The Complexity of Approximate Counting
(How hard is it to evaluate, or approximately evaluate, generating functions?)

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Warm up: The independence polynomial

Graph $G = (V, E)$

A set $I \subseteq V$ is an independent set of $G$ if it contains no edges of $G$.

- $\emptyset$ is an independent set of $G$.
- Any size-$1$ subset of $V$ is an independent set of $G$.
- $G$ has $6$ larger independent sets.
The independence polynomial

\[ Z_G(\lambda) = \sum_{I \in \mathcal{I}_G} \lambda^{|I|}. \]

- \( \emptyset \) is an independent set of \( G \).
- Any size-1 subset of \( V \) is an independent set of \( G \).
- \( G \) has 6 larger independent sets.

\[ Z_G(\lambda) = 1 + 5\lambda + 5\lambda^2 + \lambda^3 \]
Gibbs measure: measure on independent sets where the probability of $I$ is $\propto \lambda^{|I|}$.

The probability of this independent set is $\lambda^2/Z_G(\lambda)$, where $Z_G(\lambda) = 1 + 5\lambda + 5\lambda^2 + \lambda^3$.

The normalising factor $Z_G(\lambda)$ (the independence polynomial of $G$) is also called the partition function of $G$ in statistical physics.
How hard is it to compute the independence polynomial of $G$, given a fixed “activity” $\lambda$?

$$Z_G(\lambda) = \sum_{I \in \mathcal{I}_G} \lambda^{|I|}$$

Start with $\lambda = 1$...

$Z_G(1)$ is the number of independent sets of $G$. This is known to be $\#P$-complete (Valiant, 1979), even when the graph is restricted to have degree at at most 3 (Greenhill, 2000).

But most people are more interested in approximating $Z_G(\lambda)$. 
Approximating the Partition Function

Fix $\lambda$.

Graph $G$ \[ \rightarrow \] accuracy parameter $\varepsilon$ \[ \rightarrow \] Value $\hat{Z}$

$Z_G(\lambda)(1 - \varepsilon) \leq \hat{Z} \leq Z_G(\lambda)(1 + \varepsilon)$

Running time at most $\text{poly}(n, 1/\varepsilon)$.

FPRAS or FPTAS.

Robust.

When is there an FPTAS/FPRAS?
$G_\Delta$: Graphs with max degree at most $\Delta$.

$$\lambda_c = \frac{(\Delta - 1)^{\Delta-1}}{(\Delta - 2)^\Delta} \sim \frac{e}{\Delta}. $$

- **Weitz 2006**: If $\lambda < \lambda_c$ then $Z_G(\lambda)$ can be efficiently approximated on graphs $G \in G_\Delta$. (There is an FPTAS)

- **Sly 2010; Galanis, Štefankovič, Vigoda 2012; Sly, Sun 2012**: If $\lambda > \lambda_c$ then, for some $\kappa > 1$, $Z_G(\lambda)$ cannot be efficiently approximated within a factor of $\kappa^n$ on $\Delta$-regular graphs (unless NP=RP).

What is the magic value $\lambda_c$?
Let $Z_{G,v}^{\text{in}}(\lambda) = \sum_{I \in \mathcal{I}_G; v \in I} \lambda^{|I|}$. In the Gibbs measure, the probability that $v$ is occupied is

$$p_v(G) = \frac{Z_{G,v}^{\text{in}}(\lambda)}{Z_G(\lambda)}$$

Given a $\Delta$-regular tree $T$ of height $h$ with root $r$,

The occupation ratio of the tree: $p[h] = p_r(T)$.

$p[h]$ converges to a limit as $h \to \infty$ iff $\lambda \leq \lambda_c$ (Kelly 1985)

The complexity of approximating $Z_G(\lambda)$ for $G \in \mathcal{G}_\Delta$ depends on whether $p[h]$ converges.
Another Example: Partition function of the Ising model

• “Spins” \( \{0, 1\} \)

• parameter \( \beta \) (real number, associated with the temperature of the model)

Graph \( G = (V, E) \)

A “configuration” \( \sigma \) assigns a spin to every vertex

Spins interact along the edges: Same spins contribute a factor of \( \beta \) so \( w(\sigma) = \beta \).

The partition function: \( Z_G = \sum_{\sigma \in [q]^V} w(\sigma) \)
Example: Partition function of the Ising model

\[ Z_G = \sum_{\sigma \in [q]^V} w(\sigma) \]

\[ Z_G = 2\beta^3 + 6\beta. \]

Again can consider difficulty of approximately computing \( Z_G \), or sampling from the Gibbs distribution.
Partition Functions, more generally

- Fix “Spins” $[q] = \{0, \ldots, q - 1\}$ e.g., $q = 2$ for the Ising model

- Fix symmetric matrix $A \in \mathbb{R}^{q \times q}$
  e.g., for the Ising model $A = \begin{pmatrix} \beta & 1 \\ 1 & \beta \end{pmatrix}$.

- Given a graph $G = (V, E)$

- configuration $\sigma \in [q]^V$ weight

  $$w(\sigma) = \prod_{\{u,v\} \in E} A_{\sigma(u), \sigma(v)}$$

- Partition function $Z_G$ associates $G$ with the real number

  $$Z_G = \sum_{\sigma \in [q]^V} w(\sigma)$$

Examples: Ising model, Potts model... Independent sets

$$A = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$
Example
Partition functions count graph homomorphisms

Graph $G = (V, E)$

Graph $H$

Homomorphism from $G$ to $H$: A map $\sigma \in V(H)^V$ that maps every edge of $G$ to an edge of $H$
Example
Partition functions count graph homomorphisms

Graph $G = (V, E)$

Configuration
$\sigma \in \{0, 1, 2\}^V$ with weight $w(\sigma) = 1$ is a homomorphism from $G$ to $H$.

Graph $H$

Homomorphism from $G$ to $H$: A map $\sigma \in V(H)^V$ that maps every edge of $G$ to an edge of $H$.

$A$: Adjacency matrix of $H$

$$A = \begin{pmatrix}
0 & 1 & 0 \\
1 & 1 & 1 \\
0 & 1 & 0
\end{pmatrix}$$

$Z_G$: number of homomorphisms from $G$ to $H$.

Why computing partition fns is called “counting”
Complexity of computing partition functions

**Dichotomy Theorem**: For every symmetric matrix $A$, one of the following holds:
(1) the corresponding partition function $Z_G$ can be computed in polynomial time (as a function of $n$, the number of vertices of $G$), or
(2) $Z_G$ is \#P-hard to compute.

We can tell which, given $A$.

- **Dyer and Greenhill 2000**: 0-1-matrices
- **Bulatov and Grohe 2005**: non-negative real algebraic matrices.
- **G, Grohe, Jerrum, Thurley 2010**: real algebraic matrices.
- **Cai, Chen, Lu 2013**: complex algebraic matrices.
the nonnegative real case

\[
A = \begin{bmatrix}
0 & 1 & 2 & 3 & 4 \\
0 & 0 & 3.5 & 0 & 0 & 0 \\
1 & 3.5 & 1 & 1 & 0 & 0 \\
2 & 0 & 1 & 0 & 0 & 0 \\
3 & 0 & 0 & 0 & 0 & 1 \\
4 & 0 & 0 & 0 & 1 & 0 \\
\end{bmatrix}
\]

corresponding weighted graph

Each non-bipartite connected component of this graph corresponds to one block and each bipartite connected component corresponds to two blocks.

Computing \(Z_G\) is in polynomial time if the rank of every block of \(A\) is 1 and \#P-hard otherwise.
Roughly, computing $Z_G$ is tractable if each of the blocks of $A$ can be written as a tensor product of a positive matrix of rank 1 and a *[tractable Hadamard matrix]*.

\[
\begin{pmatrix} 2 & 3 \\ 4 & 6 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 2 & 3 & 2 & 3 \\ 4 & 6 & 4 & 6 \\ -2 & -2 & -2 & -2 \\ -4 & -4 & -4 & -4 \end{pmatrix}
\]
Hadamard matrices

A Hadamard matrix is a square matrix $H$ with entries from \{-1, 1\} such that $H \cdot H^T$ is a diagonal matrix.

\[
\begin{pmatrix}
1 & 1 \\
1 & -1 \\
\end{pmatrix} \cdot \begin{pmatrix}
1 & 1 \\
1 & -1 \\
\end{pmatrix} = \begin{pmatrix}
2 & 0 \\
0 & 2 \\
\end{pmatrix}.
\]

(the order is 1, 2, or a multiple of 4 - open whether there is one for every multiple of 4)

- A symmetric Hadamard matrix $H$ is tractable if it has a “quadratic representation” and hard otherwise.
A “quadratic representation” for order $2^k$ (roughly)

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Row and column labels of $A$ over $\mathbb{F}_2^k$ (here $k = 2$)

Multivariate polynomial $h(X_1, \ldots, X_k, Y_1, \ldots, Y_k)$ over $\mathbb{F}_2$ of degree at most 2 such that

$h(0001) = 1 \Leftrightarrow H_{00,01} = -1$. 
Approximating the partition function

Open even for these special cases

- $A$ is a (symmetric) 0-1 matrix (counting graph homomorphisms)
- $A$ is $2 \times 2$.

\[ A = \begin{pmatrix} \beta & 1 \\ 1 & \gamma \end{pmatrix}. \]

Normalisation to $A_{01} = A_{10} = 1$ is wlg since easy to compute if they are 0

\[ w(\sigma) = \prod_{\{u,v\} \in E} A_{\sigma(u),\sigma(v)}. \]

\[ Z_G = \sum_{\sigma \in \{0,1\}^V} w(\sigma). \]
Above $\beta \gamma = 1$. Reduction to Ising ($\beta = \gamma$) with consistent fields

$$A = \begin{pmatrix} \beta & 1 \\ 1 & \gamma \end{pmatrix}.$$ 

$$w(\sigma) = \prod_{\{u,v\} \in E} A_{\sigma(u), \sigma(v)}.$$ 

$$Z_G = \sum_{\sigma \in \{0,1\}^V} w(\sigma).$$

No FPRAS unless NP=RP

Easiness extends below hyperbola, hardness outside of the square
understanding $\beta \gamma < 1$

1. Inputs in $G_\Delta$ (graphs of degree at most $\Delta$)
2. Generalise the notion of Gibbs distribution to infinite graphs.

$$\Pr(\cdot = \sigma) = \frac{w(\sigma)}{Z_G}.$$  

Infinite $G$: For any finite subgraph $H$, marginal distribution, conditioned on $\sigma(G \setminus H)$, is proportional to $w(\cdot)$. 
• Non-uniqueness: If the infinite $\Delta$-regular tree has multiple Gibbs measures then no FPRAS/FPTAS for $\Delta$-regular graphs $G$ (NP-hard).

• Uniqueness: If $\forall d \leq \Delta$ the infinite $d$-regular tree has a unique Gibbs measure then there is an FPTAS for $Z_G$ for $G \in \mathcal{G}_\Delta$.

Sly 2010; Galanis, Štefankovič, Vigoda 2012 Sly, Sun 2012
Weitz 2006; Sinclair, Srivastava, Thurley 2011; Li, Lu, Yin 2012
Uniqueness or not?

\[ f(x) = \left( \frac{\beta x + 1}{x + \gamma} \right)^{\Delta - 1} \]

\( x^* \) is the unique positive fixed-point — the solution to \( x^* = f(x^*) \).

Uniqueness: \( |f'(x^*)| \leq 1 \)
• $0 \leq \beta < 1$ and $0 < \gamma \leq 1$: non-uniqueness on the infinite $\Delta$-regular tree for all sufficiently large $\Delta$.
• $0 \leq \beta < 1$ and $\gamma > 1$: uniqueness holds on the infinite $\Delta$-regular tree for all sufficiently large $\Delta$.

The uniqueness threshold is not monotonic in $\Delta$. (It is possible to be in uniqueness for $\Delta$, but in non-uniqueness for some $d < \Delta$!) The boundary between hard and easy is the “in uniqueness for all $\Delta$” curve.
What if $\beta$ and $\gamma$ can be negative?

$\mathbf{Z_G} = \sum_{\sigma \in \{0,1\}^V} \prod_{\{u,v\} \in E} A_{\sigma(u),\sigma(v)}.$

$A = \begin{pmatrix} \beta & 1 \\ 1 & \gamma \end{pmatrix}.$

- sky blue points: poly-time exact (already seen)
- : pos quadrant: dotted line “is” uniqueness-for-all-$\Delta$ curve. $\beta \gamma = 1$ exact poly time.
- $\beta = \gamma$ ising: Earlier work with Jerrum, hard for $\beta = \gamma \in (-1, 0)$ (even #P-hard to find sign of $\mathbf{Z_G}$) and equivalent to counting PMs for $\beta = \gamma < -1$ (orange line).
What if $\beta$ and $\gamma$ can be negative?

Yumou Fei, LG, Pinyan Lu, ITCS 2024

$$A = \begin{pmatrix} \beta & 1 \\ 1 & \gamma \end{pmatrix}.$$  

- $\beta + \gamma = -2$, $\beta + \gamma = 2$.
- green: FPTAS on $G_\Delta$ and FPRAS (all degrees)
- blue line $\beta + \gamma = -2$ has FPRAS
- red: #P-hard even to determine sign
- yellow “strip” (width $\to 0$ as move from origin) has FPTAS on $G_\Delta$ so $\beta + \gamma = 2$ not a threshold
- white: open. There are hard points near $(1, 0)$. Conjecture: extend non-uniqueness curve?

$$Z_G = \sum_{\sigma \in \{0, 1\}^V} \prod_{\{u,v\} \in E} A_{\sigma(u), \sigma(v)}.$$
How to approximate $Z_G$

Theorem. Fix $\beta \neq \gamma$ with $|\beta + \gamma| > 2$.

1. There is an FPRAS for $Z_G$
2. For any positive integer $\Delta$ there is an FPTAS for $Z_G$ for $G \in \mathcal{G}_\Delta$. 
A polynomial generalising $Z_G$ (recall the independence polynomial)

$$A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} = \begin{pmatrix} \beta & 1 \\ 1 & \gamma \end{pmatrix}.$$  

For $G = (V, E)$ and $x \in \mathbb{R}^V$, let

$$Z_G(x) = \sum_{\sigma \in \{0,1\}^V} \left( \prod_{\{u,v\} \in E} A_{\sigma(u), \sigma(v)} \prod_{v \in V} x_{\sigma(v)} \right).$$

$x$ is the vector of external fields.

$Z_G = Z_G(1)$.

Setting $x_v = x$ for all $v \in V$, we get a univariate polynomial $Z_G(x)$. 
The method of Barvinok 2016

\[ p(z) = a_0 + a_1 x + \cdots + a_d x^d, \quad a_i \text{'s complex} \]

Suppose \( p(x) \neq 0 \) in disk of radius \( r > 1 \) around origin

Fix a branch of \( f(x) = \ln p(x) \) for \( |x| \leq 1 \)

truncation Taylor expansion of \( f \) around \( x = 0 \):

\[ f_N(x) = \sum_{j=0}^{N} \frac{x^j}{j!} f^{(j)}(0). \]

For \( |x| \leq 1 \), \( f_N(x) \) is additively close to \( f \) (as a fn of \( d, N, r \)) so \( |f(1) - f_N(1)| < \varepsilon \) for \( N = O(\ln(d/\varepsilon)) \)

e.g., fix the value of \( \log(p(0)) \) to lie in \((-\pi, \pi]\)
For

\[ p(x) = Z_G(x) = \sum_{\sigma \in \{0,1\}^V} \left( \prod_{\{u,v\} \in E} A_{\sigma(u),\sigma(v)} \prod_{v \in V} x^{\sigma(v)} \right). \]

can compute the coefficients of \( f_N(x) \) for graphs \( G \in \mathcal{G}_\Delta \) by reduction to counting induced subgraphs from certain fixed graphs \( H \) into \( G \).

So to get a FPTAS we just need to prove that there are no complex zeroes in a disk of radius \( > 1 \) in the complex plane.

**Theorem.** Fix \( \beta \neq \gamma \) with \( |\beta + \gamma| > 2 \).

1. There is an FPRAS for \( Z_G \)
2. For any positive integer \( \Delta \) there is an FPTAS for \( Z_G \) for \( G \in \mathcal{G}_\Delta \).

\[ A = \begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{pmatrix} = \begin{pmatrix} \beta & 1 \\ 1 & \gamma \end{pmatrix}. \]
FPTAS for $G \in \mathcal{G}_\Delta$ when $|\beta + \gamma| > 2$ from zero-freeness in a disk of radius $r > 1$

Contraction method of Asano 1970 (used to give simple proof of Lee-Yang circle theorem and extended by Ruelle 1971) Suffices to show that $\gamma x_u x_v + x_u + x_v + \beta$ has no zeroes when $|x_u| < r$ and $|x_v| < r$

$$Z_G(x) = \sum_{\sigma \in \{0,1\}^V} \left( \prod_{\{u,v\} \in E} A_{\sigma(u), \sigma(v)} \prod_{v \in V} x_v^{\sigma(v)} \right)$$

$$A = \begin{pmatrix} \beta & 1 \\ 1 & \gamma \end{pmatrix}.$$
A typical case: $\beta > \gamma$, $\beta + \gamma > 2$. Showing $\gamma x_u x_v + x_u + x_v + \beta$ has no zeroes when $|x_u| < r$ and $|x_v| < r$

The unique sol’n to $\gamma x g(x) + x + g(x) + \beta = 0$ is $g(x) = -(x + \beta)/(\gamma x + 1)$.

But $g$ maps the open disk of radius $r$ around the origin to the outside of this circle...
FPRAS for all $G$ when $\beta \neq \gamma$, $|\beta + \gamma| \geq 2$

\[
Z_G = \sum_{\sigma \in \{0,1\}^V} \prod_{\{u,v\} \in E} A_{\sigma(u), \sigma(v)}
\]

$A = \begin{pmatrix} \beta & 1 \\ 1 & \gamma \end{pmatrix}$. 