Partition functions: complex zeros and algorithms

Part 1

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Summer school on algorithms, dynamics, and information flow in networks

Introduction

Is there an efficient algorithm to count

1) spanning trees in a graph?
2) independent sets of a graph?
3) proper q-colourings of a graph?

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- Part I, II - Efficient approximation algorithms
- Part III, IV - Hardness

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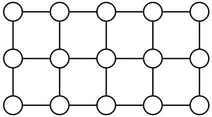
Connection to statistical physics

Example: Hard-core model

Graph $G = (V, E)$

$S \subseteq V$ is an independent set if $\forall u, v \in S$, $uv \notin E$.



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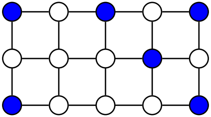

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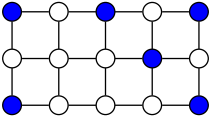

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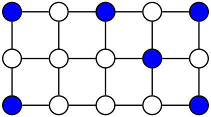

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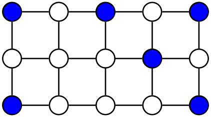

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- For $S \subseteq V$ independent, we have $\mathbb{P}(S) \propto \lambda^{|S|}$
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$$Z_G(\lambda) = \sum_{S \subseteq V \text{ independent}} \lambda^{|S|}$$

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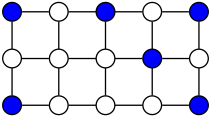

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is the partition function of the hard-core model (a.k.a the independence polynomial)

$G = (V, E)$ a graph

Independence polynomial

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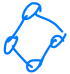
$G = (V, E)$ a graph  $1 + 4\lambda + 2\lambda$

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Examples

$$Z_{G_1 \cup G_2}(\lambda) = Z_{G_1}(\lambda)\, Z_{G_2}(\lambda)$$

$$\|$$

$$\sum_{\substack{S \text{ ind} \\ \text{in } G_1 \cup G_2}} \lambda^{|S|} = \sum_{\substack{S_1 \text{ ind in } G_1 \\ S_2 \text{ ind in } G_2}} \lambda^{|S_1|} \cdot \lambda^{|S_2|}$$

$$= \sum_{S_1 \text{ ind in } G_1} \lambda^{|S_1|} \sum_{\substack{S_2 \text{ ind} \\ \text{in } G_2}} \lambda^{|S_2|}$$

$$\underbrace{\circ \; \cdots \; \circ}_{k} \qquad (1+\lambda)^k$$

Graph polynomials / partition functions

We will look at

- Independence polynomial (hard-core model)
- Matching polynomial (monomer-dimer model)
- Chromatic polynomial
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Perspectives

- Enumeration - generating functions for counting objects in graphs
- Statistical physics - partition functions

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Questions

- Where are the roots of the graph polynomials?
- What is the computational complexity of evaluating the graph polynomials (approximately)?

Fully Polynomial Time Approximation Scheme (FPTAS)

Suppose f is a graph parameter,
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An FPRAS is a randomised algorithm that, given input G and $0 < \varepsilon < 1$,

- estimates $f(G)$ within a multiplicative factor $1 \pm \varepsilon$
- in time polynomial in $n = |V|$ and ε^{-1}
- with probability $\geq \frac{3}{4}$.

Independence Polynomial

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$\Delta(G) \leq \Delta$

- $0 \leq \lambda < \lambda_c \implies \exists$ FPTAS for $Z_G(\lambda)$ (Weitz)
- $\lambda > \lambda_c \implies \nexists$ FPTAS for $Z_G(\lambda)$ unless P = NP

(Sly and Sun)

(Galanis, Štefankovič, Vigoda)

where

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

Three methods for approximate counting

Markov chain Monte Carlo (Broder, Jerrum, Sinclair)

- randomised algorithms
- generally faster algorithms

Correlation decay (Weitz)

- deterministic algorithm

Taylor polynomial interpolation (Barvinok)

- deterministic
- complex evaluations

Taylor Polynomial Interpolation Method (Barvinok)

- Let $p = p_G$ be a (graph) polynomial of degree $\leq n$.
- Assume $p(z) \neq 0$ for all $|z| \leq R$ for some $R > 0$. ($z \in \mathbb{C}$)
- Let $f(z) = \ln p(z)$ for $|z| < R$ and let

$$T_m(z) = \sum_{k=0}^{m} f^{(k)}(0) \frac{z^k}{k!}.$$

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$$\begin{aligned} \text{i.e.} \quad & T_m(z) = f(z) + t \qquad\qquad \text{with } |t| \leq \varepsilon \\ \implies \quad & e^{T_m(z)} = e^t e^{f(z)} \approx (1+t)p(z). \end{aligned}$$

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Recipe for FPTAS

- Identify zero-free region of p containing z (inc. non-disks).
- Efficiently compute $f^{(k)}(0)$ for $k = 0, \ldots, O(\ln n/\varepsilon)$.

How to compute derivatives

Let p be a graph polynomial and G an n-vertex graph. Suppose

$$p_G(z) = a_0 + a_1 z + \cdots + a_n z^n.$$

Wish to compute $f^{(k)}(0)$ for $k = 1, \ldots, m = \ln(n/\varepsilon)$ where

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upper triangular linear system in unknowns $f^{(0)}(0), f^{(1)}(0), \ldots, f^{(m)}(0)$. Can be solved in terms of $a_0, \ldots, a_m$

$$p'(z) = p(z) f'(z)$$

Repeatedly differentiate and evaluate at zero

$$k! a_k = \sum_{j=0}^{k-1} \binom{k-1}{j} a_j f^{(m-j)}(0) \qquad k = 1, \ldots, m$$

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- Check all sets of size $\leq m$: takes $n^{O(m)} = n^{O(\ln n - \ln \varepsilon)}$ time.
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Lemma implies the following

Theorem (Patel, Regts)

Suppose $Z_G(z) \neq 0$ for all $|z| \leq C$ and $\Delta(G) \leq \Delta$.

Then $\exists$ FPTAS to compute $Z_G(z)$ for $|z| < C$ and $\Delta(G) \leq \Delta$.

This holds for more general regions than just the disk.

Lemma (Patel, Regts)

If $\Delta(G) \leq \Delta$, we can compute

$$a_k = a_k(G) = \mathrm{ind}(\circ^k, G)$$

k isolated vertices

in time $c^k n^{O(1)}$, where $c = c(\Delta)$.

Write $\mathrm{ind}(H, G) := \#$ induced copies of H in G

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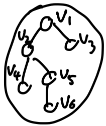
Three observations

Can compute $\mathrm{ind}(H, G)$ in time $c^k n^{O(1)}$ where

$|H| = k$, H connected and $|G| = n$, $\Delta(G) \leq \Delta$.

H



T spanning tree in H

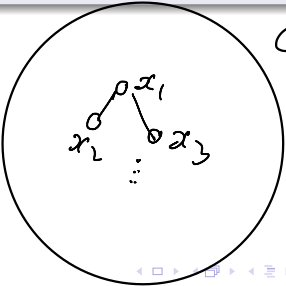
n choices for x_1

$\leq \Delta$ choices for x_2

$\leq \Delta$ choices for x_3

$\vdots$

$\leq \Delta$ choices for x_k



G

$\leq n\Delta^{k-1}$

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$$\mathrm{ind}(H_1, \cdot)\mathrm{ind}(H_2, \cdot) = \sum_{|H| \leq |H_1| + |H_2|} c_H \, \mathrm{ind}(H, \cdot)$$

$$\| \{ S_1 \subseteq V : G[S_1] = H_1 \} | \, | \{ (S_2 \subseteq V : G[S_2] = H_2 \} |$$

$$= | \{ (S_1, S_2) : G[S_1] = H_1, G[S_2] = H_2 \} |$$

$$\|$$

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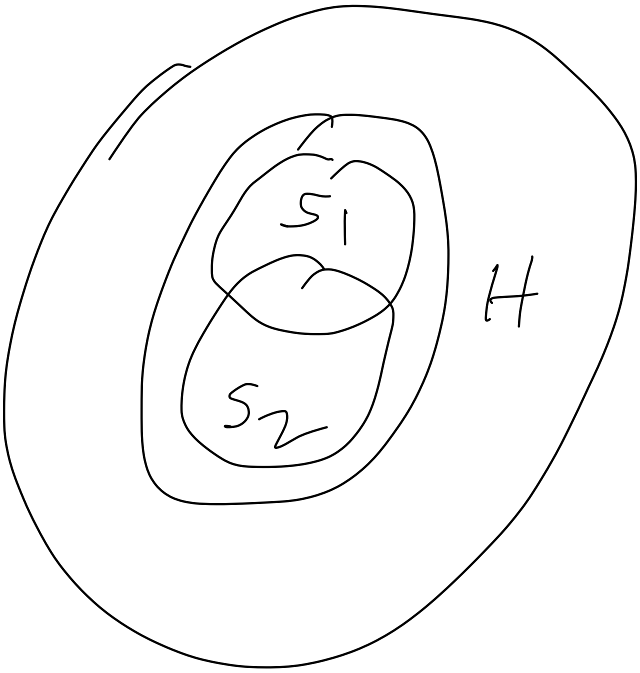

$$\left\{(S_1, S_2) : S_1, S_2 \subseteq V(H),\ H[S_1] = H_1,\ H[S_2] = H_2,\ S_1 \cup S_2 = V(H)\right\}$$

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$$\mathrm{ind}(H_1, \cdot)\mathrm{ind}(H_2, \cdot) = \sum_{|H| \leq |H_1| + |H_2|} c_H\, \mathrm{ind}(H, \cdot)$$

Suppose $\tau(G) = \sum \mu_H\, \mathrm{ind}(H, G)$

and $\tau(G_1 \cup G_2) = \tau(G_1) + \tau(G_2) \quad \forall G_1, G_2$

$\implies \mu_H = 0$ for all disconnected H. (Csikvári and Frenkel)

If H is connected then

$$f(G) = \text{ind}(H,G) \quad \text{is additive}$$

$\tau(G) - \lambda f(G)$ is additive for any λ.

$$\tau'(G) = \sum_{H \text{ disconnected}} \mu_H \, \text{ind}(H,G) \quad \text{additive}$$

Look at smallest disconnected H^* for which $\mu_{H^*} \neq 0$

$H^* = H_1 \cup H_2$

$$\tau'(H^*) = \tau'(H_1) + \tau'(H_2)$$
$$= \sum_{\text{dis } H} \mu_H \, \text{ind}(H, H_1)$$
$$+ \sum_{\text{dis } H} \mu_H \, \text{ind}(H, H_2) = 0$$

Since H bigger than H_1 and H_2 by minimality of H^*

$$\tau'(H^*) = \sum_{H \text{ discon}} \mu_H \, \text{ind}(H, H^*) = \mu_{H^*} \quad \text{by minimality of } H^*$$

$\Rightarrow \mu_{H^*} = 0$, a contradiction

i.e. there is no smallest disconnected H^* for which $\mu_{H^*} \neq 0$, i.e. $\mu_H = 0$ for all disconnected H.

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Let $p_i = \eta_1^{-i} + \cdots + \eta_d^{-i}$.

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Newton identities

$$a_0 p_t + a_1 p_{t-1} + \cdots + a_{t-1} p_1 = -t a_t \quad \forall t \geq 1$$

using second clos

$$\implies p_i(G) = \sum_{|H| \leq k} c_H \cdot \mathrm{ind}(H, G)$$

$p_1 = -a_1$

$p_2 + a_1 p_1 = -a_2$

$p_3 + a_1 p_2 + a_2 p_1 = -a_3$

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$$a_0 p_t + a_1 p_{t-1} + \cdots + a_{t-1} p_1 = -t a_t \quad \forall t \geq 1$$

$$p_i(G_1 \cup G_2) = p_i(G_1) + p_i(G_2)$$

$$\implies p_i(G) = \sum_{\substack{|H| \leq k \\ H \text{ connected}}} c_H \cdot \mathrm{ind}(H, G)$$

using third observation

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If $\Delta(G) \leq \Delta$, we can compute $a_k = a_k(G) = \mathrm{ind}(\circ^k, G)$ in time $c^k n^{O(1)}$, where $c = c(\Delta)$.

Proof.

Let $\eta_1, \ldots, \eta_d$ be the roots of $Z_G(z) = \sum a_r z^r$
Let $p_i = \eta_1^{-i} + \cdots + \eta_d^{-i}$.

$$a_0 p_t + a_1 p_{t-1} + \cdots + a_{t-1} p_1 = -t a_t \quad \forall t \geq 1$$

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- all c_H for which $\mathrm{ind}(H, G)$ non-zero
- $p_1, \ldots, p_k$ hence $a_1, \ldots, a_k$

□

Theorem (Patel, Regts)

Suppose $Z_G(z) \neq 0$ *for all* $|z| \leq C$ *and* $\Delta(G) \leq \Delta$.

Then $\exists$ *FPTAS to compute* $Z_G(z)$ *for* $|z| < C$ *and* $\Delta(G) \leq \Delta$.

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$\lambda^*(\Delta) := \frac{(\Delta-1)^{\Delta-1}}{\Delta^\Delta}$ $\quad \lambda_c(\Delta) = \frac{(\Delta-1)^{\Delta-1}}{(\Delta-2)^\Delta}$ $\quad$ (Note $\lambda^* < \lambda_c$)

Theorem

We have $Z_G(z) \neq 0$ for all $z \in D$ and $\Delta(G) \leq \Delta$ where

(1) $D = \{z \ : \ |z| \leq \lambda^*\}$ *(Dobushin, Shearer)*

(2) $D =$ *open region containing* $[0, \lambda_c)$ *(Peters, Regts)*

(3) $D = \{z : \Re(z) \geq 0, \ |z| \leq \frac{7}{8} \tan\left(\frac{\pi}{2(\Delta-1)}\right)\}$ *(Csikvári, Bencs)*

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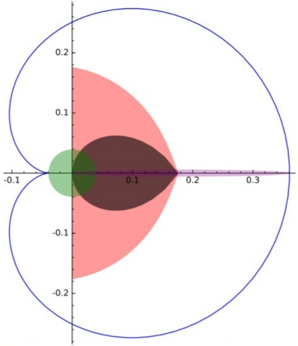
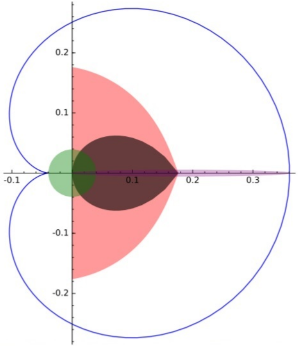
- Recover result of Weitz and more



Zero-free regions for Z_G where $\Delta(G) \leq d \quad (d = 10)$

- Green region (Shearer, Dobrushin)
- Brown/purple regions (Peters, Regts)
- Red region (Csikvári, Bencs)

Explain non-disks



Zeros of Z_G and hardness (for $\Delta(G) \le d$)

- Zeros of $Z_{T_{k,d}}$ are dense outside blue curve (de Boer, Buys, Guerini Peters, Regts)
- NP-hard to approximate $Z_G(z)$ outside blue curve (Bezáková, Galanis, Goldberg, Stefankovic)

Computing approximation for $Z_G(z)$

Summary

Idea: Approximate $f(z) = \ln(Z_G(z))$ by $\ln(n)$ term Taylor approx

1) Need to identify zero-free region
2) Compute $f^{(k)}(0)$ in time $poly(n)c^k$

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Summary

Idea: Approximate $f(z) = \ln(Z_G(z))$ by $\ln(n)$ term Taylor approx

1) Need to identify zero-free region
2) Compute $f^{(k)}(0)$ in time $poly(n)c^k$

For step 2), note that

- Compute $f^{(k)}(0) \leftrightarrow$ compute kth inverse power sum p_k
- $$p_k(G) = \sum_{\substack{|H| \leq k \\ H \text{ connected}}} c_H \cdot \mathrm{ind}(H, G)$$
- "Easy" to compute $\mathrm{ind}(H, G)$ when H connected

Matching polynomial

Graph $G = (V, E)$.

Call $M \subseteq E$ a matching if no edges in M are incident.

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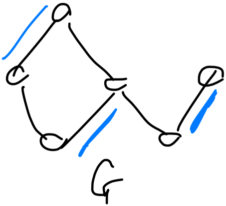
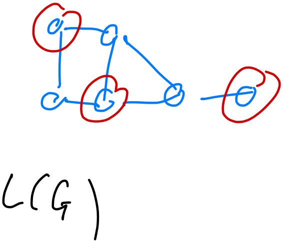
- partition function of monomer-dimer model
- special independence polynomials: $M_G(\lambda) = Z_{L(G)}(\lambda)$





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Using correlation decay

Theorem (Bayati, Gamarnik, Katz, Nair, and Tetali)

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Using MCMC

Theorem (Jerrum, Sinclair)

There is an FPRAS to evaluate $M_G(\lambda)$ for all G and $\lambda \in [0, \infty)$.

General result

Definition

Let $p = p_G$ be a graph polynomial, i.e.

$$p_G(z) = \sum_k a_k(G) z^k.$$

Call p a bounded induced graph counting polynomial (BIGCP) if

- $p_{G_1 \cup G_2} = p_{G_1} \cdot p_{G_2}$
- $a_k(G) = \sum_{|H| = O(k)} s_{H,k} \cdot \mathrm{ind}(H, G)$
- $s_{H,k}$ can be computed in $\exp(O(k))$-time

c.f. independence polynomial

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Theorem (Patel, Regts)

Let p be a BIGCP with $p_G(z) \neq 0$ for $|z| \leq K = K(\Delta)$.

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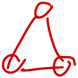
Chromatic polynomial

For a graph $G = (V, E)$

$$\chi_G(q) = \#\ \text{proper q-colourings of G};$$



$$q(q-1)(q-2) = \chi_{triangle}(q)$$

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Random cluster model formulation

$$\chi_G(q) = \sum_{A \subseteq E} (-1)^{|A|} q^{k(A)} =: \sum_i a_i(G) q^i,$$

where

- $a_n = 1$
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Hence $z^n \chi_G(z^{-1})$ is a BIGCP

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The polynomial $z^n \chi_G(z^{-1})$ is a BIGCP

Theorem (Jackson, Procacci and Sokal)

$\chi_G(z) \neq 0$ *whenever* $\Delta(G) \leq \Delta$ *and* $|z| \geq K(\Delta) = 6.91\Delta$.

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There is an FPTAS to evaluate $\chi_G(z)$ for graphs of maximum degree Δ whenever $|z| \geq K(\Delta) = 6.91\Delta$.

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Many results

- FPTAS for $q \geq 2\Delta(G)$ (Liu-Srivastava-Sinclair)
- FPRAS for $q \geq \frac{11}{6}\Delta(G)$ (Vigoda)
  $q \geq (\frac{11}{6} - \varepsilon)\Delta(G)$ (CDMPP)
- No FPTAS for $q < \Delta(G)$ unless $P = NP$
- **FP(RT)AS conjectured for** $q > \Delta(G)$

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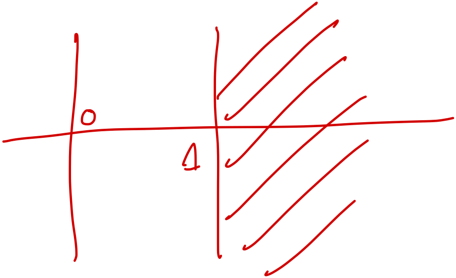
The polynomial $z^n \chi_G(z^{-1})$ is a BIGCP

Conjecture (Sokal)

$\chi_G(z) \neq 0$ *if* $\Re(z) > \Delta(G)$.



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Conjecture (Folklore)

There is an FPTAS for $\chi_G(q)$ whenever $q > \Delta(G)$.

- ~~Not quite immediate, but not too hard: requires some conformal mapping~~