

CS 59300 – Algorithms for Data Science

Classical and Quantum approaches

Lecture 5 (09/16)

Tensor Methods (V)

https://ruizhezhang.com/course_fall_2025.html

Recap

We introduced the tensor network diagram

We discussed some applications in quantum computing (simulating quantum circuits) and quantum physics (MPS, DMRG, etc)

Today: we'll talk about a classical application of tensor network: **orbit recovery**

Today's plan

- Problem setup and examples
- Some easy algorithms
- Heterogeneous setting
 - Main result: a spectral algorithm for heterogeneous MRA
- The trace method
- The blueprint of the algorithm
- Proof: the signal part
- Proof: the noise part
- Generalizations

Orbit recovery

Setup:

- Let $x \in \mathbb{R}^n$ be an unknown signal
- Let G be a group with **group action** $\mathcal{P}: G \rightarrow \mathbb{R}^{n \times n}$
- We get measurements of the form:

$$y_i = \mathcal{P}(g_i)x + \eta_i$$

- g_i is an independent, uniformly random element from G (under the Haar measure)
- η_i is an independent Gaussian noise $\mathcal{N}(0, \sigma^2 I)$

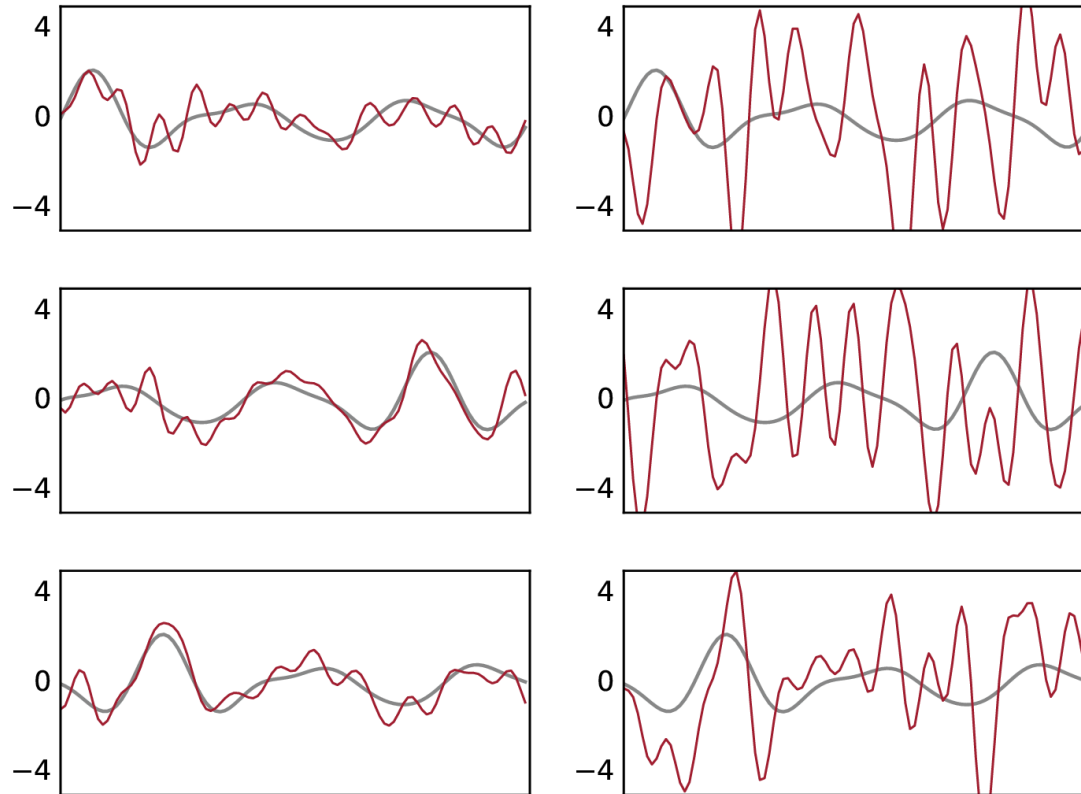
Goal: recover \hat{x} close to some element in the **orbit**

$$\{\mathcal{P}(g)x \mid g \in G\}$$

For simplicity, we'll use $g \cdot x$ to denote the group action

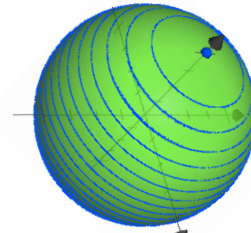
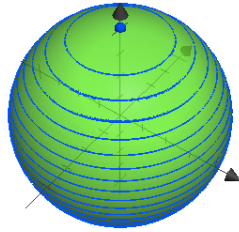
Example 1: multi-reference alignment (MRA)

- Discrete MRA: $G = \mathbb{Z}_n$ (random shift)
- Continuous MRA: $G = SO(2)$ (2D random rotation)



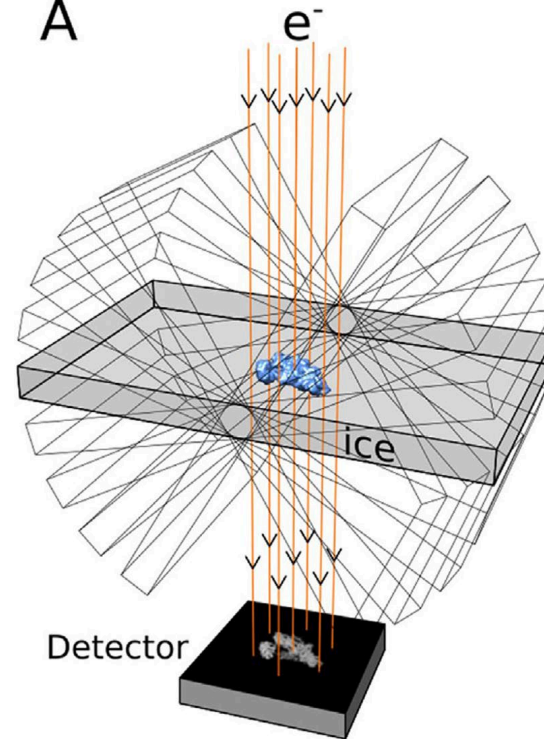
Example 2: cryo-electron tomography (cryo-ET)

- $G = SO(3)$

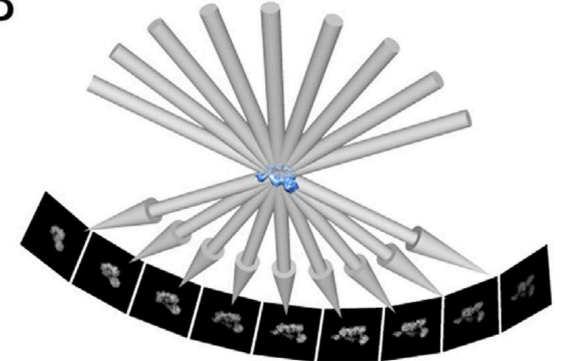


+ noise

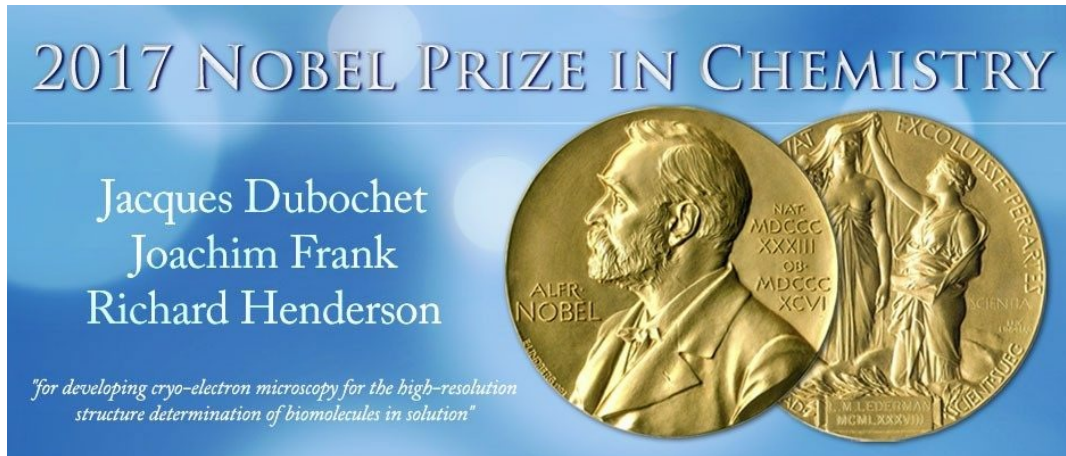
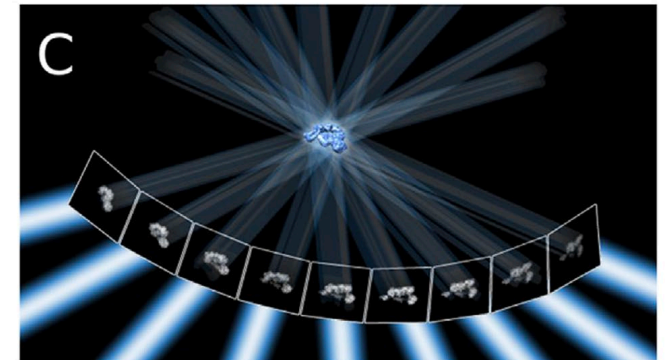
A



B



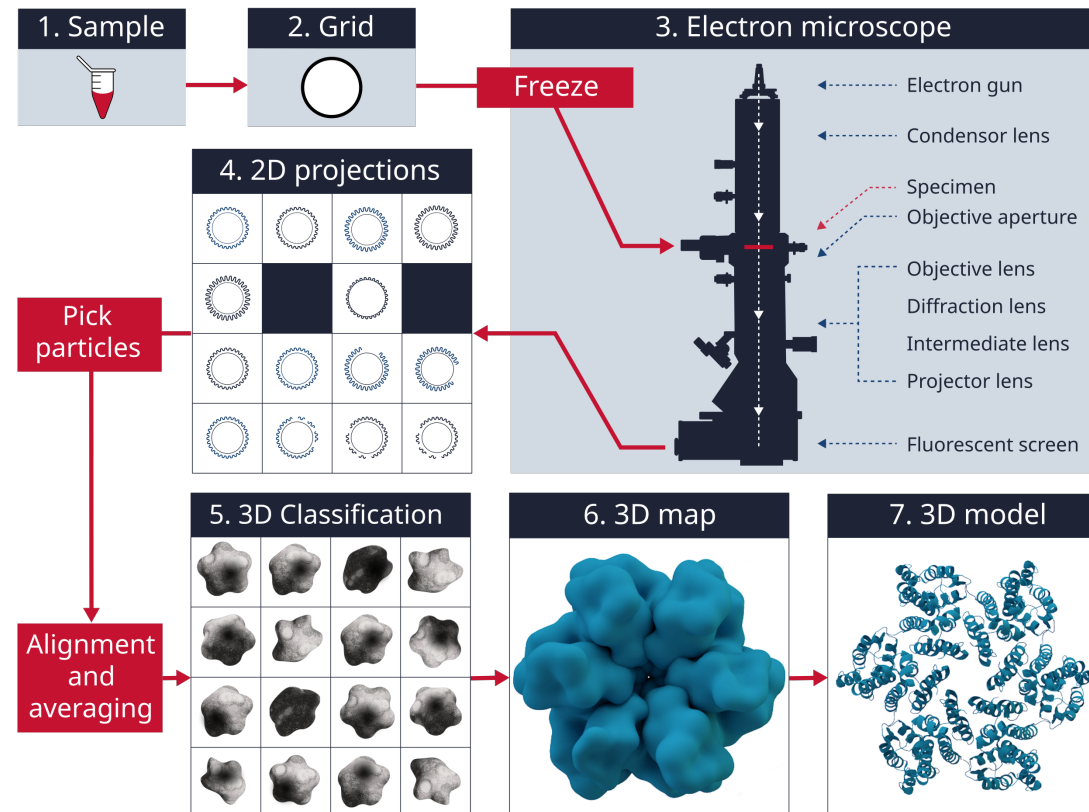
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Cryo-electron microscopy (cryo-EM)

- Cryo-ET + 2D projection

$$y_i = \Pi(g_i \cdot x) + \eta_i$$



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Discrete MRA

- For $g \in G = \mathbb{Z}_n$, we have

$$(g \cdot x)_i = x_{i-g \pmod n}$$

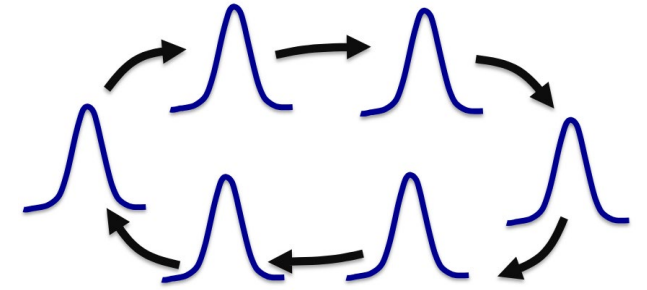
- Perry-Weed-Bandeira-Rigollet-Singer, 2017**: algorithm for discrete MRA with optimal sample complexity ($m \sim \sigma^6$)
- We have seen this algorithm: [learning mixtures of Gaussians](#)
- Each sample $y_i = g_i \cdot x + \eta_i$. If g_i is fixed, then

$$y_i \sim \mathcal{N}(g_i \cdot x, \sigma^2 I)$$

- Thus, the sample distribution can be expressed as a mixture of Gaussian with n components:

$$\mu_i = g_i \cdot x \quad \forall i \in [n]$$

- To apply Jennrich's algorithm, we compute the **3rd-moment**, which needs $\sim \sigma^6$ samples



Continuous MRA

For $g \in G = SO(2)$, what is $g \cdot x$ for $x \in \mathbb{R}^n$?

- $$x = \begin{bmatrix} x_1 & x_2 & x_3 & x_4 & \cdots & x_{\frac{n}{2}} \\ x_{-1} & x_{-2} & x_{-3} & x_{-4} & \cdots & x_{-\frac{n}{2}} \end{bmatrix}$$

$$\begin{pmatrix} x_j \\ x_{-j} \end{pmatrix} \xrightarrow{g} \begin{bmatrix} \cos(jg) & -\sin(jg) \\ \sin(jg) & \cos(jg) \end{bmatrix} \begin{pmatrix} x_j \\ x_{-j} \end{pmatrix}$$

- G can be parameterized by $g \in (0, 2\pi]$
- It is convenient to work in the **Fourier basis**:

The linear map $g \in \mathbb{R}^{n \times n}$ is **block-diagonal**

$$\hat{x}_j := \frac{1}{\sqrt{2}}(x_j + \mathbf{i}x_{-j}), \quad \hat{x}_{-j} := \frac{1}{\sqrt{2}}(x_j - \mathbf{i}x_{-j}) \quad \forall j > 0$$

- You can check that in the Fourier basis, g is a **diagonal** matrix ($\hat{x}_j \mapsto e^{\mathbf{i}jg} \hat{x}_j$)

Method of moments



- Define the p -th moment in the Fourier basis:

$$\hat{T}_p(\hat{x}) := \mathbb{E}_g[(g \cdot \hat{x})^{\otimes p}] \in \mathbb{R}^{n \times p}$$

- For any coordinates $j_1, \dots, j_p \in [n]$, we have

$$\begin{aligned}\hat{T}_p(\hat{x})_{j_1, \dots, j_p} &= \mathbb{E}_g \left[(g \cdot \hat{x})_{j_1} (g \cdot \hat{x})_{j_2} \cdots (g \cdot \hat{x})_{j_p} \right] \\ &= \mathbb{E}_g \left[e^{\mathbf{i} g j_1} \hat{x}_{j_1} e^{\mathbf{i} g j_2} \hat{x}_{j_2} \cdots e^{\mathbf{i} g j_p} \hat{x}_{j_p} \right] \\ &= \mathbb{E}_g \left[e^{\mathbf{i} g (j_1 + \cdots + j_p)} \right] \hat{x}_{j_1} \cdots \hat{x}_{j_p} \\ &= \mathbf{1}_{j_1 + \cdots + j_p = 0} \cdot \hat{x}_{j_1} \cdots \hat{x}_{j_p}\end{aligned}$$

- Given access to $\hat{T}_1, \dots, \hat{T}_p$, can we reverse-engineer \hat{x} ?

Frequency marching



$$\hat{T}_p(\hat{x})_{j_1, \dots, j_p} = \mathbf{1}_{j_1 + \dots + j_p = 0} \cdot \hat{x}_{j_1} \cdots \hat{x}_{j_p}$$

- Consider the **second moment**:

$$\hat{T}_2(\hat{x})_{j, -j} = \hat{x}_j \hat{x}_{-j} = |\hat{x}_j|^2 \quad \forall j > 0$$

- Thus, we can learn $|\hat{x}_j|$ for every j from \hat{T}_2
- To learn the phases, consider the **third moment**:

$$\hat{T}_3(\hat{x})_{j_1, j_2, -(j_1 + j_2)} = \hat{x}_{j_1} \hat{x}_{j_2} \hat{x}_{-(j_1 + j_2)}$$

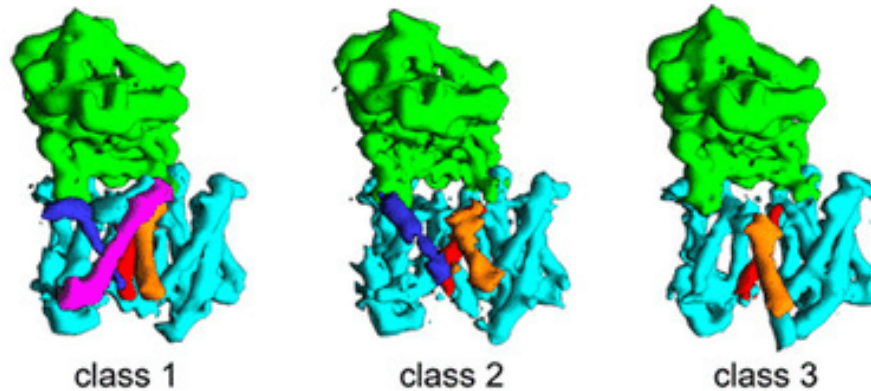
- Since $(g \cdot \hat{x})_1 = e^{ig} \hat{x}_1$, there exists an orbit such that \hat{x}_1 's phase $\phi_1 = 0$
- Then, using $\hat{T}_3(\hat{x})_{-1, -1, 2} = |\hat{x}_1|^2 \hat{x}_2$ and $|\hat{x}_1|$, we learn ϕ_2
- Next, using $\hat{T}_3(\hat{x})_{-1, -2, 3} = \hat{x}_1 \hat{x}_{-2} \hat{x}_3$ and $\hat{x}_{-2} = \hat{x}_2^*$, we learn ϕ_3
- We can repeat this procedure until we have learned all the phases

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Heterogeneous MRA

What if there are multiple molecules (or multiple conformations of the same molecule)?



- Suppose there are K unknown vectors x^1, x^2, \dots, x^K
- We observe $y_i = g_i \cdot x^{k_i} + \eta_i$, where $k_i \sim_u [K]$, $g_i \sim_u G$, and $\eta_i \sim \mathcal{N}(0, \sigma^2 I)$
- Can we still use frequency marching to recover $\{x^k\}$?

Frequency marching does not work

- Consider the Fourier transform of the p -th moment:

$$\hat{T}_p(\{\hat{x}^k\}) := \mathbb{E}_{k,g} \left[(g \cdot \hat{x}^k)^{\otimes p} \right] = \frac{1}{K} \sum_{k=1}^K \mathbb{E}_g [(g \cdot \hat{x})^{\otimes p}]$$

- Thus, we have

$$\hat{T}_p(\{\hat{x}^k\})_{j_1, \dots, j_p} = \mathbf{1}_{j_1 + \dots + j_p = 0} \cdot \frac{1}{K} \sum_{k=1}^K \hat{x}_{j_1}^k \cdots \hat{x}_{j_p}^k$$

- Frequency marching breaks down from the first step:

$$\hat{T}_2(\{\hat{x}^k\})_{j, -j} = \frac{1}{K} \sum_{k=1}^K |x^k|^2$$

Signals are entangled!

Does tensor decomposition help?

- Consider the third moment:

$$T_3(\{x^k\}) := \frac{1}{K|G|} \sum_{k=1}^K \sum_{g \in G} (g \cdot x^k)^{\otimes 3}$$

- If G is a **finite group**, then this is a rank- $K|G|$ tensor
- If undercomplete, then we can just run Jennrich's algorithm, and we're done!
- If overcomplete, we may either use higher moments (e.g., T_5) or assume x^k are random vectors
- Unfortunately, $SO(2)$ is a **continuous group** (or Lie group) \rightarrow this tensor has ∞ rank
- Moreover, the decomposition is not unique: if $T_3 = \sum_{i=1}^r a_i^{\otimes 3}$ is a solution, then there are **∞ -many solutions** $T_3 = \sum_{i=1}^r (g \cdot a_i)^{\otimes 3}$ for any $g \in [G]$

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List recovery for average-case heterogeneous MRA

Theorem (Moitra-Wein, 2018).

Let $x^1, \dots, x^K \in \mathbb{R}^n$ be drawn independently from $\mathcal{N}\left(0, \frac{1}{n}I\right)$.

We are given the tensor $\mathcal{T} = T + E \in \mathbb{R}^{n \times n \times n}$ where $\|E\| \leq 1/\text{poly}(n)$ and

$$T = \sum_{k=1}^K \mathbb{E}_g[(g \cdot x^k)^{\otimes 3}]$$

There is an algorithm that runs in time $\text{poly}(n)$ and **outputs a list of unit vectors** $\tau_1, \dots, \tau_L \in \mathbb{R}^n$ **with** $L = \text{poly}(n)$ that has the following guarantee. With high probability over both x^1, \dots, x^K and the algorithm's randomness,

$$\forall k \in [K], \exists i \in [L] \text{ s.t. } \langle \tau_i, x^k \rangle^2 \geq 0.99$$



General recipe for spectral methods

Given input tensor T

- **Step 1:** Construct a new tensor B by contracting multiple copies of T according to a tensor network
- **Step 2:** Flatten B to form a symmetric matrix M
- **Step 3:** Compute the leading eigenvector of M

We use the **trace method** to show that the top eigenvector is close to the orbit of x^k

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Interlude: the trace method

Let M be a random matrix, and our goal is to bound its spectral norm

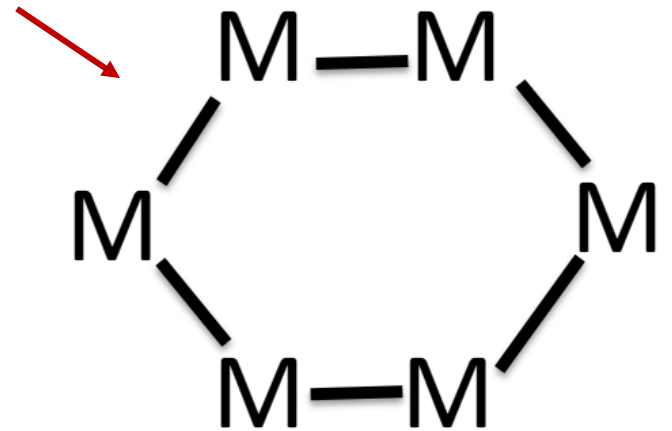
Basic idea:

$$\mathrm{tr}[M^{2k}] = \sum_i \lambda_i^{2k} \geq \|M\|^{2k}$$

Applying Markov's inequality, we get the bound

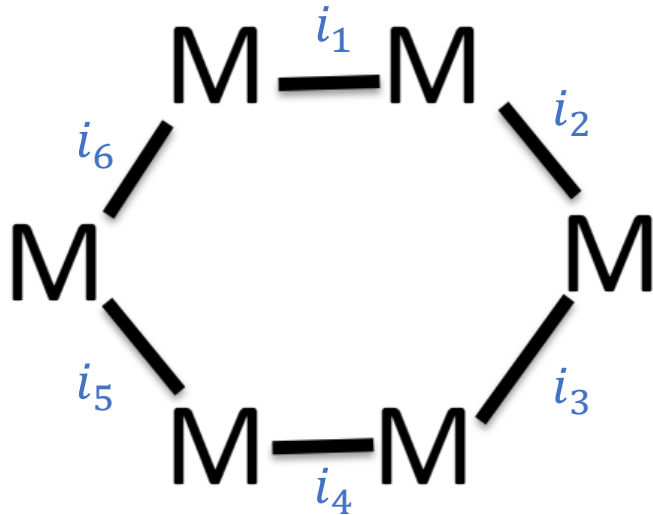
$$\Pr[\|M\| \geq t] = \Pr[\|M\|^{2k} \geq t^{2k}] \leq \frac{\mathbb{E}[\mathrm{tr}[M^{2k}]]}{t^{2k}}$$

Tensor network!



Example

Suppose M is an $n \times n$ symmetric matrix with *i.i.d.* Rademacher entries and zeros along the diagonal



$$\mathbb{E} M_{i_1,i_2} M_{i_2,i_3} M_{i_3,i_4} M_{i_4,i_5} M_{i_5,i_6} M_{i_6,i_1} = 1$$

iff every $\{i_j, i_{j+1}\}$ occurs **even** number of times

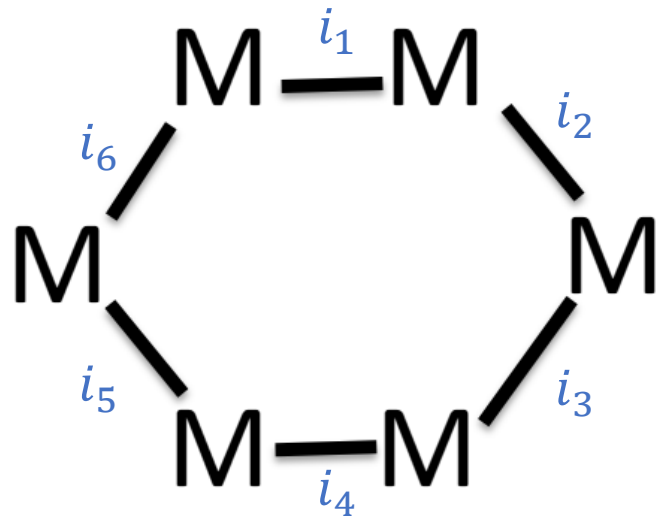
Combinatorial problem: $\text{tr}[M^{2k}]$ equals to the number of sequences $(i_1, \dots, i_{2k}) \in [n]^{2k}$ such that every $\{i_j, i_{j+1}\}$ occurs in the sequence an even number of times

- At most $k + 1$ distinct labels in the sequences

$k = 2$: $(i_1, \dots, i_4) = (a, b, c, b)$ a b c $(i_1, \dots, i_4) = (a, b, a, c)$ b c

Example

Suppose M is an $n \times n$ symmetric matrix with *i.i.d.* Rademacher entries and zeros along the diagonal



$$\mathbb{E} M_{i_1, i_2} M_{i_2, i_3} M_{i_3, i_4} M_{i_4, i_5} M_{i_5, i_6} M_{i_6, i_1} = 1$$

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Combinatorial problem: $\text{tr}[M^{2k}]$ equals to the number of sequences $(i_1, \dots, i_{2k}) \in [n]^{2k}$ such that every $\{i_j, i_{j+1}\}$ occurs in the sequence an even number of times

- At most $k + 1$ distinct labels in the sequences
- $\text{tr}[M^{2k}] \leq n^{k+1} \cdot (k + 1)^{2k}$
- $\|M\| \leq \sqrt{n} \log n$ (by taking $k \sim \log n$)

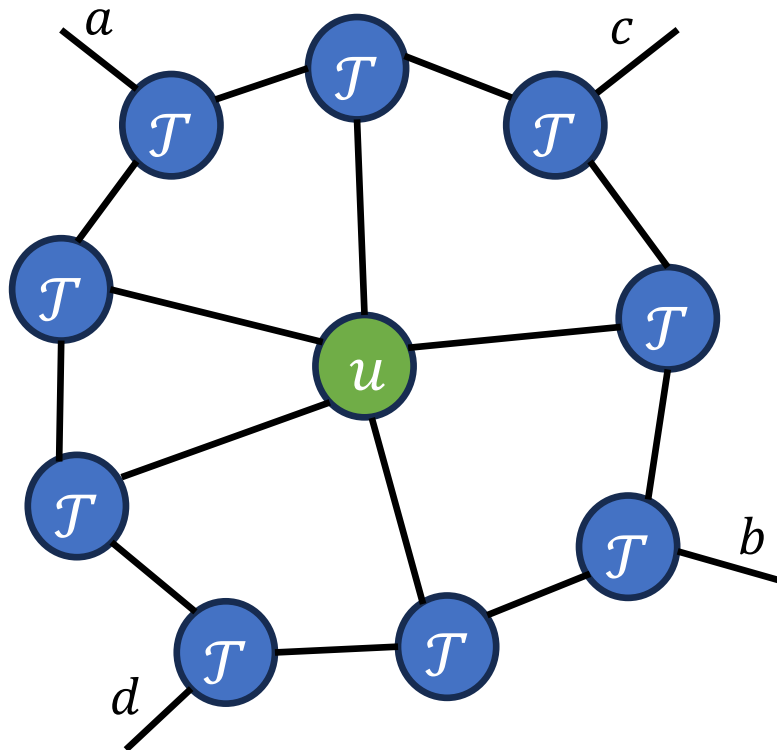
Furedi-Komlos: $\|M\| \simeq \sqrt{n}$

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The blueprint

- The algorithm takes a random order-5 tensor u (with i.i.d. $\mathcal{N}(0,1)$ entries)
- The hope is that u has non-trivial correlation with some x in the orbit of one of x^1, \dots, x^K
- Compute the following tensor network:



Q: Why do we need a random tensor u ?

A: Symmetry-breaking

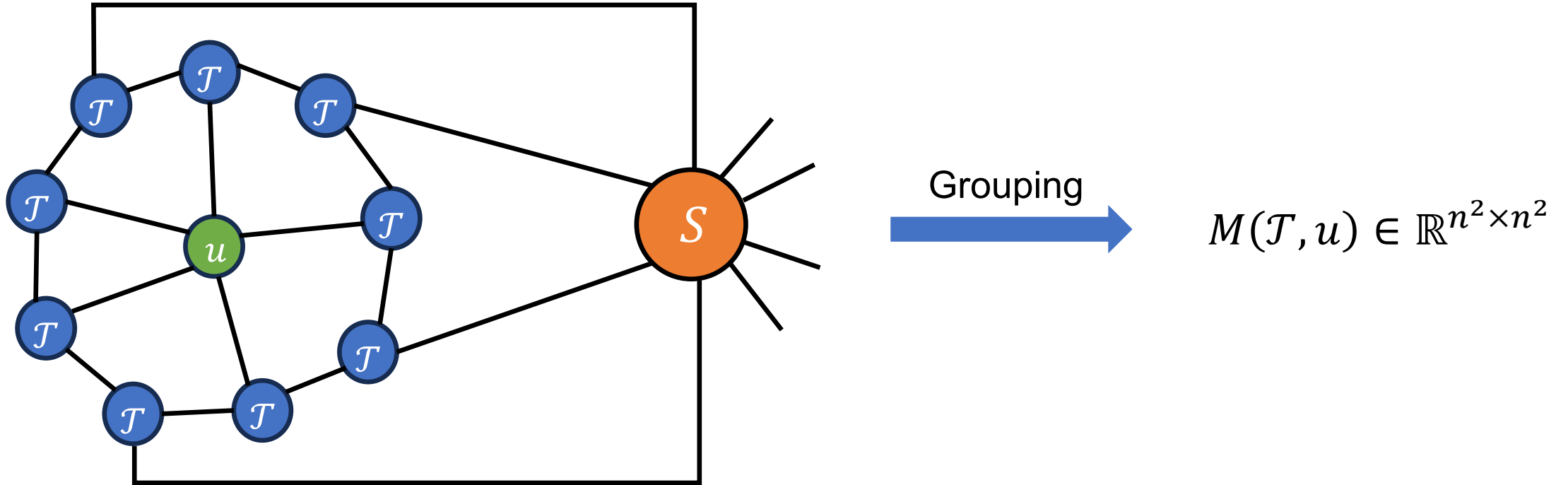
Grouping $\rightarrow \tilde{M}(\mathcal{T}, u) \in \mathbb{R}^{n^2 \times n^2}$
 $\{(a, b), (c, d)\}$

We want to show that if $u = x^{\otimes 5}$, then
 $\tilde{M}(\mathcal{T}, u) \approx x^{\otimes 2} (x^{\otimes 2})^\top$



The blueprint

- Use a simple tensor $S \in \mathbb{R}^{n \times 8}$ to correct the tensor network:



Main technical step

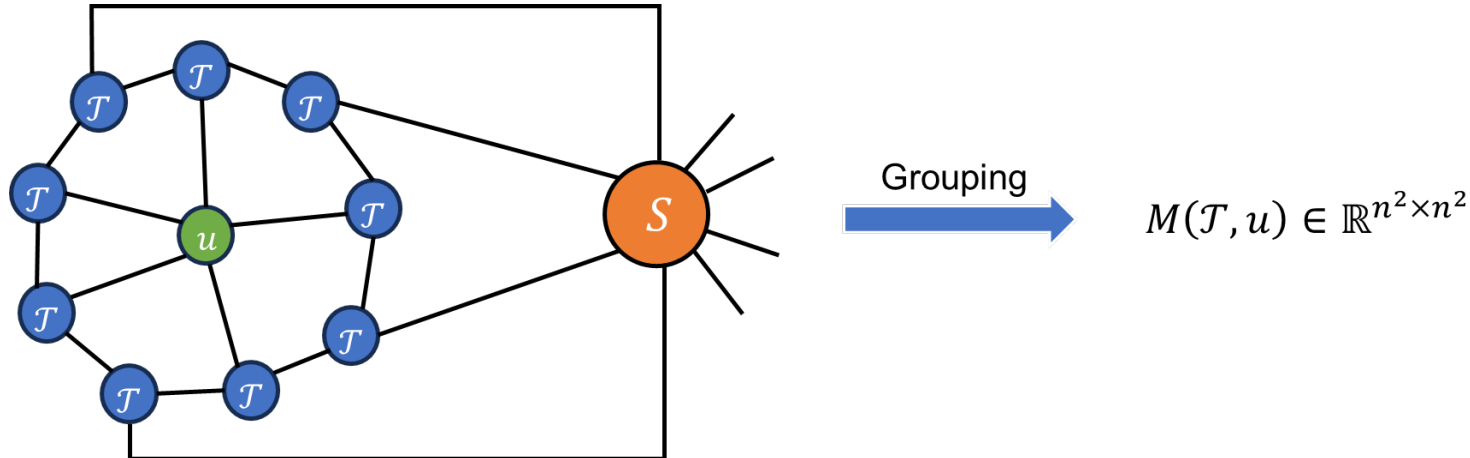
Technical theorem.

There is a matrix $M(\mathcal{T}, u) \in \mathbb{R}^{n^2 \times n^2}$ (computable in poly-time from \mathcal{T} and u) with the following guarantee.

Let $v \in \mathbb{R}^{n^2}$ be the leading eigenvector of $(M(\mathcal{T}, u) + M(\mathcal{T}, u)^\top)/2$.

Let $V = \text{mat}(v) \in \mathbb{R}^{n \times n}$ and let $\tau \in \mathbb{R}^n$ be the top eigenvector of $(V + V^\top)/2$.

With high probability over $\{x^k\}$, for **any** $k \in [K]$, we have $\langle \tau, x^k \rangle^2 \geq 0.99$ with probability $1/\text{poly}(n)$.



Main technical step

Technical theorem.

There is a matrix $M(\mathcal{T}, u) \in \mathbb{R}^{n^2 \times n^2}$ (computable in poly-time from \mathcal{T} and u) with the following guarantee. Let $v \in \mathbb{R}^{n^2}$ be the leading eigenvector of $(M(\mathcal{T}, u) + M(\mathcal{T}, u)^\top)/2$. Let $V = \text{mat}(v) \in \mathbb{R}^{n \times n}$ and let $\tau \in \mathbb{R}^n$ be the top eigenvector of $(V + V^\top)/2$. With high probability over $\{x^k\}$, for any $k \in [K]$, we have $\langle \tau, x^k \rangle^2 \geq 0.99$ with probability $1/\text{poly}(n)$.

Proof of the main theorem:

- Sample u_1, \dots, u_L and use the technical theorem to obtain τ_1, \dots, τ_L
- For any k , the overall failure probability is $\leq (1 - 1/\text{poly}(n))^L = \exp(-L/\text{poly}(n))$
- By union bound over all $k \in [K]$, the total failure probability is $\leq K \exp(-L/\text{poly}(n)) = o(1)$



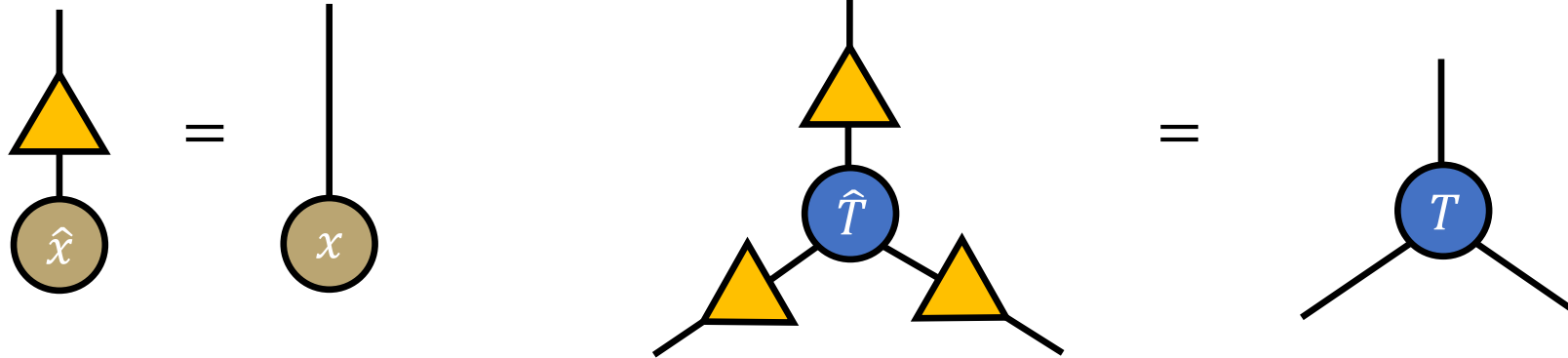
Fourier transform in tensor network

$$\hat{x}_j := \frac{1}{\sqrt{2}}(x_j + \mathbf{i}x_{-j})$$

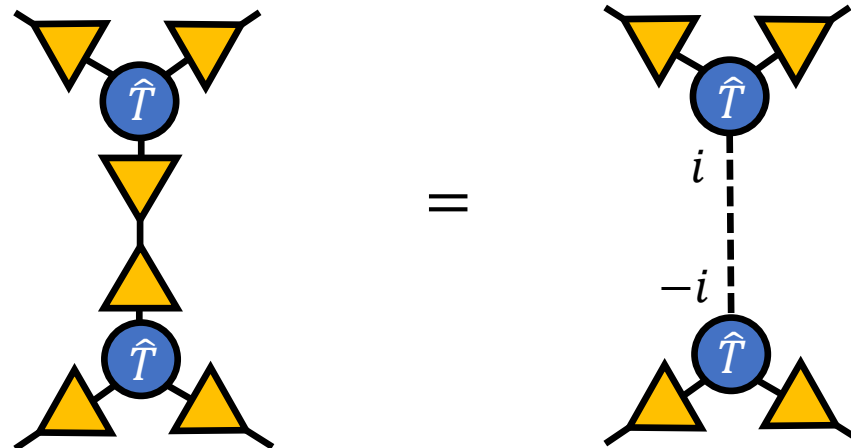
$$, \quad \hat{x}_{-j}$$

$$:= \frac{1}{\sqrt{2}}(x_j - \mathbf{i}x_{-j})$$

We first define Δ to be the Fourier transform unitary matrix that transforms \hat{x} to x

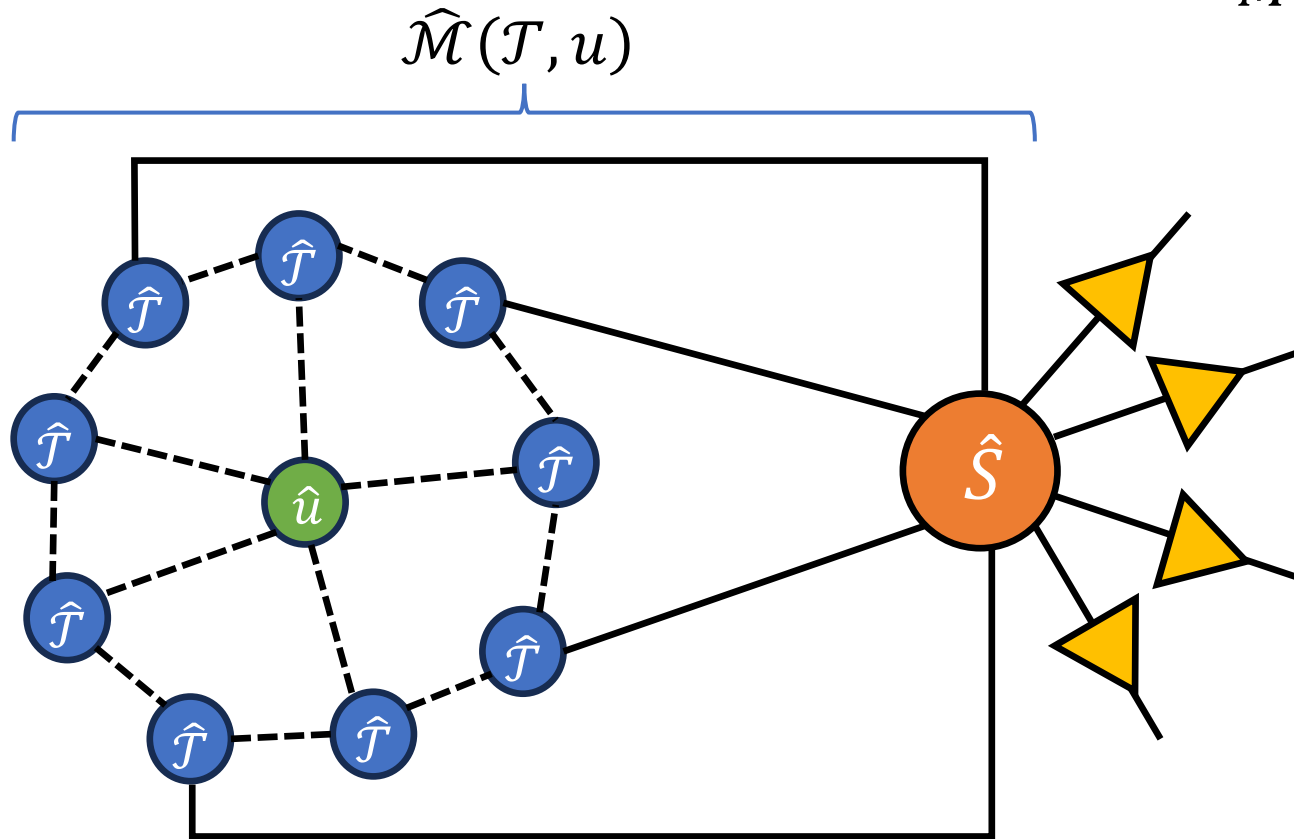


You can check that $(\Delta^\top \Delta)_{ij} = \mathbf{1}_{i=-j}$



Corrected tensor network

$$M(\mathcal{T}, u) = (\Delta \otimes \Delta) \hat{M}(\mathcal{T}, u) (\Delta \otimes \Delta)^\top$$



$$(\hat{S}T)_{abcd} = S_{abcd}T_{abcd}$$

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Correcting the signal

Goal: If we correctly guess $u = (x^k)^{\otimes 5}$, then $M(\mathcal{T}, u) \approx (x^k \otimes x^k)(x^k \otimes x^k)^\top \equiv X^k$

- Wlog, we can write $u = \alpha(x^1)^{\otimes 5} + \tilde{u}$, where $\tilde{u} \perp (x^1)^{\otimes 5}$ (noise)
- Let $T^1 := \mathbb{E}_g[(g \cdot x^1)^{\otimes 3}]$ denote the 3rd moment of x^1 . Then

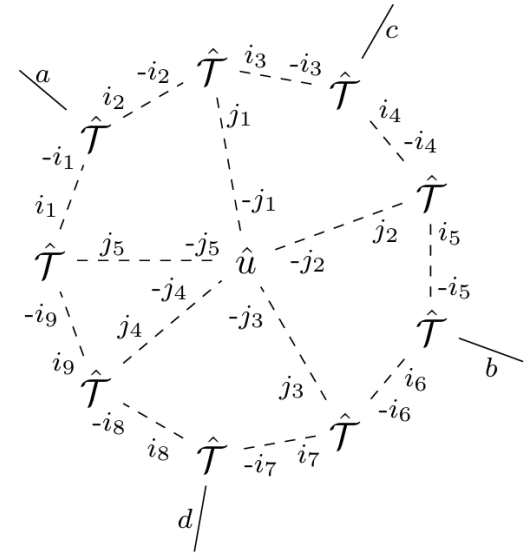
Pure signal

$$(\hat{T}^1)_{j_1 j_2 j_3} = \mathbf{1}_{j_1 + j_2 + j_3 = 0} \hat{x}_{j_1}^1 \hat{x}_{j_2}^1 \hat{x}_{j_3}^1$$

We want to match $M(T^1, (x^1)^{\otimes 5})$ to X^1 :

- $\hat{M}(T^1, (x^1)^{\otimes 5})_{ab,cd} = S_{abcd} \cdot s_{abcd} \cdot \hat{x}_a^1 \hat{x}_b^1 \hat{x}_c^1 \hat{x}_d^1$, where

$$s_{abcd} := \sum_{i_1, \dots, i_9} \sum_{j_1, \dots, j_5} (\mathbf{1}_{a+i_2=i_1} \cdots \mathbf{1}_{i_1+j_5=i_9}) |\hat{x}_{i_1}^1|^2 \cdots |\hat{x}_{i_9}^1|^2 |\hat{x}_{j_1}^1|^2 \cdots |\hat{x}_{j_5}^1|^2$$



$$s_{abcd} := \sum_{i_1, \dots, i_9} \sum_{j_1, \dots, j_5} (\mathbf{1}_{a+i_2=i_1} \cdots \mathbf{1}_{i_1+j_5=i_9}) |\hat{x}_{i_1}^1|^2 \cdots |\hat{x}_{i_9}^1|^2 |\hat{x}_{j_1}^1|^2 \cdots |\hat{x}_{j_5}^1|^2$$

$$(\hat{M})_{ab,cd} := \mathbf{S}_{abcd} s_{abcd} \cdot \hat{x}_a^1 \hat{x}_b^1 \hat{x}_c^1 \hat{x}_d^1$$

- Define

$$S_{abcd} := \begin{cases} 0 & \text{if } a = -b \text{ or } c = -d \\ \frac{1}{\mathbb{E}_{x^1}[S_{abcd}]} & \text{otherwise} \end{cases}$$

- We will show that s_{abcd} is **concentrated** around its mean (which is independent of x^1)

Proposition.

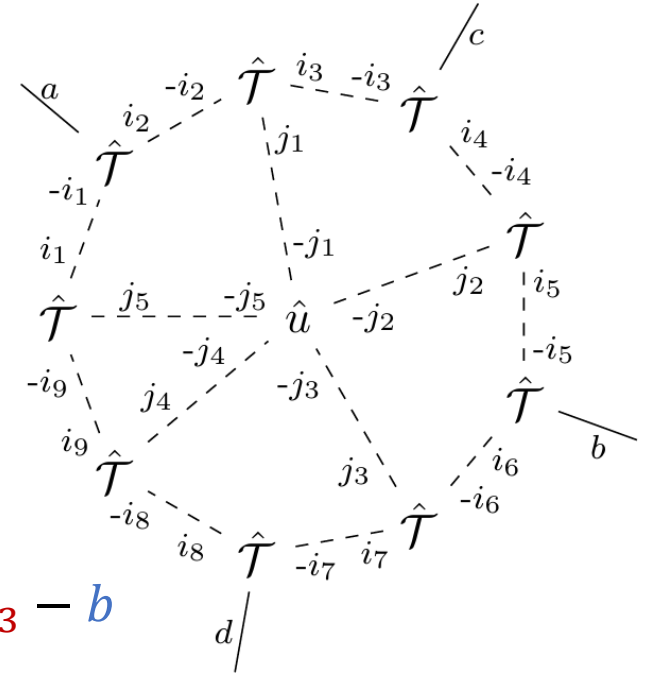
For $a \neq -b$ and $c \neq -d$, we have $|S_{abcd}s_{abcd} - 1| = \mathcal{O}(n^{-0.1})$ with overwhelming probability over x^1 . Therefore, $\|M(T^1, (x^1)^{\otimes 5}) - X^1\| = o(1)$.

Linear constraints on the indices

- $i_1 - i_2 = a$
- $i_1 + j_5 - i_9 = 0$
- $i_9 + j_4 - i_8 = 0$
- $i_7 - i_8 = d$
- $i_7 + j_3 - i_6 = 0$
- $i_5 - i_6 = b$
- $i_5 + j_2 - i_4 = 0$
- $i_3 - i_4 = c$
- $i_3 + j_1 - i_2 = 0$



- $i_1 = i_9 - j_5$
- $i_2 = i_9 - j_5 - a$
- $i_3 = i_9 - j_5 - a - j_1$
- $i_4 = i_9 - j_5 - a - j_1 - c$
- $i_5 = i_9 + j_4 + d + j_3 + b$
- $i_6 = i_9 + j_4 + d + j_3$
- $i_7 = i_9 + j_4 + d$
- $i_8 = i_9 + j_4$
- $j_2 = -j_5 - a - j_1 - c - j_4 - d - j_3 - b$



For any fixed (a, b, c, d) , there are 5 “free” indices $(i_9, j_1, j_3, j_4, j_5)$

- Thus, the number of solutions is upper-bounded by n^5
- We can also prove that the number of valid solution is lower-bounded by cn^5 for some small constant c , by a careful counting argument

Moments of random vector

Lemma. Let $x^1 \sim \mathcal{N}(0, I/n)$. Then, we have

- $\mathbb{E}_{x^1} \left[|\hat{x}_i^1|^{2k} \right] = k! n^{-k}$
- If $k_1 \neq k_2$, then $\mathbb{E}_{x^1} \left[(\hat{x}_i^1)^{k_1} (\hat{x}_{-i}^1)^{k_2} \right] = 0$
- If $i \neq \pm j$, then \hat{x}_i^1 and \hat{x}_j^1 are independent



$$\mathbb{E}_{x^1} \left[|\hat{x}_{i_1}^1|^2 \cdots |\hat{x}_{i_9}^1|^2 |\hat{x}_{j_1}^1|^2 \cdots |\hat{x}_{j_5}^1|^2 \right] \\ = \Theta(n^{-14})$$

Proof.

- $\hat{x}_i^1 \sim \mathcal{N}(0, I/(2n)) + \mathbf{i}\mathcal{N}(0, I/(2n))$ and $\hat{x}_{-i}^1 = (\hat{x}_i^1)^*$
- $|\hat{x}_i^1|^2 \sim \frac{1}{2n} \chi^2$

- Expectation:

$$\begin{aligned}
 \mathbb{E}_{x^1}[s_{abcd}] &= \sum_{i_1, \dots, i_9} \sum_{j_1, \dots, j_5} (\mathbf{1}_{a+i_2=i_1} \cdots \mathbf{1}_{i_1+j_5=i_9}) \mathbb{E}_{x^1} \left[|\hat{x}_{i_1}^1|^2 \cdots |\hat{x}_{i_9}^1|^2 |\hat{x}_{j_1}^1|^2 \cdots |\hat{x}_{j_5}^1|^2 \right] \\
 &= \sum_{i_1, \dots, i_9} \sum_{j_1, \dots, j_5} (\mathbf{1}_{a+i_2=i_1} \cdots \mathbf{1}_{i_1+j_5=i_9}) \Theta(n^{-14}) \quad S_{abcd} \text{ only depends on } n \\
 &= \Theta(n^5 \cdot n^{-14}) = \Theta(n^{-9})
 \end{aligned}$$

- Variance:

$$\begin{aligned}
 \text{Var}[s_{abcd}] &= \text{Var} \left[\sum_t Z_t \right] = \sum_t \text{Var}[Z_t] + \sum_{t \neq t'} \text{Cov}(Z_t, Z_{t'}) \\
 &\leq \Theta(n^5) \cdot \mathcal{O}(n^{-28}) + \mathcal{O}(n^9) \cdot \mathcal{O}(n^{-28}) = \mathcal{O}(n^{-19})
 \end{aligned}$$

- By Chebyshev's inequality, they imply that $|s_{abcd} - \mathbb{E}[s_{abcd}]| \leq n^{-9.1}$ with probability $1 - 1/\text{poly}(n)$
- Note that s_{abcd} is a **degree-14 polynomial** of Gaussian variables. **Gaussian hypercontractivity** can boost the probability to **$1 - \exp(-\text{poly}(n))$**

Proposition.

For $a \neq -b$ and $c \neq -d$, we have $|S_{abcd}S_{abcd} - 1| = \mathcal{O}(n^{-0.1})$ with overwhelming probability over x^1 . Therefore, $\|M(T^1, (x^1)^{\otimes 5}) - X^1\| = o(1)$.

- We have proved that for $a \neq -b$ and $c \neq -d$,

$$(\widehat{M})_{ab,cd} = S_{abcd}S_{abcd} \cdot \hat{x}_a^1 \hat{x}_b^1 \hat{x}_c^1 \hat{x}_d^1 = (1 \pm n^{-0.1}) \hat{x}_a^1 \hat{x}_b^1 \hat{x}_c^1 \hat{x}_d^1$$

- Thus, we have

$$\begin{aligned} \|M(T^1, (x^1)^{\otimes 5}) - X^1\| &= \|M(T^1, (x^1)^{\otimes 5}) - (x^1 \otimes x^1)(x^1 \otimes x^1)^\top\| \\ &= \|\widehat{M}(T^1, (x^1)^{\otimes 5}) - (\hat{x}^1 \otimes \hat{x}^1)(\hat{x}^1 \otimes \hat{x}^1)^\top\| \\ &\leq \|\widehat{M}(T^1, (x^1)^{\otimes 5}) - (\hat{x}^1 \otimes \hat{x}^1)(\hat{x}^1 \otimes \hat{x}^1)^\top\|_F \\ &\leq \sqrt{n^4 \cdot (n^{-0.1} \cdot n^{-2})^2 + 2n^3 \cdot (n^{-2})^2} \\ &= o(1) \end{aligned}$$

- The proposition is then proved



If correctly guess $u = x^k$, then

$$M \approx (x^k \otimes x^k)(x^k \otimes x^k)^\top$$

Road map



$$u = \alpha x^1 + \tilde{u}, \quad \tilde{u} \perp x^1$$

$$M(\mathcal{T}, u) = \alpha M(T^1, (x^1)^{\otimes 5}) + \alpha \left(M(T, (x^1)^{\otimes 5}) - M(T^1, (x^1)^{\otimes 5}) \right) + (M(\mathcal{T}, u) - M(T, u)) + M(T, \tilde{u})$$

If correctly guess $u = x^k$, then M
 $\approx (x^k \otimes x^k)(x^k \otimes x^k)^\top$

Road map



$$u = \alpha x^1 + \tilde{u}, \quad \tilde{u} \perp x^1$$

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$$= (1 \pm o(1))(x^k \otimes x^k)(x^k \otimes x^k)^\top$$

If correctly guess $u = x^k$, then M
 $\approx (x^k \otimes x^k)(x^k \otimes x^k)^\top$

Road map



$$u = \alpha x^1 + \tilde{u}, \quad \tilde{u} \perp x^1$$

$$M(\mathcal{T}, u) = \alpha M(T^1, (x^1)^{\otimes 5}) + \alpha \left(M(T, (x^1)^{\otimes 5}) - M(T^1, (x^1)^{\otimes 5}) \right) + (M(\mathcal{T}, u) - M(T, u)) + M(T, \tilde{u})$$



$$\|M(T, (x^1)^{\otimes 5}) - M(T^1, (x^1)^{\otimes 5})\| = o(1)$$

$$\|M(\mathcal{T}, u) - M(T, u)\| = o(1)$$

If correctly guess $u = x^k$, then

$$M \approx (x^k \otimes x^k)(x^k \otimes x^k)^\top$$

Road map



$$u = \alpha x^1 + \tilde{u}, \quad \tilde{u} \perp x^1$$

$$M(\mathcal{T}, u) = \alpha M(T^1, (x^1)^{\otimes 5}) + \alpha \left(M(T, (x^1)^{\otimes 5}) - M(T^1, (x^1)^{\otimes 5}) \right) + (M(\mathcal{T}, u) - M(T, u)) + M(T, \tilde{u})$$



Non-negligible!

- Random tensor contraction ($\tilde{u} \sim \mathcal{N}(0, \Sigma)$)
- The **trace method** to upper bound $\|\tilde{W}\|$
- **Combinatorial problem** of counting labels

$$\tilde{W} =$$



$$\|M(T, \tilde{u})\| = \sqrt{\log n}$$

If correctly guess $u = x^k$, then

$$M \approx (x^k \otimes x^k)(x^k \otimes x^k)^\top$$

Road map



$$u = \alpha x^1 + \tilde{u}, \quad \tilde{u} \perp x^1$$

$$M(\mathcal{T}, u) = \alpha M(T^1, (x^1)^{\otimes 5}) + \alpha \left(M(T, (x^1)^{\otimes 5}) - M(T^1, (x^1)^{\otimes 5}) \right) + (M(\mathcal{T}, u) - M(T, u)) + M(T, \tilde{u})$$



x^1 can be recovered from the **top eigenvector** of $M(\mathcal{T}, u)$

As long as we sample sufficiently many u 's, we can “hit” all x^k w.h.p.

Today's plan

- Problem setup and examples
- Some easy algorithms
- Heterogeneous setting
 - Main result: a spectral algorithm for heterogeneous MRA
- The trace method
- The blueprint of the algorithm
- Proof: the signal part
- **Proof: the noise part**
- Generalizations

Towards proving the technical theorem

Recall that $u = \alpha(x^1)^{\otimes 5} + \tilde{u}$, and our final goal is to analyze

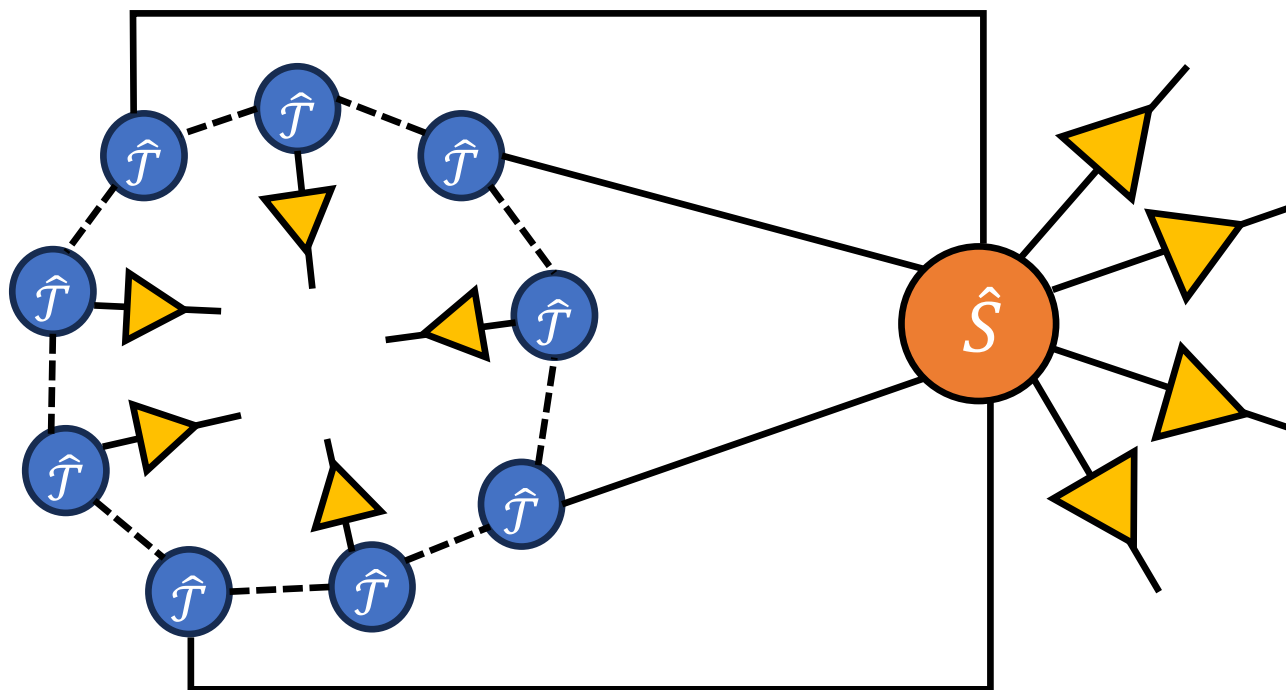
$$M(\mathcal{T}, u) = \underbrace{\alpha M(T^1, (x^1)^{\otimes 5})}_{\approx X^1} + \underbrace{\alpha \left(M(T, (x^1)^{\otimes 5}) - M(T^1, (x^1)^{\otimes 5}) \right)}_{\text{heterogeneous signal term}} + \underbrace{M(T, \tilde{u})}_{\text{noise term}} + \underbrace{\left(M(\mathcal{T}, u) - M(T, u) \right)}_{\text{error term}}$$

Key Proposition.

There is an event \mathcal{E} depending only on $\{x^k\}$ that happens with high probability over the randomness of $\{x^k\}$. Conditioned on \mathcal{E} , we have $\|M(T, \tilde{u})\| = \mathcal{O}(\sqrt{\log n})$ with high probability over the randomness of \tilde{u} .

$$M(T, \tilde{u}) = (I_{d^2} \otimes I_{d^2} \otimes \tilde{u})W$$

$$W \in \mathbb{R}^{n^2 \times n^2 \times n^5} :=$$



Interlude: random tensor contraction

Theorem (Ma-Shi-Steurer, 2016).

Let $W \in \mathbb{R}^p \times \mathbb{R}^q \times \mathbb{R}^r$ be an order-3 tensor. Let $\tilde{u} \sim \mathcal{N}(0, \Sigma)$ with $r \times r$ covariance matrix satisfying $0 \preceq \Sigma \preceq I$. Define

$$L := \max\{\|W_{\{1\},\{23\}}\|, \|W_{\{13\},\{2\}}\|\} .$$

Then for any $t \geq 0$,

$$\Pr_{\tilde{u}}[\|(I_p \otimes I_q \otimes \tilde{u})W\| \geq t] \leq 4(p + q)e^{-\frac{t^2}{2L^2}}$$

- L serves as the **Lipschitz parameter**

Lipschitz property

- Define $A(u) := (I_p \otimes I_q \otimes u)W = \sum_{k \in [r]} u_k W_k$
- For any $u, v \in \mathbb{R}^r$, we have

$$\begin{aligned} \|A(u) - A(v)\| &= \left\| \sum_{k \in [r]} (u_k - v_k) W_k \right\| \\ &= \sup_{\substack{x \in \mathbb{R}^p: \|x\|=1, \\ y \in \mathbb{R}^q: \|y\|=1}} \left| \sum_{k \in [r]} (u_k - v_k) \langle W_k, xy^\top \rangle \right| \\ &\leq \sup_{\substack{x \in \mathbb{R}^p: \|x\|=1, \\ y \in \mathbb{R}^q: \|y\|=1}} \|u - v\| \cdot \left(\sum_{k \in [r]} \langle W_k, xy^\top \rangle^2 \right)^{1/2} \end{aligned}$$

$$\begin{aligned}
\sup_{\substack{x \in \mathbb{R}^p: \|x\|=1, \\ y \in \mathbb{R}^q: \|y\|=1}} \left(\sum_{k \in [r]} \langle W_k, xy^\top \rangle^2 \right)^{1/2} &= \sup_{\|x\|=1} \sup_{\|y\|=1} \left(\sum_{k \in [r]} (x^\top W_k y)^2 \right)^{1/2} \\
&\leq \sup_{\|x\|=1} \left(\sum_{k \in [r]} \sup_{\|y\|=1} (x^\top W_k y)^2 \right)^{1/2} \\
&= \sup_{\|x\|=1} \left(\sum_{k \in [r]} \|W_k^\top x\|^2 \right)^{1/2} = \|W_{\{1\},\{23\}}\|
\end{aligned}$$

$$\begin{aligned}
\sup_{\substack{x \in \mathbb{R}^p: \|x\|=1, \\ y \in \mathbb{R}^q: \|y\|=1}} \left(\sum_{k \in [r]} \langle W_k, xy^\top \rangle^2 \right)^{1/2} &= \sup_{\|y\|=1} \sup_{\|x\|=1} \left(\sum_{k \in [r]} (x^\top W_k y)^2 \right)^{1/2} \\
&\leq \sup_{\|y\|=1} \left(\sum_{k \in [r]} \sup_{\|x\|=1} (x^\top W_k y)^2 \right)^{1/2} \\
&= \sup_{\|y\|=1} \left(\sum_{k \in [r]} \|W_k y\|^2 \right)^{1/2} = \|W_{\{13\},\{2\}}\|
\end{aligned}$$



$$\|A(u) - A(v)\| \leq L \cdot \|u - v\|$$

$u \mapsto \|A(u)\|$ is L -Lipschitz

Back to the proof of Key Proposition

- Applying that theorem to $M(T, \tilde{u}) = (I_{n^2} \otimes I_{n^2} \otimes \tilde{u})W$, we have

$$\Pr_{\tilde{u}}[\|M(T, \tilde{u})\| \geq tL] \leq n^2 e^{-t^2/2},$$

where

$$L := \max\{\|W_{ab,cdj_1 \dots j_5}\|, \|W_{abj_1 \dots j_5,cd}\|\}$$

- By symmetry, we just consider the first one, and define $\tilde{W} \in \mathbb{R}^{n^2 \times n^7}$:

$$\tilde{W}_{ab,cdj_1 \dots j_5} := W_{ab,cd,j_1 \dots j_5}$$

- We need to upper bound $\|\tilde{W}\|$

Recap: the trace method

Theorem.

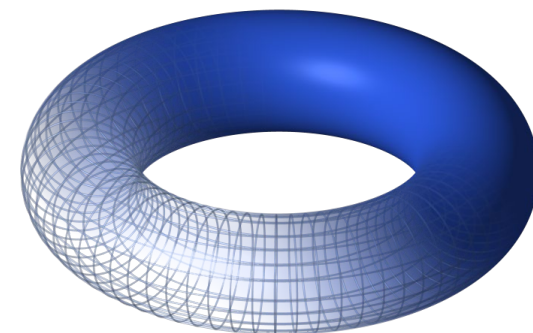
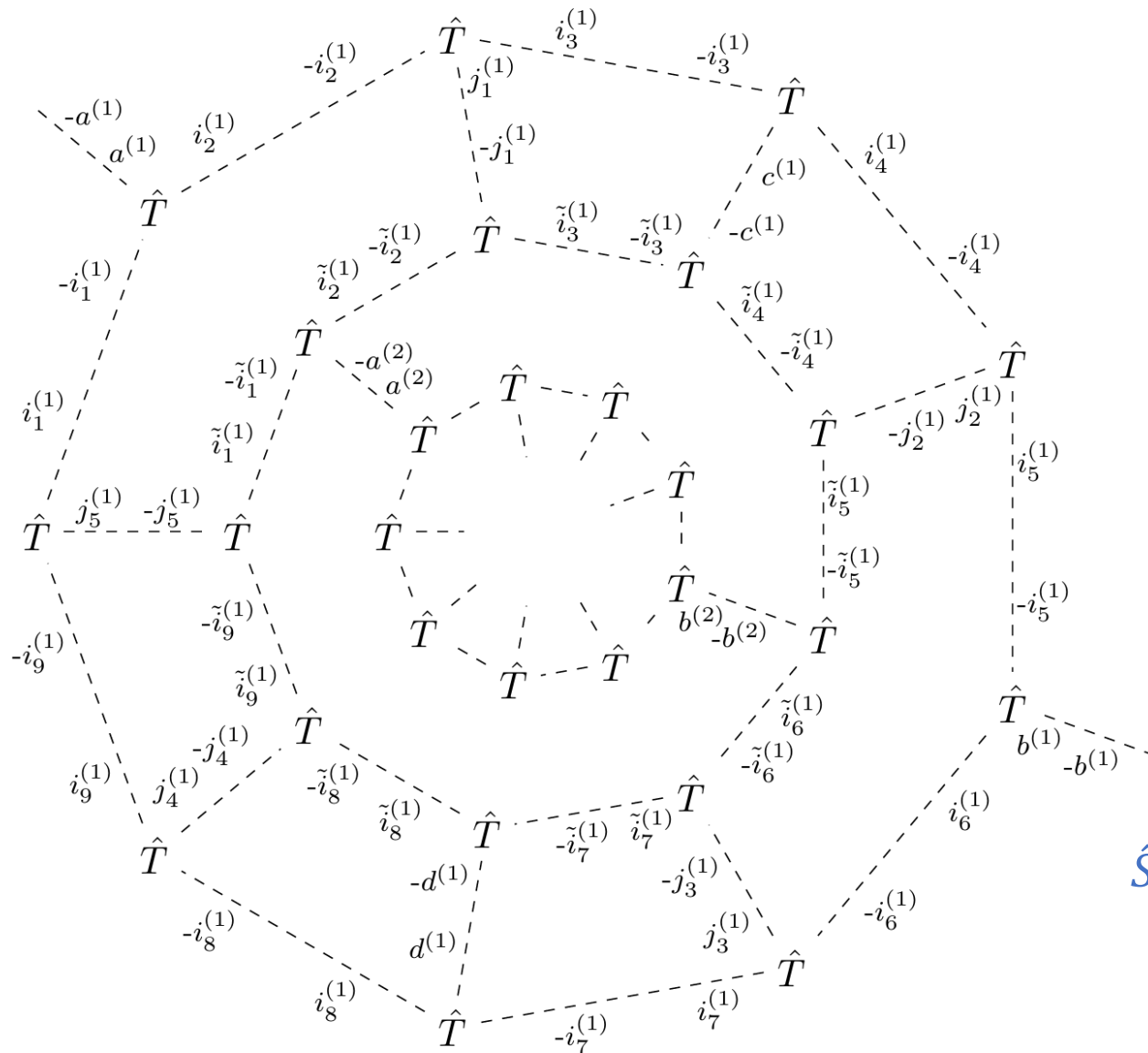
For any real-valued random matrix Y , for any integer $q \geq 1$ and any $\epsilon > 0$,

$$\Pr \left[\|Y\| > \left(\frac{\mathbb{E}[\text{tr}[(YY^\top)^q]]}{\epsilon} \right)^{\frac{1}{2q}} \right] \leq \epsilon$$

- $\text{tr}[(\tilde{W}\tilde{W}^\top)^q]$ can be represented as a **huge TN** \mathcal{G}_q by connecting $2q$ copies of the TN for \tilde{W} in a ring
- Computing $\mathbb{E}[\text{tr}[(\tilde{W}\tilde{W}^\top)^q]]$ is reduced to a **combinatorial problem** of labeling \mathcal{G}_q

Tensor network for the trace method

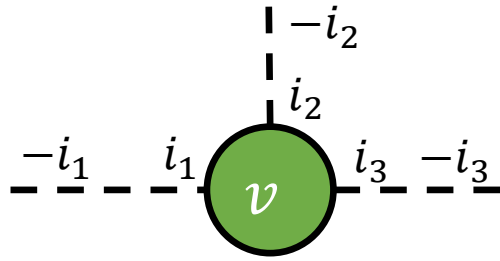
$$\text{tr} \left[(\tilde{W} \tilde{W}^\top)^q \right]$$



\hat{S} is not shown

Labeling the TN graph

A **labeling** \mathcal{L} of \mathcal{G}_q is to assign every edge a pair of indices $(i_e, -i_e)$ for any $i_e \in [n/2]$, and assign every vertex v (i.e., \hat{T} in the graph) an index $k_v \in [K]$.



$$\mathcal{L}(v) := \mathbf{1}_{i_1+i_2+i_3=0} x_{i_1}^{k_v} x_{i_2}^{k_v} x_{i_3}^{k_v}$$

$$\mathbb{E} \left[\text{tr} \left[(\tilde{W} \tilde{W}^\top)^q \right] \right] = \mathbb{E} \left[\sum_{\mathcal{L}} S_{\mathcal{L}} \prod_v \mathcal{L}(v) \right]$$

where

$$S_{\mathcal{L}} := \prod_{l=1}^q S_{a^{(l)} b^{(l)} c^{(l)} d^{(l)}} \cdot S_{(-a^{(l+1)}) (-b^{(l+1)}) (-c^{(l)}) (-d^{(l)})}$$

Labeling the TN graph

$$\mathbb{E} \left[\sum_{\mathcal{L}} S_{\mathcal{L}} \prod_v \mathcal{L}(v) \right] = \sum_{\mathcal{L}} S_{\mathcal{L}} \mathbb{E} \left[\prod_v \mathcal{L}(v) \right]$$

- Let $c(\mathcal{L})$ be the number of repeated labels:

$$c(\mathcal{L}) := \sum_{i \in [p/2]} \max\{0, (\text{\#edges with label } \pm i) - 1\}$$

- The vertices with the same label k_v form a region. Let $r(\mathcal{L})$ be the number of regions:

$$r(\mathcal{L}) := \text{\#distinct } k_v \text{ values}$$

- A labeling \mathcal{L} is **valid** if:

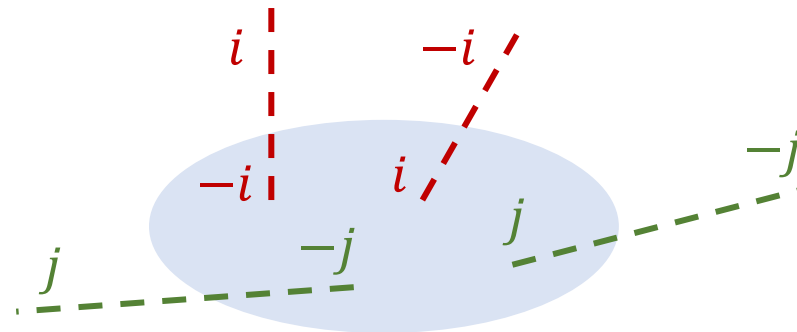
- 1) $i_1 + i_2 + i_3 = 0$ at every vertex ➡ $\mathcal{L}(v) \neq 0$
- 2) $a^{(l)} \neq -b^{(l)}$ and $c^{(l)} \neq -d^{(l)}$ for every layer l ➡ $S_{\mathcal{L}} \neq 0$
- 3) Each region has as many incident i labels as incident $-i$ labels ➡ $\mathbb{E}[\dots] \neq 0$

Labeling the TN graph

Claim. For any valid labeling \mathcal{L} with $r(\mathcal{L}) > 1$, we have $c(\mathcal{L}) \geq r(\mathcal{L})/2$.

Proof.

- Since the number of regions > 1 , and each region has an even number of cut edges (otherwise condition (3) is violated)
- So, the total number of cut edges is $\geq r(\mathcal{L})$
- Since every cut edge with label $(i, -i)$ can be matched to another edge with label $(-i, i)$, the number of repeated edges is at least $r(\mathcal{L})/2$



Counting the valid labelings

Lemma. The number of valid **edge-labelings** with exactly $c(\mathcal{L})$ repeated labels is at most

$$q^{\mathcal{O}(c(\mathcal{L}))} n^{1+9q-c(\mathcal{L})/25}$$

Lemma. For a valid edge-labeling with c repeated labels, the number of valid **vertex-labelings** is at most

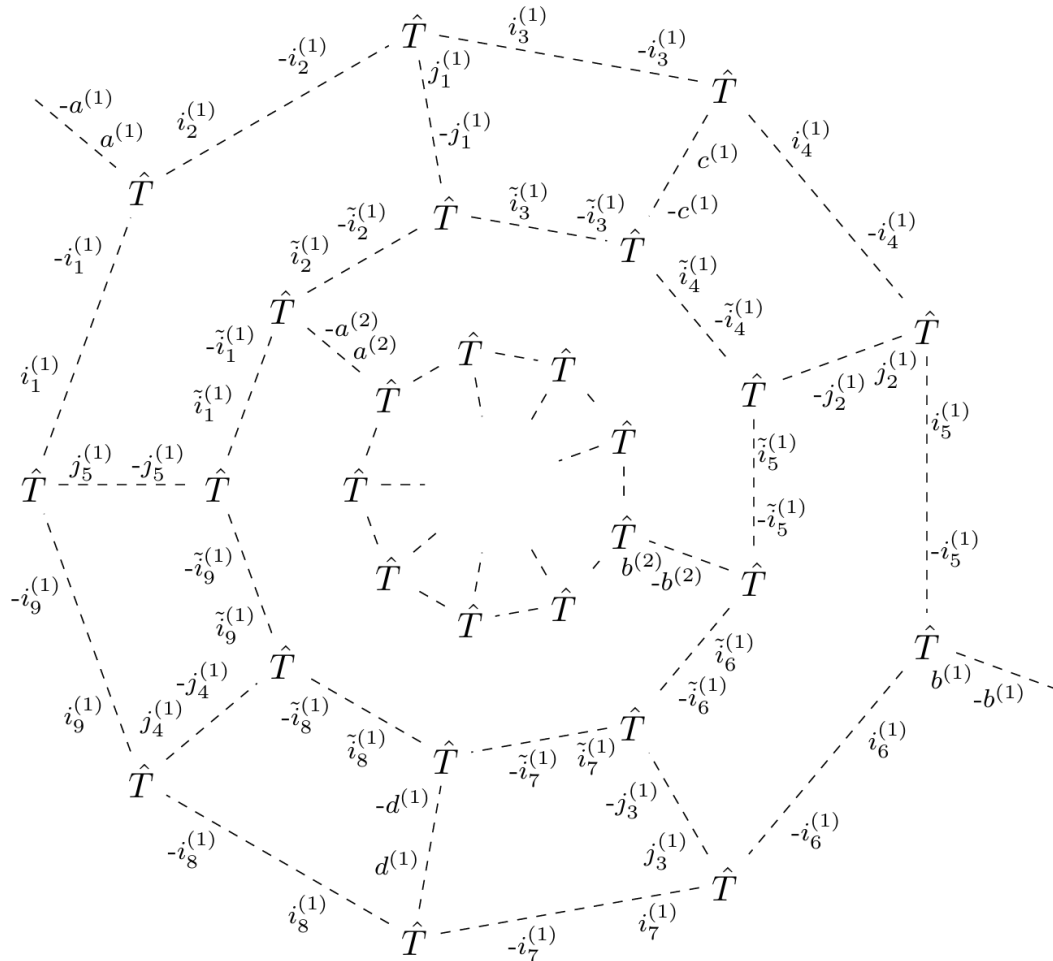
$$c(\mathcal{L})^{\mathcal{O}(q)} \exp(c(\mathcal{L}))$$

Proof.

- $r(\mathcal{L}) \leq 2c(\mathcal{L}) + 1$
- #vertices = $18q$, and the number of ways to assign regions is $\leq (2c + 1)^{18q}$
- #labelings for regions is $\leq K^{2c+1}$



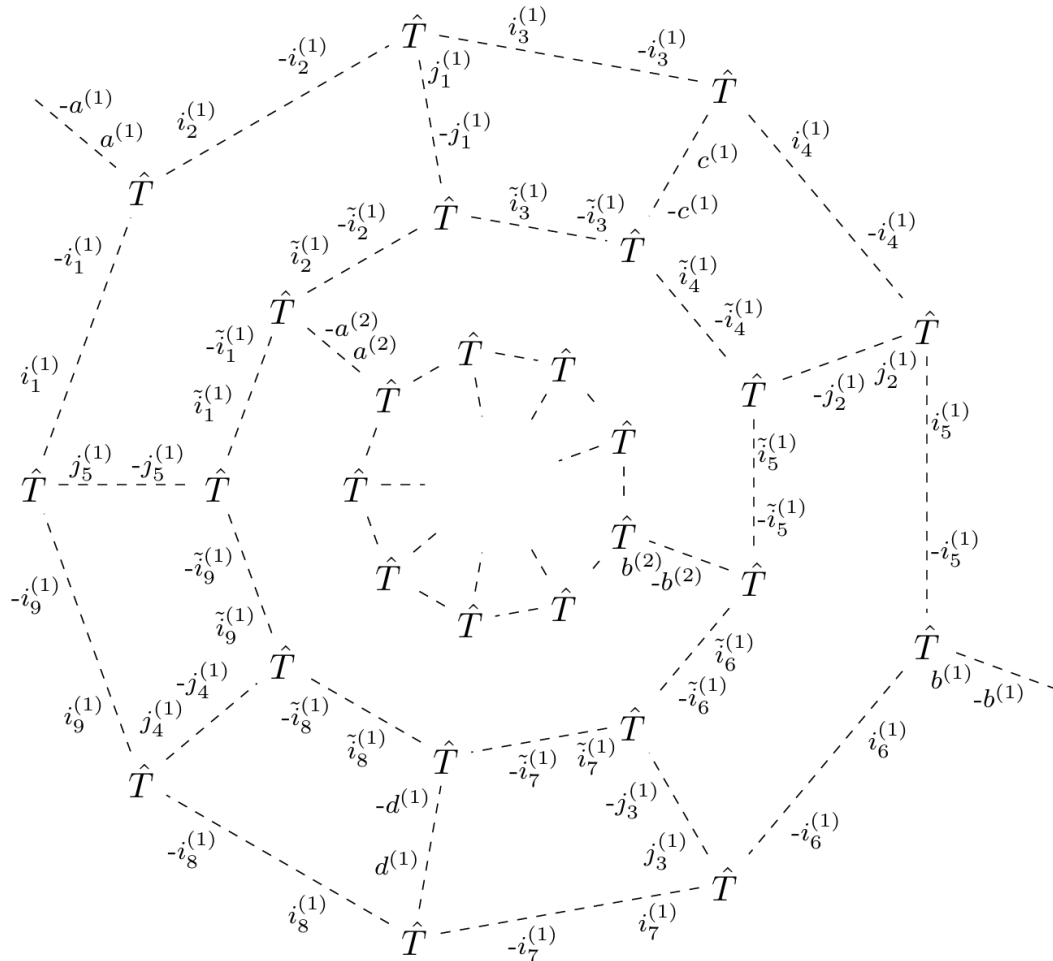
Linear constraints in the TN graph



- $a^{(1)} + j_1^{(1)} + c^{(1)} + j_2^{(1)} + b^{(1)} + j_3^{(1)} + d^{(1)} + j_4^{(1)} + j_5^{(1)} = 0$
- $-a^{(2)} - j_1^{(1)} - c^{(1)} - j_2^{(1)} - b^{(2)} - j_3^{(1)} - d^{(1)} - j_4^{(1)} - j_5^{(1)} = 0$

$$\begin{aligned}
 \text{www} &= a^{(1)} + b^{(1)} \\
 &= j_1^{(1)} - c^{(1)} - j_2^{(1)} - j_3^{(1)} - d^{(1)} - j_4^{(1)} - j_5^{(1)} \\
 &= a^{(2)} + b^{(2)} + b^{(l+1)}
 \end{aligned}$$

Number of free labels



$$\begin{aligned}
 w &:= a^{(l)} + b^{(l)} \\
 &= -j_1^{(l)} - c^{(l)} - j_2^{(l)} - j_3^{(l)} - d^{(l)} - j_4^{(l)} - j_5^{(l)} \\
 &= a^{(l+1)} + b^{(l+1)}
 \end{aligned}$$

- w has $(2d + 1)$ choices
- $a^{(l)}$ is free
- $c^{(l)}, d^{(l)}, j_1^{(l)}, j_2^{(l)}, j_3^{(l)}, j_4^{(l)}$ are free
- $i_1^{(l)}$ is free
- $\tilde{i}_1^{(l)}$ is free
- So, each l has **9** free labels

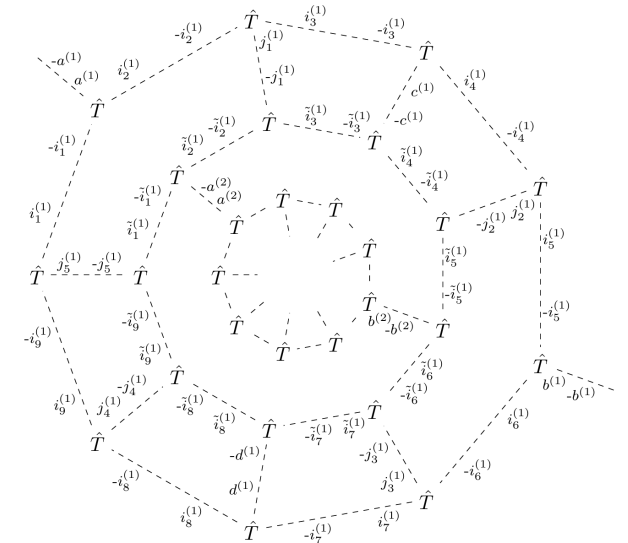
Number of repetition patterns

- \mathcal{L} is required to have $c(\mathcal{L})$ repeated edge labels
- Suppose we label the edges layer-by-layer, and within a layer, there is an ordering for the edges
- We say an edge is repeated if its label equal to a previous label up to sign in the ordering

repetition pattern:



- The total number of edges is $27q$
- At most $(27q)^{c(\mathcal{L})}$ ways to choose which edges are repeated
- At most $(2 \times 27q)^{c(\mathcal{L})}$ ways to choose which previous edges to repeat
- So, there are $q^{O(c(\mathcal{L}))}$ repetition patterns



Repetition pattern reduces free labels

Fix w and fix a repetition pattern. We need to bound the number of labelings

- For each l , the labels are partitioned into two classes: $\{ab\}$ and $\{cdji\tilde{i}\}$
- Each class has ≤ 25 edges, while there are $c(\mathcal{L})$ repeated edges in total. So, at least $c(\mathcal{L})/25$ classes has repeated edges
- By a case study, you can check that each class with a repeated edge will has **one fewer free label**

If $\{a^{(l)}, b^{(l)}\}$ has a repeated edge, there are three cases:

- If $a^{(l)}$ or $b^{(l)}$ repeats a previous edge outside of this class, then the other label is determined, since $a^{(l)} + b^{(l)} = w$
- If $a^{(l)} = b^{(l)}$, then the labels are also determined ($= w/2$)
- If $a^{(l)} = -b^{(l)}$, then it violates the condition (2) and the labeling is not valid

Thus, $a^{(l)}$ is no longer a free label

Total number of valid edge-labelings

$$\underbrace{(2n + 1)}_w \cdot \underbrace{q^{O(c(\mathcal{L}))}}_{\text{\#repetition patterns}} \cdot \underbrace{n^{9q - c(\mathcal{L})/25}}_{\text{\#free labelings}} = q^{O(c(\mathcal{L}))} n^{1 + 9q - c(\mathcal{L})/25}$$

Now, we are ready to compute the q -th moment

$$\begin{aligned}
\mathbb{E} \left[\text{tr} \left[(\tilde{W} \tilde{W}^\top)^q \right] \right] &= \sum_{\text{valid } \mathcal{L}} S_{\mathcal{L}} \mathbb{E} \left[\prod_v \mathcal{L}(v) \right] \\
&\leq (n^9)^{2q} \sum_{\text{valid } \mathcal{L}} \mathbb{E} \left[\prod_v \mathcal{L}(v) \right] \\
&\leq n^{18q} \sum_{c=0}^{27q} \underbrace{(n^{-27q} \cdot (c+1)!)}_{\text{Gaussian moments}} \cdot \underbrace{(c^{\mathcal{O}(q)} \exp(c))}_{\text{\#vertex-labelings}} \cdot \underbrace{(q^{\mathcal{O}(c)} n^{1+9q-c/25})}_{\text{\#edge-labelings}} \\
&= \exp(q) \cdot n \cdot \sum_{c=0}^{27q} (n^{-1/25} q^{\mathcal{O}(1)})^c c^q
\end{aligned}$$

- If we set $q = \log n$, then we have

$$\mathbb{E} \left[\text{tr} \left[(\tilde{W} \tilde{W}^\top)^q \right] \right] = n^{\mathcal{O}(1)}$$

- So,

$$\mathbb{E} \left[\text{tr} \left[(\tilde{W} \tilde{W}^\top)^q \right] \right]^{\frac{1}{2q}} = n^{\frac{\mathcal{O}(1)}{\log n}} = \mathcal{O}(1)$$

Bound the noise term

Key Proposition.

There is an event \mathcal{E} depending only on $\{x^k\}$ that happens with high probability over the randomness of $\{x^k\}$. Conditioned on \mathcal{E} , we have $\|M(T, \tilde{u})\| = \mathcal{O}(\sqrt{\log n})$ with high probability over the randomness of \tilde{u} .

Proof.

- $\Pr \left[\|\tilde{W}\| > \left(\frac{\mathbb{E}[\text{tr}[(\tilde{W}\tilde{W}^\top)^{\log n}]]}{1/n} \right)^{1/(2 \log n)} \right] \leq \frac{1}{n}$
- We have with probability $1 - 1/n$, $\|\tilde{W}\| = \mathcal{O}(1)$. Let \mathcal{E} be this event
- Conditioned on \mathcal{E} ,

$$\Pr_{\tilde{u}}[\|M(T, \tilde{u})\| \geq t\mathcal{O}(1)] \leq n^2 e^{-t^2/2}$$

- Thus, with probability $1 - 1/\text{poly}(n)$,
$$\|M(T, \tilde{u})\| = \mathcal{O}(\sqrt{\log n})$$



Technical theorem.

There is a matrix $M(\mathcal{T}, u) \in \mathbb{R}^{n^2 \times n^2}$ (computable in poly-time from \mathcal{T} and u) with the following guarantee. Let $v \in \mathbb{R}^{n^2}$ be the leading eigenvector of $(M(\mathcal{T}, u) + M(\mathcal{T}, u)^\top)/2$. Let $V = \text{mat}(v) \in \mathbb{R}^{n \times n}$ and let $\tau \in \mathbb{R}^n$ be the top eigenvector of $(V + V^\top)/2$. With high probability over $\{x^k\}$, for any $k \in [K]$, we have $\langle \tau, x^k \rangle^2 \geq 0.99$ with probability $1/\text{poly}(n)$.

Proof.

We have proved that, for any $k \in [K]$,

$$M(\mathcal{T}, u) = \underbrace{\alpha M\left(T^k, (x^k)^{\otimes 5}\right)}_{(1 \pm o(1))(x^k \otimes x^k)(x^k \otimes x^k)^\top} + \underbrace{\alpha \left(M\left(T, (x^k)^{\otimes 5}\right) - M\left(T^1, (x^k)^{\otimes 5}\right) \right)}_{\leq o(1)} + \underbrace{M(T, \tilde{u})}_{o(\sqrt{\log n})} + \underbrace{(M(\mathcal{T}, u) - M(T, u))}_{\leq o(1)}$$

To conclude the proof,

1. Show that the top eigenvector of $M_{\text{sym}} := (M(\mathcal{T}, u) + M(\mathcal{T}, u)^\top)/2$ is close to $(x^k)^{\otimes 2}$
2. Show that the top eigenvector of $V_{\text{sym}} := (V + V^\top)/2$ is close to x^k

(Possibly in your problem set)

Today's plan

- Problem setup and examples
- Some easy algorithms
- Heterogeneous setting
 - Main result: a spectral algorithm for heterogeneous MRA
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- Proof: the signal part
- Proof: the noise part
- **Generalizations**

Generalizations

- Orbit recovery with other groups?
 - **Bandeira-Blum-Smith-Kileel-Perry-Wein-Weed**: the sample complexity of list recovery for a compact group G is $\Theta(\sigma^{2d^*})$ generically, where σ is the noise-level, and d^* is the degree of the **invariant ring** for G
 - **Liu-Moitra**: Smoothed analysis for $SO(3)$ orbit recovery (cryo-ET)

Invariant theory and orbit recovery

- The ring of invariant polynomials consists of all polynomials q that satisfy
$$q(g \cdot x) = q(x) \quad \forall g \in G$$
- The invariant ring determines x up to its orbit, i.e., $y \in \text{orbit}(x) \iff q(y) = q(x) \quad \forall \text{ invariant } q$
- **Method of moment with group symmetry**: How many moments suffices \iff At what degree do invariant polynomials generate the full invariant ring