $C_2 > 0$ s.t.

$$\left\|\boldsymbol{E}_{ij}^{(\boldsymbol{k})}\right\|_{\infty} \leq C_2 \sigma \sqrt{\frac{\log n}{n}}.$$

Putting Everything Together, with a Union Bound

With high probability, uniformly for all $i, j \in [n]$, $\hat{\theta}_{ij}$ is close to the true offset $\theta_i - \theta_j$ as long as

$$1 - \frac{1}{2k_{\max}\sin\left(\frac{\pi}{2k_{\max}+1}\right)} \ge \left\| \mathbf{E}_{ij}^{(k)} \right\|_{\infty}$$

$$\Leftrightarrow 1 - \frac{1}{2k_{\max}\sin\left(\frac{\pi}{2k_{\max}+1}\right)} > C_2 \sigma \sqrt{\frac{\log n}{n}}$$

$$\Leftrightarrow k_{\max} > \max\left\{ 5, \frac{1}{\sqrt{2}\pi - 2 - 4\sqrt{2}\pi C_2 \sigma \sqrt{\log n/n}} \right\}$$

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New Theory: Strong Recovery

Theorem (G.–Zhao 2019). Under (mild) assumptions, with high probability, the multi-frequency phase synchronization algorithm produces an estimate \hat{x} satisfying

$$|\operatorname{Corr}(\hat{x},z)| \geq 1 - rac{C'}{k_{\max}^2}$$

provided that

$$k_{\max} > \max\left\{5, \frac{1}{\sqrt{2}\pi - 2 - 4\sqrt{2}\pi C_2 \sigma \sqrt{\log n/n}}\right\}$$

In particular, $|\operatorname{Corr}(\hat{x}, z)| \to 1$ as $k_{\max} \to \infty$.

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Detour: Multi-Frequency Synchronization over SO(3)

Peter–Weyl:
$$f(g) = \sum_{k=0}^{\infty} d_k \operatorname{Tr} \left[\hat{f}(k) \rho_k(g) \right], \ \forall f \in L^2(\mathrm{SO}(3))$$

Random corruption model:

$$g_{ij} = \begin{cases} g_i g_j^{-1} & \text{with probability } r \\ \text{Unif (SO(3))} & \text{with probability } 1 - r \end{cases}$$

- ► Use spectral methods to estimate ρ₁(g_{ij}),..., ρ_{kmax}(g_{ij}), denote Ĥ^(k)_{ij} for the estimator of ρ_k(g_{ij})
- ► Solve a generalized harmonic retrieval problem on SO(3):

$$\hat{g}_{ij} = rgmax_{g \in \mathrm{SO}(3)} \sum_{k=1}^{k_{\mathrm{max}}} d_k \mathrm{Tr} \left[\widehat{H}_{ij}^{(k)} \rho_k^* \left(g
ight)
ight]$$

Works fantastic in practice, but no theory yet!

Outline

Motivation

Class Averaging and Phase Synchronization

Multi-Frequency Phase Synchronization

- A Multi-Frequency Formulation
- A Proof by Picture

Multi-Frequency Class Averaging

Some Representation Theoretic Patterns

From a Fibre Bundle Point of View

Joint work with Yifeng Fan (UIUC) & Zhizhen Zhao (UIUC)

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Compute the rotation-invariant distance between all pairs of images d_{RID} (I_i, I_j) := min_{α∈[0,2π]} ||I_i − e^{ια}I_j||_F, and denote α_{ij} for the optimal alignment angle

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Fix threshold $\epsilon > 0$ and define Hermitian $W \in \mathbb{C}^{n \times n}$ by

$$W_{ij} := \begin{cases} \exp(\iota \alpha_{ij}) & \text{if } d_{\text{RID}}(I_i, I_j) < \epsilon \\ 0 & \text{otherwise} \end{cases}$$

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Solve for the top 3 eigenvectors ψ₁, ψ₂, ψ₃ of W, which embeds I₁, I₂, ... into C³ by

$$I_{i} \longmapsto \Psi(I_{i}) := \frac{(\psi_{1}(i), \psi_{2}(i), \psi_{3}(i))}{\|(\psi_{1}(i), \psi_{2}(i), \psi_{3}(i))\|}$$

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► Use correlation in the embedded C³ space to determine the closeness between viewing directions

Multi-Frequency Class Averaging

- Compute the rotation-invariant distance between all pairs of images d_{RID} (I_i, I_j) := min_{α∈[0,2π]} ||I_i − e^{ια}I_j||_F, and denote α_{ij} for the optimal alignment angle
- ▶ Fix threshold $\epsilon > 0$ and define Hermitian $W \in \mathbb{C}^{n \times n}$ by

$$W_{ij}^{(k)} := \begin{cases} \exp(\iota k \alpha_{ij}) & \text{if } d_{\text{RID}}(I_i, I_j) < \epsilon \\ 0 & \text{otherwise} \end{cases}$$

Solve for the top 2k + 1 eigenvectors ψ₁^(k), ..., ψ_{2k+1}^(k) of W^(k), which embeds I₁, I₂,... into C^{2k+1} by

$$I_{i} \longmapsto \Psi^{(k)}(I_{i}) := \frac{(\psi_{1}(i), \dots, \psi_{2k+1}(i))}{\|(\psi_{1}(i), \dots, \psi_{2k+1}(i))\|}$$

► Use all correlations in the embedded C^{2k+1} (k = 1,..., k_{max}) spaces to determine the closeness between viewing directions

Why 2k + 1? Some Representation Theoretic Patterns

► (G., Fan, Zhao 2019) For sufficiently large sample size n and appropriately small ε > 0, the top eigenspace of W^(k) is (2k + 1)-dimensional, and the spectral gap grows linearly in k:

$$\lambda_k^{(k)} - \lambda_{k+1}^{(k)} \sim \frac{1+k}{4}\epsilon^2$$

• Larger $k \Rightarrow$ larger spectral gap \Rightarrow better numerical stability!

• Tingran Gao, Yifeng Fan, Zhizhen Zhao. Representation Theoretic Patterns in Multi-Frequency Class Averaging for Three-Dimensional Cryo-Electron Microscopy. arXiv:1906.01082.

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More Representation Theoretic Patterns.....

 (G.–Fan–Zhao 2019) The viewing angle θ_{ij} between image i and image j satisfies

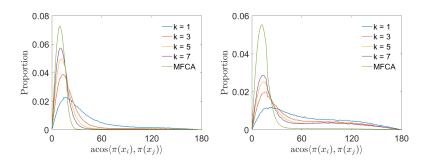
$$\left|\left\langle \Psi^{\left(k
ight)}\left(I_{i}
ight),\Psi^{\left(k
ight)}\left(I_{j}
ight)
ight
angle
ight|=\left(rac{1+\cos heta_{ij}}{2}
ight)^{k}$$

• Larger $k \Rightarrow$ easier thresholding

Can also jointly use k = 1, · · · , k_{max} to construct polynomial filters for cos θ_{ij}

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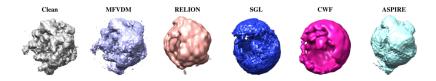
Multi-Frequency Information Improves Class Averaging



Histograms of true viewing angles between each image and its 50 nearest neighboring images

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Multi-Frequency Information Improves Class Averaging



• Yifeng Fan & Zhizhen Zhao. Cryo-Electron Microscopy Image Analysis Using Multi-Frequency Vector Diffusion Maps. arXiv:1904.07772.

• Tingran Gao, Yifeng Fan, Zhizhen Zhao. Representation Theoretic Patterns in Multi-Frequency Class Averaging for Three-Dimensional Cryo-Electron Microscopy. arXiv:1906.01082.

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Synchronization Problems

- Data:
 - graph $\Gamma = (V, E)$
 - ▶ topological group *G*, equipped with a norm $\|\cdot\|$, and a *G*-module *F*
 - edge potential $g: E \to G$ satisfying $g_{ij} = g_{ji}^{-1}, \ \forall (i,j) \in E$

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 Goal:
 - find a vertex potential $f: V \to G$ or F such that

$$f_i = g_{ij}f_j, \quad \forall (i,j) \in E$$

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- The goal can be achieved if and only if $g_{ij} = f_i f_i^{-1}$
- Not always feasible!

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- The goal can be achieved if and only if $g_{ij} = f_i f_i^{-1}$
- Not always feasible!
- If infeasible, find the "closest solution" in the sense of

$$\min_{\substack{f:V \to G \\ \|f\| \neq 0}} \frac{1}{2} \frac{\sum_{i,j \in V} \|f_i - g_{ij}f_j\|^2}{\sum_{i \in V} \|f_i\|^2} (=: \eta(f))$$

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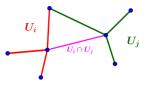
Geometric Picture

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 - edge potential $g: E \to G$ satisfying $g_{ij} = g_{ji}^{-1}, \forall (i,j) \in E$
- Flat Principal G-Bundle:
 - Let 𝔅 = {U_i | 1 ≤ i ≤ |V|} be an open cover of Γ (viewed as a 1-dimensional simplicial complex), where U_i is the (open) star neighborhood of vertex i.

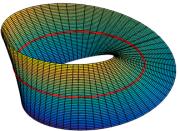


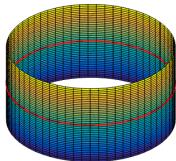
• Triplet (g, G, Γ) defines a *flat principal G-bundle* \mathscr{B}_{ρ} over Γ

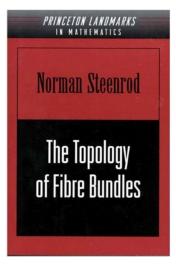
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Fibre Bundle: $\mathscr{E} = (E, M, F, \pi)$ is called a *F*-bundle over *M* if

- M: base manifold
- ► F: fibre manifold
- E: total manifold
- $\pi: E \to M$: smooth surjective map (bundle projection)
- Iocal triviality: for "small" open set U ⊂ M, π⁻¹(U) is diffeomorphic to U × F



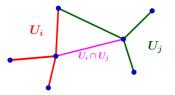




Theorem (Steenrod 1951, §2). If Lie group *G* acts on *Y*, $\mathfrak{U} = \{U_i\}$ is an open cover of *X*, $\{g_{ij} \in G \mid U_i \cap U_j \neq \emptyset\}$ satisfies

$$\begin{split} g_{ii} &= e \in G \quad \text{for all } U_i \\ g_{ij} &= g_{ji}^{-1} \quad \text{if } U_i \cap U_j \neq \emptyset \\ g_{ij}g_{jk} &= g_{ik} \quad \text{if } U_i \cap U_j \cap U_k \neq \emptyset \end{split}$$

then there exists a fibre bundle \mathscr{B} with base space X, fibre Y, group G, and bundle transformations $\{g_{ii}\}$.



No triple intersections!

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Representation and Associated Bundles

If M is a principal G-bundle over B, ρ : G → Aut (F) is a representation of G over a vector space F. Then ρ induces an associated F-bundle over B:

$$M \times_{\rho} F := M \times F / \sim$$

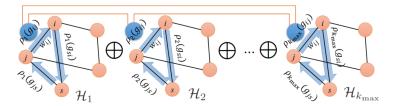
where the equivalence relation is defined by

$$(m \cdot g, v) \sim (m, \rho(g) v)$$

 Non-equivalent irreducible representations gives rise to distinct associated bundles

Multi-Frequency \leftrightarrow Multiple Associated Bundles

- ▶ All irreducible representations of U(1): $\{\theta \to e^{\iota k \theta} \mid k \in \mathbb{Z}\}$
- Entrywise power: Inducing multiple irreducible representations, effectively creating many associated bundles
- Multi-frequency phase synchronization and class averaging both strive to distill features across multiple associate bundles (associated with different principal bundles)



How Far Can We Push This idea Further?

Faster ways than arg max Peter–Weyl?

$$\hat{g}_{ij} = \arg\max_{g \in G} \sum_{k=1}^{k_{\max}} d_k \operatorname{Tr} \left[\widehat{H}_{ij}^{(k)} \rho_k^*(g) \right]$$

Alternative ways to leverage the algebraic consistency across irreducible representations / associated bundles?

Example: Construct invariant features such as the bispectrum, using algebraic constraints such as

 $e^{\iota k_1 \theta_{ij}} \cdot e^{\iota k_2 \theta_{ij}} = e^{\iota (k_1 + k_2) \theta_{ij}}$

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► In phase synchronization, this amounts to comparing 1 with $\left| W_{ij}^{(k_1)} W_{ij}^{(k_2)} \overline{W_{ij}^{(k_1+k_2)}} \right|$ for each pair (i,j)

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- ► In general, with the help of Clebsch–Gordan coefficients C_{k1,k2}, compare the following with the identity matrix I_{d1d2}:

$$\left[F_{ij}^{(k_1)}\bigotimes F_{ij}^{(k_2)}\right]C_{k_1,k_2}\left[\bigoplus_{k\in k_1\bigotimes k_2}F_{ij}^{(k)}\right]C_{k_1,k_2}^*$$

where $F_{ij}^{(k_1)}$, $F_{ij}^{(k_2)}$, $F_{ij}^{(k)}$ estimate $\rho_{k_1}(g_{ij})$, $\rho_{k_2}(g_{ij})$, $\rho_k(g_{ij})$

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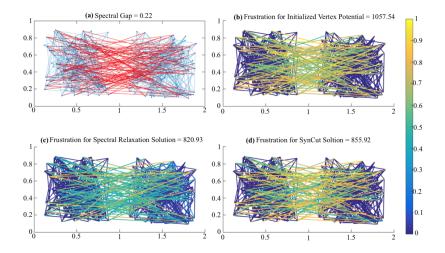
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where F^(k₁)_{ij}, F^(k₂)_{ij}, F^(k)_{ij} estimate ρ_{k₁}(g_{ij}), ρ_{k₂}(g_{ij}), ρ_k(g_{ij})
Can use this to construct invariant moment features of arbitrary order; more details in (Fan–G.–Zhao 2019)

Detour: A Variant of Community Detection



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Open Problems

- ► Algorithm works for SO(3) seamlessly, but theory?
- Possible extension to other synchronization and multireference alignment problems over compact/noncompact Lie groups?

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- Fundamental statistical/computational limits in the community detection setting?
- Mult-frequency vector diffusion maps?
- A learning paradigm on sheaves?

Thank You!

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