Math 270: Geometry of Polynomials **Fall 2015**

Lecture 15: Lee Yang Theory of Phase Transitions

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Lee Yang Theory of Phase Transitions

Monomer-Dimer model

Let G be a graph with the vertice and edge set as V and E respectively and M be any matching. Let u(M) denote the number of unmatched vertices (or monomers) in M which is just $|V| - 2|M|$

Define $Z(x) = \sum_M x^{u(m)}$ where the summation runs over all possible matchings.

Now the average fraction of monomers, $M(x) = \frac{\sum_M u(M)x^{u(M)}}{|V|Z(x)} = \frac{x\frac{dZ(x)}{dt}}{|V|Z(x)} = \frac{x}{|V|}\frac{d\ln Z(x)}{dx}$.

Then if we call the polynomial $\frac{\ln Z(x)}{|V|}$ to be the free energy of the system, $F(x)$, our $M(x)$ becomes simply $x\frac{dF(x)}{dx}$

Ising Model

Now let us consider a slightly different model. Let G be a graph with the vertice and edge set as V and E respt. Consider some function $\sigma : V \to \{+, -\}$. We call σ a spin function.

Now define $d(\sigma)$ = # edges of G with opposite spins at endpoints.

And $m(\sigma)$ = # vertices of G with positive spin.

Now for some real number $0 < \beta < 1$ define the polynomial $Z_\beta(x) = \sum_\sigma \beta^{d(\sigma)} x^{m(\sigma)}$ where the summation runs over all possible functions $\sigma : V \to \{1, -1\}$. Since $m(\sigma)$ is at most $|V_G|$, $Z_\beta(x)$ is a polynomial in x with degree at most $|V|$.

As before we want to find the average magnetization of the graph per volume. In this case we write it as, $M_\beta(x) = \frac{\sum_\sigma m(\sigma)\beta^{d(\sigma)}x^{m(\sigma}}{|V|Z_\beta(x)}$. Similarly if we define the free energy of the graph, $F_\beta(x) = \frac{\ln Z_\beta(x)}{|V|}$, then our equation simplifies to $M_\beta(x) = x\frac{dF_\beta(x)}{dx}$

Firstly a value of x physically corresponds to the magnitude of a magnetic field. Thus we will only consider the case when $x > 0$. What we are interested in are the phase transitions or points of discontinuities of $M_\beta(x)$, which is same as the zeroes of $Z_\beta(x)$. If we consider finite graphs, as $Z_\beta(x)$ has all positive coefficients , these do not have any phase transition. Thus we need to generalize to infinite graphs. We do this by taking a sequence of finite graphs and looking at the uniform limit of the Z_β polynomials created by them (assuming of course that such a limit exists). In such a case it is also known that if each Z_β doesn't have any roots inside an open region in $\mathbb{C}$, then the limiting polynomial doesn't have any zeroes in that set. Thus the following theorem is important.

Lee-Yang Thm : Let G be a finite graph, and let $Z_\beta(x)$ be the partition function of the ferromagnetic Ising model on G (for some $\beta \in (0,1)$). Then all zeroes of Z_β lie on the unit circle.

Corollary : Thus any limiting polynomial will also have no zeroes outside of the unit circle. Thus as we are only considering real x, the only possible phase transition is at $x = 1$

Lemma 1 : Consider $Z_\beta(x_1, x_2, ..., x_n) = \sum_\sigma \beta^{d(\sigma)} \prod_{v:\sigma(v)=+} x_v$, the multivariate version of $Z_\beta(x)$. Then this multinomial has no roots when $\forall i, |x_i| > 1$

proof : Whenever G is a graph by $Z_{(\beta,G)}$ we mean the Z_β multinomial for G. First we show a few elementary identities involving Z_β. Let G_1, G_2 be two disjoint graphs. Let G be $G_1 \cup G_2$. Then if $\Omega_1, \Omega_2, \Omega$ are the set of all spin functions on G_1, G_2, G respectively, there is a obvious canonical bijection from $\Omega_1 \times \Omega_2 \to \Omega$. Thus $Z_{(\beta,G)} = \sum_{\sigma\in\Omega} \beta^{d(\sigma)} \prod_{v:\sigma(v)=+} x_v$
$= \sum_{(\sigma_1,\sigma_2)\in\Omega_1\times\Omega_2} \beta^{d(\sigma_1)+d(\sigma_2)} \prod_{v:\sigma_1(v)=+} x_v \prod_{v:\sigma_2(v)=+} x_v$
$= (\sum_{\sigma_1\in\Omega_1} \beta^{d(\sigma_1)} \prod_{v:\sigma_1(v)=+} x_v).(\sum_{\sigma_2\in\Omega_2} \beta^{d(\sigma_2)} \prod_{v:\sigma_2(v)=+} x_v)$
$= Z_{(\beta,G_1)} Z_{(\beta,G_2)}$.

Next suppose, that v_1 and v_2 are two non-neighbouring vertices of G. Then let G' denote the graph obtained by contracting v_1 and v_2 to v_2. Let Ω_3 denote the set of all partition functions on $G - \{v_1, v_2\} = G' - \{v_2\}$, and Ω' that of G'. Then any element of Ω' can be constructed uniquely by taking a element of Ω_3 and then assigning a spin value to v_2 $+or-$. Thus there is a canonical bijection from $\Omega_3 \times \{+,-\} \to \Omega'$.

Similarly there is canonical bijection from $\Omega_3 \times \{+,-\} \times \{+,-\} \to \Omega$.

Using this and a calculation similar to the previous one, we find the following;

If $Z_{(\beta,G)}(x_1, x_2, ...x_n) = Ax_1.x_2 + Bx_1 + Cx_2 + D$, where A, B, C, D are multinomials in $(x_3, ..., x_n)$, then $Z_{(\beta,G')}(x_2, x_3, ..., x_n) = Ax_2 + D$. In fact $A = Z_{(\beta,G_3)}(y_3, y_4, ...y_n)$ where $y_i = x_i/\beta$ if v_i is a neighbour of v_1 or v_2 and $y_i = x_i$ otherwise.

Now say a graph G satisfies Lee-Yang Property(LYP) if above lemma is true for G and all induced subgraphs of G. Then first we show that G' satisfies LYP. So suppose G satisfies LYP, then $Z_{(\beta,G)}$ is non zero whenever $|x_i| > 1 \forall i \leq n$. Then fix some values for $x_3, x_4, ..., x_n$ with modulus greater than 1, and set $x_1 = x_2 = x$. Then the quadratic $Ax^2 + (B + C)x + D$ has no roots for $|x| > 1$ ($\because Z_{(\beta,G)}(x_1, x_2, ...x_n) = Ax_1x_2 + Bx_1 + Cx_2 + D$ is nonzero for all values of x_i with $|x_i| > 1$).

Also as $A = Z_{(\beta,G_3)}(y_3, y_4, ...y_n)$ where $y_i = x_i/\beta$ if v_i is a neighbour of v_1 or v_2 and $y_i = x_i$ otherwise, and $\beta < 1 \Rightarrow |x_i/\beta| > 1$, and G_3 is a subgraph of G, we have that $A \neq 0$ (by LYP).

$\therefore$ the product of its roots $D/A \leq 1$. Thus $Ax + D$ is nonzero when $|x| > 1$ ($\because Ax + D = 0 \Rightarrow x = -D/A$).

$\therefore Z_{(\beta,G')}(x_2, x_3, ..., x_n)$ is nonzero when $|x_i| > 1 \forall 2 \leq i \leq n$.

Similarly for all subgraphs of G' same thing holds. So G' satisfies LYP.

Now the rest of the proof follows an inductive method. First we show that a single point and the single edge satisfies LYP. For a single isolated vertice there is nothing to show. For a single edge E

the polynomial $Z_{(\beta,E)}(x_1, x_2) = 1 + \beta(x_1 + x_2) + x_1x_2$.

$\therefore Z_{(\beta,E)}(x_1, x_2) = 0 \Rightarrow x_1 = \frac{1+\beta x_2}{\beta+x_2}$.

$\because$ the right hand side is a Mobius transform which sends the outside of the unit disc to the inside, if (x_1, x_2) is a root then $|x_2| > 1 \Rightarrow |x_1|leq1$. Thus no root has both modulus more than 1. As all sub graphs of E is singletons, this means E satisfies LYP.

Now for a arbitrary graph G, start with a disjoint collection of edges and as many isolated points as G has, G_0. Then since $Z_{(\beta,G_0)}$ is the product of the Z_β functions of each edge and single tons, we have that $Z_{(\beta,G_0)}$ satisfies LYP. Now by repeatedly contracting we can get G back from G_0. Thus as contraction preserves LYP, $Z_{(\beta,G)}$ has LYP. In particular $Z_{(\beta,G)}$ satisfies above lemma.

Proof of Lee-Yang Theorem : By lemma 1, we have that $Z_{(\beta,G)} \neq 0$ whenver $|x_i| > 1 \forall i$. Then observe that $Z_{(\beta,G)}(x_1^{-1}, ..., x_n^{-1}) = \sum_{\sigma\in\Omega} \beta^{d(\sigma)} \prod_{v:\sigma(v)=+} x_v{}^{-1} = \frac{\sum_{\sigma\in\Omega} \beta^{d(\sigma)} \prod_{v:\sigma(v)=-} x_v}{\prod x_v}$.

But for any sign function we have a unique sign function with exactly opposite signs,

$\therefore Z_{(\beta,G)}(x_1^{-1}, ..., x_n^{-1}) = \frac{\sum_{\sigma\in\Omega} \beta^{d(\sigma)} \prod_{v:\sigma(v)=-} x_v}{\prod x_v} = \frac{Z_{(\beta,G)}(x_1,.....,x_n)}{\prod x_v}$

$\therefore Z_{(\beta,G)}(x_1, ..., x_n) \neq 0$ whenever $|x_i| < 1 \forall i$.

finally observe that the univariate version of Z_β is just the diagonal restriction of the multivariate version. Hence proved.

This method can be generalised to prove other things. For instance one can prove that $M_\beta(x) = \frac{xZ_\beta{}'(x)}{|V|Z_\beta(x)}$ is $\#p$ hard to compute.

To prove this we shall use two known results :

1) Computing $Z_\beta(x)$ is $\#p$ hard.

2) Suppose $R(x) = p(x)/q(x)$ where $deg(p) = deg(q) = n$ then if $gcd(p, q) = 1$, we have that p and q can be computed efficiently from $2n + 2$ evaluations of $R(x)$. (Macon, Dupree)

Thus to prove that M_β is $\#p$ hard to compute we only need to prove that Z_β has no repeated roots. First of observe that if G is disconnected, then this is clearly not true. After all if $G = G_1 \cup G_2$ and $G_1 \simeq G_2$ then as $Z_{(\beta,G)}(x) = Z_{(\beta,G_1)}(x)Z_{(\beta,G_2)}(x)$, clearly $Z_{(\beta,G)}$ has a repeated root. So we assume that G is connected.

Then we have the theorem by Sinclair and Srivastava : **Theorem :** If G is a connected graphs then zeroes of $Z'_{(\beta,G)}(x)$ are in the open unit disc. Thus as all zeroes of $Z_{(\beta,G)}(x)$ are on the circumference, their roots never coincide.

Proof Sketch : The argument for this is precisely the same as before. Say a graph has property SSG if it and all of its subgraphs satisfy a multivariate version of the above theorem, i.e. $DZ_{(\beta,G)}(x_1, x_2, ..., x_n) \neq 0$ whenever $|x_i| \geq 1 \forall i$ where $D = \sum_{v\in V} fracx_v\partial\partial x_v$.

Then first show that if $Ax_1x_2 + Bx_1 + Cx_2 + D$ has no roots outside unit disc (corresponds to G satisfying SSG)then $Az^2 + B$ has no roots outside unit disc (corresponds to contraction of G by v_1, v_2 satisfying SSG).

Finally show that adding a single new edge or vertex also preserves the property and we will be done via induction.