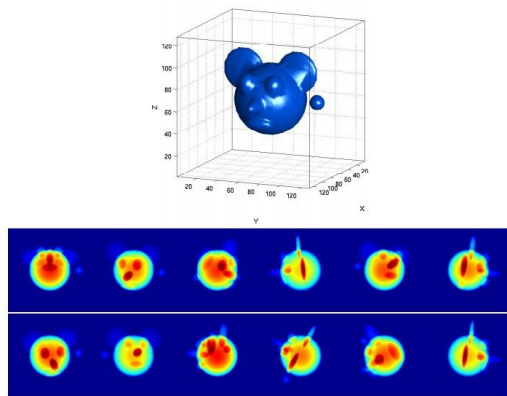

Message-passing algorithms for synchronization problems

Amelia Perry (MIT Mathematics)

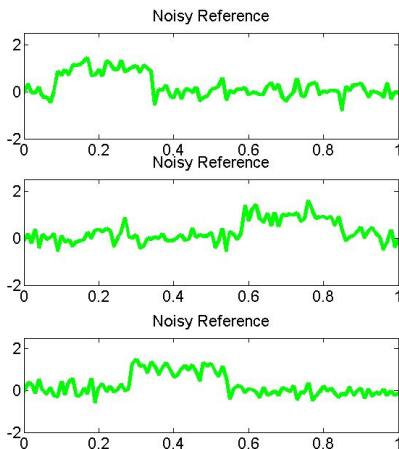
with Afonso Bandeira, Ankur Moitra, and Alex Wein

Motivation

Cryo-EM



Multireference alignment



Angular synchronization

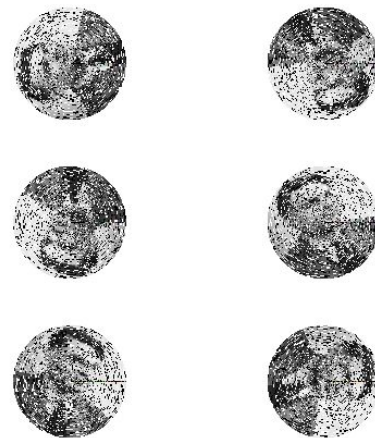
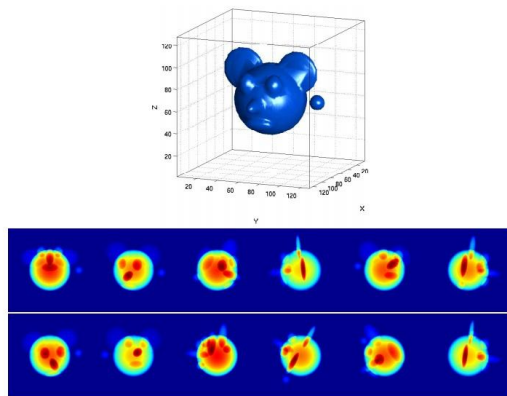


Figure: courtesy of Amit Singer and Yoel Shkolnisky

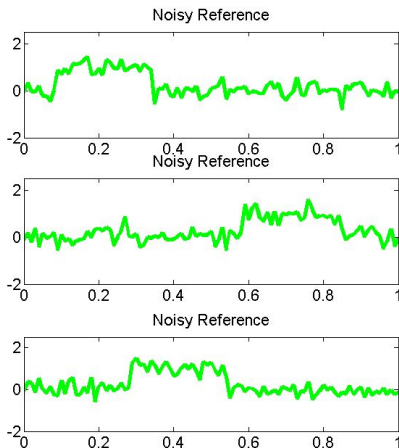
Figure: A. S. Bandeira, M. Charikar, A. Singer, and A. Zhu.
Multireference alignment using semidefinite programming. *5th Innovations in Theoretical Computer Science (ITCS 2014)*, 2014.

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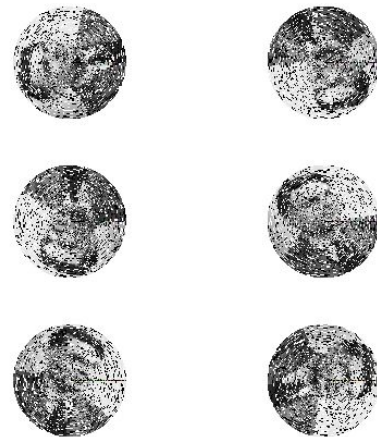
Cryo-EM



Multireference alignment



Angular synchronization



Samples are random group actions on a true signal, plus noise.

Estimation of signal vs. shifts

In Jon's and Nicolas's talks yesterday: shifts are sometimes hard to estimate; just estimate the signal directly.

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- Simultaneous localization and mapping [RCBL16]: the shifts tell us where our robot is (localization)

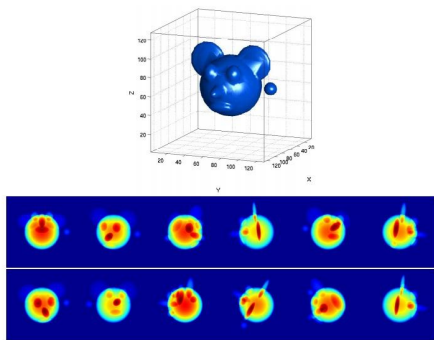
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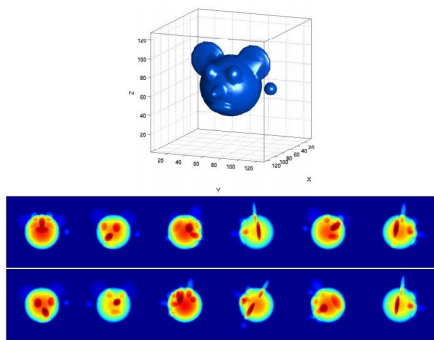
- Simultaneous localization and mapping [RCBL16]: the shifts tell us where our robot is (localization)
- Cryo-EM: the invariant theory approach is not yet developed...

Synchronization: shifts from comparisons



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

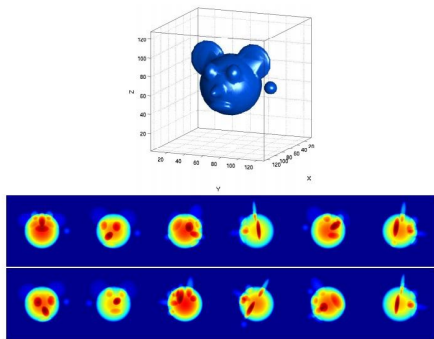
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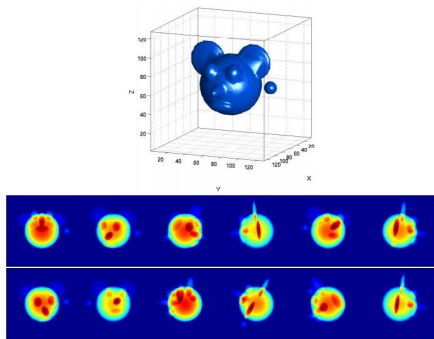


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One answer: spectral methods (PCA) [CSSS10]

Synchronization & PCA

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

Trouble:

- PCA ignores the constraint to valid group elements.

Synchronization & PCA

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How do we make better use of this structure?
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We apply Approximate Message Passing, an existing framework for structured linear problems.

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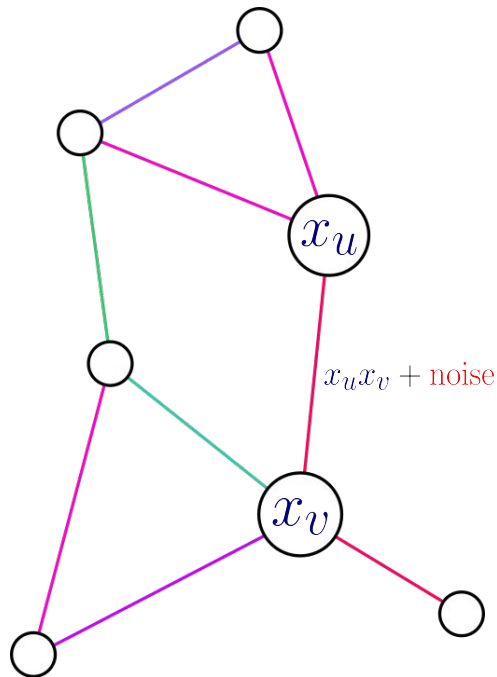
We will build up towards cryo-EM via simpler problems.

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

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

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

from noisy pairwise measurements...



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

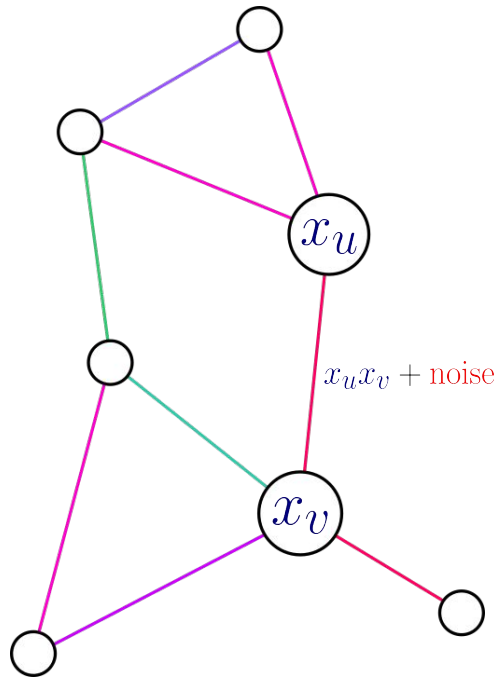
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Learn $\mathbf{x} \in \{\pm 1\}^n$

from a matrix of noisy pairwise measurements:

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

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



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

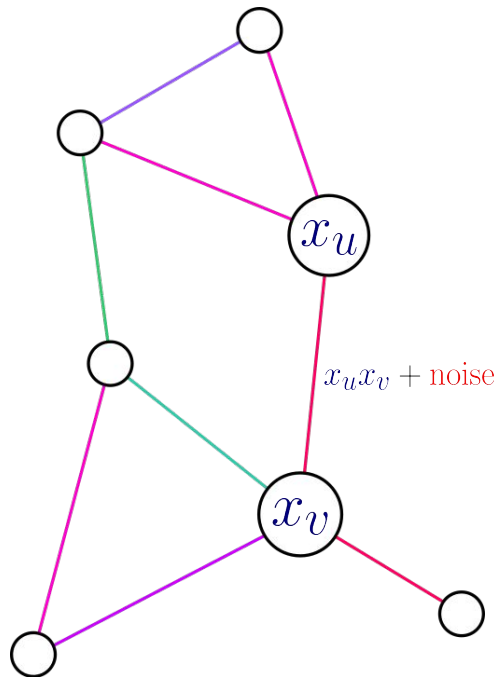
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Learn $x \in \{\pm 1\}^n$ (up to a global flip)

from a matrix of noisy pairwise measurements:

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



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

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

PCA: top eigenvector of Y [Sin11]

Power iteration: $v \leftarrow Yv$

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Projected power iteration (“majority dynamics”) [Bou16]

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Semidefinite programming [Sin11, BCS15]

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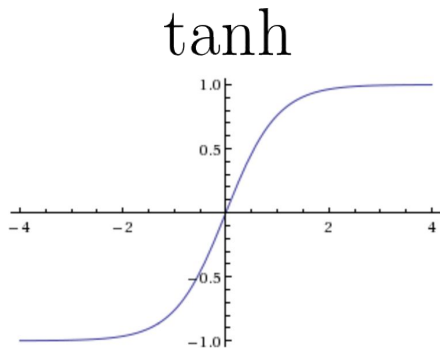
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[BCS15] A. S. Bandeira, Y. Chen, and A. Singer. “Non-unique games over compact groups and orientation estimation in cryo-EM.” *arXiv:1505.03840* (2015).

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

Soft thresholding: $v \leftarrow Yf(v)$
(f is applied entry-wise to v)

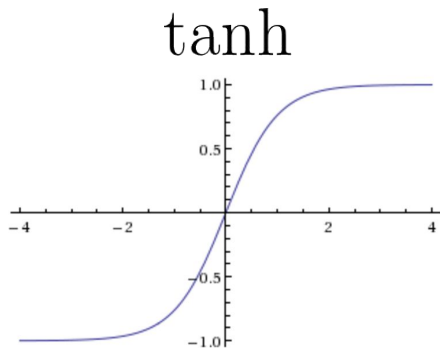
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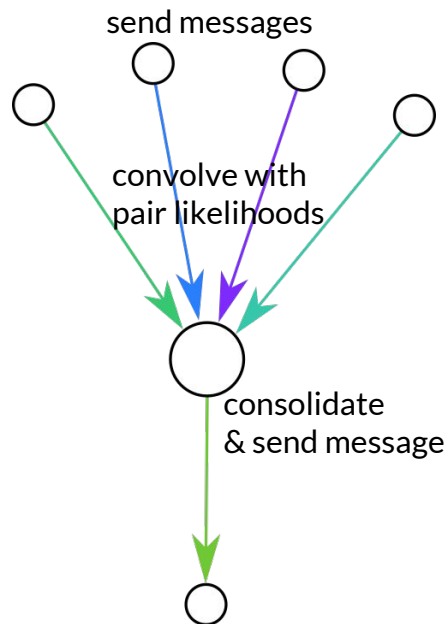
Optimal: $f(v) = \tanh(\lambda v)$

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

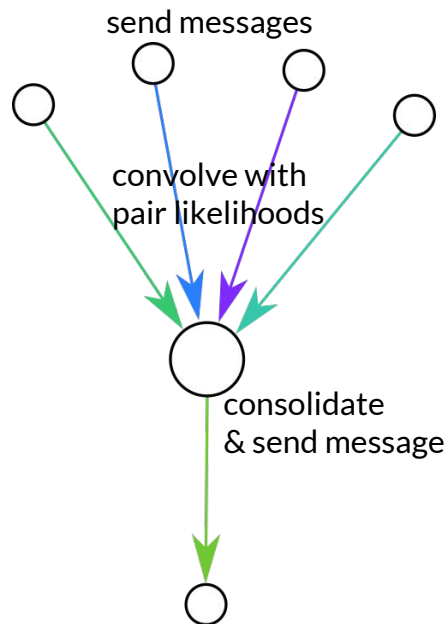
So this iterative algorithm passes around distributions...

Belief Propagation (BP)

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



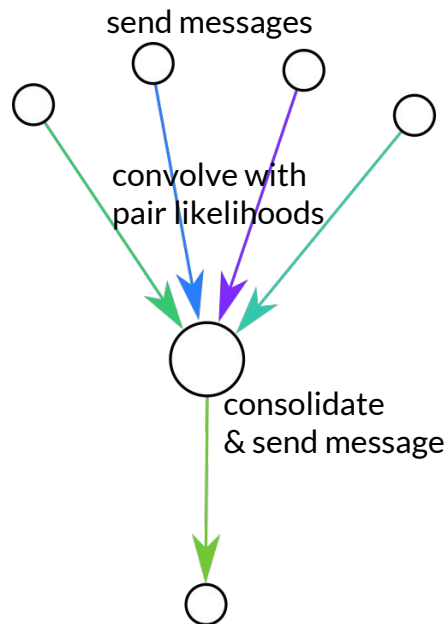
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Belief Propagation (BP)



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Caveat: no backtracking!

Arose simultaneously as ‘cavity equations’ in physics.

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

Approximate Message Passing (AMP)

Simplifies belief propagation

- Exploits central limit theorems for dense graphs
- Encodes messages (distributions) in a few parameters

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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).

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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]

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

—Onsager correction—

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

—soft thresholding—

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

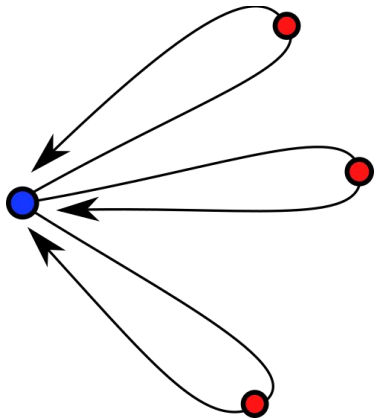
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Onsager term corrects for backtracking, to leading order.

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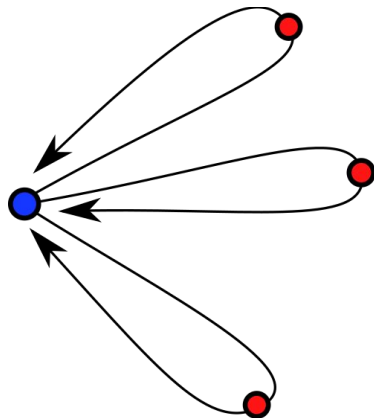
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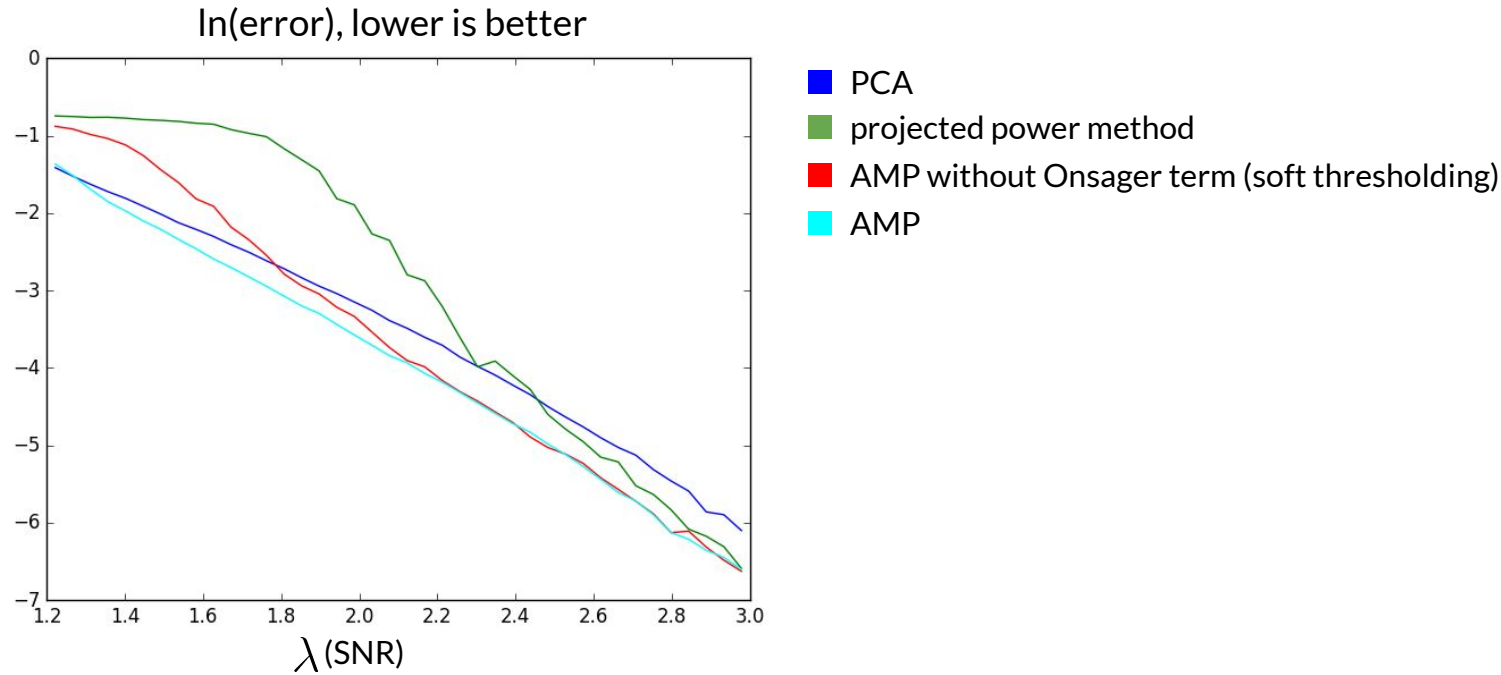
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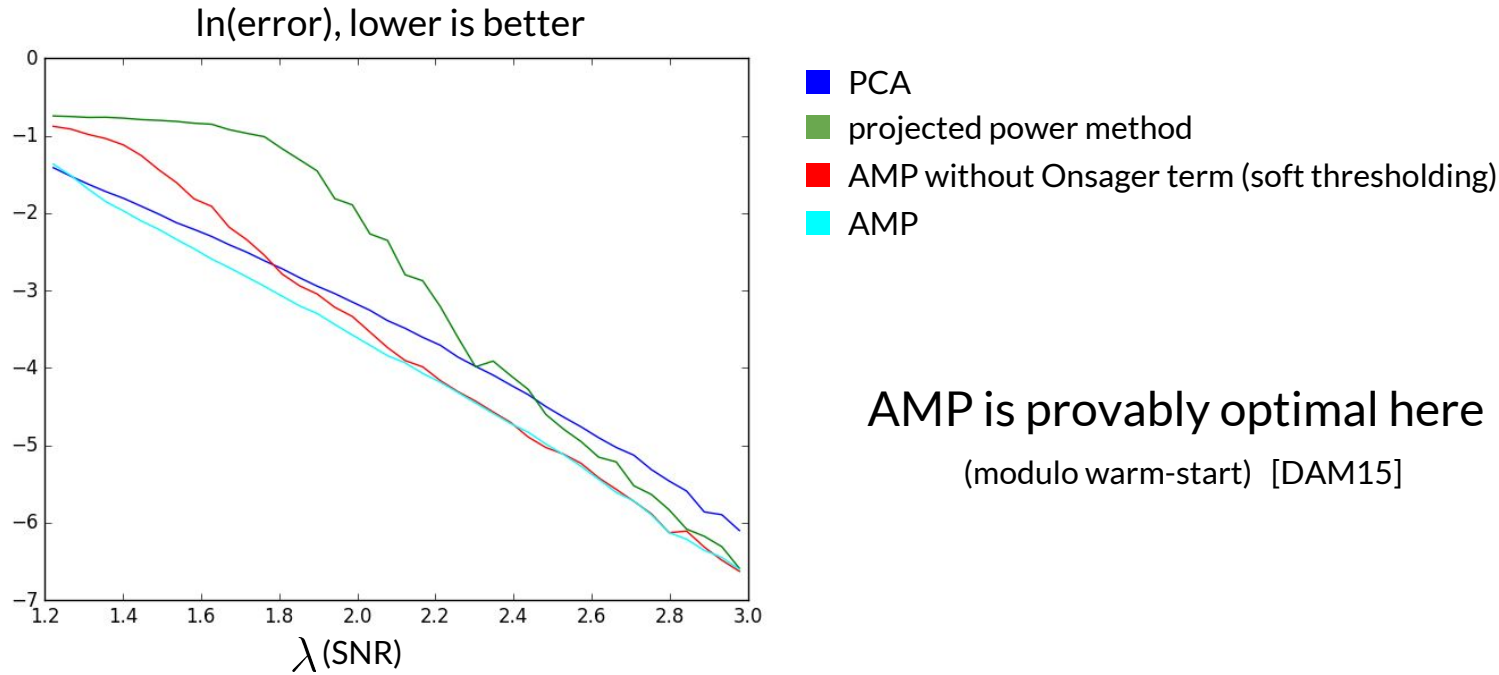
Onsager term corrects for backtracking, to leading order.

Each entry of v^t encodes a distribution over $\{\pm 1\}$.
(as the expectation)

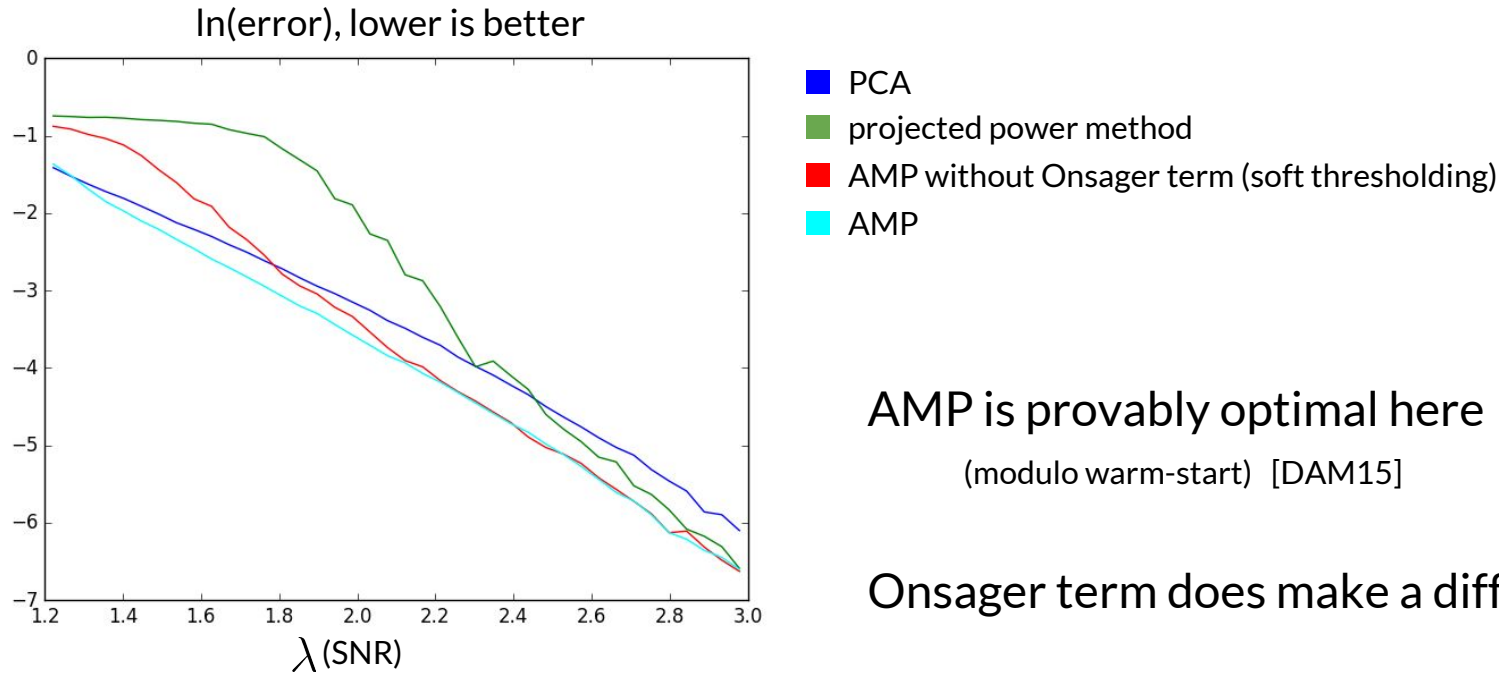
Comparison of Methods



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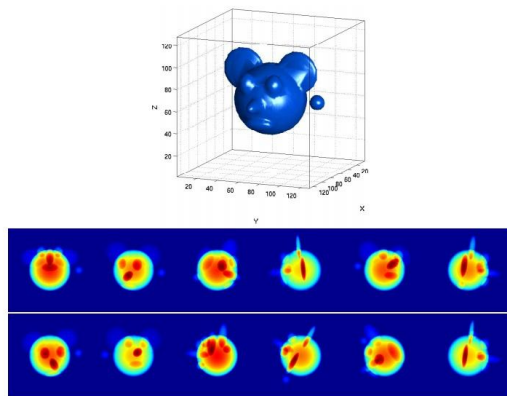
AMP is provably optimal here

(modulo warm-start) [DAM15]

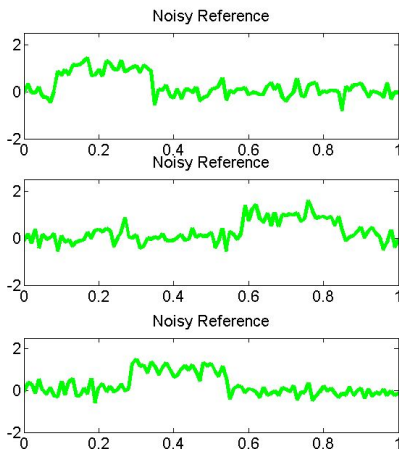
Onsager term does make a difference!

Motivation

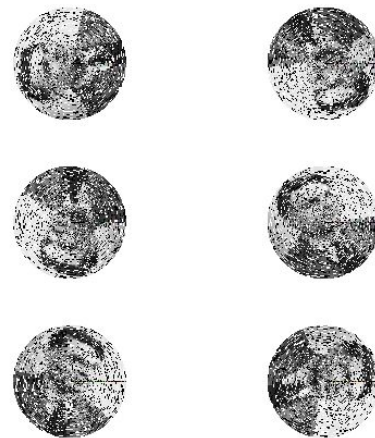
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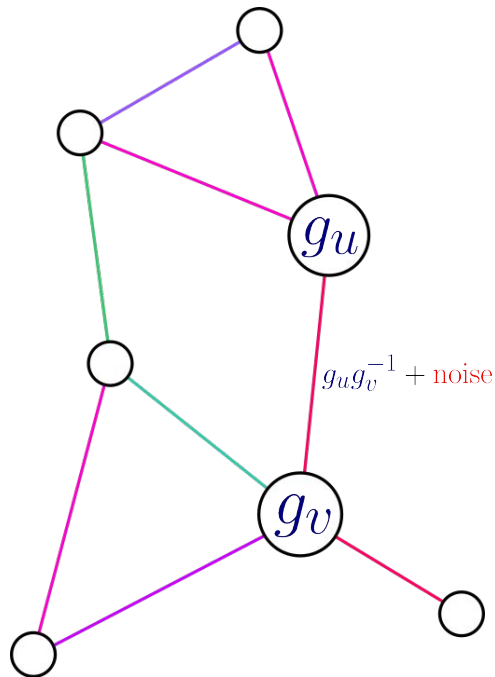
Angular synchronization



Synchronization over any group

[BCS15]

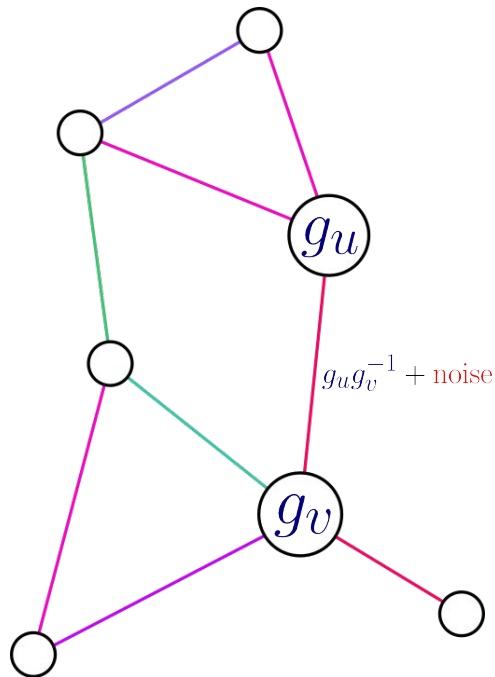
Learn a vector g of group elements
from noisy observations of $g_u g_v^{-1}$.
(up to global right-multiplication by a group element)



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)



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

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

U(1) synchronization

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

SDP is tight [BNS14]

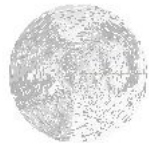
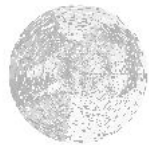
U(1) with two frequencies

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

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

—signal— —noise—

Multiple channels of
pairwise information.



U(1) with multiple frequencies

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

Multiple channels of pairwise information.

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

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—signal— —noise—



U(1) with multiple frequencies

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

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

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

—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?

U(1): AMP algorithm

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?

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

U(1): AMP algorithm

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

log-likelihood?

$$\log \frac{d\mathbb{P}(g_u)}{d\theta} + \text{const} = \sum_k c_u^{(k)} e^{ik\theta}$$



U(1): AMP algorithm

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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)

U(1): AMP algorithm

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

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

U(1): the nonlinear transformation

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

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

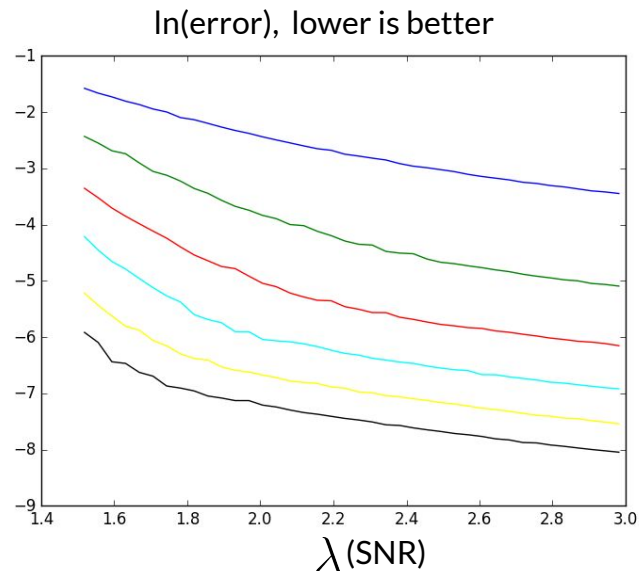
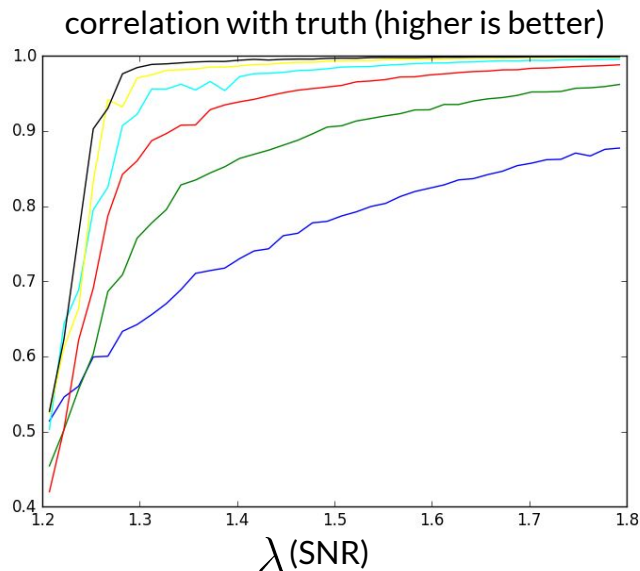
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$\mathbb{Z}/2$: On the “Fourier coefficient” $g(1) - g(-1)$, this is \tanh .

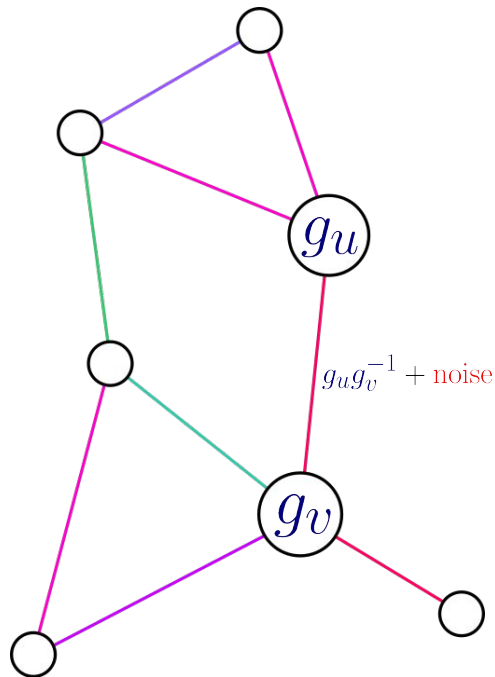
U(1): empirical results



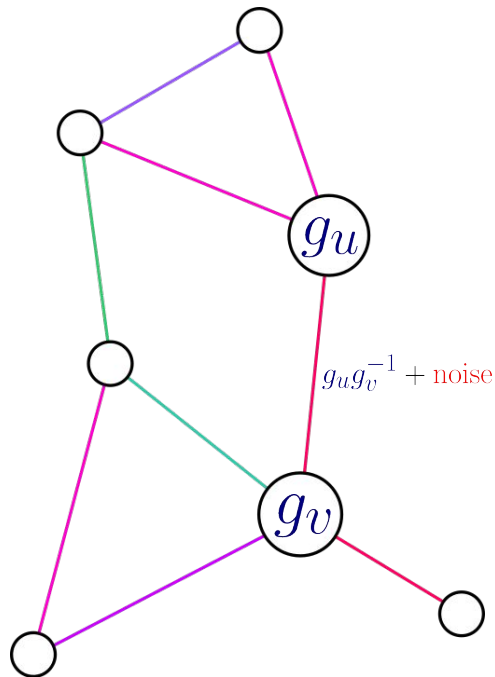
AMP can synthesize information across multiple frequencies.

Synchronization over any* group

Fourier theory becomes **representation theory**.



Synchronization over any* group

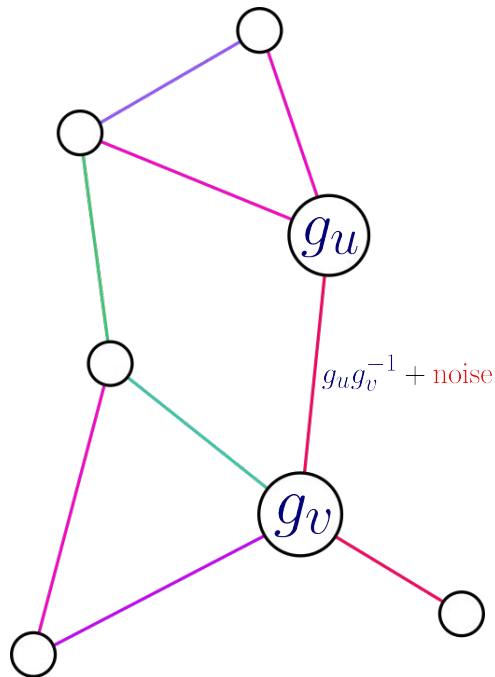


Fourier theory becomes **representation theory**.

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

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Synchronization over any* group



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Apply this to distributions to describe the AMP iterations.

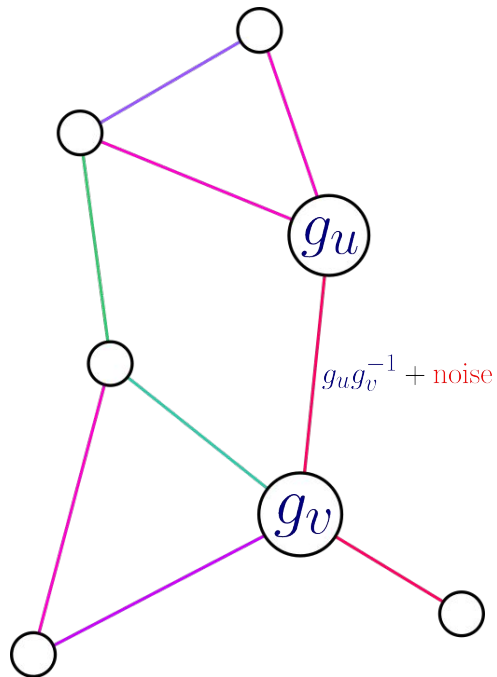
$$C^{(\rho)} \leftarrow Y^{(\rho)} V^{(\rho)} + \text{onsager}$$

(messaging)

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

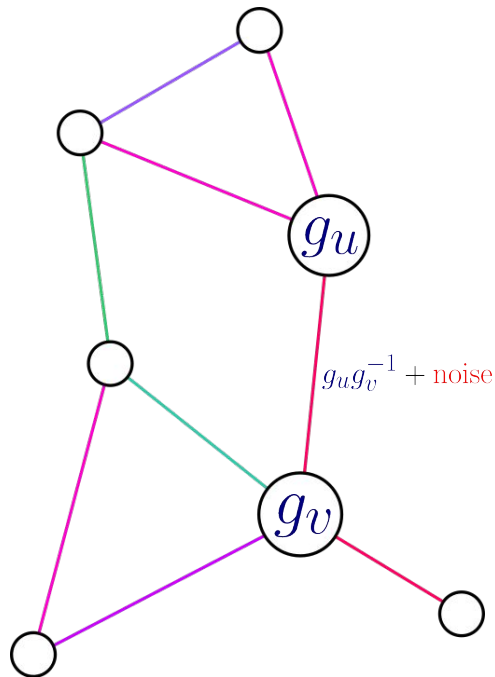
(consolidation: exp & normalize)

Noise models & non-unique games



What sort of **noise**?

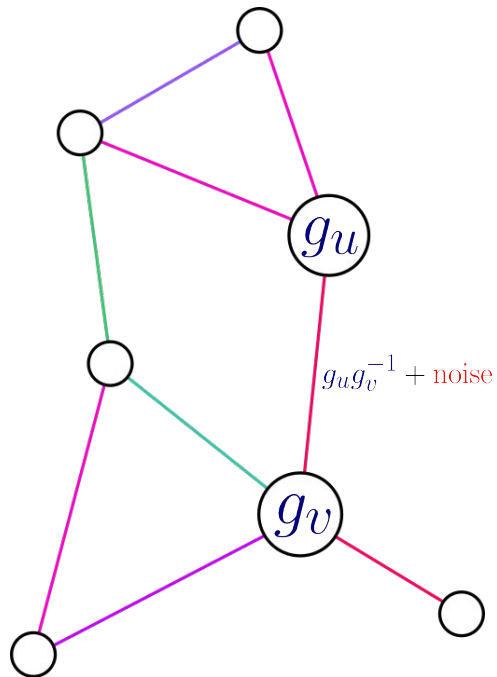
Noise models & non-unique games



We assume pair measurements have independent noise.

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

Noise models & non-unique games



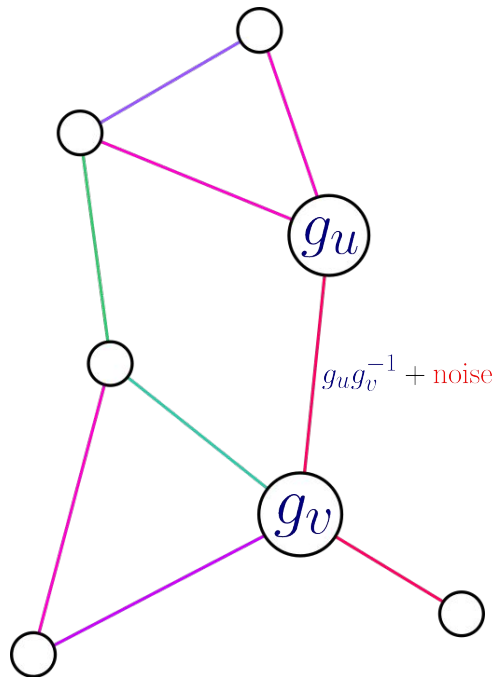
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Likelihood factors over edges: $\log \mathcal{L}(g) = \sum_{u,v} \ell_{u,v}(g_u g_v^{-1})$

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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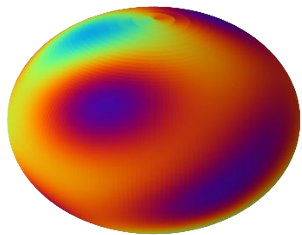
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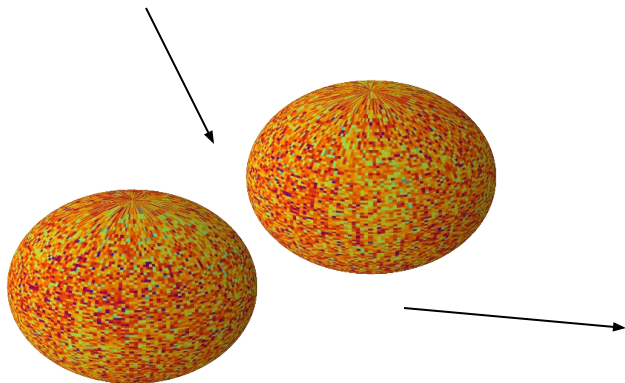
$$\begin{aligned} C^{(\rho)} &\leftarrow Y^{(\rho)} V^{(\rho)} + \text{onsager} \\ V_u^{(\bullet)} &\leftarrow f(C_u^{(\bullet)}) \end{aligned}$$

AMP for $SO(3)$ synchronization

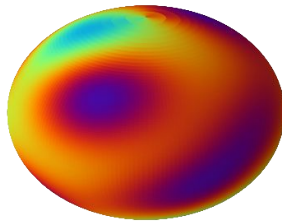
ground truth



Example: aligning noisy copies of images on the sphere.



noisy rotated copies

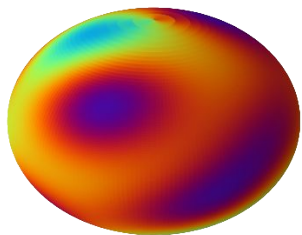


recovery result



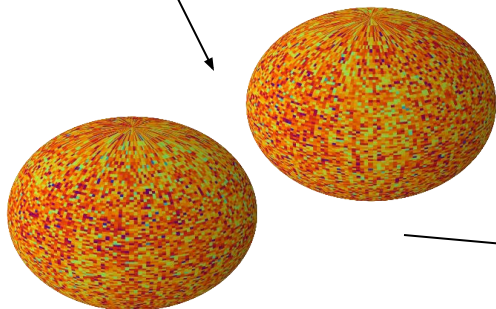
AMP for $SO(3)$ synchronization

ground truth

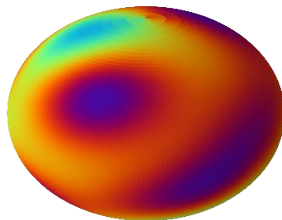


Example: aligning noisy copies of images on the sphere.

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



noisy rotated copies



recovery result



Thanks!

Preprint: A. Perry, A. S. Wein, A. S. Bandeira, A. Moitra,
*Message-passing algorithms for synchronization problems over
compact groups*. arXiv:1610.04583, 2016.
