Counting Without Sampling. New Algorithms for Enumeration Problems Using Statistical Physics

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Two Counting Problems

Definition 1 (Independent Set) *Suppose* $G := (V, E)$ *be a finite graph. We will say a subset* $I \subseteq V$ *is an* independent set *of* G*, if for any two vertices* $u, v \in I$ *there is no edge between* u *and* v*.*

We will denote by $\mathcal{I}_G$*, the set of all independent sets of* G*.*

Problem 1 : Given a finite graph G find out the cardinality of the set $\mathcal{I}_G$. In other words, count the *number of independent sets* of G.

Definition 2 (Proper q-Coloring) *Fix* $q \geq 2$ *an integer, and suppose* $G := (V, E)$ *be a finite graph. A map* $C : V \to [q]$ *is called a* proper q-coloring *of* G *if for each* $k \in [q]$ *the subset of vertices with color* k*, namely* $C^{-1}(\{k\})$*, is an an independent set of* G *(in other words, no two vertices of same color share an edge).*

We will denote by $\mathcal{C}_G(q)$*, the set of all proper* q*-colorings of* G*.*

Problem 2 : Given a graph G, and $q \geq 2$ an integer, find out the cardinality of the set $\mathcal{C}_G(q)$. In other words, count the *number of proper* q*-colorings* of G.

Exact/Approximate Counting

Q: Can we do exact counting ?

A:
- Perhaps not !
- The sets are typically exponentially large.
- No polynomial time algorithm, [Valiant 1979].

Q: So what do we do ?

A: We can try “approximate” counting.

Q:
- How do we approximate ?
- What kind of approximation ?

A:
- Typical approach : *Markov chain Monte Carlo* techniques.
- One need to prove *rapid mixing* for the chain.

Some Known Results

Some notable breakthroughs and success stories for the Markov chain based approximation schemes :

- Computing the permanent :
  - Jerrum and Sinclair (1989, 1997).
  - Jerrum, Sinclair and Vigoda (2004).
- Computing the volume of a convex body :
  - Dyer, Frieze and Kannan (1991).
  - Kannan, Lovasz and Simonovits (1997).
  - Lovasz and Vempala (2003).
- Counting independent set :
  - Luby and Vigoda (1997).

Remark : Such MCMC techniques typically provide a randomized ε-approximation to the counting problem, which runs in time which is a polynomial in the size of the problem (e.g. the size of V), and also in the error ε.

What Do We Propose to Do ?

- We will give *deterministic* approximation schemes, which will use no sampling.

- But we will provide ε-approximation to $\log |\mathcal{I}_G|$ and $\log |\mathcal{C}_G(q)|$. (Unfortunately, this is *obviously* less efficient !)

- Moreover, we will need restrictions on our graphs ! For example, we will need low degree graphs, and a "*large girth*" assumption (will be more specific later).

Get lost !!!! : Then we *obviously* are not doing a good job ! In fact, we are doing worse than what is already known !

Then why am I here ?

- Well well ... Alden Biesen is a nice place, and AofA is a great conference :-)

- But there are few other reasons as well ... :-)

Motivation and Achievements

- Our motivation comes from *statistical physics*.

- Computation of $\log|\mathcal{I}_G|$ or $\log|\mathcal{C}_G(q)|$ are interesting, because they correspond to the *free energy* for certain models in statistical physics (details will be given).

- We can achieve (nice) explicit results for regular graphs ! To give some example :

  - ▶ We can show that for every 4-regular graph of n vertices and large girth, the number of independent sets is approximately $(1.494\ldots)^n$.

  - ▶ We can also show that if $q \geq r+1$ then for every r-regular graph with large girth, the number of proper q-coloring is approximately

$$\left[q\left(1-\frac{1}{q}\right)^{\frac{r}{2}}\right]^n .$$

- We can drop the "large girth" assumption and work with random regular graphs to get concentration results.

Two Statistical Physics Models

Hard-Core Model : Given a finite graph G and a real number $\lambda > 0$, consider a (discrete) probability distribution on $\mathcal{I}_G$ given by

$$\mathbb{P}(I) \propto \lambda^{|I|}, \quad I \in \mathcal{I}_G .$$

Thus

$$\mathbb{P}(I) = \frac{\lambda^{|I|}}{Z(\lambda, G)}, \quad I \in \mathcal{I}_G ,$$

where

$$Z(\lambda, G) := \sum_{I \in \mathcal{I}_G} \lambda^{|I|} .$$

Remarks :

- $\mathbb{P}$ is called the *Gibbs distribution* on $\mathcal{I}_G$.
- $Z(\lambda, G)$ is called the *partition function*.
- λ is called the *activity parameter*.
- Observe $Z(\lambda, G) = |\mathcal{I}_G|$ when $\lambda = 1$, then we are back to the original counting problem.

Counting Proper q-Colorings : Given $q \geq 2$ an integer, and a finite graph G, let $\lambda_k > 0$, for $1 \leq k \leq q$. Consider a (discrete) probability distribution on $\mathcal{C}_G(q)$ given by

$$\mathbb{P}(C) \propto \prod_{1 \leq k \leq q} \lambda_k^{|C^{-1}(\{k\})|}, \quad C \in \mathcal{C}_G(q) .$$

Thus

$$\mathbb{P}(C) = \frac{\prod_{1 \leq k \leq q} \lambda_k^{|C^{-1}(\{k\})|}}{Z(\lambda, q, G)}, \quad C \in \mathcal{C}_G(q) ,$$

where

$$Z(\lambda, q, G) := \sum_{C \in \mathcal{C}_G(q)} \prod_{1 \leq k \leq q} \lambda_k^{|C^{-1}(\{k\})|} .$$

Remarks :

- $\mathbb{P}$ is called the *Gibbs distribution* on $\mathcal{C}_G(q)$.
- $Z(\lambda, q, G)$ is called the *partition function*.
- λ_k's are called the *activity parameters*.
- Observe $Z(\lambda, q, G) = |\mathcal{C}_G(q)|$ when $\lambda_k = 1$, for all $1 \leq k \leq q$, then we are back to the original counting problem.
- Let $Z(q, G) := |\mathcal{C}_G(q)|$.

Some Families of Graphs

- **[Large girth] :** An infinite family of graphs $\mathcal{G}_{\text{lg}}$ is defined to have *large girth*, if there exists an increasing function $f : \mathbb{N} \to \mathbb{N}$ with $\lim_{s\to\infty} f(s) = \infty$, such that for every $G \in \mathcal{G}_{\text{lg}}$ with n vertices, we have

$$\text{girth}\,(G) \geq f(n)\,.$$

- **[Low degree] :** Let $\mathcal{G}\,(n, r, g)$ be the family of graphs on n vertices, such that the maximum degree of any vertex is bounded by r and each graph has girth at least g.

- **[Regular] :** Let $\mathcal{G}_{\mathtt{reg}}\,(n, r, g)$ be the family of r-regular graphs on n vertices, such that each graph has girth at least g.

Main Results for the Two Counting Problems

Theorem 1 (Independent Sets) *For every family of graphs $\mathcal{G}$ with maximum degree at most 4 and large girth, there is an algorithm $\mathcal{A}$, such that for any $\varepsilon > 0$ and $G \in \mathcal{G}_{lg}$, $\mathcal{A}$ produces a quantity $\hat{Z}$ in time polynomial in $n := |V|$, such that*

$$(1-\varepsilon)\frac{\log|\mathcal{I}_G|}{n} \leq \hat{Z} \leq (1+\varepsilon)\frac{\log|\mathcal{I}_G|}{n}.$$

Theorem 2 (Colorings) *Fix $q \geq r+1$ be two integers then*

$$\lim_{g\to\infty} \sup_{G\in\mathcal{G}(n,r,g)} \left| \frac{\log|\mathcal{C}_G(q)|}{n} - \frac{1}{n}\sum_{1\leq k\leq n} \log\left[q\left(1-\frac{1}{q}\right)^{r_{G_{k-1}}(v_k)}\right]\right| = 0.$$

where $V := \{v_1, v_2, \ldots, v_n\}$ and $G_k := G \setminus \{v_1, v_2, \ldots, v_k\}$, and by $r_G(v)$ we mean the degree of vertex v in graph G.

In particular, we can get an algorithm result for counting the number of proper q-colorings, which is similar to the previous theorem.

Main Results for Regular Graphs

Theorem 3 (Independent Sets) *Suppose* $\lambda < \lambda_c(r)$ *where* $\lambda_c(r) = (r-1)^{r-1}/(r-2)^r$. *Then the partition function* $Z(\lambda, G)$ *corresponding to independent sets satisfies*

$$\lim_{g\to\infty} \sup_{G\in\mathcal{G}_{\mathtt{reg}}(n,r,g)} \left| \frac{\log Z(\lambda, G)}{n} - \log\left(x^{-\frac{r}{2}}(2-x)^{-\frac{r-2}{2}}\right)\right| = 0\,,$$

where x *is the unique positive solution of*

$$x = 1/(1+\lambda x^{r-1})\,.$$

In particular, if $r = 2, 3, 4, 5$ *and* $\lambda = 1$, *then the corresponding limits for* $\frac{\log|\mathcal{I}_G|}{n}$ *are respectively,* $\log 1.618\ldots$, $\log 1.545\ldots$, $\log 1.494\ldots$ *and* $\log 1.453\ldots$.

Theorem 4 (Colorings) *For every* $q \geq r+1$, *the number of* q*-colorings of graphs* $G \in \mathcal{G}_{\mathtt{reg}}(n, r, g)$ *satisfies*

$$\lim_{g\to\infty} \sup_{G\in\mathcal{G}_{\mathtt{reg}}(n,r,g)} \left| \frac{\log Z(q, G)}{n} - \log\left[q\left(1-\frac{1}{q}\right)^{\frac{r}{2}}\right]\right| = 0\,.$$

Results for Random Regular Graphs

Theorem 5 (Independent Sets) *For every $r \geq 2$ and every $\lambda < (r-1)^{r-1}/(r-2)^r$, the (random) partition function $Z(\lambda, G_r(n))$ of a random r-regular graph $G_r(n)$ corresponding to the Gibbs distribution on independent sets satisfies*

$$\frac{\log Z(\lambda, G_r(n))}{n} \to \log\left[x^{-\frac{r}{2}}(2-x)^{-\frac{r-2}{2}}\right],$$

with high probability (w.h.p.), as $n \to \infty$, where x is the unique positive solution of $x = 1/(1+\lambda x^{r-1})$.

Theorem 6 (Colorings) *For every $r \geq 2$ and $q \geq r+1$, the (random) partition function $Z(q, G_r(n))$ of a random r-regular graph $G_r(n)$ corresponding to the uniform distribution on proper q-colorings satisfies*

$$\frac{\log Z(q, G_r(n))}{n} \to \log\left[q\left(1-\frac{1}{q}\right)^{\frac{r}{2}}\right].$$

w.h.p. as $n \to \infty$.

Remark : Theorem 6 was proved earlier by Achlioptas and Moore (2004) using second moment method.

Our Main Approach (Four Steps)
(Illustrated only for the Independent Sets)

STEP - 1 (The Cavity Equation) :

- In this step we relate the computation of the partition function to the computation of the marginal probabilities.
- This is done by creating a *cavity* in the original graph.

Proposition 7 *Let* $V := \{v_1, v_2, \ldots, v_n\}$*, and for* $1 \leq k \leq (n-1)$ *we define* $G_k := G \setminus \{v_1, v_2, \ldots, v_k\}$ *as the graph obtained from* G *after creating* k cavities. *Put* $G_0 = G$. *Then the following relation holds*

$$\frac{Z(\lambda, G_1)}{Z(\lambda, G_0)} = \mathbb{P}_{G_0}(v_1 \notin \mathbf{I}) \ ,$$

where $\mathbf{I}$ *is a random independent set distributed according the Gibbs measure* $\mathbb{P}$. *As a result we get*

$$Z(\lambda, G) = \prod_{k=1}^{n} \left(\mathbb{P}_{G_{k-1}}(v_k \notin \mathbf{I})\right)^{-1} \ .$$

Remark : This proposition is well known in Physics literature and also in the Markov chain based approximation algorithms for counting.

STEP - 2 (Computation on Trees) :

- Note our *large girth* assumption makes our graphs "*locally*" tree like !

- So in this step we only make computation for the marginal probabilities when the graph is a finite tree.

- This can be done easily by a recursive method.

Proposition 8 *Suppose T be a finite rooted tree with root v_0, and let $\{v_1, v_2, \ldots, v_k\}$ be $k \geq 0$ children of v_0. For each $1 \leq j \leq k$, let $T(v_j)$ denote the tree rooted at v_j consists of only the descendants of v_j (if any). Then the following recursion holds*

$$\mathbb{P}_T\left(v_0 \notin \mathbf{I}\right) = \frac{1}{1 + \lambda \prod_{1 \leq j \leq k} \mathbb{P}_{T(v_j)}\left(v_j \notin \mathbf{I}\right)}.$$

STEP - 3 (Strong Correlation Decay) :

- This is the crucial step !

- In this step we prove that under certain assumptions, e.g., $\lambda < (r-1)^{r-1}/(r-2)^r$ (for the r-regular case), or $r \leq 4$ (for the counting problem algorithm), etc, the *influence* of the boundary at the root decreases exponentially fast.

- A statistical physics consequence of this is the Gibbs measure on the limiting infinite graph is unique (Dobrushin's uniqueness criterion).

- For r-regular trees this was shown by Kelly (1985).

- We further extends this result to the class of finite trees with maximum degree at most 4, which is the most crucial result for our algorithm to succeed.

Remark : The correlation decay for the counting of proper q-colorings was proved by Jonasson (2002) for finite depth r-regular tree, but his result extends to any finite tree with bounded degree, which we use for the coloring case.

STEP - 4 (From Tree to the Original Graph) :

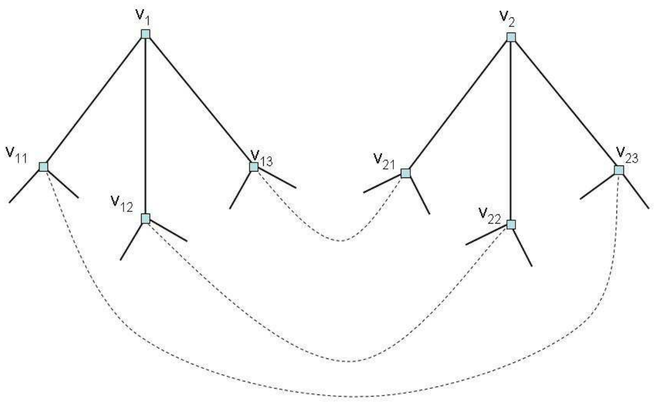
- In this step we show that the error we make in the *approximation* by taking a *local tree* around a vertex is *small*.

  Note : The *local tree* comes from the *large girth* assumption.

- This is again done by using the strong correlation decay property and the (spacial) Markovian nature of the Gibbs distribution.

Special Cavity Trick for Regular Graphs

- For regular graphs creating a *cavity* destroy the regularity !
- Instead we do the following which we call the *rewiring*. Similar idea has been used in Physics literature [Mezard and Parisi, 2005].



Lemma 9 *Given an r-regular graph G, and $\lambda > 0$, the graph G^o obtained from G by rewiring on nodes $v_1, v_2 \in G$, the following relation holds*

$$\frac{Z(\lambda, G^o)}{Z(\lambda, G)} = \mathbb{P}_G(v_1, v_2 \notin \mathbf{I})\mathbb{P}_{G\setminus\{v_1,v_2\}}\left(\wedge_{1\le j\le r}\left(v_{1j} \notin \mathbf{I} \vee v_{2j} \notin \mathbf{I}\right)\right)$$

where $v_{ij}, j = 1, \ldots, r$ is the set of neighbors of $v_i, i = 1, 2$ in G.

Few Final Remarks

- Recent work of Weitz (2006) provides a *fully polynomial approximation scheme* for any finite graph with low degree for the problem of counting the independent sets. The novel approach was to associate with any graph G, a tree which is obtained from all the *self avoiding walks* on G. And to prove the (strong) correlation decay for any general tree.

- Recent work of Gamarnik and Katz (2006) (personal communication) extends the work of Weitz (2006) in case of counting colorings, and matchings for general graphs.

- It seems to me that each of this is a "success story" for making a rigorous argument for a very powerful method of statistical physics, called the **cavity method** ! But the full math picture is yet to be discovered.