Complexity of slightly positive tensor networks

CCQ Tensor Meeting 04/30/2025

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Based on: Sign problem in tensor network contraction (arXiv:2404.19023)

Positive bias makes tensor network contraction tractable (arXiv:2410.05414)







Sign problem and tensor networks

In quantum Monte Carlo (QMC) simulations, especially for fermions, "sign problem" exponentially increases the number of samples needed.

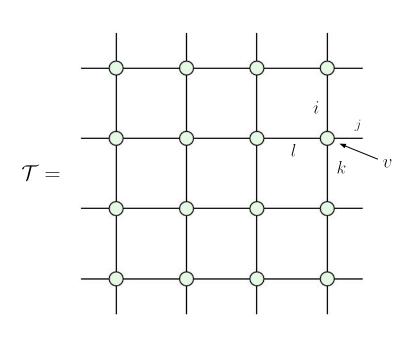
It has often been narrated that tensor networks can circumvent the sign problem, since by construction they do not depend on local basis choices.

We try to understand this aspect rigorously by studying:

Random tensor networks with controlled sign structure.

Tensor networks (TNs)

2D square-lattice graph with n vertices



Edges: $i \in \{1,...,d\}$, d is called bond-dimension

Vertices: M_{ijkl}^v , order-4 tensor

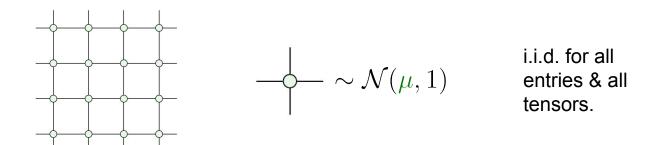
Edge labeling: an assignment of values to all edges

e.g.
$$c = (..., i = 3, j = 2, k = 1, l = 1, ...)$$

Contraction of a TN yields a number:

$$\mathcal{C}(\mathcal{T}) \;\; = \sum_{ ext{edge labeling } c} \;\; \prod_v M_c^v$$

The problems we study



Contracting a tensor network with random entries. Larger mean → more positive.

- Is the contraction easier when the mean increases?
- If yes, when does the contraction become easy/hard?

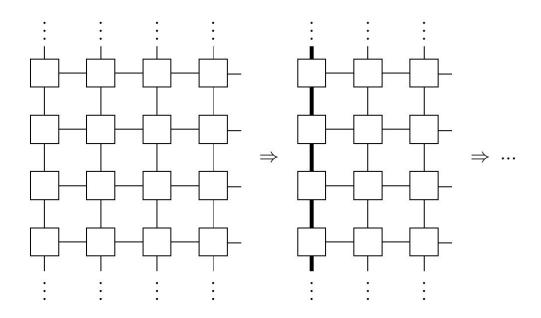
Part I: Sign problem in tensor network contraction (arXiv:2404.19023)

We predicted the complexity **transition point** through an effective classical statistical model, and numerically verified the transition.

Transition point: mean = 1/bond-dimension

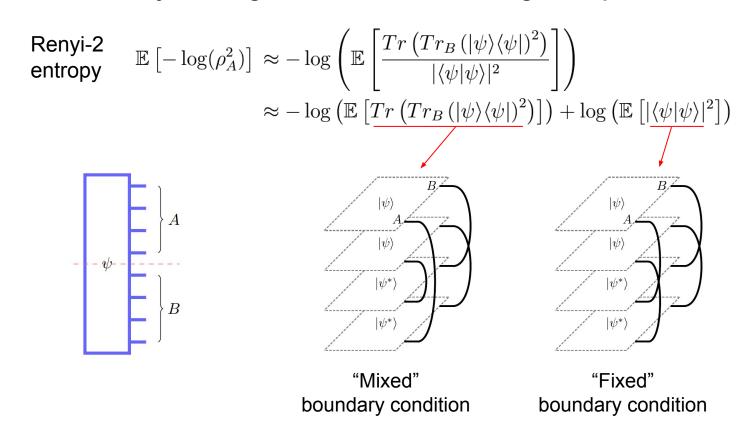
This transition happens **much earlier** than "sign problem" disappears. In other words, the entries only need to be **slightly positive**.

Contractability ≈ entanglement in the TN



Increased bond-dimension

Contractability ≈ entanglement in the TN ⇔ Average of copies of random TNs



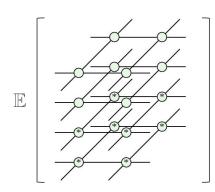
Contractability ≈ entanglement in the TN ⇔ Average of copies of random TNs

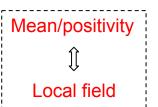


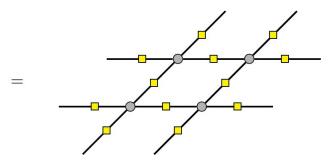
Partition function of classical stats model

Average of copies of random tensors can be computed analytically.

E.g. Isserlis/Wick's theorem







Partition function of a **ferromagnetic**Potts model with external field

$$\sum_{\{\sigma^{(s)}\}} e^{-\sum_s h(\sigma^{(s)}) - \sum_{\langle s,s'\rangle} k(\sigma^{(s)},\sigma^{(s')})}$$

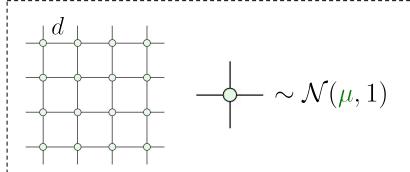
Contractability ≈ entanglement in the TN ⇔ Average of copies of random TNs

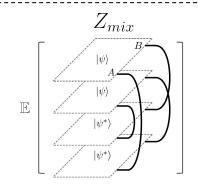
Phase transition point: $\mu d=1 \Leftrightarrow$ Partition function of classical stats model

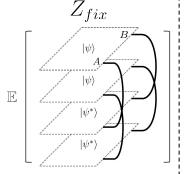
$$\mu d = 1$$

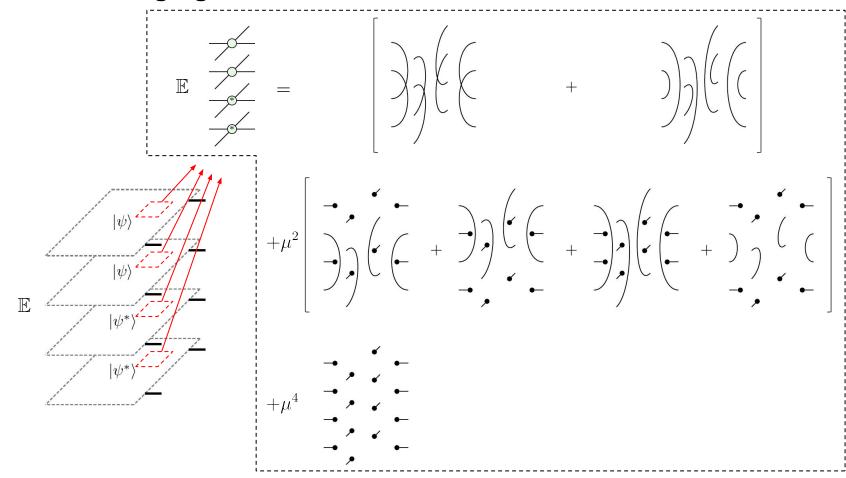
$$\label{eq:multiple}$$
 No local field

$$\left| \begin{array}{c} \mu d < 1: Z_{mix} \ll Z_{fix} & -\log\left(rac{Z_{mix}}{Z_{fix}}
ight) \gg 0 \end{array} \right| \right|$$
 high entanglement

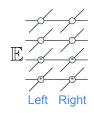


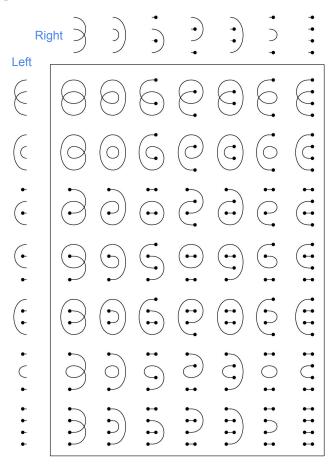




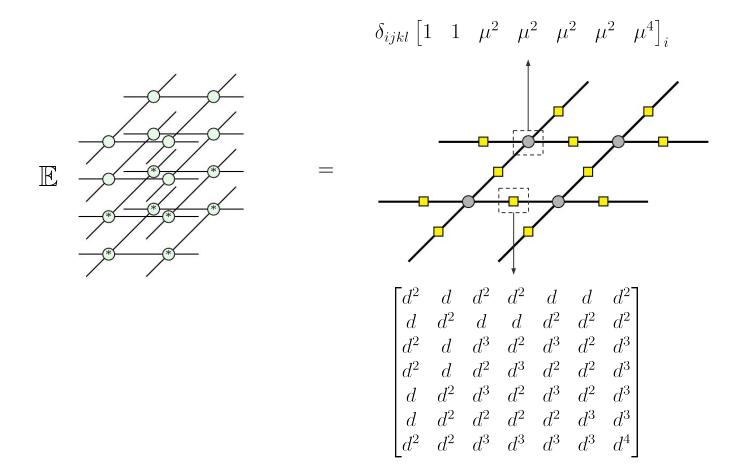


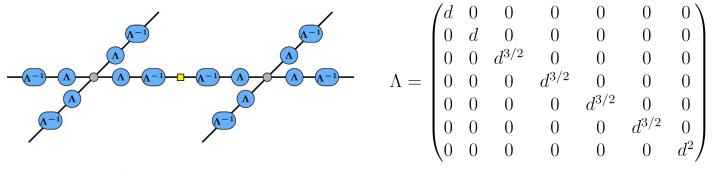
Contracting adjacent tensors introduces a scalar depending on the number of loops & lines





$$= \begin{bmatrix} d^2 & d & d^2 & d^2 & d & d & d^2 \\ d & d^2 & d & d & d^2 & d^2 & d^2 \\ d^2 & d & d^3 & d^2 & d^3 & d^2 & d^3 \\ d^2 & d & d^2 & d^3 & d^2 & d^2 & d^3 \\ d & d^2 & d^3 & d^2 & d^3 & d^2 & d^3 \\ d & d^2 & d^2 & d^2 & d^2 & d^3 & d^3 \\ d^2 & d^2 & d^3 & d^3 & d^3 & d^3 & d^4 \end{bmatrix}$$

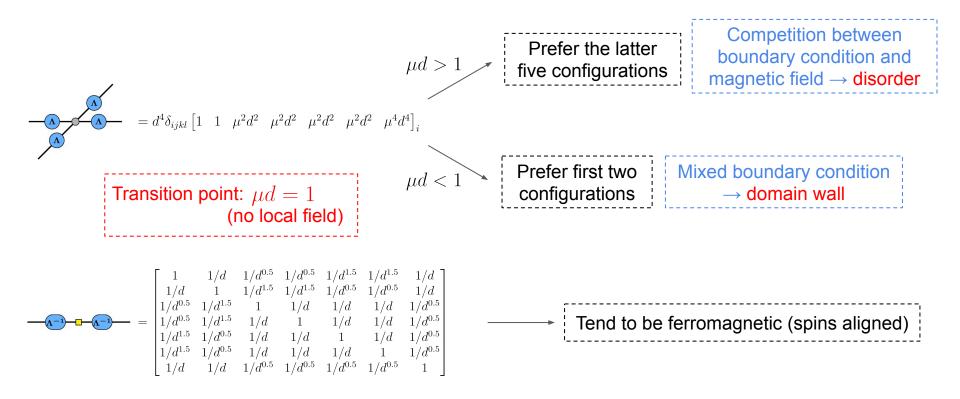




$$= d^4 \delta_{ijkl} \begin{bmatrix} 1 & 1 & \mu^2 d^2 & \mu^2 d^2 & \mu^2 d^2 & \mu^2 d^2 & \mu^4 d^4 \end{bmatrix}_i$$

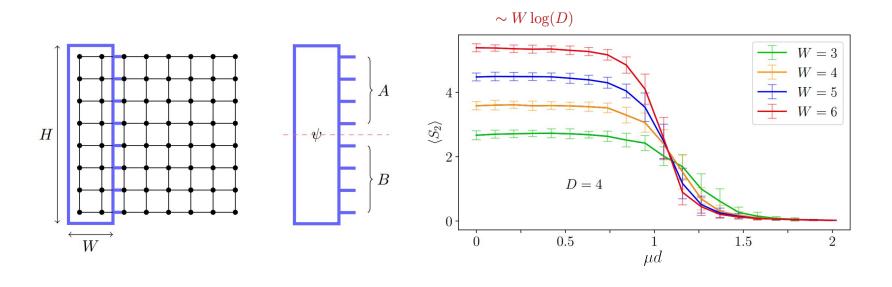
$$= \begin{bmatrix} 1 & 1/d & 1/d^{0.5} & 1/d^{0.5} & 1/d^{1.5} & 1/d^{1.5} & 1/d \\ 1/d & 1 & 1/d^{1.5} & 1/d^{1.5} & 1/d^{0.5} & 1/d^{0.5} & 1/d \\ 1/d^{0.5} & 1/d^{1.5} & 1 & 1/d & 1/d & 1/d & 1/d^{0.5} \\ 1/d^{0.5} & 1/d^{1.5} & 1/d & 1 & 1/d & 1/d & 1/d^{0.5} \\ 1/d^{1.5} & 1/d^{0.5} & 1/d & 1/d & 1 & 1/d & 1/d^{0.5} \\ 1/d^{1.5} & 1/d^{0.5} & 1/d & 1/d & 1/d & 1 & 1/d^{0.5} \\ 1/d & 1/d & 1/d^{0.5} & 1/d^{0.5} & 1/d^{0.5} & 1/d^{0.5} & 1/d^{0.5} \end{bmatrix}$$

Becomes ferromagnetic as $D \rightarrow \infty$!



Numerical simulation

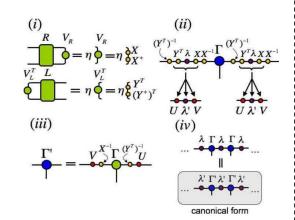
We observed the same transition in finite-size simulation. We choose $H \gg W$ so the entropy saturates (H = 4W in our simulation).



iMPS simulation of the effective model

iMPS - iMPO algorithm

Roman Orus and Guifre Vidal, The iTEBD algorithm beyond unitary evolution, Phys. Rev. B 78, 155117 (2008)

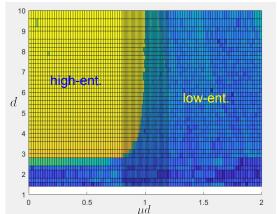


Overlap between left/right dominant eigenvectors of fixed-point iMPS

$$\left| \frac{\langle l_1 | \lambda | r_0 \rangle}{\langle l_0 | \lambda | r_0 \rangle} \right|$$

$$|r_i\rangle = v_{\max}^r(\Gamma_i\lambda)$$

 $\langle l_i| = v_{\max}^l(\lambda\Gamma_i)$



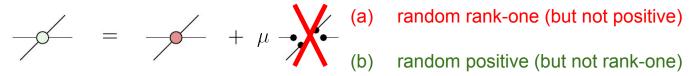
μ = 0 case also relates to previous results:

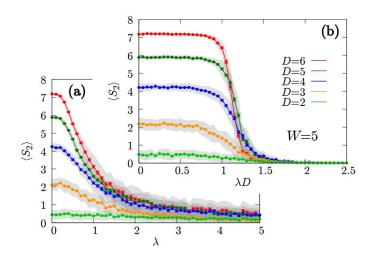
[1] Romain Vasseur, Andrew C. Potter, Yi-Zhuang You, Andreas W. W. Ludwig, Entanglement Transitions from Holographic Random Tensor Networks, Phys. Rev. B 100, 134203 (2019) [2] Ryan Levy, Bryan K. Clark, Entanglement Entropy Transitions with Random Tensor Networks,

[2] Ryan Levy, Bryan K. Clark, Entanglement Entropy Transitions with Random Tensor Networks arXiv:2108.02225

Role of positivity?

Does "rank-one" ness cause the complexity transition instead of positiveness?





The "positivity" part is important to observe the transition!

Or in other words, the rank-one states need to be "aligned".

Sign problem in QMC

$$\langle O \rangle = \frac{1}{Z} \mathrm{Tr}[Oe^{-\beta H}] = \frac{1}{Z} \mathrm{Tr}[O(e^{-\beta H/M})^M]$$

$$= \frac{1}{Z} \sum_{\{x_i\}} \langle x_0 | O | x_1 \rangle \langle x_1 | e^{-\beta H/M} | x_2 \rangle \langle x_2 | ... | x_M \rangle \langle x_M | e^{-\beta H/M} | x_0 \rangle$$

$$= \frac{1}{Z} \sum_{x} O(x) T(x)$$

$$T(x) = \mathrm{sign}(T(x)) | T(x) |$$

$$T(x) \geq 0$$

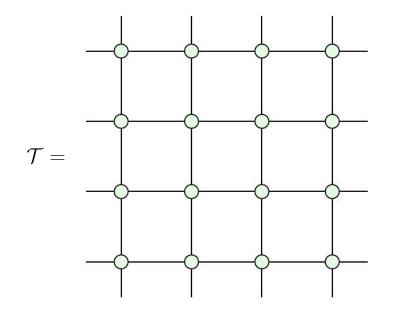
$$T(x) \text{ varying signs}$$

$$\langle \mathrm{sign} \rangle = \frac{\sum_{x} T(x)}{\sum_{x} |T(x)|} = e^{-\beta N \Delta f}$$
sample $x_i^* \sim \frac{|T(x)|}{\sum_{x} |T(x)|}$
estimate by $\frac{1}{K} \sum_{i=1}^K O(x_i^*)$ estimate by $\frac{1}{K} \frac{1}{\langle \mathrm{sign} \rangle} \sum_{i=1}^K O(x_i^*) \mathrm{sign}(T(x_i^*))$
error $\sim \frac{e^{\beta N \Delta f}}{\sqrt{K}}$ "sign problem": exponential dependence on N caused by $\langle \mathrm{sign} \rangle$

Sign problem in random TN

"Sign problem" in TN:

$$e^{-N\Delta f} := \frac{\sum_{\text{edge labeling } c} \frac{\prod_{v} M_c^v}{\sum_{\text{edge labeling } c} \frac{\prod_{v} M_c^v}{\prod_{v} |M_c^v|}}$$



$$\mathcal{C}(\mathcal{T}) = \sum_{ ext{edge labeling } c} \prod_{v} M_c^v$$

Sign problem in random TN

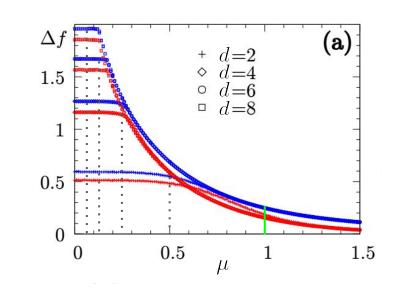
$$e^{-N\Delta f} := \frac{\sum_{\text{edge labeling } c} \prod_{v} M_c^v}{\sum_{\text{edge labeling } c} \prod_{v} |M_c^v|}$$

Sign problem is

 $\mu \lesssim 1/d$: worse for large d

 $1/d \lesssim \mu \lesssim 1$: independent of d

 $1 \lesssim \mu$: rapidly vanishing



Sign problem only disappears when $\,\mu\gtrsim 1$, where entries are mostly positive

Part II: Positive bias makes tensor network contraction tracatable (arXiv:2410.05414)

We give a series of more rigorous results, including a provably "efficient" algorithm to contract slightly positive random tensor networks (same transition point).

Complexity of (2D) tensor network contraction

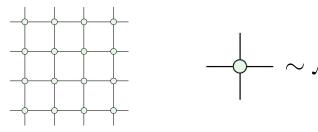
	Exact	Approximate	
Worst-case	#P-hard [SWVC07]	Empirically hard	
Average-case ($\mu=0$)	#P-hard [HHEG20]		
Average-case + small positive bias ($\mu \gtrsim 1/d$)	#P-hard [our result]	Quasi-poly time algorithm [our result]	

Main theorem

Theorem (informal): For a random 2D tensor network, if

$$\mu \gtrsim 1/d, \qquad d \gtrsim n$$

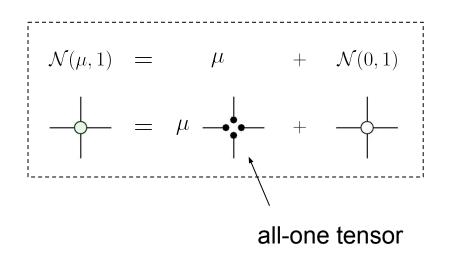
then with high probability, there exists a quasi-polynomial time algorithm which approximates the TN contraction value up to arbitrary 1/poly(n) multiplicative error.

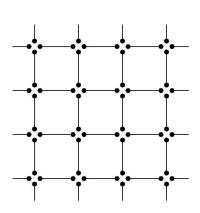


 $- \hspace{-0.2cm} \longleftarrow \sim \mathcal{N}(\mu,1) \hspace{1cm} \begin{array}{l} \text{i.i.d. for all} \\ \text{entries \& all} \\ \text{tensors.} \end{array}$

Method overview

Easy	Interpolate	Hard
$\mu \to \infty$		$\mu = 1/d$





Easy to contract!

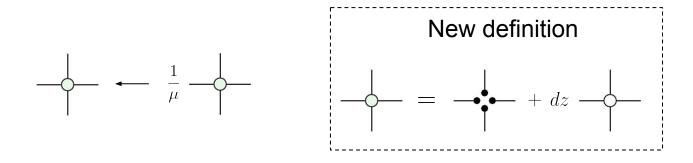
Method overview

Easy	Interpolate	Hard
$\mu \to \infty$		$\mu = 1/d$
[z=0]		[z=1]

For convenience later, introduce change of variable

$$z = \frac{1}{\mu d}$$

and rescale the tensors. No effect on multiplicative error.



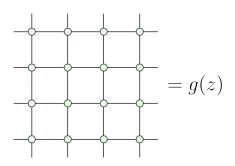
Method overview

To interpolate from z = 0 to 1, we uses **Barvinok's** method [Bar16]. It relies on two observations.

$$+ dz -$$

Observation 1

Contracted TN is a degree-n random polynomial on z, denoted as g(z).



Observation 2

k-th derivative of g(z) at z = 0 can be computed brute-forcely in $n^{O(k)}$ time.

e.g.
$$\frac{1}{4!} \frac{\partial^4 g(z)}{\partial z^4} \Big|_{z=0} =$$

+ $\,$ all other configs with four $\,$ $\!$ $\!$ $\!$

Barvinok's method [Bar16]

Originally designed for permanent

Input: degree-n polynomial g(z)

 $g^{(k)}(0)$ accessible in $n^{O(k)}$ time

Output: g(1), ε multiplicative error

 $f(z) = \ln(g(z))$, now ϵ additive error

Algorithm: $f(1) \approx \hat{f}(1) = \sum_{k=0}^{M} \frac{f^{(k)}(0)}{k!}$, output $e^{\hat{f}(1)}$, that's it!

Effectiveness depends on the roots of g(z)

Barvinok's method [Bar16]

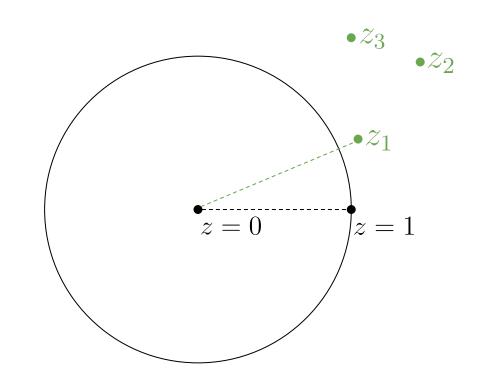
Roots of g(z) are outside the |z| = 1 disk \rightarrow small error

$$f(z) = \ln(g(z))$$

$$f(1) \approx \hat{f}(1) = \sum_{k=0}^{M} \frac{f^{(k)}(0)}{k!}$$

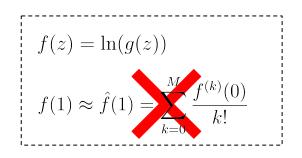
$$M = O\left(\ln\left(\frac{n}{\epsilon}\right)\right)$$

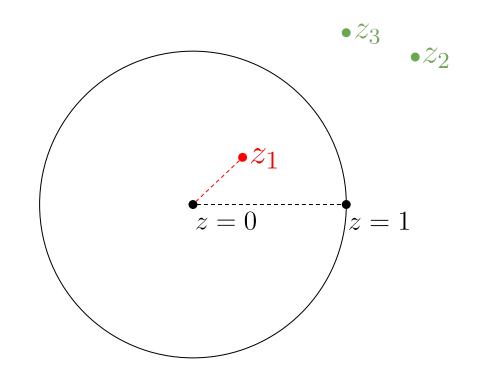
Run time $n^{O(M)}$, quasi-poly



Barvinok's method [Bar16]

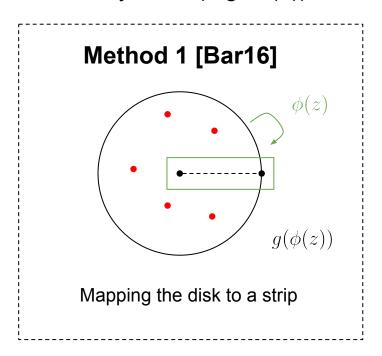
A root of g(z) is inside the |z| = 1 disk \rightarrow error blows up!

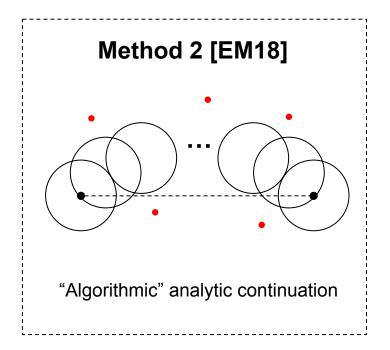




Barvinok's method via root-free path

Not many roots (e.g. O(1)) \rightarrow can interpolate along a root-free path!





Both remain quasi-polynomial time.

$$f(z) = \ln(g(z)) \\ f(1) \approx \hat{f}(1) = \sum_{k=0}^{M} \frac{f^{(k)}(0)}{k!}$$
 few roots on average \longrightarrow find a root-free path with high probability \longrightarrow flat successes with high probability

$$f(z) = \ln(g(z))$$
 few roots $f(1) \approx \hat{f}(1) = \sum_{k=0}^{M} \frac{f^{(k)}(0)}{k!}$ few roots on average in the finding a root-free path with high probability in that successes with high probability

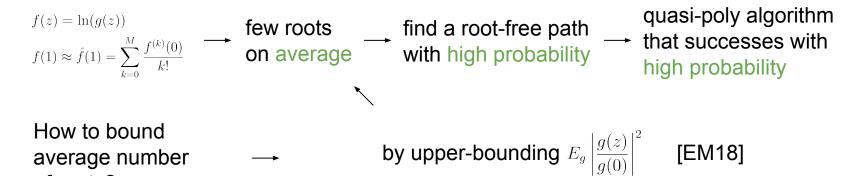
How to bound average number of roots?

$$\mathbb{E}_{g}[N_{r(1-\delta)}] \leq \frac{1}{2\delta} \mathbb{E}_{g} \left[\oint_{r} \log \left(\left| \frac{g(z)}{g(0)} \right|^{2} \right) dz \right]$$
 Jensen's formula
$$\leq \frac{1}{2\delta} \log \left(\oint_{r} \mathbb{E}_{g} \left| \frac{g(z)}{g(0)} \right|^{2} dz \right)$$
 Jensen's inequality

Jensen's formula

[EM18]

of roots?



$$f(z) = \ln(g(z)) \\ f(1) \approx \hat{f}(1) = \sum_{k=0}^{M} \frac{f^{(k)}(0)}{k!}$$
 few roots on average \longrightarrow find a root-free path with high probability \longrightarrow that successes with high probability

How to bound average number of roots?

by upper-bounding $E_g \left| rac{g(z)}{g(0)}
ight|^2$ [EM18]

$$f(z) = \ln(g(z))$$
 few roots on average \rightarrow find a root-free path with high probability \rightarrow that successes with high probability

How to bound average number of roots?

 \longrightarrow by upper-bounding $E_g \left| \frac{g(z)}{g(0)} \right|^2$ [EM18]

partition function of 2D
$$E_g|g(z)|^2= ext{ classical ising model with local magnetic field!}$$

 $z=1 \longleftrightarrow {\sf zero magnetic field}$

$$f(z) = \ln(g(z))$$
 few roots $f(1) = \sum_{k=0}^{M} \frac{f^{(k)}(0)}{k!}$ on average $f(1) = \lim_{k \to \infty} \frac{f(k)}{k!}$ few roots on average $f(1) = \lim_{k \to \infty} \frac{f(k)}{k!}$ find a root-free path with high probability $f(1) = \lim_{k \to \infty} \frac{f(k)}{k!}$ few roots on average $f(1) = \lim_{k \to \infty} \frac{f(k)}{k!}$ find a root-free path with high probability high probability

How to bound average number of roots?

by upper-bounding $E_g \left| rac{g(z)}{g(0)}
ight|^2$ [EM18]

partition function of 2D
$$E_g|g(z)|^2 =$$
 classical ising model with local magnetic field!

 $z = 1 \leftrightarrow \text{zero magnetic field}$

Onsager's solution [Ons44] for zero-field 2D ising model (finite-size variant [Kau49])

$$f(z) = \ln(g(z))$$
 few roots on average on average $f(z) = \frac{1}{k!} = \frac{f(k)(0)}{k!}$ few roots on average on average of $f(z) = \frac{1}{k!} = \frac{f(k)(0)}{k!}$ find a root-free path with high probability on a probability high probability

How to bound average number of roots?

by upper-bounding
$$E_g \left| \frac{g(z)}{g(0)} \right|^2$$
 [EM18]
$$O(1) \text{ for z} \lesssim 1$$

partition function of 2D
$$E_g|g(z)|^2 =$$
 classical ising model with local magnetic field!

 $z = 1 \longleftrightarrow \text{ zero magnetic field}$

Outlook

(Part I)

 Besides the stats model mapping, how to more intuitively understand the complexity transition?

(Part II)

- How to prove tractability with constant bond-dimension?
- Can one improve the interpolation method?
 - Interpolate from other rank-one tensors? (e.g. BP fixed point)
 - Use better interpolations?
- Can the interpolation method be used in practice? (with some modifications & heuristics)