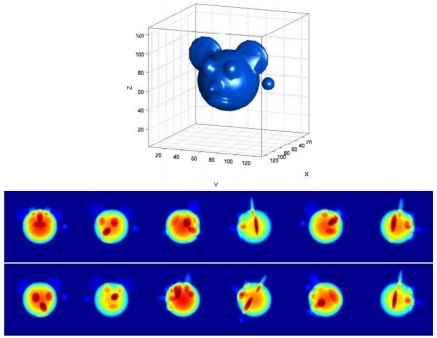
Message-passing algorithms for synchronization problems

Amelia Perry (MIT Mathematics)
with Afonso Bandeira, Ankur Moitra, and Alex Wein

Motivation: cryo-EM



Given many noisy 2D images of molecules, each with a different, unknown 3D rotation $g_u \in SO(3)$

Figure: courtesy of Amit Singer and Yoel Shkolnisky

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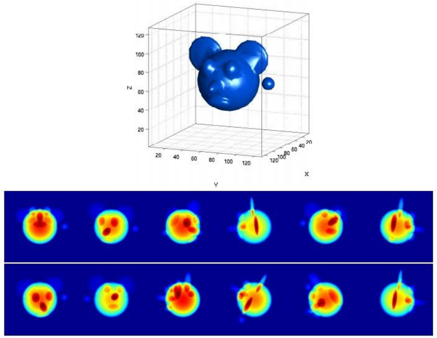

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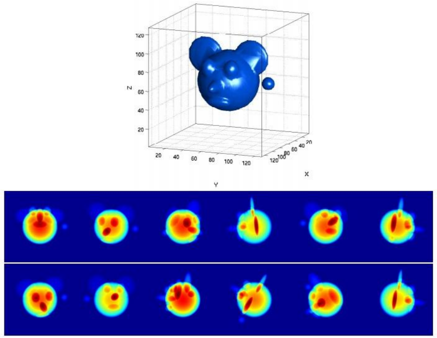

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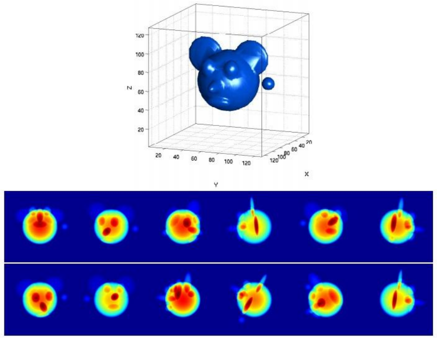

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One answer: spectral methods (PCA) [CSSS10]

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[CSSS10] R. R. Coifman, Y. Shkolnisky, F. J. Sigworth, A. Singer, "Reference free structure determination through eigenvectors of center of mass operators". Applied and Computational Harmonic Analysis, Volume 28, Issue 3 (2010).

$$\begin{pmatrix} g_1 g_1^{-1} & g_1 g_2^{-1} & g_1 g_3^{-1} & \\ g_2 g_1^{-1} & g_2 g_2^{-1} & g_2 g_3^{-1} & \\ g_3 g_1^{-1} & g_3 g_2^{-1} & g_3 g_3^{-1} & \\ & & & \ddots \end{pmatrix}$$

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Trouble:

- PCA ignores the constraint to valid group elements.

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Motivation: cryo-EM

Challenge:

- PCA ignores the constraint to valid group elements. How do we make better use of this structure?
- PCA effectively linearizes the observations, losing much of the signal. How do we fully exploit our observations?

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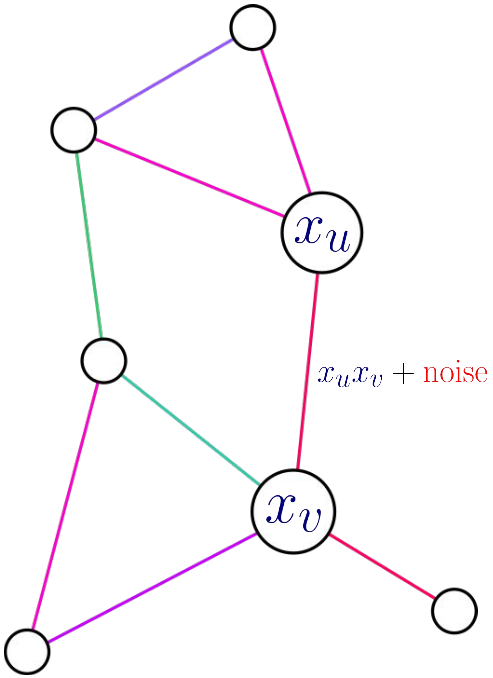
We apply Approximate Message Passing, an existing framework for structured linear problems.

We will build up towards cryo-EM via simpler problems.

Warm-up: $\mathbb{Z}/2$ synchronization

e.g. [HLL77], [Sin11], [ABBS14]



Learn $x \in \{\pm 1\}^n$

from noisy pairwise measurements...

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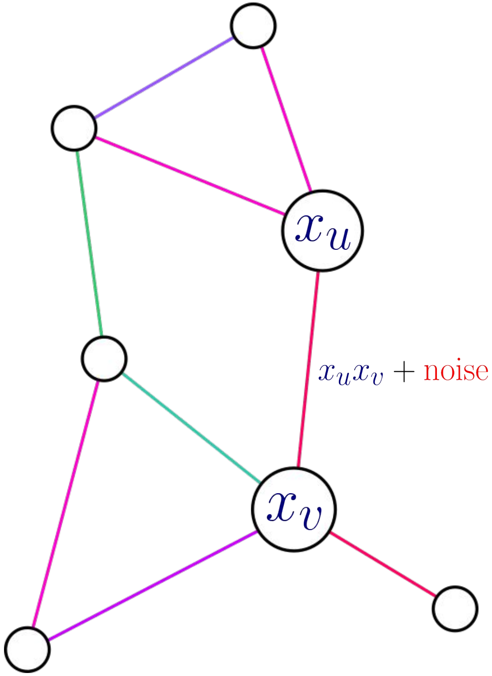

Learn $x \in \{\pm 1\}^n$

from a matrix of noisy pairwise measurements:

$$\underset{(n \times n)}{Y} = \underbrace{\frac{\lambda}{n} x x^\top}_{\text{signal}} + \underbrace{\frac{1}{\sqrt{n}} W}_{\text{noise}}$$

λ: signal-to-noise ratio, W: Gaussian noise (GOE)

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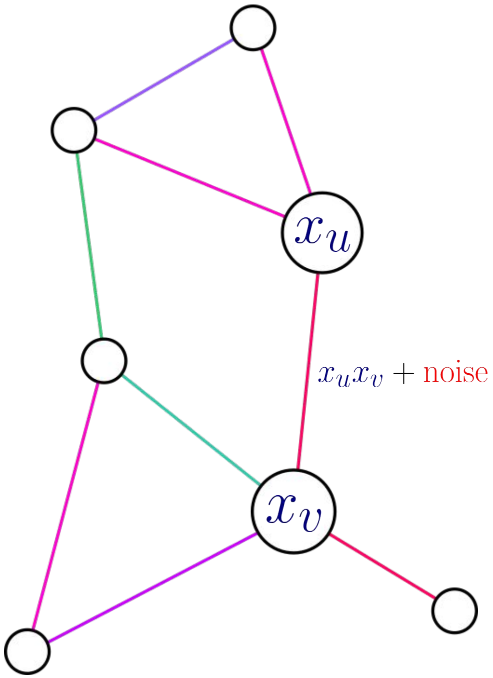

Learn $x \in \{\pm 1\}^n$ (up to a global flip)

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$\mathbb{Z}/2$: some prior methods

$$\begin{pmatrix} 1 & x_1x_2 & x_1x_3 & \\ x_2x_1 & 1 & x_2x_3 & \\ x_3x_1 & x_3x_2 & 1 & \\ & & & \ddots \end{pmatrix}$$

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PCA: top eigenvector of Y [Sin11]

Power iteration: $v \leftarrow Yv$

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Semidefinite programming [Sin11, BCS15]

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$\mathbb{Z}/2$: try soft thresholding?

Soft thresholding: $v \leftarrow Y f(v)$

(f is applied entry-wise to v)

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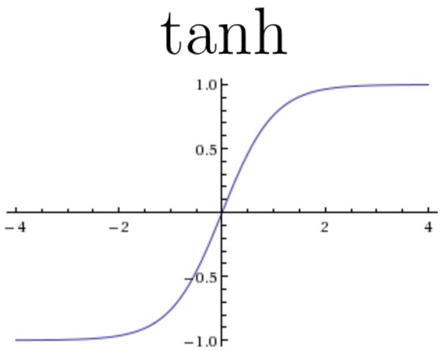

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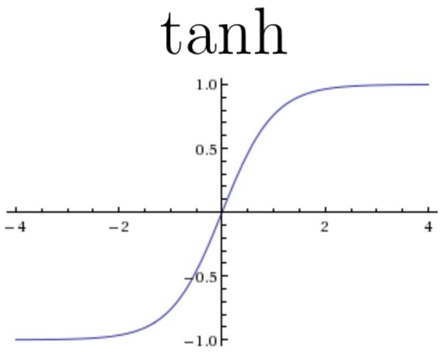

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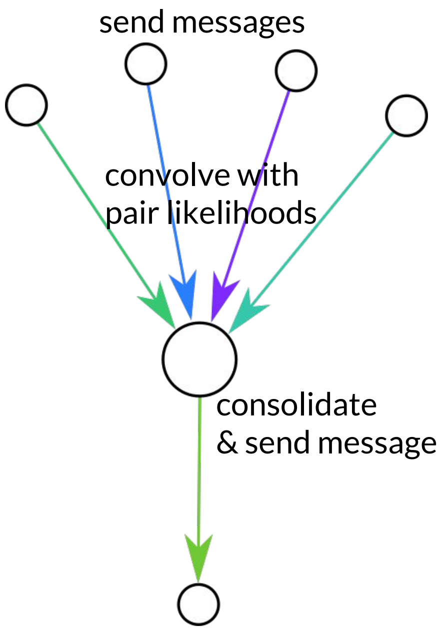
Outputs in $[-1, 1]$ capture “confidence” of estimates.

So this iterative algorithm passes around distributions...

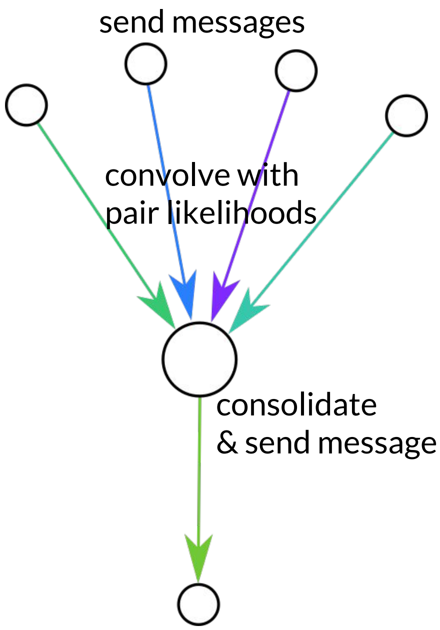
Belief Propagation (BP)



In each iteration, nodes send each other 'messages': their posterior **distributions** given the previous iteration.

[Pea86] Pearl, Judea. "Fusion, propagation, and structuring in belief networks." *Artificial intelligence* 29.3 (1986): 241-288.

[MPV86] M. Mézard, G. Parisi, and M. A. Virasoro. "SK model: The replica solution without replicas." *Europhys. Lett* 1.2 (1986): 77-82.



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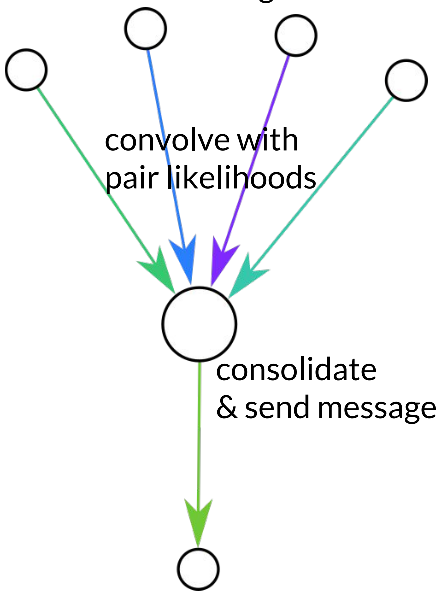

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Arose simultaneously as ‘cavity equations’ in physics.

Not rigorously well-understood.
(e.g. random SAT)

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Approximate Message Passing (AMP)

Simplifies belief propagation

- Exploits central limit theorems for dense graphs
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Frequently yields state-of-the-art statistical performance.

- Compressed sensing [DMM09]
- Sparse PCA [DM14], non-negative / cone PCA [DMR14]

[DMM09] D. L. Donoho., A. Maleki, and A. Montanari. "Message-passing algorithms for compressed sensing." *P. Natl. Acad. Sci. USA* 106.45 (2009).

[DM14] Y. Deshpande and A. Montanari. Information-theoretically optimal sparse PCA." *IEEE ISIT*, 2014.

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Rigorous proof framework [BM11]

[BM11] M. Bayati and A. Montanari. "The dynamics of message passing on dense graphs, with applications to compressed sensing." *IEEE T. Inform. Theory* 57.2 (2011).

[DMM09] D. L. Donoho., A. Maleki, and A. Montanari. "Message-passing algorithms for compressed sensing." *P. Natl. Acad. Sci. USA* 106.45 (2009).

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AMP for $\mathbb{Z}/2$ synchronization

[DAM15]

$$c^t = \lambda Y v^{t-1} - \lambda^2(1 - \langle v^{t-1} \rangle^2) v^{t-2}$$

—Onsager correction—

$$v^t = \tanh(c^t)$$

—soft thresholding—

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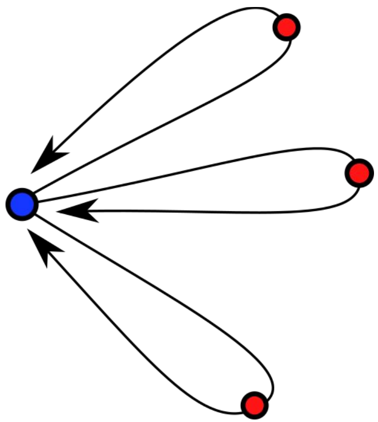

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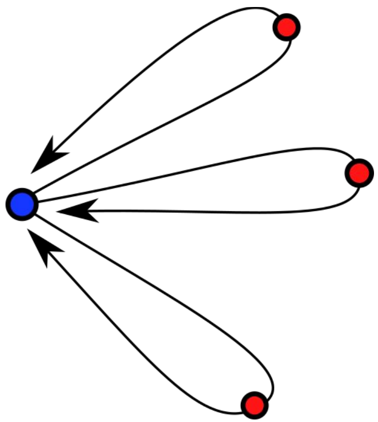

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Each entry of v^t encodes a distribution over $\{\pm 1\}$.

(as the expectation)

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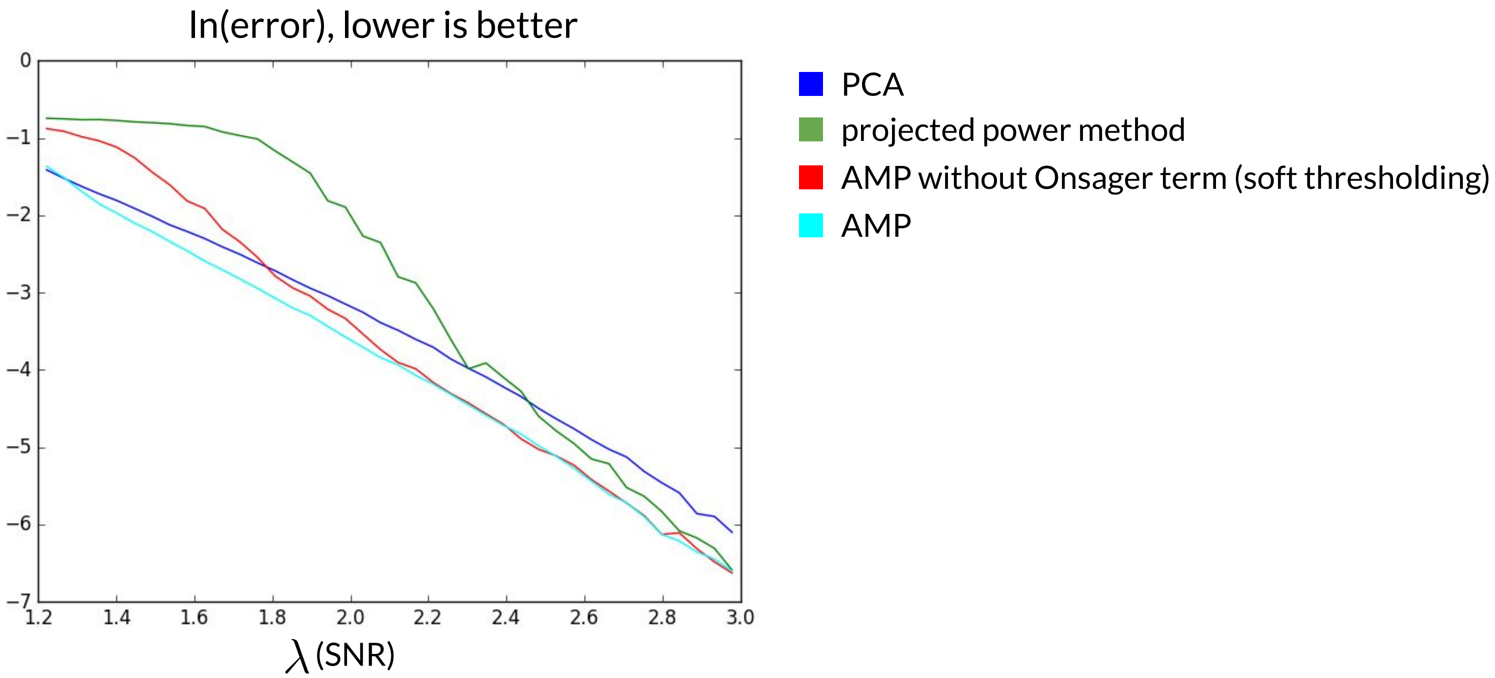
Comparison of Methods



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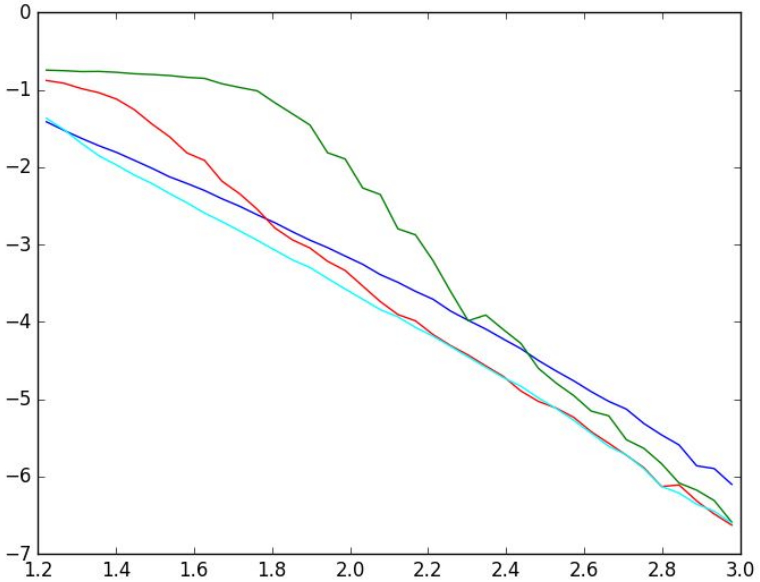
Comparison of Methods

ln(error), lower is better



λ (SNR)

- PCA
- projected power method
- AMP without Onsager term (soft thresholding)
- AMP

AMP is provably optimal here

(modulo warm-start) [DAM15]

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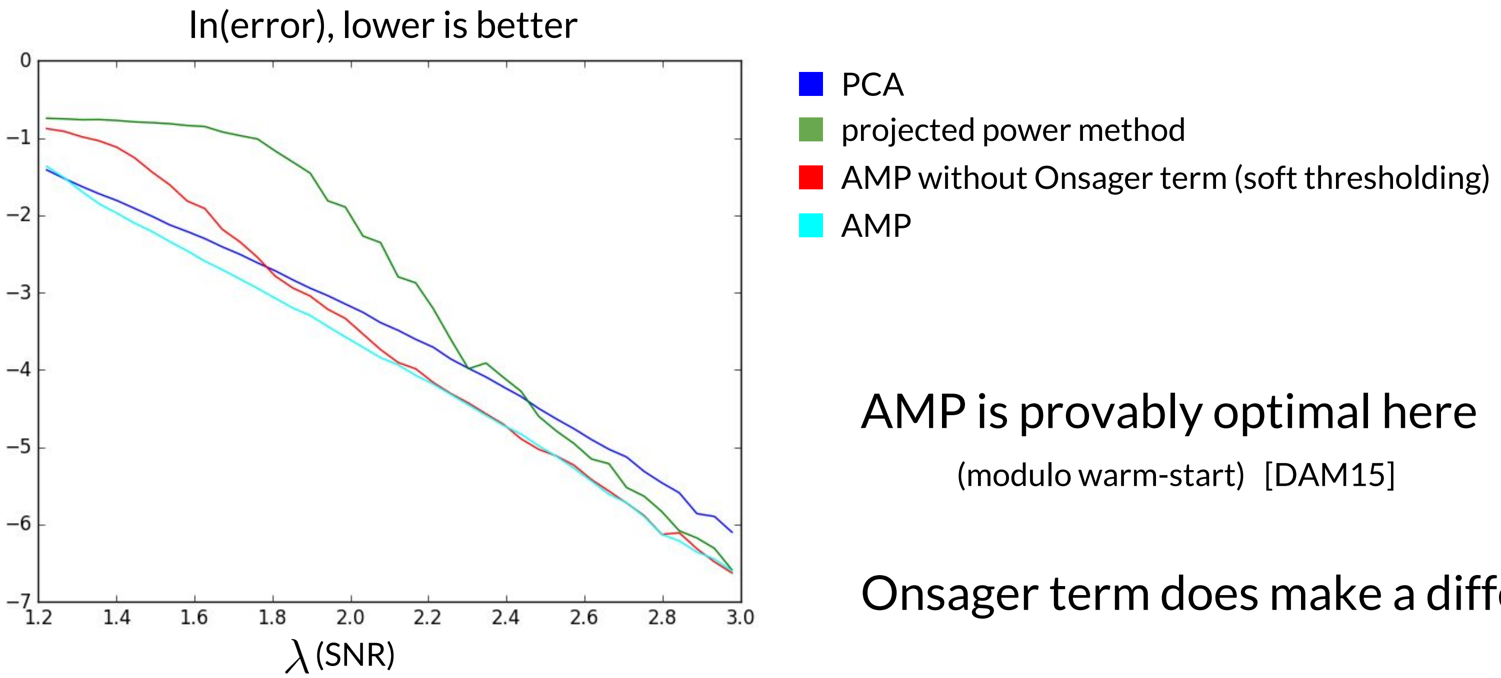

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Onsager term does make a difference!

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Motivation: multireference alignment

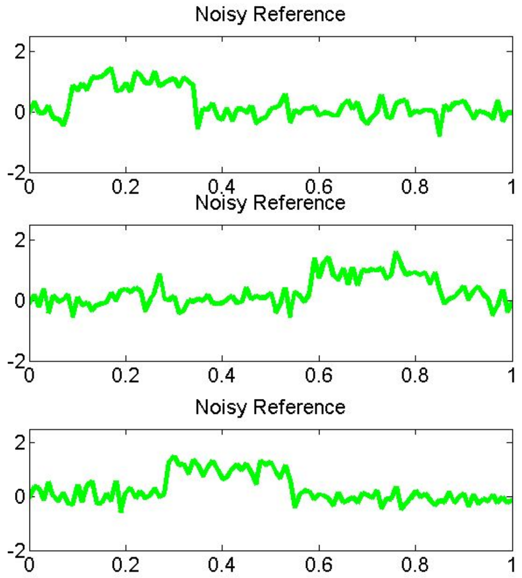
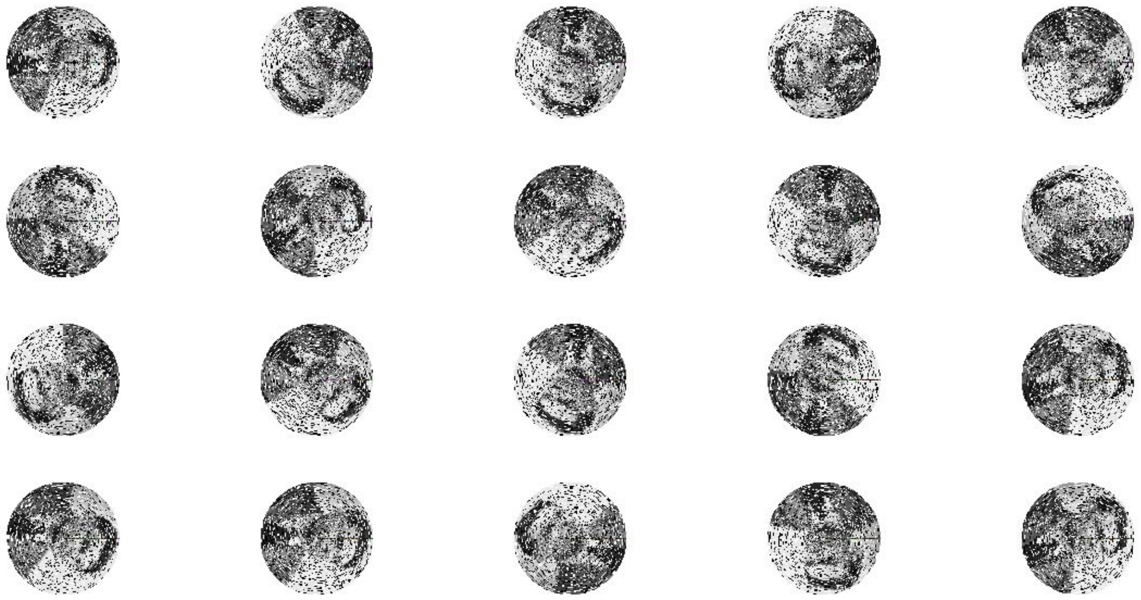


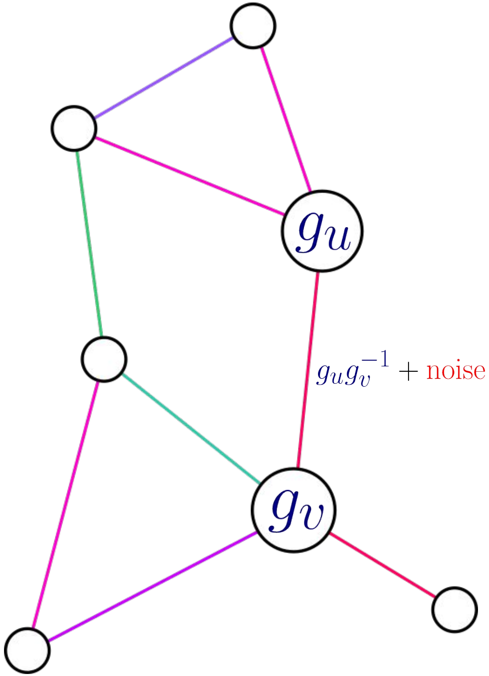
Figure: A. S. Bandeira, M. Charikar, A. Singer, and A. Zhu. Multireference alignment using semidefinite programming. *5th Innovations in Theoretical Computer Science (ITCS 2014)*, 2014.

Motivation: angular synchronization



Synchronization over any group

[BCS15]



Learn a vector g of group elements
from noisy observations of $g_u g_v^{-1}$.
(up to global right-multiplication by a group element)

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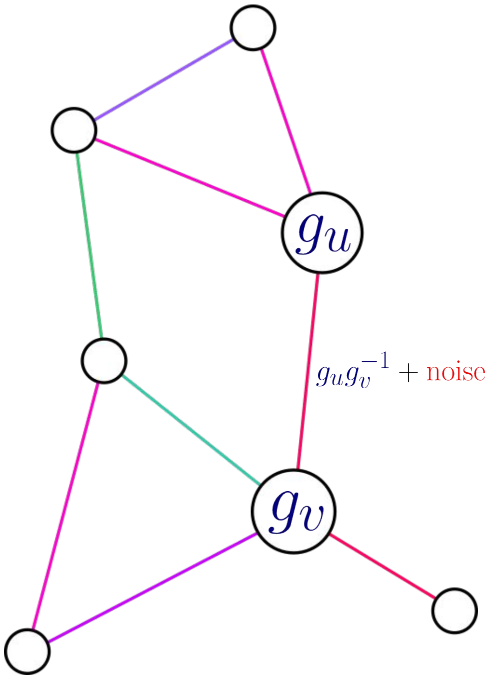

Synchronization over any group

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Learn a vector g of group elements
from noisy observations of $g_u g_v^{-1}$.
(up to global right-multiplication by a group element)

Our contribution: AMP for synchronization over any* group, with any* noise model

(e.g. $\mathbb{Z}/L,\ U(1),\ SO(3),$ compact Lie groups)

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U(1) synchronization

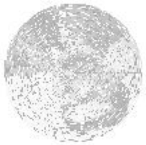
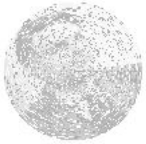
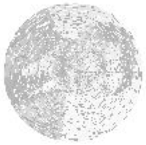
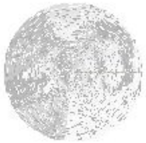
Observe $Y^{(1)} = \frac{\lambda}{n} x x^* + \frac{1}{\sqrt{n}} W^{(1)}$

—signal— —noise—

SDP is tight [BNS14]

[BNS14] A. S. Bandeira, N. Boumal, and A. Singer. "Tightness of the maximum likelihood semidefinite relaxation for angular synchronization." *arXiv:1411.3272* (2014).

U(1) with two frequencies

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$$Y^{(1)} = \frac{\lambda}{n} x x^* + \frac{1}{\sqrt{n}} W^{(1)}$$
$$Y^{(2)} = \frac{\lambda}{n} x^2 (x^2)^* + \frac{1}{\sqrt{n}} W^{(2)}$$

—signal— —noise—

Multiple channels of pairwise information.

U(1) with multiple frequencies

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$$Y^{(2)} = \frac{\lambda}{n} x^2 (x^2)^* + \frac{1}{\sqrt{n}} W^{(2)}$$

...

$$Y^{(k)} = \underbrace{\frac{\lambda}{n} x^k (x^k)^*}_{\text{signal}} + \underbrace{\frac{1}{\sqrt{n}} W^{(k)}}_{\text{noise}}$$

—signal— —noise—

Multiple channels of pairwise information.

U(1) with multiple frequencies

Observe
$$Y^{(1)} = \frac{\lambda}{n} x x^* + \frac{1}{\sqrt{n}} W^{(1)}$$
$$Y^{(2)} = \frac{\lambda}{n} x^2 (x^2)^* + \frac{1}{\sqrt{n}} W^{(2)}$$
$$\cdots$$
$$Y^{(k)} = \frac{\lambda}{n} x^k (x^k)^* + \frac{1}{\sqrt{n}} W^{(k)}$$

—signal— —noise—

Multiple channels of pairwise information.

Multiple frequencies corresponds to nonlinear observations.

No clear PCA approach that couples them.

U(1): AMP algorithm

Represent distributions by discretizations?

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Represent distributions by discretizations?

Discretizing $SO(3)$ is awkward: impossible without breaking symmetry.

Rotating a discretized function is lossy.

U(1): AMP algorithm

Represent distributions by Fourier coeffs of...

density?

$$\frac{d\mathbb{P}(g_u)}{d\theta} = \sum_k v_u^{(k)} e^{ik\theta}$$

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Iteration:

$$x^{(k)} \leftarrow \lambda Y^{(k)} v^{(k)} + \text{onsager}$$ (messaging)

$$v_u^{(\bullet)} \leftarrow f(x_u^{(\bullet)})$$ (consolidation)

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Iteration: $c^{(k)} \leftarrow \lambda Y^{(k)} v^{(k)} + \text{onsager}$ (messaging)

$v_u^{(\bullet)} \leftarrow f(c_u^{(\bullet)})$ (consolidation)

f is the transformation from $c_u^{(\bullet)}$ to $v_u^{(\bullet)}$!

U(1): the nonlinear transformation

f converts Fourier coefficients of $g : U(1) \to \mathbb{R}$
into Fourier coefficients of $\exp(g)$, and then normalizes.

This couples Fourier components $Y^{(k)}$ of the measurements.

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c $-c$

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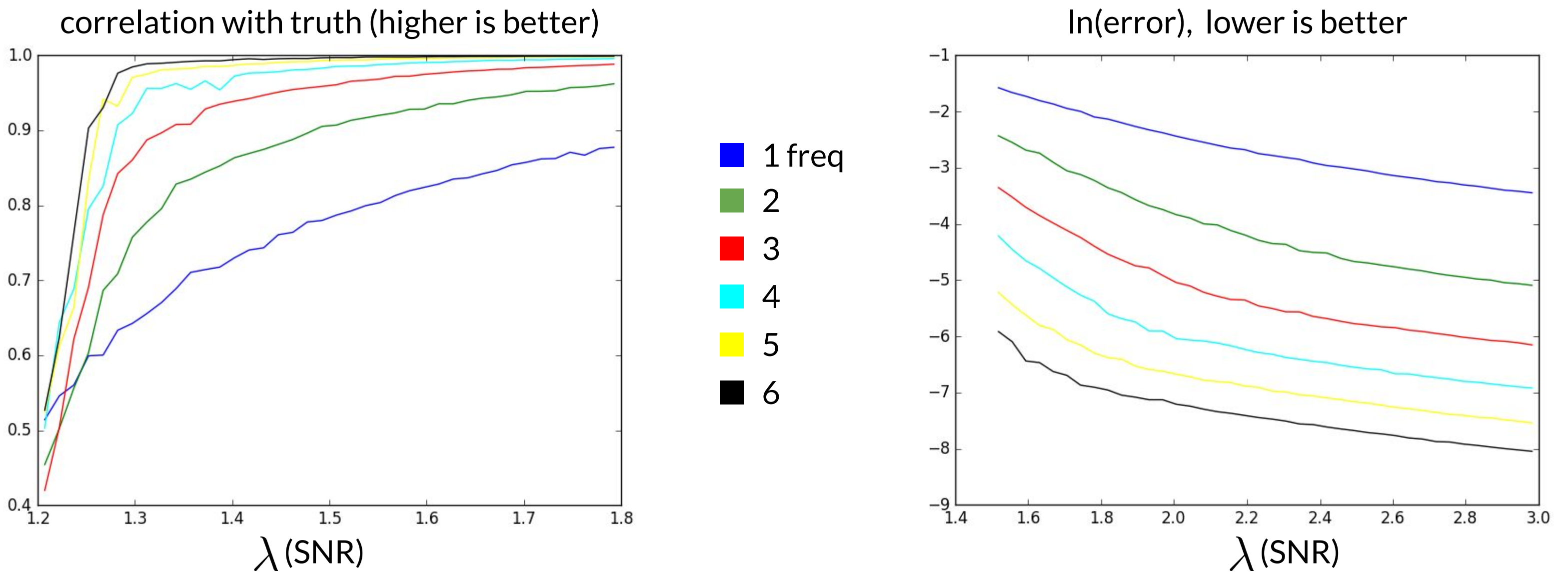
Then,

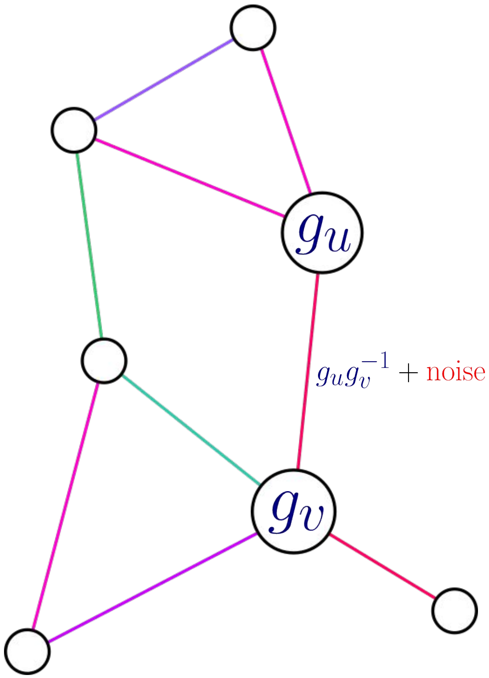
$$f(c) = \frac{e^c - e^{-c}}{e^c + e^{-c}} = \tanh(c)$$

U(1): empirical results

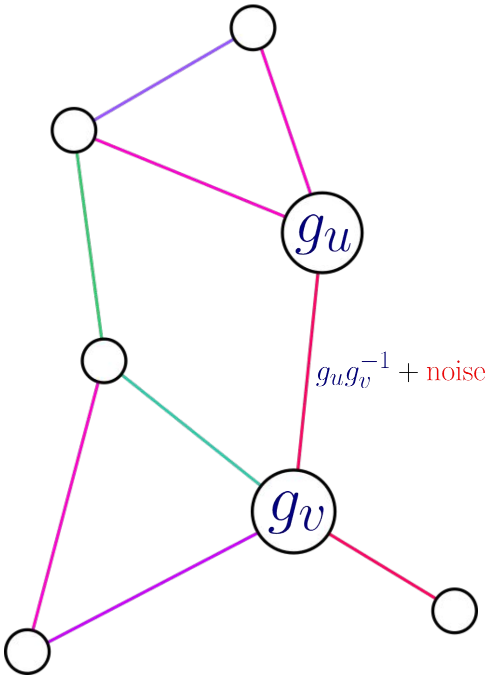


AMP can synthesize information across multiple frequencies.

Synchronization over any* group



Fourier theory becomes **representation theory**.



Synchronization over any* group

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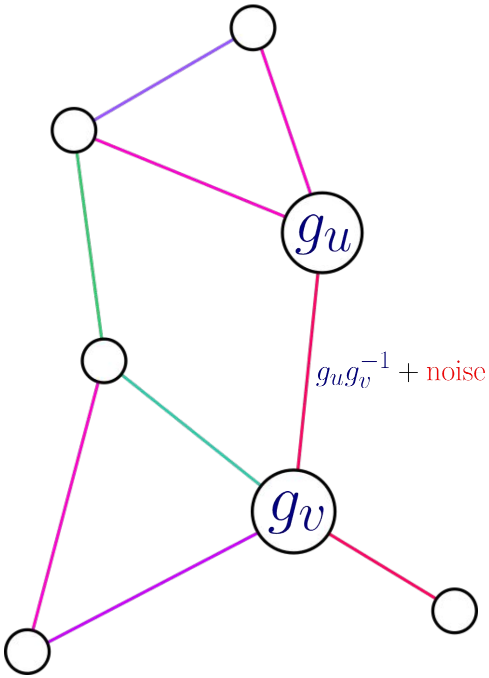
Peter–Weyl theorem: any* $f : G \to \mathbb{C}$ decomposes into normal modes:

$$f(g) = \sum_{\text{irreps } \rho} \left\langle C^{(\rho)}, \rho(g) \right\rangle$$



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Apply this to distributions to describe the AMP iterations.

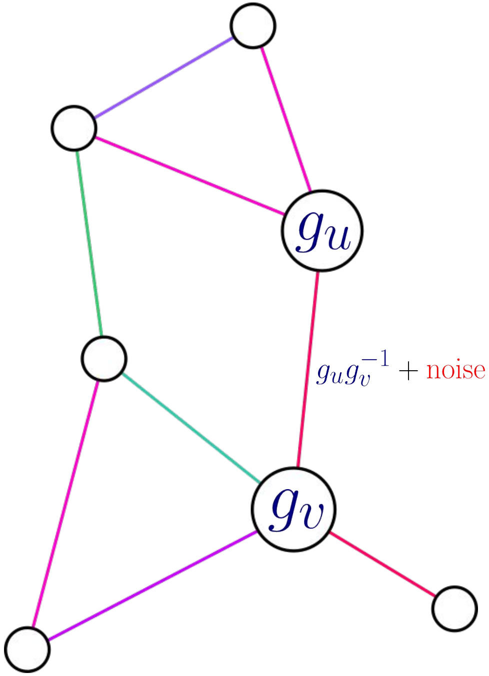
$$C^{(\rho)} \leftarrow Y^{(\rho)} V^{(\rho)} + \text{onsager}$$

(messaging)

$$V_u^{(\bullet)} \leftarrow f(C_u^{(\bullet)})$$

(consolidation: exp & normalize)

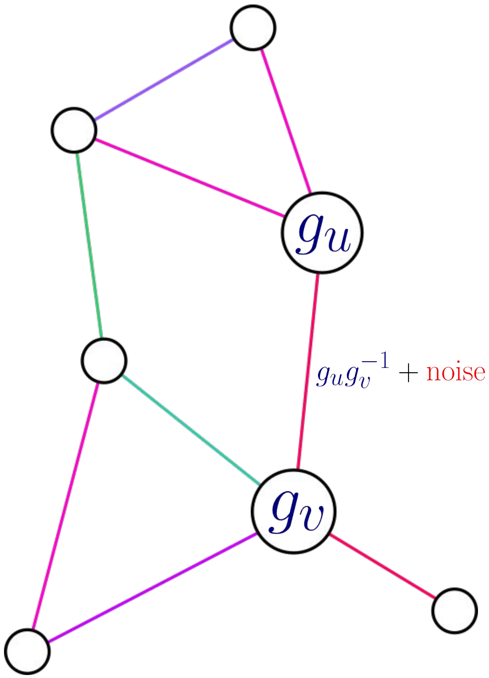
Noise models & non-unique games



What sort of noise?

[BCS15] A. S. Bandeira, Y. Chen, and A. Singer. "Non-unique games over compact groups and orientation estimation in cryo-EM." *arXiv:1505.03840* (2015).

Noise models & non-unique games



We assume pair measurements have independent noise.

Likelihood factors over edges: $$\log \mathcal{L}(g) = \sum_{u,v} \ell_{u,v}(g_u g_v^{-1})$$

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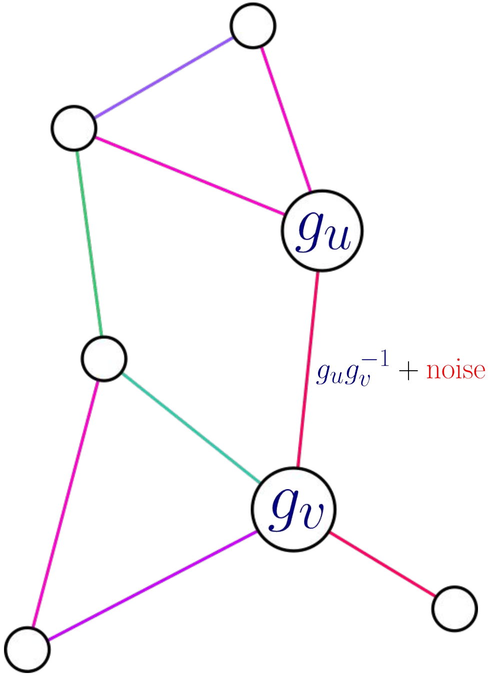

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Likelihood factors over edges: $\log \mathcal{L}(g) = \sum_{u,v} \ell_{u,v}(g_u g_v^{-1})$

Assemble matrix coefficients of $\ell_{u,v}$ into matrices $Y^{(\rho)}$.

$$Y^{(\rho)} = \begin{pmatrix} \hat{\ell}_{1,1}(\rho) & \hat{\ell}_{1,2}(\rho) & \hat{\ell}_{1,3}(\rho) & \\ \hat{\ell}_{2,1}(\rho) & \hat{\ell}_{2,2}(\rho) & \hat{\ell}_{2,3}(\rho) & \\ \hat{\ell}_{3,1}(\rho) & \hat{\ell}_{3,2}(\rho) & \hat{\ell}_{3,3}(\rho) & \\ & & & \ddots \end{pmatrix}$$

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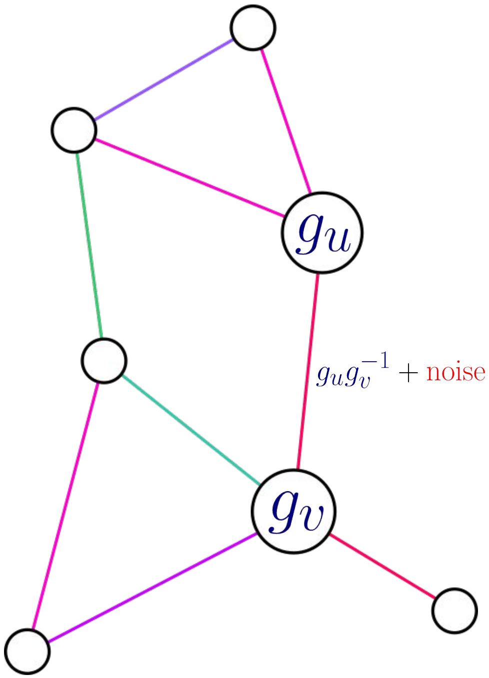

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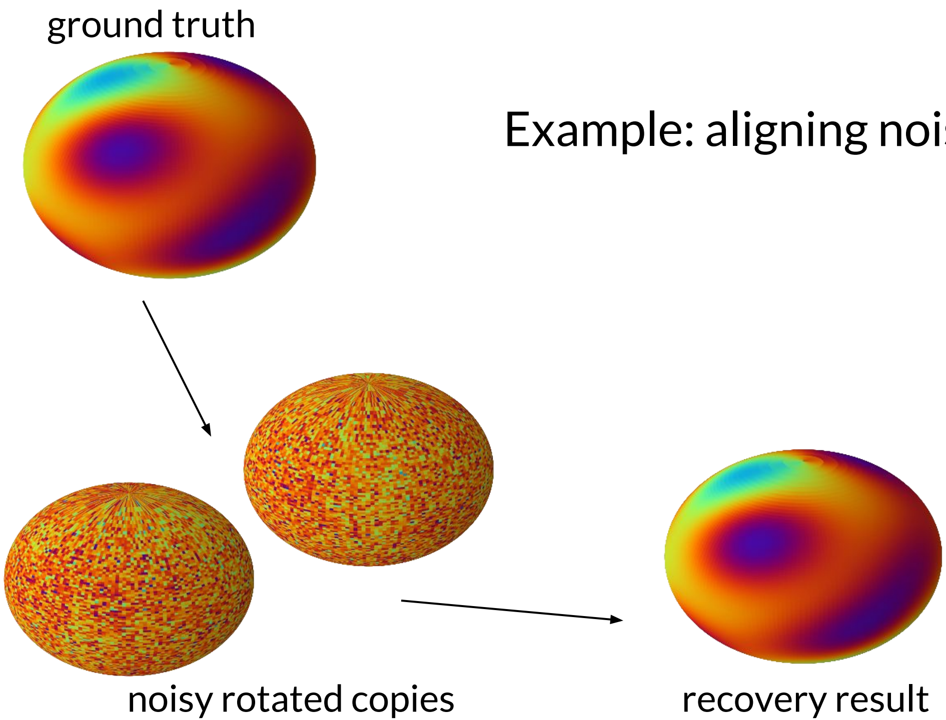
AMP for SO(3) synchronization

Example: aligning noisy copies of images on the sphere.



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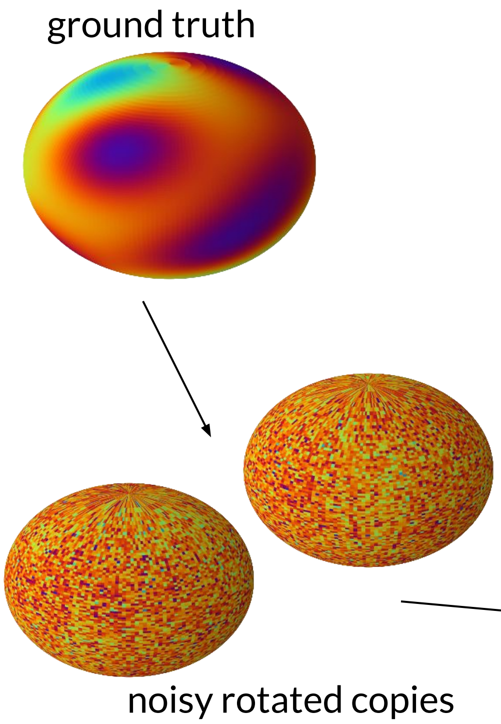
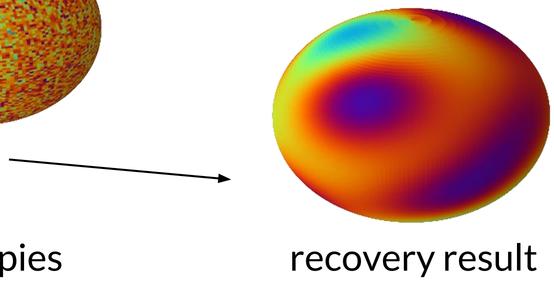


Example: aligning noisy copies of images on the sphere.

To form $Y^{(\rho)}$: decompose images into spherical harmonics.
j^{th} representation compares the degree j harmonics.



Ongoing work:

Correct AMP for per-vertex noise

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What are the information limits of synchronization problems?

Does AMP match them?

Thanks!

Any questions?