The complexity of computing averages

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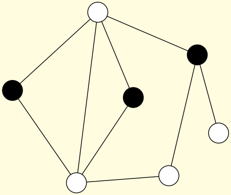
Based on joint work with Leonard J. Schulman and Alistair Sinclair

Independent sets



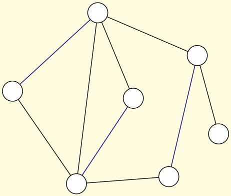
MAX-IND-SET	NP-hard
#IND-SET	#P-hard

[Karp, 1972; Valiant, 1979a]

Question

What is the complexity of computing the average size of an independent set?

Matchings



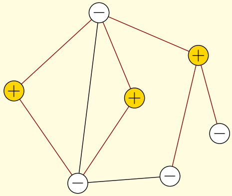
MAX-MATCHING	P
#MATCHING	#P-hard

[**Edmonds, 1965; Valiant, 1979a**]

Question

What is the complexity of computing the average size of a matching?

Ising model [Ising, 1925]



Vertex activity

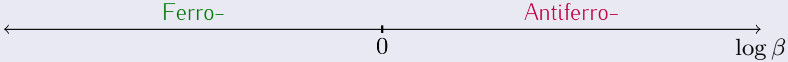
$$w(C) = \lambda^{\#(+)} \beta^{|C|}$$

Edge activity

Partition function $Z(\beta, \lambda) := \sum_{\text{cuts C}} w(C)$

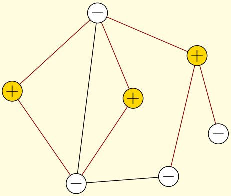
- $Z(\beta, \lambda)$ is #P-hard for fixed (β, λ)

Ferromagnetic vs. Antiferromagnetic Ising



$\beta < 1$ and $\beta > 1$ are qualitatively very different

Ising model [Ising, 1925]



$$w(C) = \lambda^{\#(+)} \beta^{|C|}$$

Vertex activity: λ

Edge activity: β

Partition function $Z(\beta, \lambda) := \sum_{\text{cuts C}} w(C)$

- $Z(\beta, \lambda)$ is #P-hard for fixed (β, λ)

Questions (for both ferro- and antiferromagnetic Ising)

Mean magnetization	Mean energy ("Avg. cut size")
$\mathbb{E}_{C \sim w}[\#(+)]$	$\mathbb{E}_{C \sim w}[\lvert C \rvert]$

What is the complexity of computing the above?

Why averages?

Approximation

- **Very extensively studied:** a major application of sampling

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Exact computation

- Ising model: Computing magnetization is trivial for $\lambda = 1$ (spins are symmetric, so magnetization $= 1/2$). Other λ? Mean energy? Other models

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Technical reasons

Interesting questions about zeros of partition functions

Results

All these averages are #P-hard to compute, even on bdd. degree graphs

[**Schulman, Sinclair, S., IEEE FOCS 2015**]

Avg. size of independent sets

Holds also for the "Hard core lattice gas"

Avg. size of matchings

Holds also for the "Monomer-dimer model"

Ising mean magnetization

For both Ferro- and Antiferro- Ising

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Earlier results [**Sinclair, S., *Comm. Math. Phys.* 2014**]

#P hardness for Ferromagnetic Ising magnetization and for Monomer-dimer with edge weights

- ...using new extensions to Lee-Yang type theorems

Proving #P-hardness: Partition functions

Recall that

$$Z(\beta, \lambda) = \sum_{\sigma \in \{+,-\}^V} \beta^{\#(+,-)} \lambda^{\#(+)}$$

Interpolation [Valiant, 1979b; …Vadhan, 2001; …Dyer and Greenhill, 2000; …]

- View $Z(\beta, \lambda) = \sum_{k=1}^{|V|} \alpha_k \lambda^k$ as a polynomial in λ
- Coefficients α_k encode the solution to a #P-hard problem (e.g. #Max-Cut)
- Find the coefficients α_k using polynomial interpolation

- Shows that computing $Z(\beta, \lambda)$ is hard—at least when λ is part of the input

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- Shows that computing $Z(\beta, \lambda)$ is hard—at least when λ is part of the input
- Complexity of partition functions is very well understood via dichotomy theorems [e.g. Bulatov and Grohe, 2005; ...Cai, Chen, and Lu, 2010...]

Proving #P-hardness: Magnetization

Magnetization $\mu(\beta, \lambda)$ can be written as

$$\mu(\beta, \lambda) := \frac{\sum_\sigma \#(+) w(\sigma)}{\sum_\sigma w(\sigma)} = \frac{\lambda Z'}{Z}, \quad \because\ w(\sigma) = \lambda^{\#(+)} \beta^{C(\sigma)},$$

where $Z' = \frac{\partial}{\partial \lambda} Z(\beta, \lambda)$

Interpolation

- View $\mu(\beta, \lambda)$ as a rational function in λ
- Coefficients of Z, Z' encode the solution to a #P-hard problem
- Find the coefficients of Z (and Z') using rational interpolation

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Interpolation

✓ View $\mu(\beta, \lambda)$ as a rational function in λ

✓ Coefficients of Z, Z' encode the solution to a #P-hard problem

? Find the coefficients of Z (and Z') using rational interpolation

But...

Cannot interpolate $\frac{p(x)}{q(x)}$ when $p(x)$ and $q(x)$ share common factors!

Rest of the talk: Ensuring rational interpolation succeeds

Approach 1: Show there are no common factors

New results for zeros of partition functions

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Approach 1: Show there are no common factors

New results for zeros of partition functions

Approach 2: Interpolate with common factors

Integrate the mean

Rest of the talk: Ensuring rational interpolation succeeds

Approach 1: Show there are no common factors

New results for zeros of partition functions

Rational interpolation and #P-hardness

Rational Interpolation [Macon and Dupree, 1962]

Suppose $R(x) = \frac{p(x)}{q(x)}$ where $\deg(p(x)) = \deg(q(x)) = n$.
If

$$\gcd(\mathrm{p}(\mathrm{x}), \mathrm{q}(\mathrm{x})) = 1$$

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We had

$$\mu(\beta, \lambda) = \lambda \frac{Z'}{Z}$$

Requirement: No common zeros for Z and Z'

#P-hardness will follow if $\gcd(Z'(\beta,\lambda), Z(\beta,\lambda)) = 1$,

$\iff Z(\beta,\lambda)$ and $Z'(\beta,\lambda)$ have no common complex zeros

Rational interpolation and #P-hardness (contd...)

Conclusion

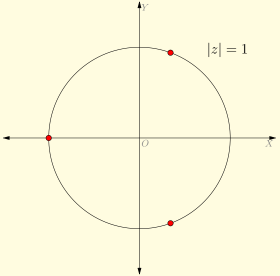
Z, Z' have no common zeros $\Longrightarrow$ magnetization μ is as hard to compute as Z (and hence #P-hard)

- Disconnected graphs can have common zeros:
  - e.g., $Z_{G \dot\cup G} = Z_G^2$, so that $Z_{G \dot\cup G}$ and $Z'_{G \dot\cup G}$ have lots of common zeros

Complex zeros and Ferromagnetic Ising

Theorem [Lee and Yang, 1952]

When $0 < \beta \leq 1$, the zeros of $Z(\beta, z)$ satisfy $|z| = 1$.



Lee-Yang theorem: Zeros of Z

- **Gauss-Lucas lemma**: $Z'(\beta, z) = 0 \implies |z| \leq 1$
    - …but this is not sufficient for showing that Z and Z' have no common zeros
- Original motivation for the theorem was studying phase transitions in the Ising model

An extension of the Lee-Yang theorem

Theorem [Sinclair, S., 2014]

For a connected graph with $0 < \beta < 1$, the zeros of $Z'(\beta, z) = \frac{\partial}{\partial z} Z(J, z)$ satisfy $|z| < 1$. In particular, $\gcd\left(Z(\beta, z), Z'(\beta, z)\right) = 1$.

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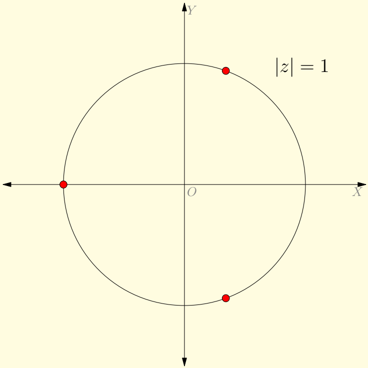

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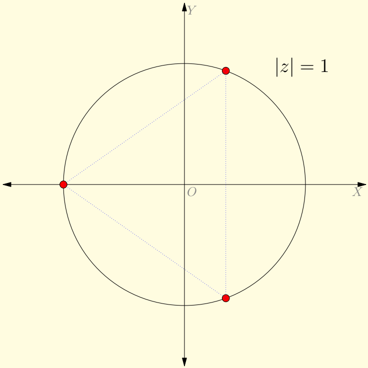
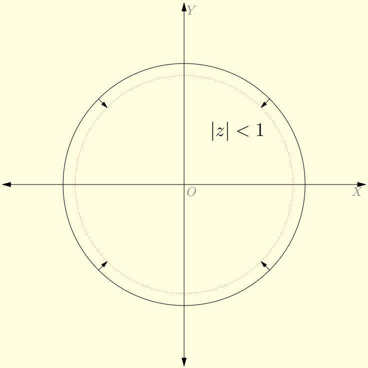


Lee-Yang theorem: Zeros of Z



Our theorem: Zeros of Z'

Proving Lee-Yang theorems

New approach

Multivariate Lee-Yang theorems

- Consider the scenario where the vertex activities can vary across vertices:

$$w(\sigma) = \beta^{\#(+,-)} \prod_{v:\sigma(v)=+} z_v$$

Multivariate Lee-Yang theorems

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Magnetization operator

$$\mathcal{D} := \sum_v z_v \frac{\partial}{\partial z_v}$$

so that

$$\mathcal{D}Z(\beta, z_1, z_2, \dots z_n)|_{z_1=z_2=\dots=z_n=x} = z\frac{\partial}{\partial z}Z(\beta, z)|_{z=x}$$

- The magnetization itself is given by

$$\mu(\beta, z_1, z_2, \dots z_n) = \frac{\mathcal{D}Z(\beta, z_1, z_2, \dots z_n)}{Z(\beta, z_1, z_2, \dots z_n)}$$

- Agrees with the univariate case: $\mu(\beta, \lambda) = \frac{\lambda Z'}{Z}$

Multivariate Lee-Yang theorems (contd...)

Theorem [Lee and Yang, 1952; Asano, 1970]

Suppose $0 < \beta \leq 1$, and $|z_i| > 1$ for $1 \leq i \leq n$. Then,

$$Z(\beta, z_1, z_2, \ldots, z_n) \neq 0.$$

- The univariate Lee-Yang theorem follows by setting $z_i = z$ for all i

Multivariate Lee-Yang theorems (contd...)

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Our theorem

On a connected graph, the conditions $0 < \beta < 1$ and $|z_i| \geq 1$ for all $1 \leq i \leq n$ imply that

$$\mathcal{D}Z(\beta, z_1, z_2, \ldots, z_n) \neq 0.$$

- Our univariate theorem follows from the above by setting $z_i = z$ for all i

Proof Sketch

Theorem

On a connected graph, the conditions $0 < \beta < 1$ and $|z_i| \geq 1$ for all $1 \leq i \leq n$ imply that

$$\mathcal{D}Z(\beta, z_1, z_2, \ldots, z_n) \neq 0.$$

- Say that $Z(\beta, z_1, z_2, \ldots, z_n)$ has property $\mathcal{G}$ if it satisfies the conclusion of the above theorem
- The proof proceeds by induction:
  - Each step maintains the connectedness of the graph, and the property $\mathcal{G}$ for its partition function
  - Asano's proof of the Lee-Yang theorem as a warm-up

Asano's Proof of the Lee-Yang theorem

Property $\mathcal{A}$

Z_G has property $\mathcal{A}$ (denoted $Z \in \mathcal{A}$) if

$$0 < \beta \leq 1 \text{ and } |z_i| > 1 \text{ for all } i$$
$$\implies Z_G(\beta, z_1, z_2, \ldots, z_n) \neq 0$$

- If G and H are disjoint graphs with $Z_G, Z_H \in \mathcal{A}$, then

$$Z_{G \dot\cup H} = Z_G Z_H \in \mathcal{A}$$

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- If G and H are disjoint graphs with $Z_G, Z_H \in \mathcal{A}$, then

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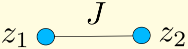
- **Single edge:**



$$z_1 z_2 + \beta(z_1 + z_2) + 1 \in \mathcal{A}$$

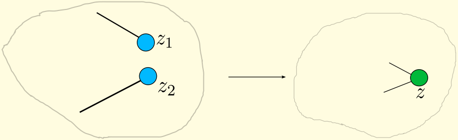
Proof

$$z_1 z_2 + \beta(z_1 + z_2) + 1 = 0 \implies |z_2| = \left| \frac{1 + \beta z_1}{\beta + z_1} \right|$$

For $0 < \beta \leq 1$, this is a Möbius transform mapping the exterior of the unit disk to its interior. Thus, if $|z_1| > 1$ then $|z_2| \leq 1$ $\square$

Asano's proof of the Lee–Yang theorem (contd.)

- **Merging vertices:**



$$Az_1z_2 + Bz_1 + Cz_2 + D \in \mathcal{A} \implies Az + D \in \mathcal{A}$$

Proof

Let $z_3, z_4, \ldots z_n$ be fixed so that $|z_i| > 1$ for $i \geq 3$.

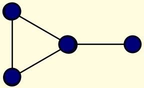
$$\begin{aligned} Az_1z_2 + Bz_1 + Cz_2 + D \in \mathcal{A} &\implies Az_1z_2 + Bz_1 + Cz_2 + D \neq 0, \text{ for } |z_1|, |z_2| > 1 \\ &\implies Az^2 + Bz + Cz + D \neq 0 \text{ for } |z| > 1 \\ &\implies \left|\frac{D}{A}\right| \leq 1 \text{ (Product of zeros)} \end{aligned}$$

Thus, $Az + D = 0 \implies |z| = |D| / |A| \leq 1$ $\square$

Asano's proof: Putting it together

Repeated use of above operations implies that $G \in \mathcal{A}$ for all graphs G

Example:



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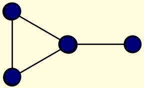
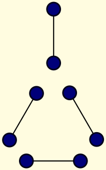
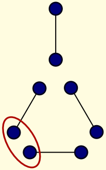




$\in \mathcal{A}$



Single edges and disjoint products

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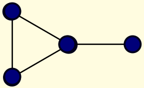
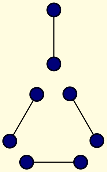
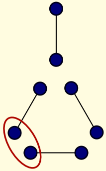


 $\in \mathcal{A}$ $\Longrightarrow$  $\in \mathcal{A}$

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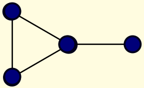

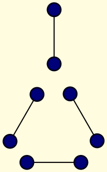

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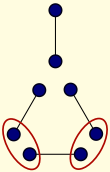

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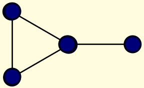
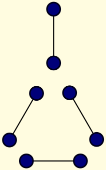
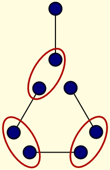


 $\in \mathcal{A}$ $\Longrightarrow$  $\in \mathcal{A}$

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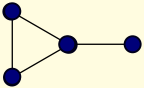

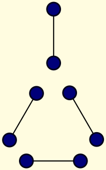

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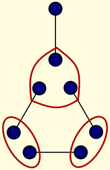

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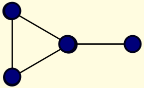

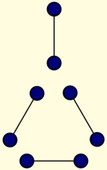

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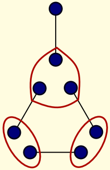

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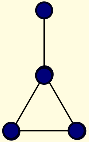

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$\square$

Proof of our theorem: In Asano's footsteps

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$$0 < \beta < 1 \text{ and } |z_i| \geq 1 \text{ for all } i \implies \mathcal{D}Z_G(\beta, z_1, z_2, \ldots, z_n) \neq 0$$

(Recall that $\mathcal{D} = \sum_{v \in V} z_v \frac{\partial}{\partial z_v}$)

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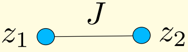
Property $\mathcal{G}$

Z_G has property $\mathcal{G}$ (denoted $Z \in \mathcal{G}$) if

$$0 < \beta < 1 \text{ and } |z_i| \geq 1 \text{ for all } i \implies \mathcal{D}Z_G(\beta, z_1, z_2, \ldots, z_n) \neq 0$$

(Recall that $\mathcal{D} = \sum_{v \in V} z_v \frac{\partial}{\partial z_v}$)

- **Single edge:**



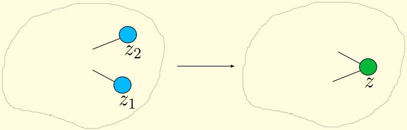
$$z_1 z_2 + \beta(z_1 + z_2) + 1 \in \mathcal{G}$$

  - $\mathcal{D}Z = 2z_1z_2 + \beta(z_1 + z_2) = 0$ implies that $\frac{1}{|z_1|} + \frac{1}{|z_2|} \geq \frac{2}{\beta}$: contradiction

- But things become too complicated when we try to merge graphs

Proof of our theorem: The two inductive steps

- Contracting vertices:



$$Az_1z_2 + Cz_1 + Dz_2 + B \in \mathcal{G} \implies Az^2 + B \in \mathcal{G}$$

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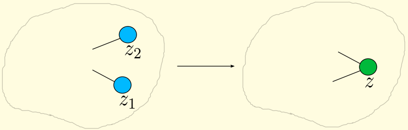
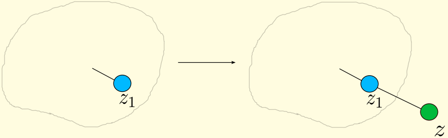


$$Az_1z_2 + Cz_1 + Dz_2 + B \in \mathcal{G} \implies Az^2 + B \in \mathcal{G}$$

- Adding a single new edge and a new vertex:



$$Az_1 + B \in \mathcal{G} \implies Az_1^2(\beta + z) + B(1 + \beta z) \in \mathcal{G}$$

Proof of our theorem: The two inductive steps

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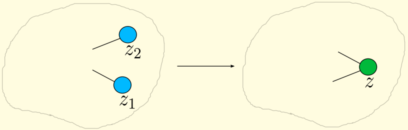

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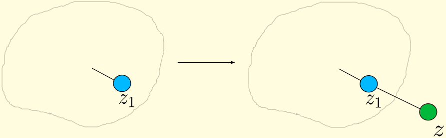

$$Az_1 + B \in \mathcal{G} \implies Az_1^2(\beta + z) + B(1 + \beta z) \in \mathcal{G}$$

- Unlike Asano's proof, each of the above steps requires a somewhat technical argument relying on a correlation inequality due to Newman [1974]
- Another technical problem is the change in degree of the activities

Finishing the proof

- Our proof works via an induction on the number of edges, using the above operations to construct the graph
  - See paper for details

...or `arXiv:1407.5991` [**S., Szegedy**] for a shorter, more analytic proof of a weaker (but sufficient) version

Finishing the proof

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- The main theorem then immediately implies the hardness result

Theorem

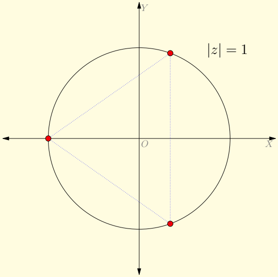
For any $0 < \beta < 1$ and $\lambda \neq 1$ computing the magnetization of the Ising model is #P-hard. This is true even for bounded degree graphs (with degree ≥ 4)

Complex zeros and Ferromagnetic Ising magnetization

Theorem

For a connected graph with $0 < \beta < 1$, (and $Z'(\beta, z) = \frac{\partial}{\partial z} Z(\beta, z)$)

- $Z(\beta, z) = 0 \Longrightarrow |z| = 1$. [Lee and Yang, 1952]



Zeros of Z

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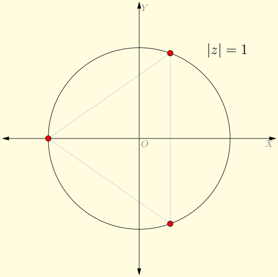
In particular, $\gcd\left(Z(\beta, \lambda), Z'(\beta, \lambda)\right) = 1$



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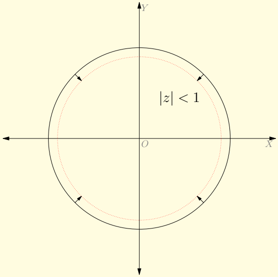

Zeros of Z'

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- $Z'(\beta, z) = 0 \implies |z| < 1$. [Sinclair, S., 2014]

In particular, $\gcd(Z(\beta, \lambda), Z'(\beta, \lambda)) = 1$

Theorem [Sinclair, S., 2014]

- Computing the mean magnetization of the ferromagnetic Ising model is #P-hard
- Similar strategy for matchings using the **Heilmann-Lieb** theorem [1972]

Complex zeros and Ferromagnetic Ising magnetization

Theorem

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In particular, $\gcd(Z(\beta, \lambda), Z'(\beta, \lambda)) = 1$

But...

- This strategy fails for Antiferromagnetic Ising ($\beta > 1$) and independent sets
- Z and $\frac{\partial}{\partial \beta} Z$ can have common factors as polynomials in β
  - ...so also does not apply to mean energy ("avg. cut size")

Such detailed information on zeros of Z is available only for very specific models

Circumventing Lee-Yang theorems

Averages and $\log Z$ ("free energy")

$$\mu(\beta,\lambda) = \lambda \frac{Z'}{Z} = \lambda \frac{\partial}{\partial \lambda} \log Z$$

$$\implies \log Z = \int \frac{1}{\lambda} \mu(\beta,\lambda) \mathrm{d}\lambda + c$$

- Exactly analogous relationships hold for all other models

Possible strategy for reduction

Numerically integrate evaluations of μ to find $\log Z$ and hence Z

- Can only evaluate μ at $\mathrm{poly}(n)$ points
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Attempt symbolic integration using evaluations of μ?

Coping with common factors

Suppose $\gcd(Z(\beta,\lambda), Z'(\beta,\lambda)) = g(\lambda)$, then

$$\frac{1}{\lambda}\mu(\beta,\lambda) = \frac{a(\lambda)}{b(\lambda)}, \text{ where } a(\lambda) = \frac{Z'(\beta,\lambda)}{g(\lambda)},\ b(\lambda) = \frac{Z(\beta,\lambda)}{g(\lambda)}.$$

If $Z(\beta,\lambda) = \prod_{i=1}^{k} p_i(\lambda)^{d_i}$, where $p_i(\lambda)$ are irreducible in $\mathbb{Q}[\lambda]$,

then $$g(\lambda) = \prod_{i=1}^{k} p_i(\lambda)^{d-1}, \qquad b(\lambda) = \prod_{i=1}^{k} p_i(\lambda).$$

Observation

Symbolic integration of $\mu(\beta,\lambda)/\lambda$ amounts to finding $p_i(\lambda)$ and d_i

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Observation

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Lemma

[Well known, or follows from Macon and Dupree, 1962]

$a(\lambda)$ and $b(\lambda)$ can be efficiently computed using evaluations of $\mu(\beta,\lambda) = \lambda\frac{a(\lambda)}{b(\lambda)}$ at poly (n) values $\lambda = \lambda_1, \lambda_2, \ldots, \lambda_{\mathrm{poly}(n)}$

Coping with common factors

$$Z(\beta,\lambda) = \prod_{i=1}^{k} p_i(\lambda)^{d_i}, \text{ where } p_i(\lambda) \text{ are irreducible in } \mathbb{Q}[\lambda],$$

$$\frac{1}{\lambda}\mu(\lambda) = \frac{a(\lambda)}{b(\lambda)}$$

$$a(\lambda) = Z'(\beta,\lambda)/\gcd(Z,Z'), \quad b(\lambda) = \prod_{i=1}^{d} p_i(\lambda)$$

Determining p_i and d_i (sketch)

- Compute $a(\lambda)$ and $b(\lambda)$ from $\operatorname{poly}(n)$ evaluations of μ at $\lambda = \lambda_1, \lambda_2, \ldots, \lambda_{\operatorname{poly}(n)}$
- p_i are uniquely (and efficiently) determined by factoring $b(\lambda)$ in $\mathbb{Q}[\lambda]$
- d_i are uniquely (and efficiently) determined via a partial fraction expansion of $a(\lambda)/b(\lambda)$

Coping with common factors

$$Z(\beta, \lambda) = \prod_{i=1}^{k} p_i(\lambda)^{d_i}, \text{ where } p_i(\lambda) \text{ are irreducible in } \mathbb{Q}[\lambda],$$

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Conclusion

Can symbolically integrate μ to obtain $Z(\beta, \lambda)$ using evaluations of μ at $\mathrm{poly}(n)$ values of λ

Completing the proof

- The above reduction requires evaluations of μ at several values of λ

- To prove hardness for a fixed value of λ, different values of λ are simulated by modifying the input graph
  - …similar to techniques used previously for partition functions
  - but some care is needed while extending these to averages

- The same proof strategy works for the other averages as well
  - …the only model specific details appear in the above "simulation" step

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Precluding common factors

Leads to new results about zeros of partition functions, potentially of independent interest

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