Approximating Partition Functions

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Partition Functions

Given a family $\mathcal{F}$, of subsets of the set $[n]$, we define the *partition function* of $\mathcal{F}$ (a polynomial in n real or complex variables $x_1, \ldots, x_n$) as:
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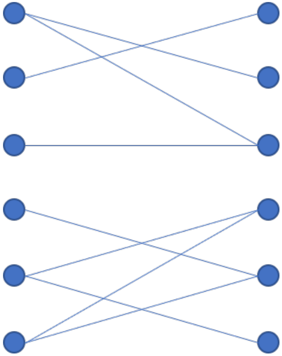
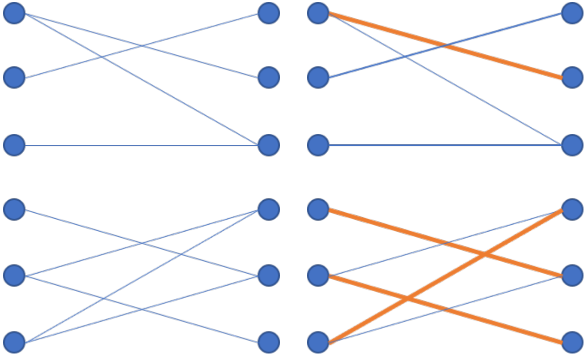
Difficulties:

- Typically, it is unrealistic to try to write $p_{\mathcal{F}}$ as a sum of monomials explicitly as the size of $\mathcal{F}$ is large (or the size is unknown).
- It is believed that in general, efficient and exact computation of $p_{\mathcal{F}}$ is impossible (unless $\mathbf{P} = \#\mathbf{P}$). For this reason, we shift focus to *approximating* partition functions.

Bipartite Matchings



(a) A Bipartite Graph G.



(a) A Bipartite Graph G. (b) A Matching of G.

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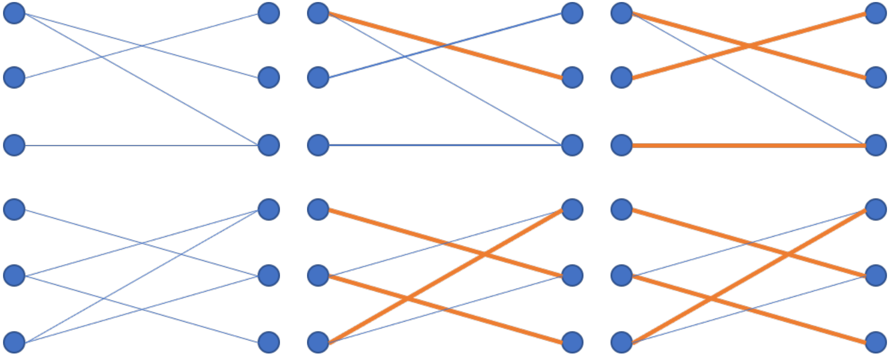

(a) A Bipartite Graph G. (b) A Matching of G. (c) A Perfect Matching.

Example

Permanent

Given a real or complex matrix $A = (a_{ij})$ of dimension $n \times n$, we define the permanent:

$$\mathrm{Per}(A) = \sum_{\sigma \in S_n} \prod_{i=1}^{n} a_{i\sigma(i)}.$$

If A is a real matrix with $a_{ij} \in \{0, 1\}$, then a combinatorial interpretation is that $\mathrm{Per}(A)$ counts the number of perfect matchings in a bipartite graph G with biadjacency matrix A. This is a known $\#\mathbf{P}$ problem in complexity theory.

Computing permanents of complex matrices has applications in physics.

Random Sampling and Markov Chains

In 2004 Jerrum, Sinclair, and Vigoda gave a fully polynomial randomized approximation algorithm for the permanent of non-negative matrices. In particular:

Theorem (Jerrum-Sinclair-Vigoda)

There exists a randomized algorithm, which given an input $n \times n$ nonnegative matrix A together with an accuracy parameter $\epsilon \in (0, 1]$, outputs a number Z such that:

$$\mathbb{P}[\exp(-\epsilon)Z \leq \mathrm{Per}(A) \leq \exp(\epsilon)Z] \geq \frac{3}{4}.$$

More Random Sampling

The proof of Jerrum, Sinclair, and Vigoda's result (and their algorithm) rely on constructing a fully polynomial almost uniform sampler for perfect matchings in a weighted graph corresponding to A.

Specifically, a Markov chain whose states are matchings in the corresponding graph is considered. The mixing time of the chain will determine the number of steps in the simulation needed before a random sample is produced. This result applied to general nonnegative matrices generalized an earlier result by Jerrum and Sinclair which proved the result for 0-1 matrices.

Randomized Counting Continued

Let $\mu : \mathcal{P}([n]) \to \mathbb{R}_{\geq 0}$ be a probability distribution on subsets of the set $[n]$. We assign a multiaffine polynomial with variables $x_1, \ldots, x_n$ to μ,:

$$g_\mu(x) = \sum_{s \subseteq [n]} \mu(S) \prod_{i \in S} x_i.$$

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- We say p is strongly log-concave on K if for any $k \geq 0$ and any $1 \leq i_1, \ldots, 1_k \leq n$,:

$$(\partial_{i_1} \ldots \partial_{i_k} p)$$

is log-concave on K.

Approximate Counting of Bases

Anari, Liu, Gharan, and Vinzant leverage the following into a FPRAS for the number of bases of a matroid.
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- μ is $r-$homogeneous.
- g_μ is strongly log-concave.

The "natural" Markov Chain on the support of an $r-$homogeneous strongly log-concave distribution mixes rapidly. By the equivalence of approximate counting and approximate sampling given in Jerrum, Sincliar and Vigoda we have a way to approximately count the number of bases of a matroid.

The Interpolation Method

Lemma (Barvinok)

Let $g(z)$ *be a complex polynomial of degree* d *and suppose* $g(z) \neq 0$ *for all* $|z| \leq \beta$ *where* $\beta > 1$. *Choose a branch of* $f(z) = \ln g(z)$ *for* $|z| \leq 1$, *and consider the Taylor polynomial:*

$$p_n(z) = f(0) + \sum_{k=1}^{n} \left(\frac{\mathrm{d}^k}{\mathrm{d}z^k} f(z) \Big|_{z=0} \right) \frac{z^k}{k!}.$$

Then,

$$|f(z) - p_n(z)| \leq \frac{d}{(n+1)\beta^n(\beta - 1)} \text{ for all } |z| \leq 1.$$

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The "interpolation method" is then applying this lemma to a sufficiently modified partition function. For the permanent, we use the function $g(z) = \mathrm{Per}(J + z(A - J))$ where J is the all 1s matrix.

Permanent Approximation

Theorem (Barvinok)

Fix $0 < \delta < 0.5$*. Then, there is* $\gamma = \gamma(\delta) > 0$ *such that for any* $\epsilon > 0$*, and positive integer* n*, there is a polynomial* $p = p_{n,\delta,\epsilon}$ *in the entries of an* $n \times n$ *complex matrix* A *satisfying*

$$\deg p \leq \gamma(\ln n - \ln \epsilon)$$

and

$$|\ln \mathrm{Per}(A) - p(A)| \leq \epsilon$$

provided

$$|1 - a_{ij}| \leq \delta.$$

The proof relies on the interpolation method which "smoothes out" the computation allowing approximation.

Phase Transitions

The notions of partition functions above translate naturally into the physics realm by setting $x_i = e^{\beta_i / t}$. This begs the question of how to consider phase transitions for general partition functions.

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- Correlation Decay: in 2006, Weitz showed that there is decay of correlations for the independence polynomial (another popular partition function). Informally, at a high enough temperature long range correlations become absent.
- Discontinuities: a loss of smoothness in certain physical quantities may occur as we approach a critical temperature t_c – in particular, $\ln p_{\mathcal{F}}$ may encode a quantity of interest and consequently zeros of $p_{\mathcal{F}}$ lead to a singularity in measurement of our quantity.

Barvinok makes note of a slightly more general notion of the second kind of phase transition. Instead of considering only behavior as we approach real temperatures (which makes sense physically) the real difficulty in approximation arises due to an inability to "reach" 1 in a zero free domain of our interpolating function.

Another Partition Function

For a graph $G = (V, E)$, and $\beta \in \mathbb{C}$ fixed, the *partition function of the Ising model* $Z_G(\lambda, \beta)$ is defined as:

$$Z_G(\lambda, \beta) = \sum_{U \subset V} \lambda^{|U|} \beta^{|\delta(U)|}$$

where $\delta(U)$ is the set of edges with one endpoint in U and one endpoint outside of U.

We say that $\beta < 1$ corresponds to the ferromagnetic case, while $\beta > 1$ is referred to as the anti-ferromagnetic case.

Theorem (Peters & Regts)

Let $d \geq 2$ be an integer, and let $\beta \in \left(\frac{d-1}{d+1}, 1\right)$. Then there is an arc of the unit circle such that for all graphs G with maximum degree $d + 1$, $Z_G(\lambda, \beta) \neq 0$ when λ lies in this arc.

More from Peters and Regts

In 2019, Peters and Regts also verified a long standing conjecture of Sokal. Namely, for the partition function of the multivariate independence polynomial:

$$Z_G(\lambda) = \sum_{\substack{I \subset V \\ \text{independent}}} \prod_{v \in I} \lambda_v$$

is zero free in a complex neighborhood of the real interval $\left[0, (d-1)^{d-1}/(d-2)^d\right]$ on all graphs G of maximum degree d. By the interpolation method, this means we can approximate this polynomial in a sufficiently constructed neighborhood of the specified interval.

Dense Subsets of a Graph

Let $G = (V, E)$ be an undirected simple graph. For a non-empty subset $S \subseteq V$ of vertices, define the density $\sigma(S)$ as

$$\sigma(S) = \frac{\left|\binom{S}{2} \cap E\right|}{\binom{|S|}{2}}$$

Partition Function of Cliques

We define the partition function of cliques as:

$$\mathrm{den}_m(G; \gamma) = \binom{n}{m}^{-1} \sum_{S \subseteq V, |S| = m} \exp\{\gamma m \sigma(S)\}.$$

The exponential tilting of $\sigma(S)$ puts greater emphasis on sets of higher density. As γ grows this partition function approximates the density of the densest subset.

Definition

One Last Partition Function

Let $Z = (z_{ij})_{i,j=1}^{n}$ be an $n \times n$ real or complex matrix. Then for an integer $1 < m \leq n$, we define the polynomial

$$P_m(Z) = \sum_{\substack{S \subset [n] \\ |S| = m}} \exp\left\{ \prod_{\substack{i,j \subset S \\ i \neq j}} z_{ij} \right\}.$$

Note that $P_m(Z_0) = \exp\{-\gamma m/2\} \binom{n}{m} \mathrm{den}_m(G;\gamma)$ if $Z_0 = (z_{ij})$ satisfies:

$$z_{ij} = \begin{cases} \gamma/(m-1) & \text{if } \{i,j\} \in E \\ -\gamma/(m-1) & \text{if } \{i,j\} \notin E. \end{cases}$$

We approximate $P_m(Z_0)$ using the interpolation method by showing $P_m(Z) \neq 0$ in a suitable region.

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Thank You

Thank you for your attention!