Multi-Representation Manifold Learning on Fibre Bundles

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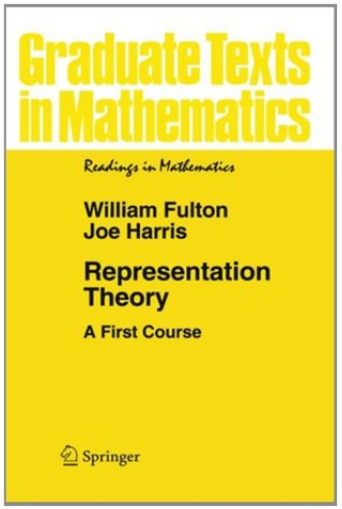
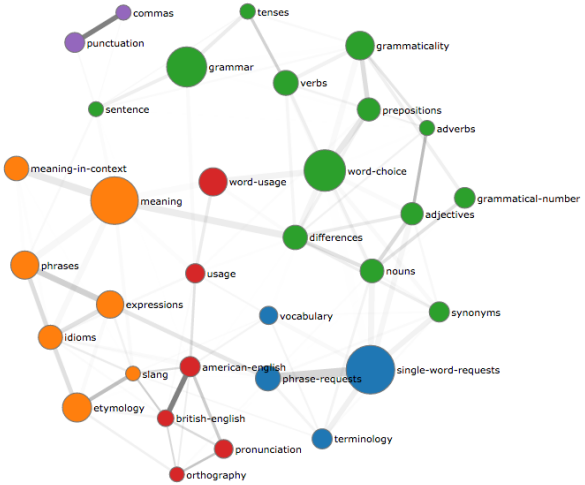
Outline

Representation?



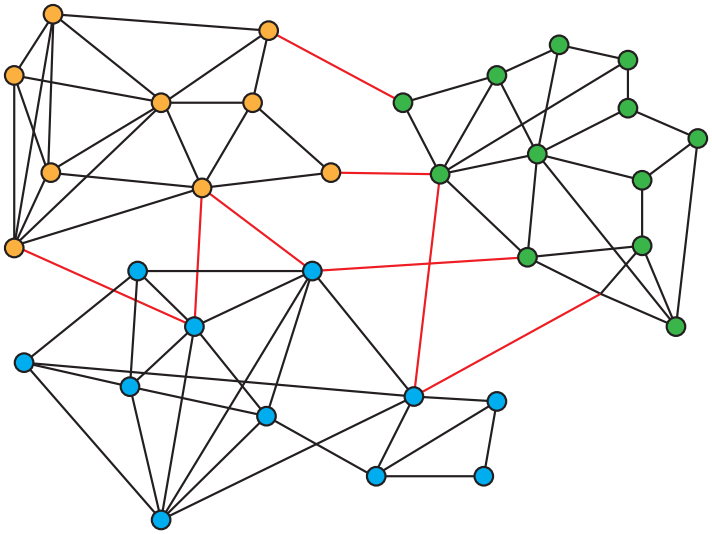
representation theory

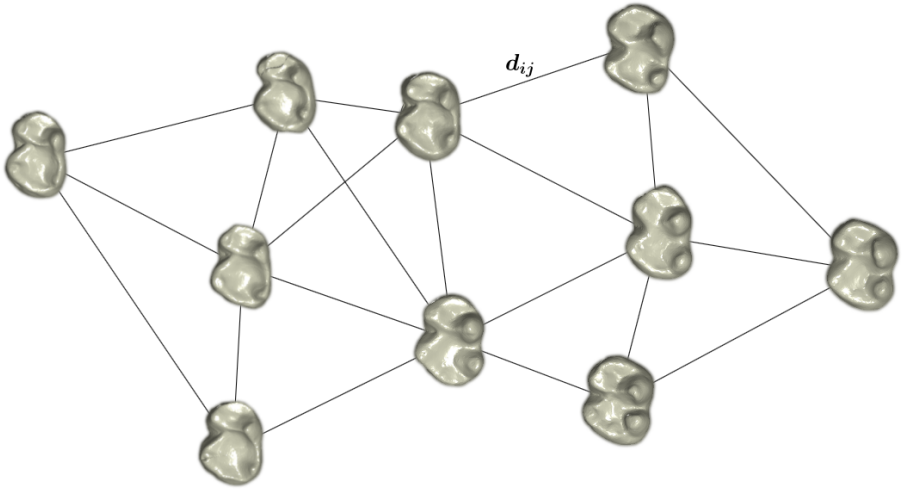
representationism

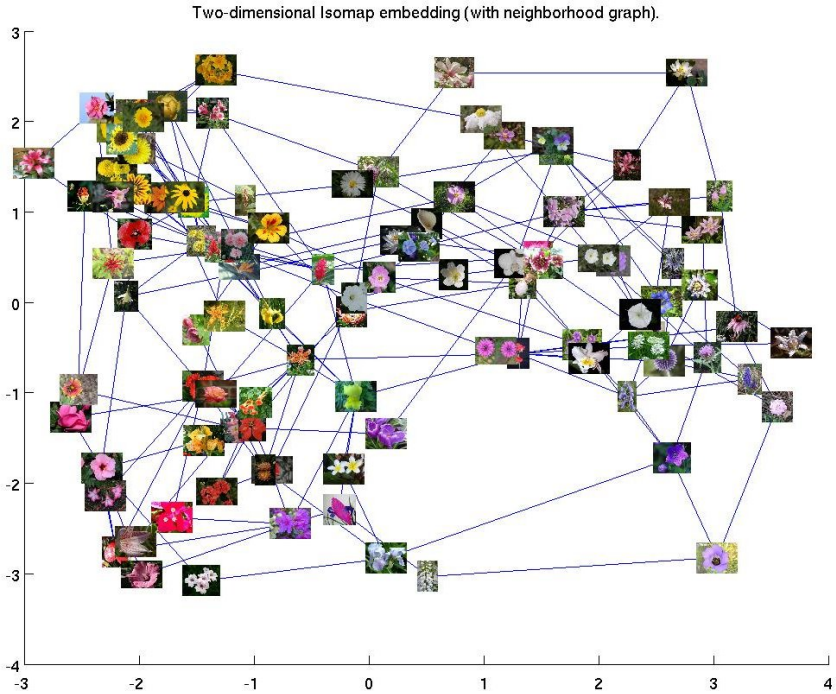


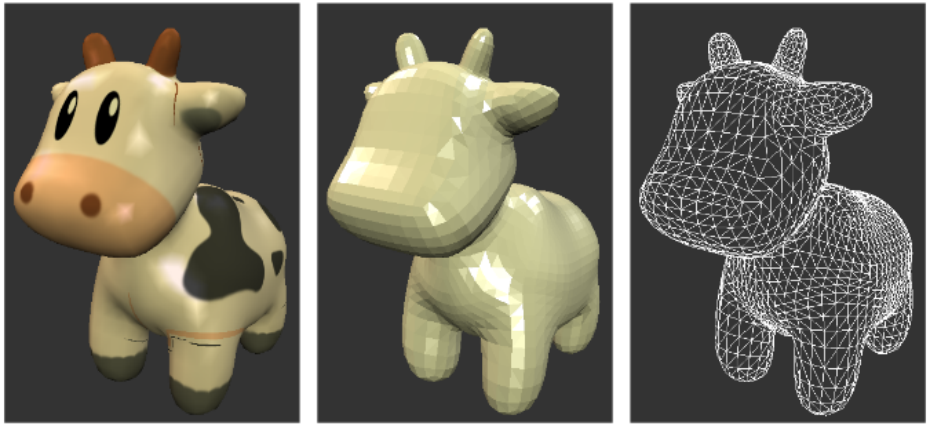
representation learning

Graph: A Flexible Data Representation





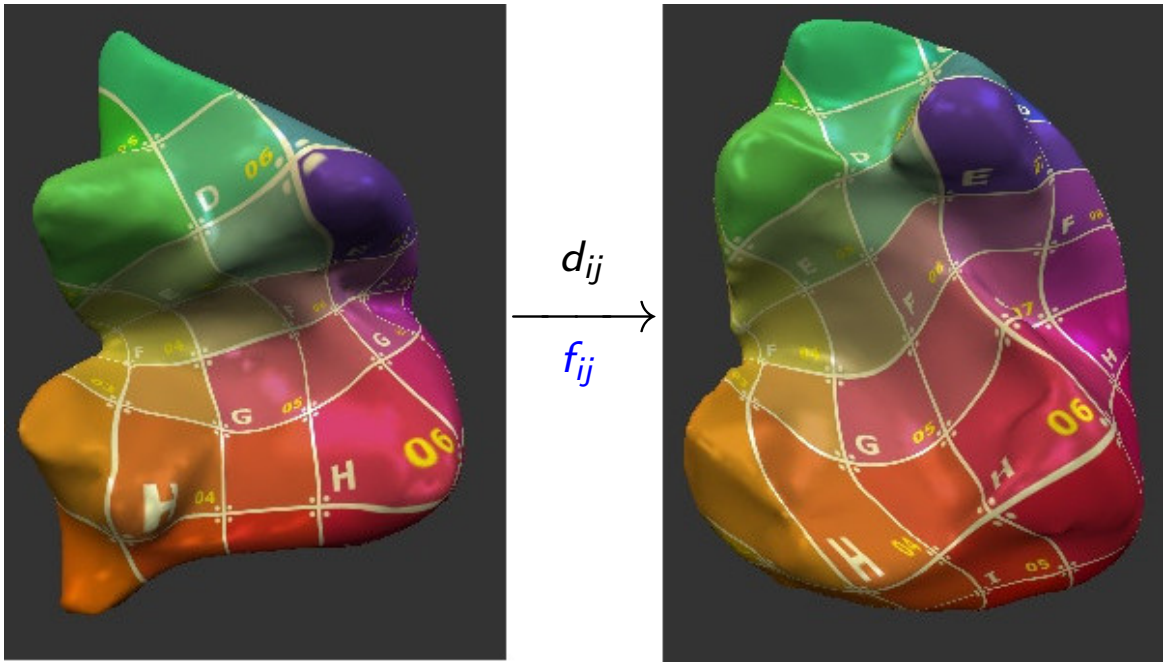




Non-Scalar Edge Weights

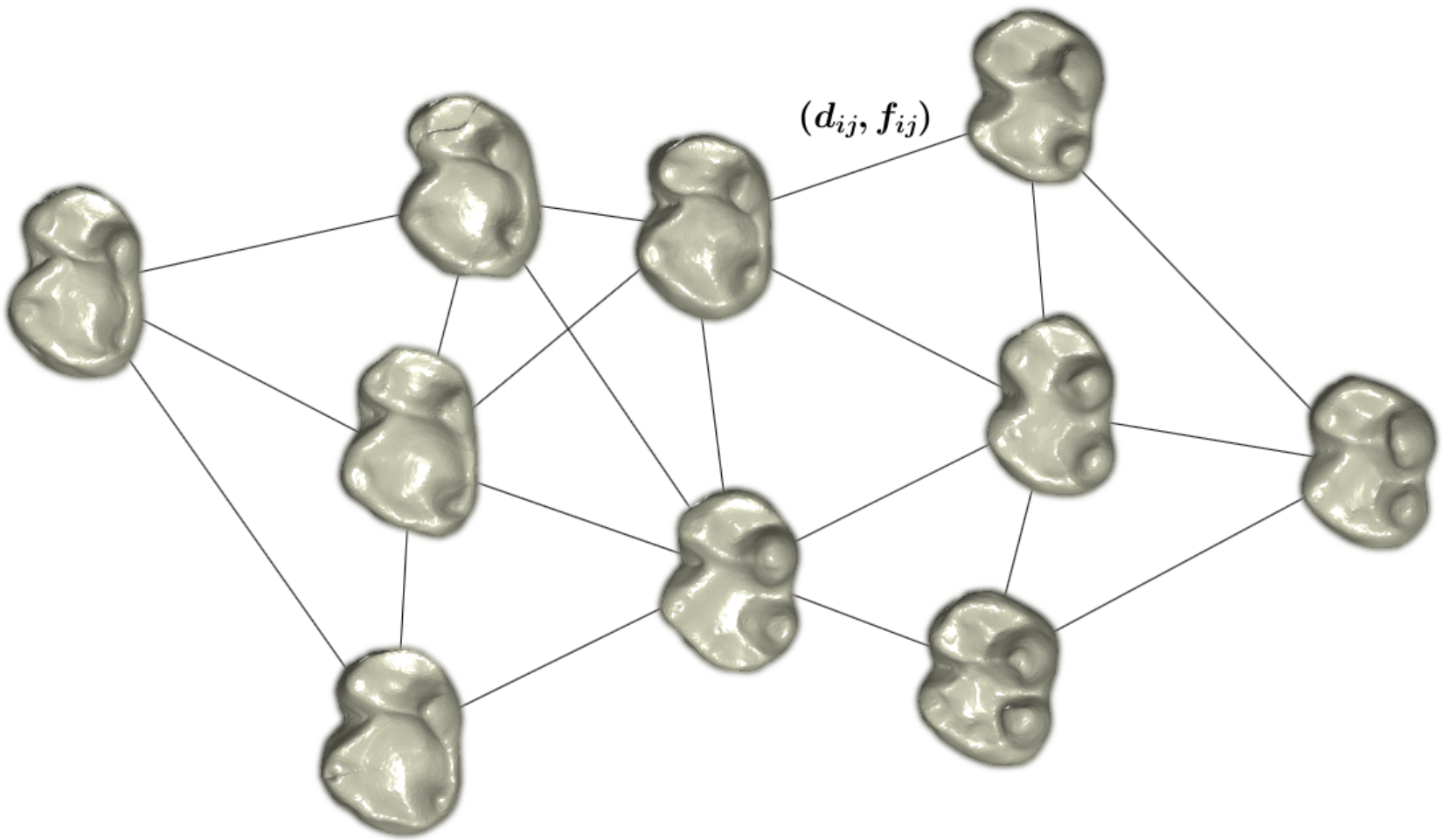
$$d_{\mathrm{cP}}\left(S_i, S_j\right) = \inf_{\mathcal{C}\in\mathcal{A}\left(S_i,S_j\right)} \inf_{R\in\mathbb{E}(3)} \left(\int_{S_i} \left\|R\left(x\right) - \mathcal{C}\left(x\right)\right\|^2 d\mathrm{vol}_{S_i}\left(x\right)\right)^{\frac{1}{2}}$$

S_i



S_j

Do Graph Representations Have Enough Expressive Power?



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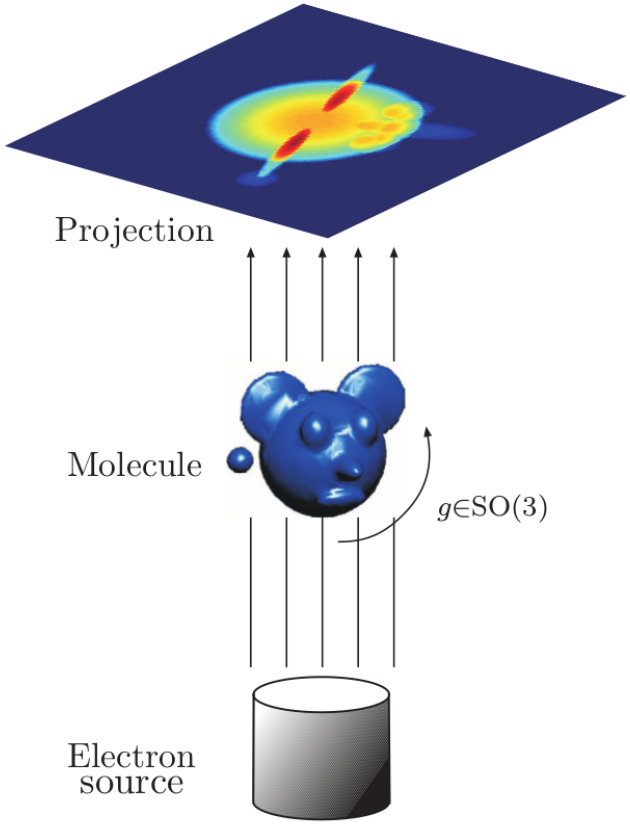
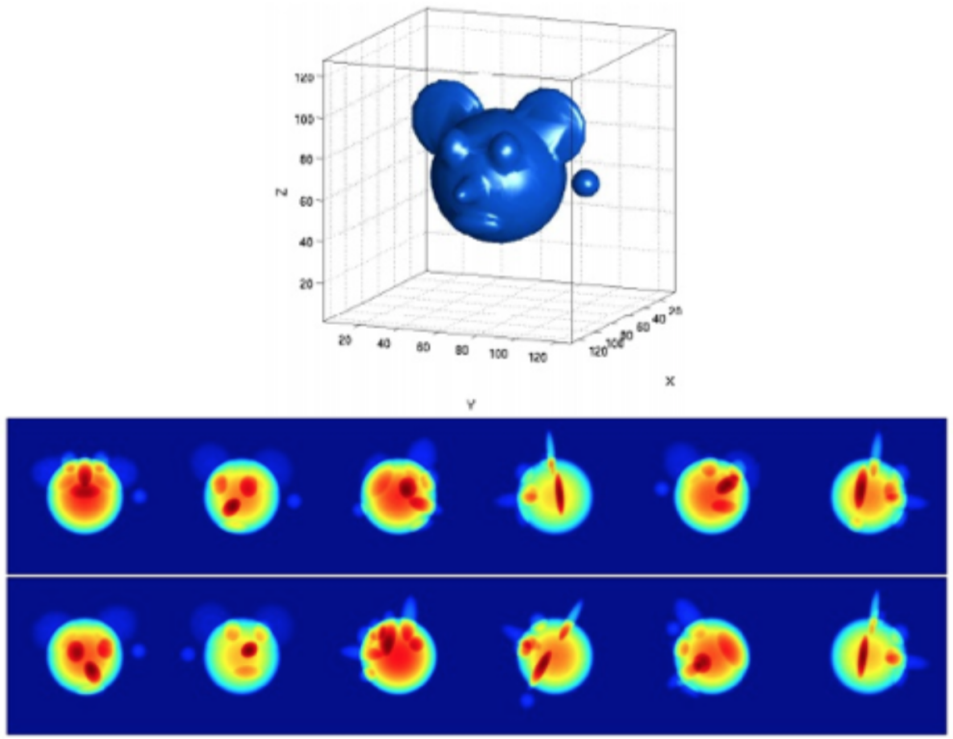
Cryo-Electron Microscopy





• 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

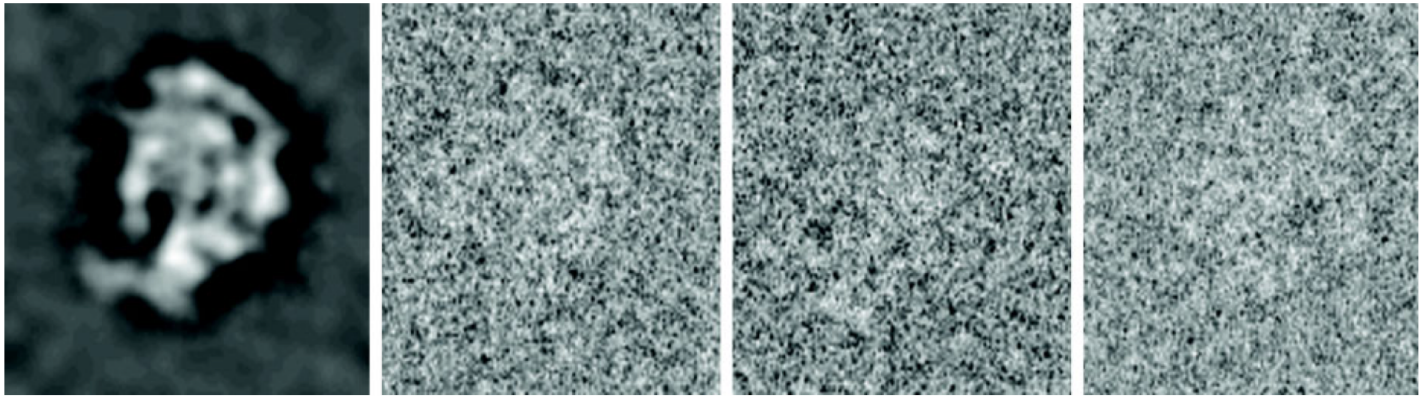


Fig. 3 The left most image is a clean simulated projection image of the E.coli 50S ribosomal subunit. The other three images are real electron microscope images of the same subunit

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).

Class Averaging

- Compute the *rotation-invariant distance* between all pairs of images $d_{\mathrm{RID}}(I_i, I_j) := \min_{\alpha \in [0,2\pi]} \|I_i - e^{\iota\alpha} I_j\|_{\mathrm{F}}$, 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

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

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- Solve for the top 3 eigenvectors ψ_1, ψ_2, ψ_3 of W, which embeds $I_1, I_2, \ldots$ into $\mathbb{C}^3$ 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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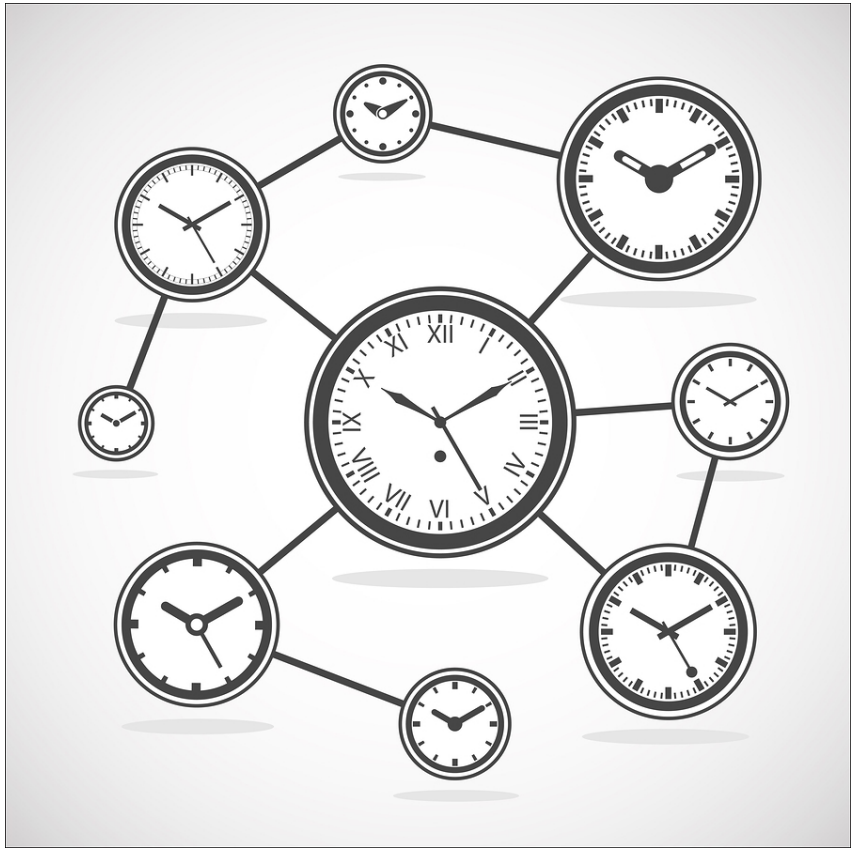
- Use correlation in the embedded $\mathbb{C}^3$ space to determine the closeness between viewing directions

Phase Synchronization (Singer'11)

- **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 (Singer'11)

- **Setup**: Phase vector $z = \left(e^{\iota\theta_1}, \ldots, e^{\iota\theta_n}\right)^\top \in \mathbb{C}_1^n$, noisy pairwise measurements in n-by-n Hermitian matrix

$$H_{ij} = \begin{cases} e^{\iota\left(\theta_i - \theta_j\right)} = z_i \bar{z}_j & \text{with prob. } r \in [0,1] \\ \text{Uniform}\left(\mathrm{U}(1)\right) & \text{with prob. } 1 - r \end{cases}$$

  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)
- **Spectral Relaxation**: solve for the top eigenvector of H, denoted as $\tilde{x}$ (scaled to $\|\tilde{x}\|_2 = \sqrt{n}$), then define $\hat{x} \in \mathbb{C}_1^n$ by

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

Phase Synchronization: Existing Methods

- Convex Relaxations: Singer'11, Chaudhury et al.'15, Bandeira et al.'16, Bandeira et al.'17
- Nonconvex Methods: Boumal'16, Zhong & Boumal'17
- Non-Unique Games: Bandeira et al.'15
- Approximate Message Passing: Perry et al.'18

• Singer, A. Angular synchronization by eigenvectors and semidefinite programming. *Applied and Computational Harmonic Analysis*, 30(1), 20–36 (2011).
• Chaudhury, K.N., Khoo, Y., Singer, A. Global registration of multiple point clouds using semidefinite programming. *SIAM Journal on Optimization*, 25(1), 468–501 (2015)
• Bandeira, A.S., Kennedy, C., Singer, A. Approximating the little Grothendieck problem over the orthogonal and unitary groups. *Mathematical Programming*, 160(1-2) pp. 433–475 (2016).
• Bandeira, A.S., Boumal, N., Singer, A. Tightness of the maximum likelihood semidenite relaxation for angular synchronization. *Mathematical Programming*, 163(1-2) pp. 145–167 (2017).
• Boumal, N. Nonconvex phase synchronization. *SIAM Journal on Optimization*, 26(4):2355–2377, 2016.
• Zhong, Y., Boumal, N. Near-optimal bounds for phase synchronization. *SIAM Journal on Optimization*, 28(2):989-1016, 2018
• Bandeira, A., Chen, Y., Singer, A. Non-unique games over compact groups and orientation estimation in cryo-EM. arXiv preprint arXiv:1505.03840, 2015.
• Perry, A., Wein, A. S., Bandeira, A. S., Moitra, A. Message-passing algorithms for synchronization problems over compact groups. *Communications on Pure and Applied Mathematics*, 2018.

Outline

Initialization: Inspired by Harmonic Retrieval

- Fix $k_{\max} \geq 1$, build $H^{(2)}, \ldots, H^{(k_{\max})}$ out of $H = H^{(1)}$ by taking entrywise powers of H

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- For each $k = 1, \ldots, k_{\max}$, find a reasonably good symmetric rank-1 approximation

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

using e.g. spectral method

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- For all $1 \leq i, j \leq n$, find the "peak location" of the spectrogram

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

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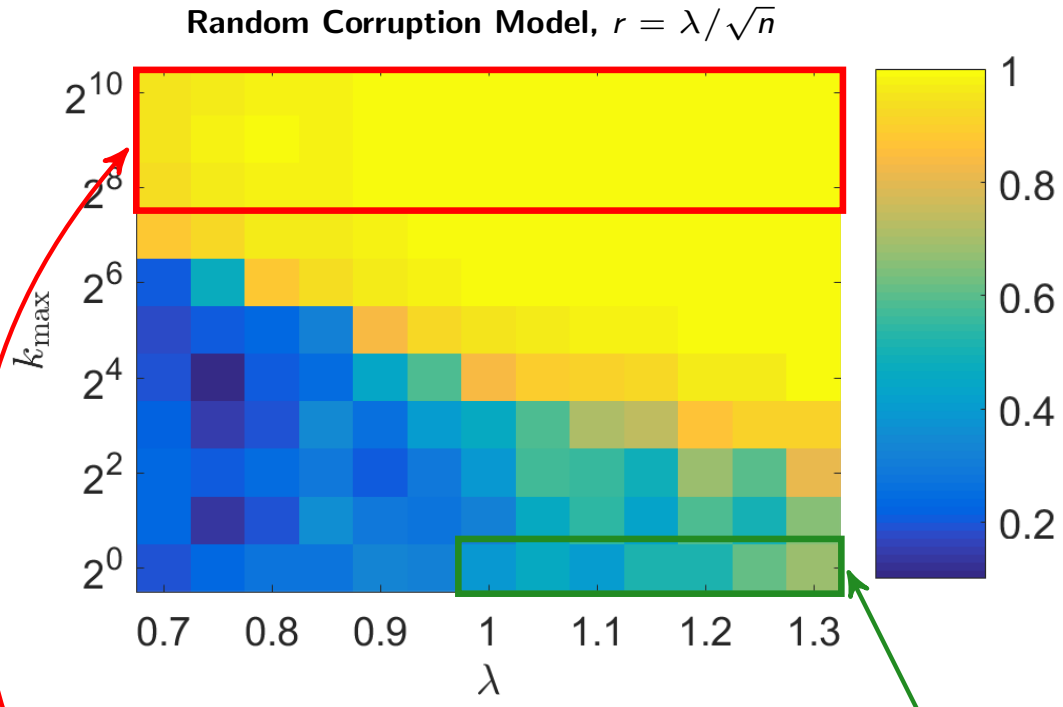
- Apply the spectral method yet again to the Hermitian matrix $\widehat{H}$ to get $\hat{x} \in \mathbb{C}_1^n$, where $\widehat{H}_{ij} = e^{\iota \hat{\theta}_{ij}}$

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



Our Method: $|\mathrm{Corr}\,(\hat{x}, z)| \longrightarrow 1$

as $k_{\max} \gg 1$, **even for** $\lambda < 1$**!**

Previous Art: Only ensures

$|\mathrm{Corr}\,(\hat{x}, z)| > \frac{1}{\sqrt{n}}$ **for** $\lambda > 1$

Outline

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

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

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, $|\mathrm{Corr}\,(\hat{x}, z)| \to 1$ **as** $k_{\max} \to \infty$**.**

Why does it work?

- By a perturbation analysis, after solving each subproblem

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

  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

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

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

Landscape Analysis of the Dirichlet Kernel

$$\sum_{k=-k_{\max}}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k \phi}$$

$$= \sum_{k=-k_{\max}}^{k_{\max}} e^{\iota k \left(\theta_i - \theta_j\right)} e^{-\iota k \phi} + \sum_{k=-k_{\max}}^{k_{\max}} E_{ij}^{(k)} e^{-\iota k \phi}$$

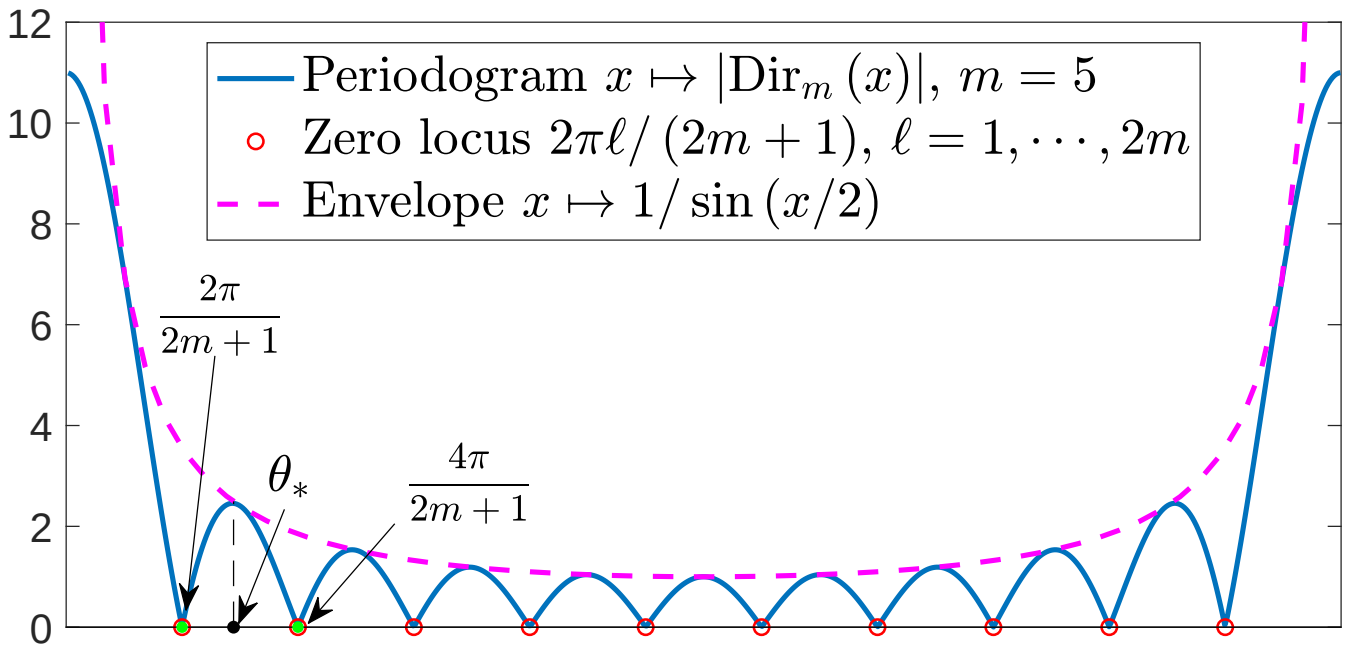
Landscape Analysis of the Dirichlet Kernel

$$
\begin{aligned}
&\sum_{k=-k_{\max}}^{k_{\max}} W_{ij}^{(k)} e^{-\iota k \phi} \\
&= \sum_{k=-k_{\max}}^{k_{\max}} e^{\iota k \left(\theta_i - \theta_j\right)} e^{-\iota k \phi} + \sum_{k=-k_{\max}}^{k_{\max}} E_{ij}^{(k)} e^{-\iota k \phi} \\
&= \frac{\sin\left[\left(k_{\max} + \frac{1}{2}\right)(\theta_i - \theta_j - \phi)\right]}{\sin\left[\frac{1}{2}(\theta_i - \theta_j - \phi)\right]} + \sum_{k=-k_{\max}}^{k_{\max}} E_{ij}^{(k)} e^{-\iota k \phi} \\
&=: \mathrm{Dir}_{k_{\max}}\left(\phi - (\theta_i - \theta_j)\right) + R_{k_{\max}}(\phi)
\end{aligned}
$$

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

Key Observation: $|\Delta\theta_{ij}| \leq \theta_* < \frac{4\pi}{2k_{\max}+1}$ whenever

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



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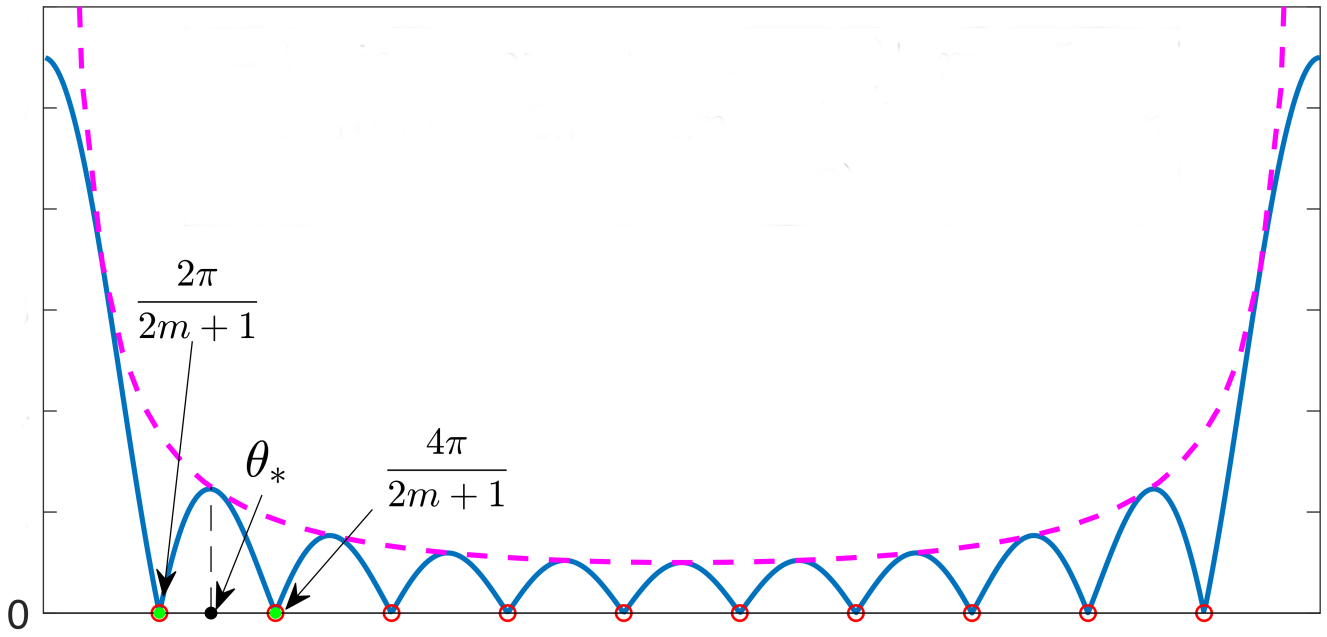

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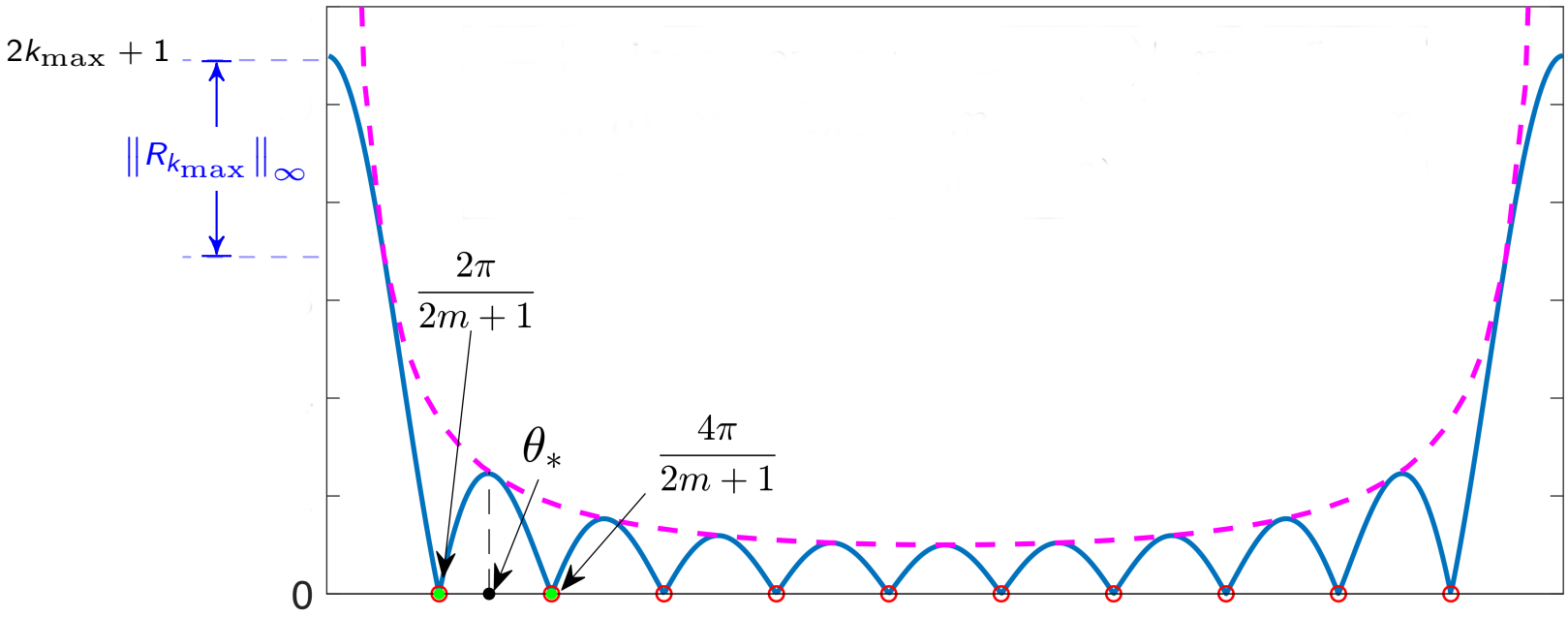

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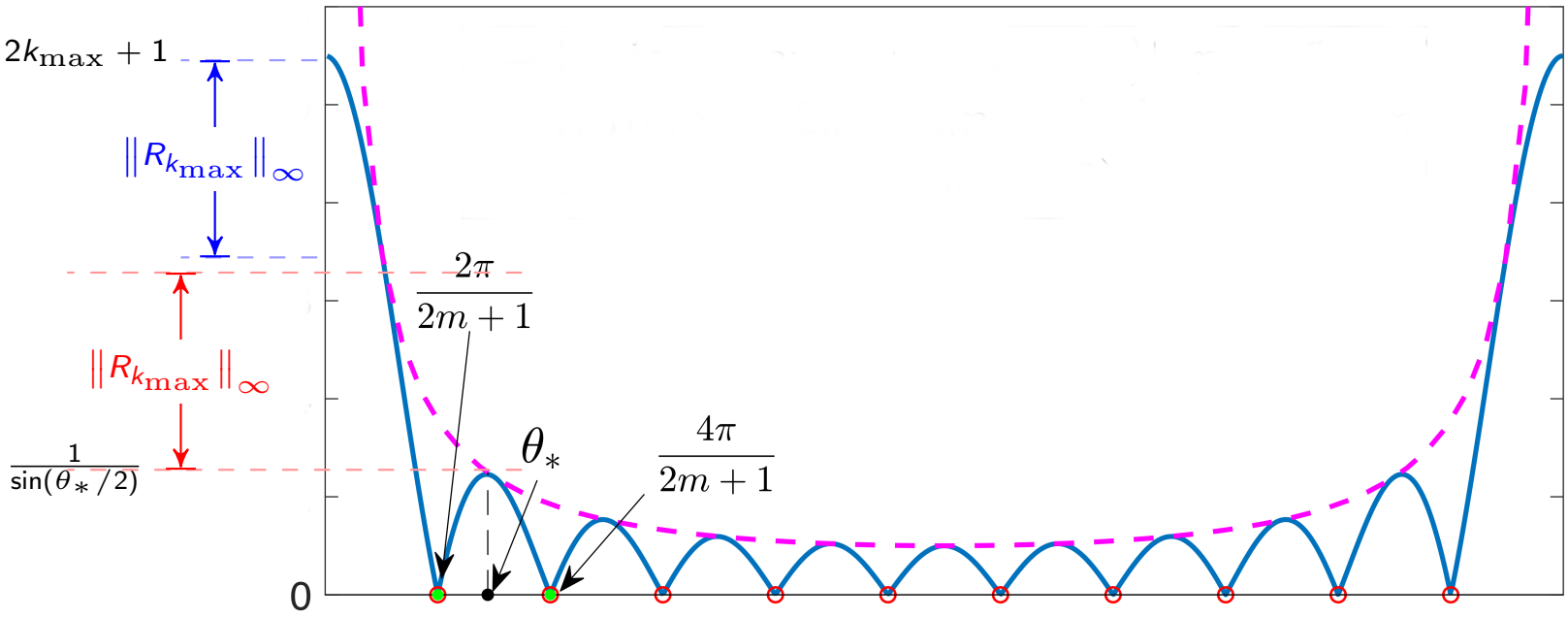

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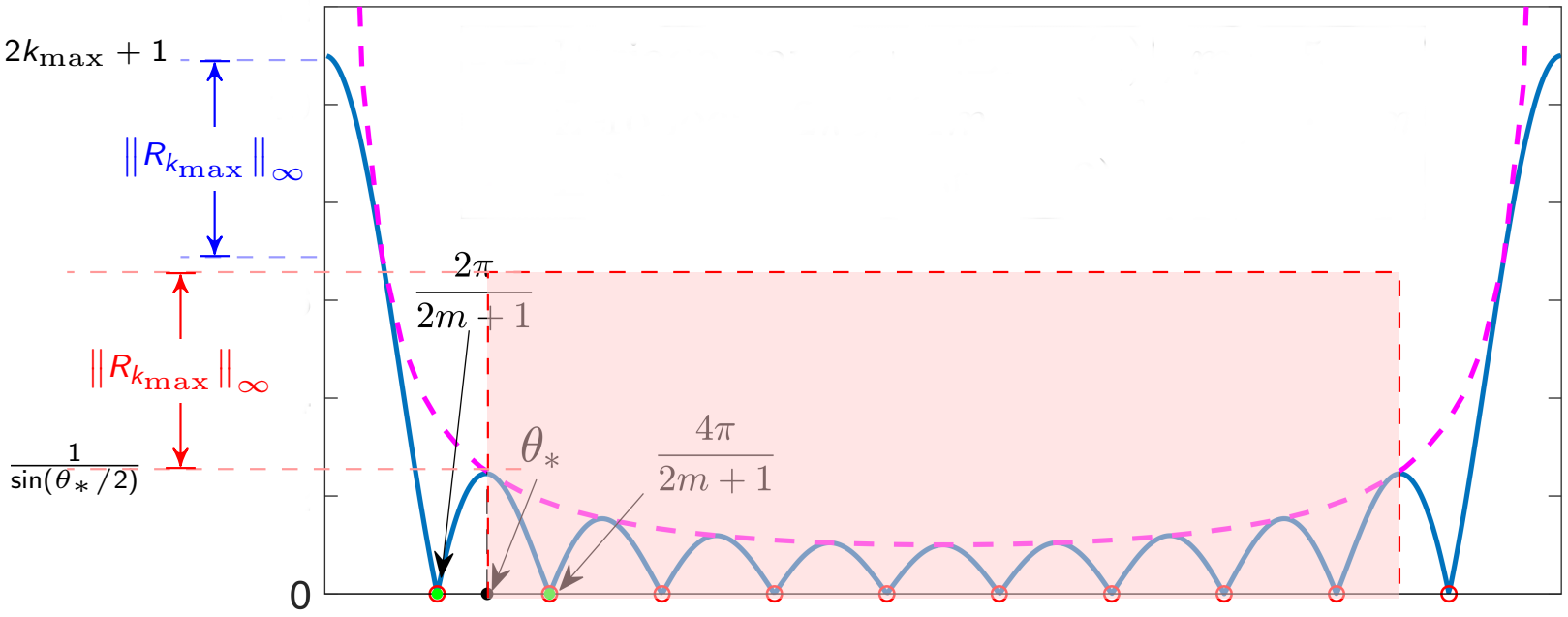

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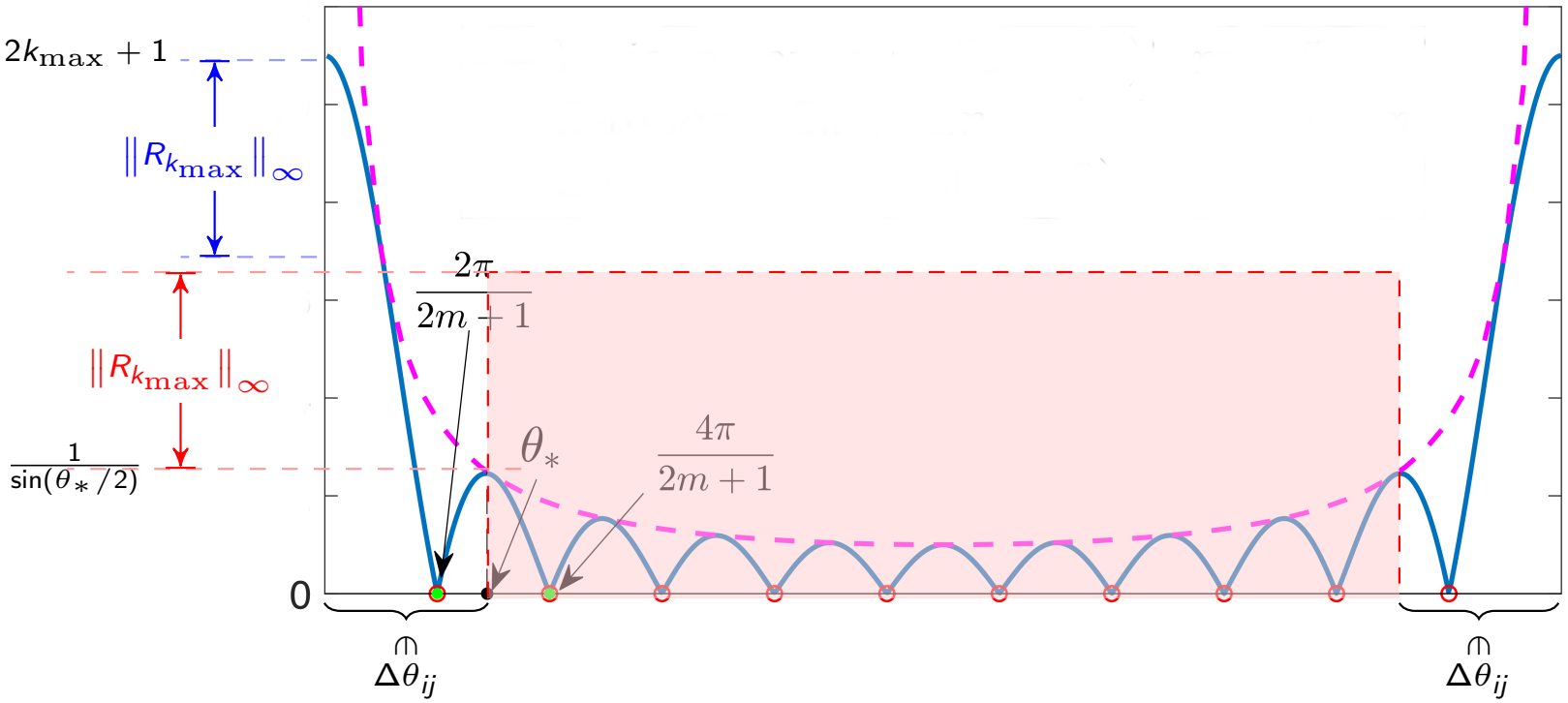

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$$\Leftarrow \; 1 - \frac{1}{2k_{\max}\sin\left(\frac{\pi}{2k_{\max}+1}\right)} > \frac{1}{k_{\max}}\|R_{k_{\max}}\|_\infty \sim \left\|E_{ij}^{(k)}\right\|_\infty$$

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

Eigenvector perturbation analysis in ℓ_∞-norm!

- Standard perturbation bounds use ℓ_2-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 $0 < \epsilon \leq 2$, with probability at least $1 - O\left(n^{-(2+\epsilon)}\right)$, there exists absolute constant $C_2 > 0$ s.t.

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

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

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

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

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

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

Detour: Multi-Frequency Synchronization over $\mathrm{SO}(3)$

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

- Random corruption model:

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

- Use spectral methods to estimate $\rho_1(g_{ij}), \ldots, \rho_{k_{\max}}(g_{ij})$, denote $\widehat{H}_{ij}^{(k)}$ for the estimator of $\rho_k(g_{ij})$
- Solve a generalized harmonic retrieval problem on $\mathrm{SO}(3)$:

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

- Works fantastic in practice, but no theory yet!

Outline

Class Averaging

- Compute the *rotation-invariant distance* between all pairs of images $d_{\mathrm{RID}}(I_i, I_j) := \min_{\alpha \in [0,2\pi]} \|I_i - e^{\iota\alpha} I_j\|_{\mathrm{F}}$, and denote α_{ij} for the optimal alignment angle
- Fix threshold $\epsilon > 0$ and define Hermitian $W \in \mathbb{C}^{n \times n}$ by

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

- Solve for the top 3 eigenvectors ψ_1, ψ_2, ψ_3 of W, which embeds $I_1, I_2, \ldots$ into $\mathbb{C}^3$ by

$$I_i \longmapsto \Psi(I_i) := \frac{(\psi_1(i), \psi_2(i), \psi_3(i))}{\|(\psi_1(i), \psi_2(i), \psi_3(i))\|}$$

- Use correlation in the embedded $\mathbb{C}^3$ space to determine the closeness between viewing directions

Multi-Frequency Class Averaging

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

- Solve for the top $2k+1$ eigenvectors $\psi_1^{(k)}, \cdots, \psi_{2k+1}^{(k)}$ of $W^{(k)}$, which embeds $I_1, I_2, \ldots$ into $\mathbb{C}^{2k+1}$ by

$$I_i \longmapsto \Psi^{(k)}(I_i) := \frac{(\psi_1(i), \ldots, \psi_{2k+1}(i))}{\|(\psi_1(i), \ldots, \psi_{2k+1}(i))\|}$$

- Use all correlations in the embedded $\mathbb{C}^{2k+1}$ $(k = 1, \ldots, k_{\max})$ spaces to determine the closeness between viewing directions

Why $2k+1$? Some Representation Theoretic Patterns

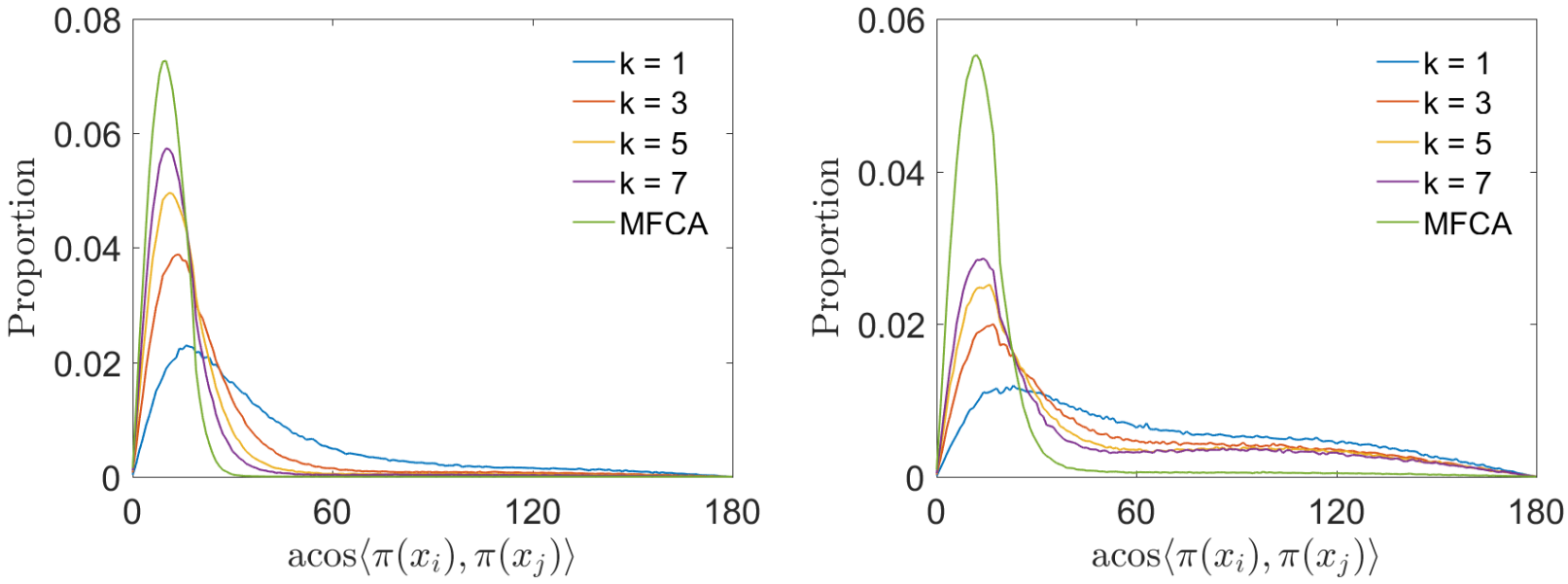
- **(G.–Fan–Zhao 2019)** The *extrinsic model* S^2 of viewing directions and the *intrinsic* model of the top eigenspace of $W^{(k)}$ are isomorphic, following (Hadani & Singer, 2011)
- For sufficiently large sample size n and appropriately small $\epsilon > 0$, the top eigenspace of $W^{(k)}$ is $(2k+1)$-dimensional, 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!

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

Multi-Frequency Information Improves Class Averaging



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

Outline

Synchronization Problems: Geometric Picture

- 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 $g_{ij} = g_{ji}^{-1}$, $\forall (i,j) \in E$

Synchronization Problems: Geometric Picture

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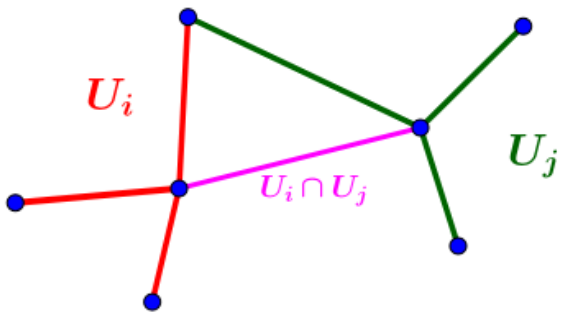
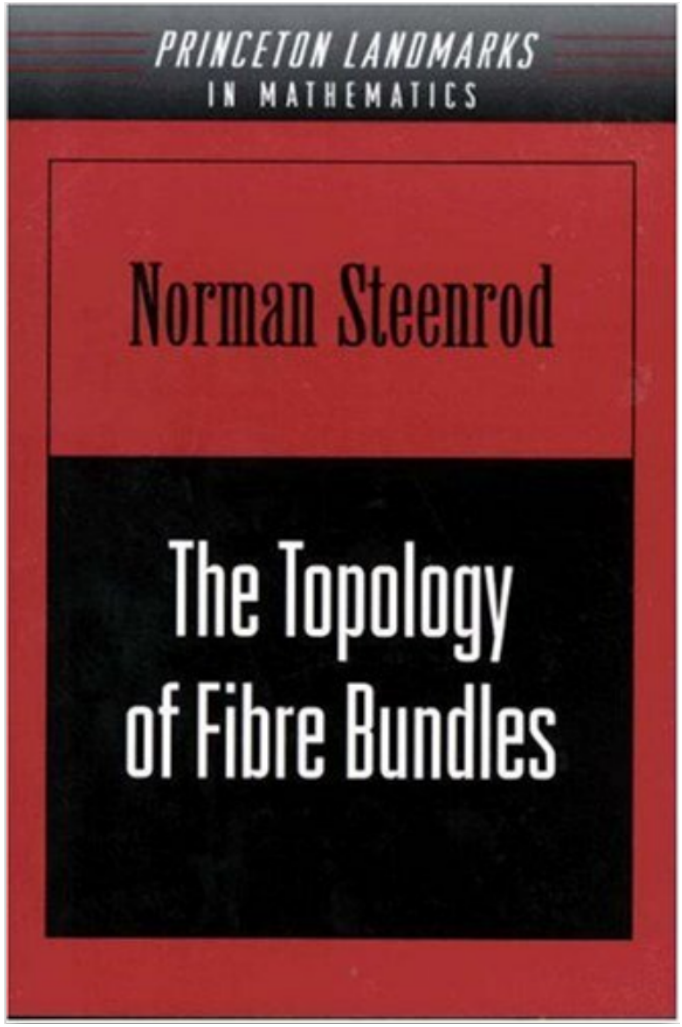
  - **edge potential** $g : E \to G$ satisfying $g_{ij} = g_{ji}^{-1}$, $\forall (i,j) \in E$
- Flat Principal G-Bundle:
  - Let $\mathfrak{U} = \{U_i \mid 1 \leq i \leq |V|\}$ be an open cover of Γ (viewed as a 1-dimensional simplicial complex), where U_i is the *(open) star neighborhood* of vertex i.



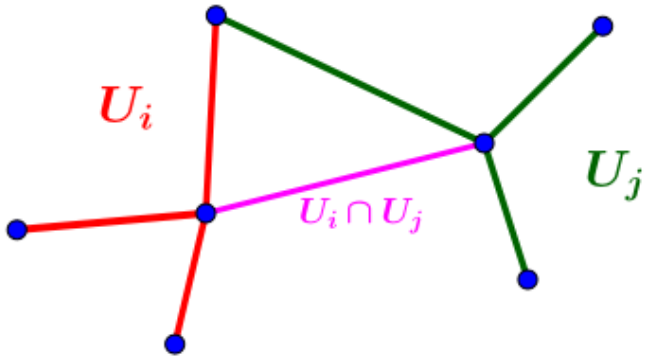
  - Triplet (g, G, Γ) defines a *flat principal G-bundle $\mathscr{B}_\rho$* over Γ



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

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

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



No triple intersections!

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$$g_{ii} = e \in G \quad \text{for all } U_i$$

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$$\cancel{g_{ij} g_{jk} = g_{ik} \quad \text{if } U_i \cap U_j \cap U_k \neq \emptyset}$$

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

Representation and Associated Bundles

- If M is a principal G-bundle over B, $\rho : G \to \mathrm{Aut}\,(F)$ is a representation of G over a vector space F. Then ρ induces an **associated** F-bundle over B:

$$M \times_\rho F := M \times F \Big/ \sim$$

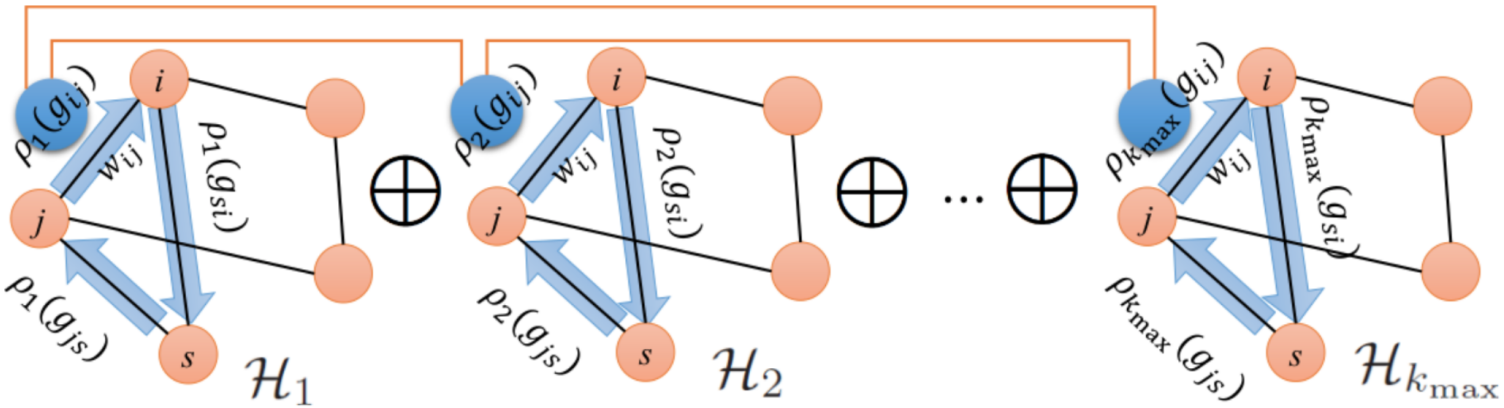
where the equivalence relation is defined by

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

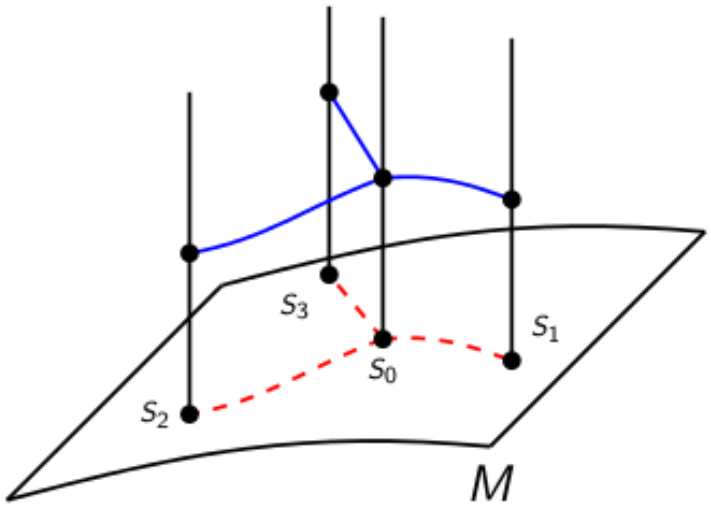
- Non-equivalent irreducible representations gives rise to distinct associated bundles

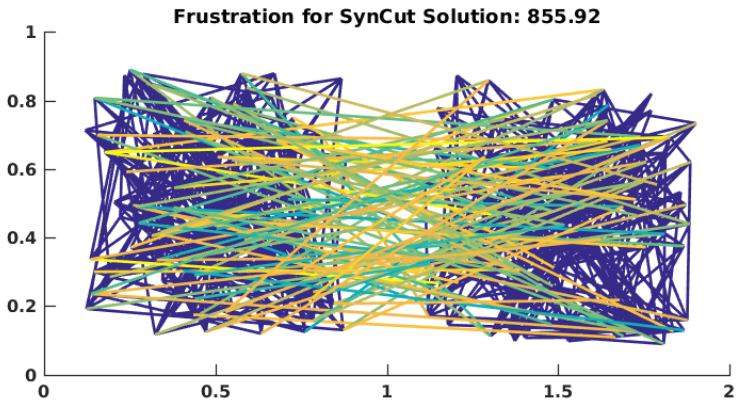
Multi-Frequency $\leftrightarrow$ Multiple Associated Bundles

- All irreducible representations of $\mathrm{U}(1)$: $\left\{\theta \to e^{\iota k\theta} \mid k \in \mathbb{Z}\right\}$
- 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 the same principal bundles)



Diffusion and Community Detection on Fibre Bundles





• Tingran Gao. *The Diffusion Geometry of Fibre Bundles: Horizontal Diffusion Maps.* Applied and Computational Harmonic Analysis, online first, pp.1–69 (2019)
• Tingran Gao, Jacek Brodzki, and Sayan Mukherjee. *The Geometry of Synchronization Problems and Learning Group Actions*, Discrete & Computational Geometry, online first, pp.1–62 (2019)

Open Problems

- Extension to other synchronization and multireference alignment problems over compact/noncompact Lie groups?
- Fundamental statistical/computational limits in synchronizability-based community detection?
- **A learning paradigm on sheaves?**

Thank You!

- AMS–Simons Travel Grant
- UChicago CDAC Data Science Discovery Seed Grant
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Center for Data and Computing

• Tingran Gao and Zhizhen Zhao. *Multi-Frequency Phase Synchronization.* Proceedings of the 36th International Conference on Machine Learning (ICML 2019), PMLR 97:2132–2141, 2019.
• Tingran Gao, Yifeng Fan, and Zhizhen Zhao. *Representation Theoretic Patterns in Multi-Frequency Class Averaging for Three-Dimensional Cryo-Electron Microscopy.* arxiv:1906.01082.
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