A Tutte polynomial for edge- and vertex-weighted graphs, list coloring, and the zero-temperature Potts model

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WHERE DISCOVERIES BEGIN

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The history…

- The zero-field Potts model partition function is an evaluation of the Tutte polynomial--1972.
- This means that results for the Tutte polynomial carry over to the Potts model and vice versa.
- This includes particularly computational complexity results, and
- locations for the zeros of the chromatic polynomial, which inform the zero-temperature, anti-ferromagnetic Potts model.

Today's connections...

- List coloring, heavily studied (hundreds of papers since introduced by Vizing in 1976)

is the same as….

- Zero-temperature anti-ferromagnetic Potts model with an external field.

(Connection is via a List Chromatic Polynomial that is a specialization of the V-polynomial.)

Again a very rich opportunity for cross-fertilization from 40 years of independently developed theory on the same object.

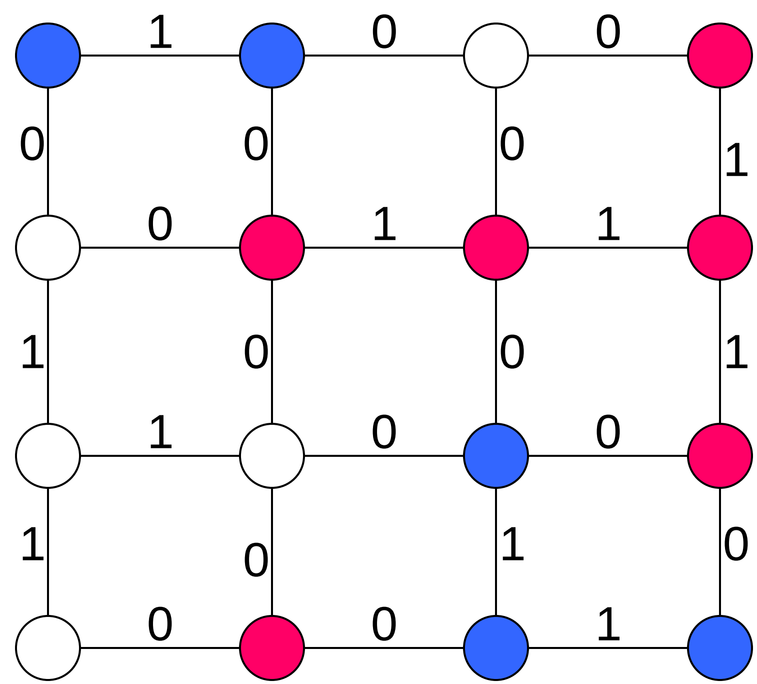
A Graph state and its Hamiltonian

The **Hamiltonian** still measures the overall energy of the a state of a system.

$$H(w) = \sum_{edges} -J\delta_{a,b}$$

Note: constant interaction energy of J and no external magnetic field (no additional terms in the Hamiltonian.

The Hamiltonian of a state of a 4 x 4 lattice with 3 choices of spins (colors) for each element.



$$H = -10J$$

Probability of a state

The probability of a particular state S occurring depends on the *temperature*, T

(or other measure of activity level in the application)

--Boltzmann probability distribution--

$$P(S) = \frac{\exp(-\beta H(S))}{\sum_{\text{all states } \mathbf{S}} \exp(-\beta H(\mathbf{S}))}$$

$\beta = \frac{1}{kT}$ where $k = 1.38 \times 10^{-23}$ joules/Kelvin and T is the temperature of the system.

The numerator is easy. The denominator, $Z = \sum_{\text{all states } \mathbf{S}} \exp(-\beta H(\mathbf{S}))$

called the *Potts Model Partition Function*,

is the interesting (hard) piece.

The classical Tutte/Potts connection

$$Z = \sum_{\text{all states } \mathbf{S}} \exp(-\beta H(\mathbf{S})) = q^{k(G)} (v)^{|V(G)|-k(G)} T\left(G; \frac{q+v}{v}, 1+v\right)$$

The Potts model partition function is a polynomial in q

$$Z(G;u,v) = \sum_{A \subseteq E(G)} u^{k(A)} v^{|A|}$$

Computational complexity results for the Tutte polynomial and Potts model partition function have built in alternation over the years:

- Ising model tractable for plane graphs (Fischer ‘66, Kastelyn ’67) → Tutte tractable along (*x*-1)(*y*-1)=2 for plane graph.
- Ising model not tractable off the plane (Jerrum, ‘87) → Tutte is not tractible along (*x*-1)(*y*-1)=2.
- Tutte polynomial is #P-complete in general, except along (*x*-1)(*y*-1)=1 and 9 trivial points (Jaeger, Vertigan & Welsh, ‘90) → Potts model is generally intractable.

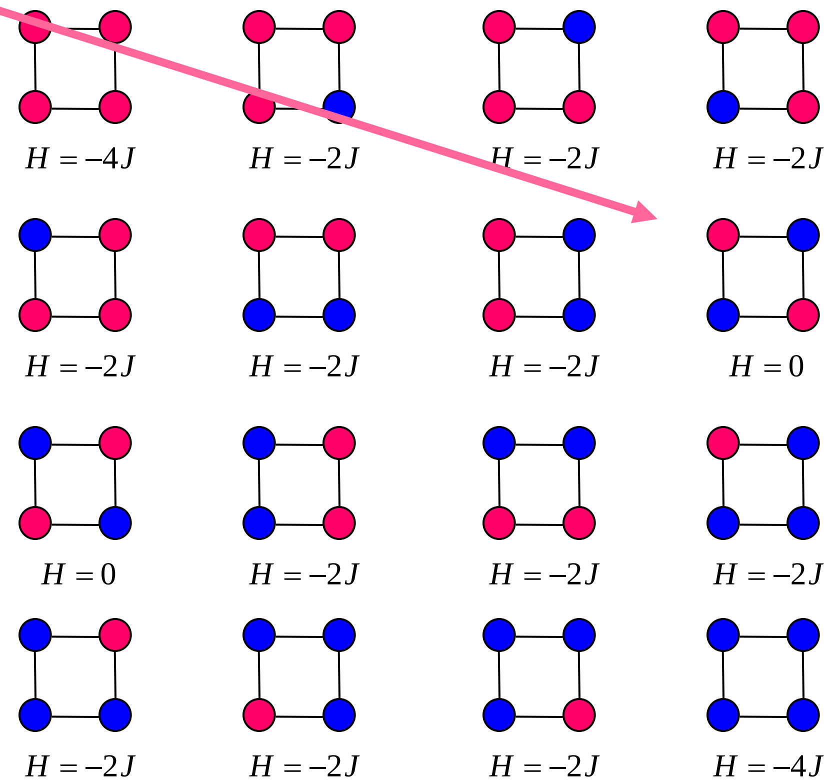
The antiferromagnetic model at zero temperature

Minimum energy states if $J < 0$ (anti-ferromagnetic)

J is negative in the antiferromagnetic model, so minimal energy states have a maximum number of zeros in the Hamiltonian, i.e. every edge has endpoints with different spins.

Such a state corresponds to a proper coloring of the graph.

The Potts model partition function of a square lattice with two possible spins



The connection

Consider the summands of

$$Z(G;q,\beta)=\sum \exp\left(\beta J\sum \delta(\sigma_i,\sigma_j)\right)$$

as $T \to 0$, and hence $\beta = 1/\kappa T \to \infty$, remembering $J < 0$

a summand is 0 except precisely when $\sum \delta\left(\sigma_i,\sigma_j\right)=0$

in which case it is 1. Thus

$Z(G)$ simply counts the number of proper colorings of G with q colors.

Zeros of the chromatic polynomial

S=Entropy (a measure of the randomness and disorder in a system):

$$S = -\kappa\beta \frac{\partial \ln(Z)}{\partial \beta} + \kappa \ln(Z)$$

In the infinite volume limit, the ground state (T=0) entropy per vertex of the Potts antiferromagnetic model then becomes:

$$S = \kappa \lim_{n\to\infty} \frac{1}{|V(G_n)|} \ln\left(C(G_n;q)\right)$$

Thus, phase transitions correspond to the accumulation points of roots of the chromatic polynomial in the infinite volume limit.

Limitation of the classical connection

Many applications

- Liquid-gas transitions
- Foam behaviors
- Magnetism
- Biological membranes
- Ghetto formation (Schnelling 2005)
- Separation in binary alloys
- Cell migration
- Spin glasses
- Neural networks
- Flocking birds

However…

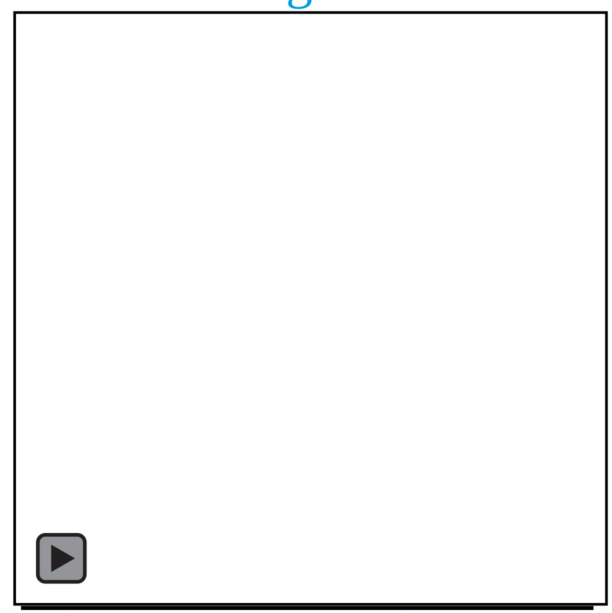
Most applications include additional terms in the Hamiltonian, and the classical theory of the Tutte-Potts connection does not encompass this.

A simple external field

The first spin is favored, and *M* is the strength of the favoritism

$$H(w)=\sum_{edges} -J\delta_{a,b} \longrightarrow H(w)=\sum_{edges} -J\delta_{a,b} + \sum_{vertices} -M\delta_{1,a}$$

- In the first sum, *a* and *b* are the spins on endpoints of the edge
- In the second sum, *a* is the spin on the vertex.



http://pages.physics.cornell.edu/sss/ising/ising.html

More encompassing model

- Allow edge-dependent interaction energies--- (**γ**).

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i,\sigma_j)$$

- Also allow q-dimensional external field contributions via a vector $(M_{i,1} \ldots M_{i,q})$ associated to each vertex v_i --**(M)**

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i,\sigma_j) - \sum_{v_i\in V(G)}\sum_{\alpha=1}^{q} M_{i,\alpha}\delta(\alpha,\sigma_i)$$

Variable (edge-dependent) energies and a variable (vertex-dependent) external field.

Appropriate choices of **M** and **γ** yield familiar models: Preferred Spin, Spin Glass, Random Field Ising Model, etc.

Catching up the Math

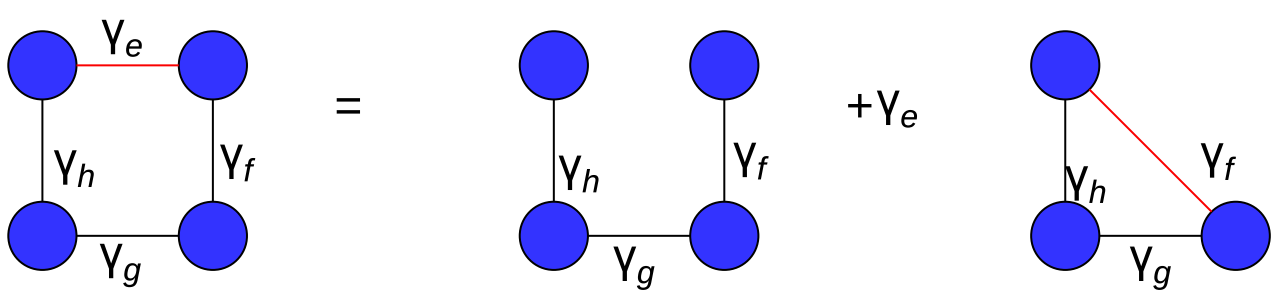
How do we extend the classical Tutte-Potts relation to these more typical (and applicable) versions of the Potts model?

- Edge-dependent interaction energies?
  - In the past 15-25 years, multivariable generalizations of the Tutte polynomial have been developed that capture this. (Traldi ‘89, Zaslavsky ‘92, Bollobas&Riordan ‘99, Sokal connections 2005, etc.)
- External magnetic fields?
  - **This is the tricky bit….**

Multivariate Tutte Polynomial

classical

$$Z(G;u,v) = \sum_{A \subseteq E(G)} u^{k(A)} v^{|A|}$$



multivariable

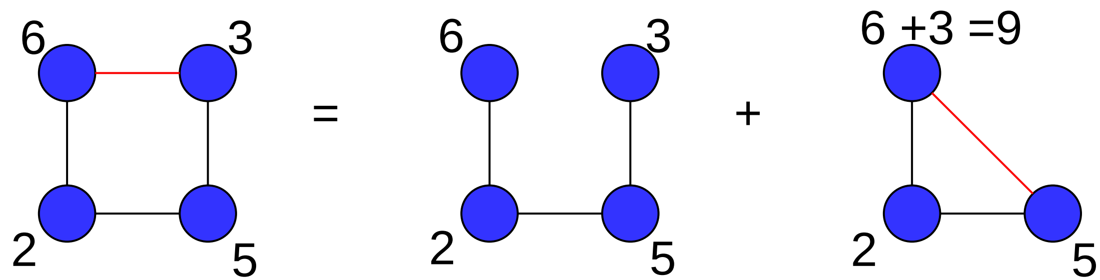
$$Z_T(G;\theta,\gamma) := \sum_{A \subseteq E(G)} \theta^{k(A)} \prod_{e \in A} \gamma_e .$$

The U- and W-polynomials

Noble and Welsh (1999) in the context of knot theory and combinatorics of Vassiliev invariants. Loebl 2007, coloring

- Take vertex weights in $\mathbf{Z}^{+}$
- Take indeterminates $x_1, x_2 \ldots$

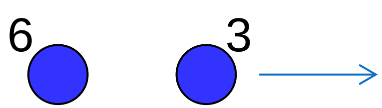
1.



2. if e is a loop, then

$$W(G) = yW(G - e);$$

3. if E_m consists of m isolated vertices of weights $\omega_1, \ldots, \omega_m$, then



$x_6 + x_3$

$$W(E_m) = \prod_{i=1}^{m} x_{\omega_i}.$$

U is the same, but all weights initialized to 1, to give an invariant of graphs rather than of vertex-weighted graphs.

The V-polynomial

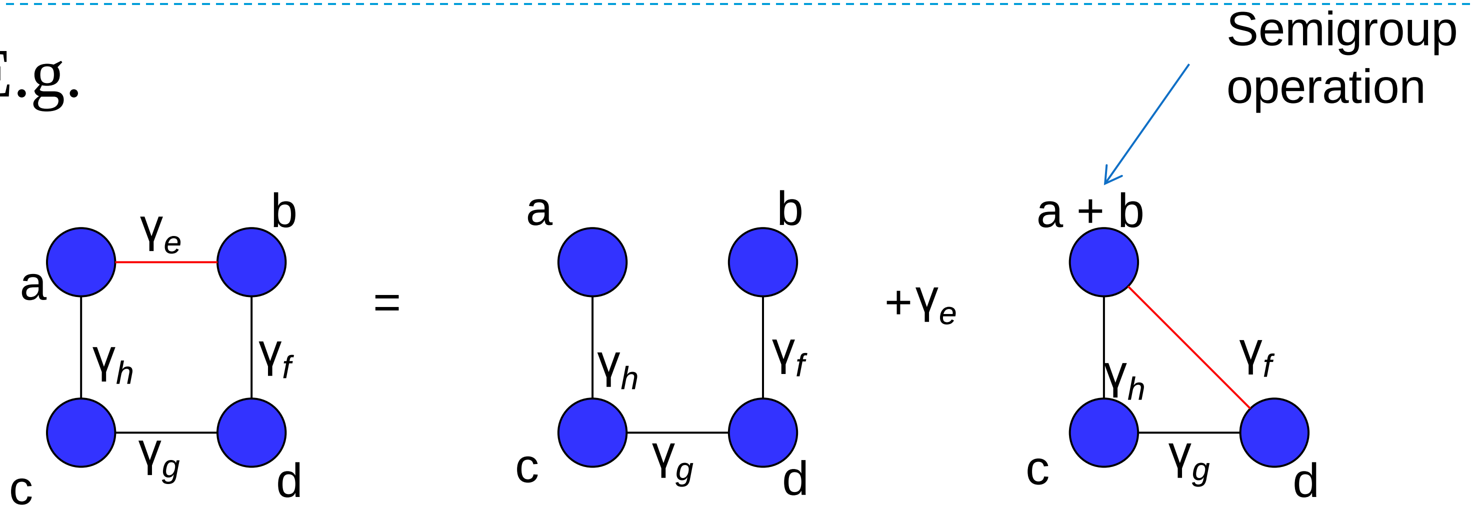
E-M, Moffatt 2011
cf Forge, Zaslavsky 2013
for gain graphs

- Edge weights/indeterminates indexed by the edges--- (γ).
- Vertex weights in a semigroup S--- (ω)
- Indeterminates indexed by S--- (***x***)

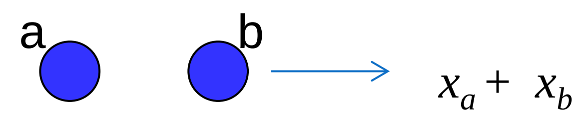
$$\boldsymbol{V}(G) = \boldsymbol{V}(G, \omega; \boldsymbol{x}, \gamma) \in \mathbb{Z}[\{\gamma_e\}_{e \in E(G)}, \{x_k\}_{k \in S}]$$

Computing the V polynomial

- E.g.



if e is a loop, then
$V(G) = (\gamma_e + 1)V(G - e)$;



State Model: $$V(G) = \sum_{A \subseteq E(G)} x_{c_1} x_{c_2} \cdots x_{c_{k(A)}} \prod_{e \in A} \gamma_e,$$ where c_i sums weights on the i^{th} component.

Also a Spanning Tree Expansion, —McDonald & Moffatt 2012

External field Potts is an evaluation of V

Let G be a graph equipped with a magnetic field vector $\boldsymbol{M}_i = (M_{i,1}, \ldots, M_{i,q}) \in \mathbb{C}^q$ *at each vertex* v_i*, and suppose*

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i, \sigma_j) - \sum_{v_i \in V(G)} \sum_{\alpha=1}^{q} M_{i,\alpha}\delta(\alpha, \sigma_i).$$

Then

$$Z(G) = \boldsymbol{V}\left(G, \omega;\ \{X_M\}_{M\in\mathbb{C}^q},\ \{\mathrm{e}^{\beta J_{i,j}} - 1\}_{\{i,j\}\in E(G)}\right),$$

where the vertex weights are given by $\omega(v_i) = \boldsymbol{M}_i$ *and, for any* $\boldsymbol{M} = (M_1, \ldots, M_q) \in \mathbb{C}^q$,

$$X_M = \sum_{\alpha=1}^{q} \mathrm{e}^{\beta M_\alpha}.$$

Basically take the semigroup to be q-dimensional complex vectors,
initialize vertex weights with the given magnetic field vectors,
and take the edge weights to be exp($\beta J_{i,j}$-1).

Polynomial expressions

Get a cluster model expansion and deletion/contraction.

The partition function, even with an external field, is a polynomial in q.

Suppose a complex value z_i is associated to each vertex v_i of a graph G, and the Hamiltonian is given by

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i,\sigma_j) - \sum_{v_i\in V(G)} z_i\delta(1,\sigma_i).$$

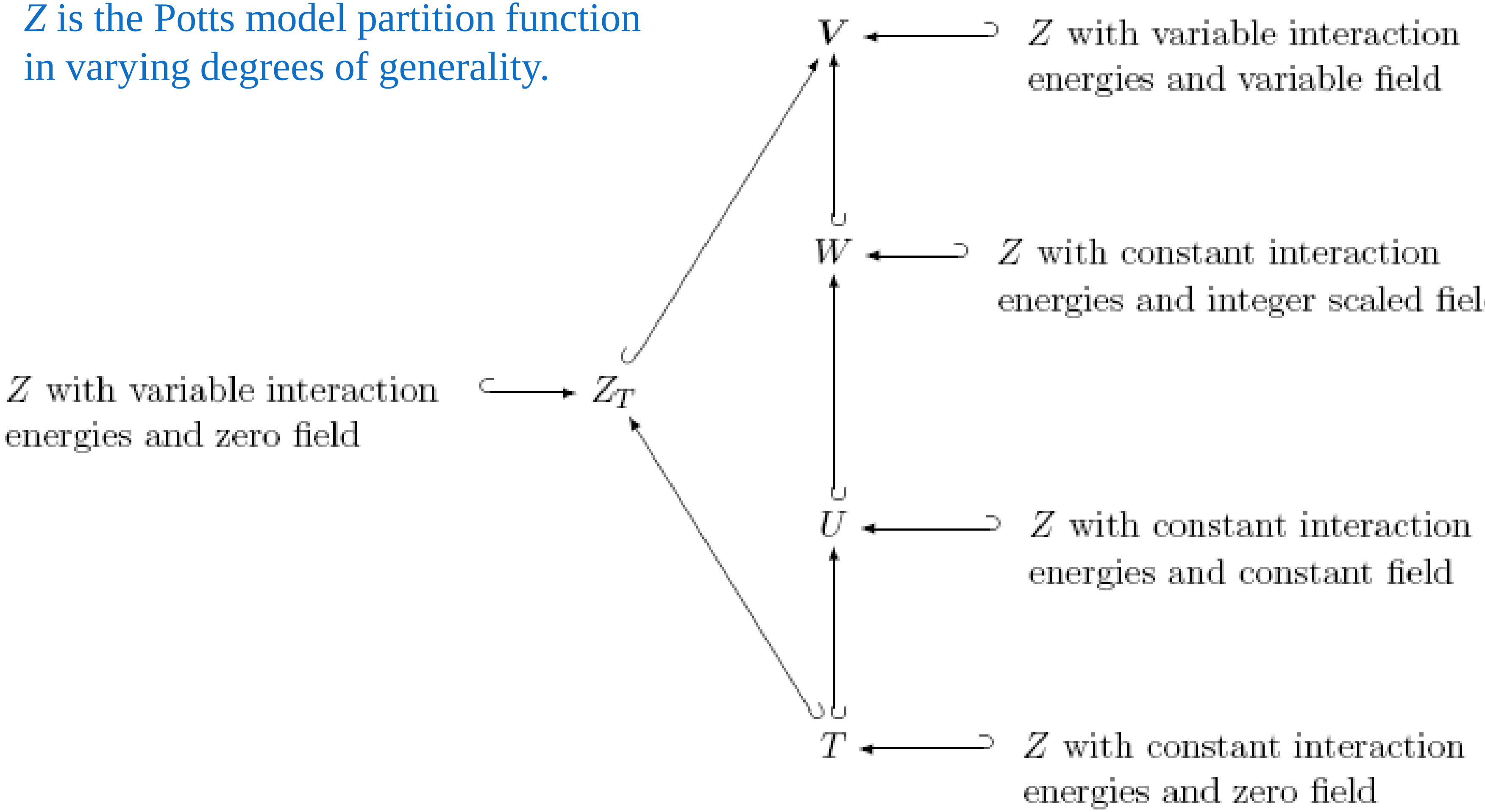
Then

$$Z(G) = \sum_{A\subseteq E(G)} X_{z_{C_1}} \cdots X_{z_{C_{k(A)}}} \left(\prod_{e\in A}(\mathrm{e}^{\beta J_e} - 1)\right),$$

where z_{C_l} is the sum of the weights, z_i, of all of the vertices v_i in the l-th connected component of the spanning subgraph $(V(G), A)$, and $X_z = q - 1 + \mathrm{e}^{\beta z}$.

A Hierarchy of Relations

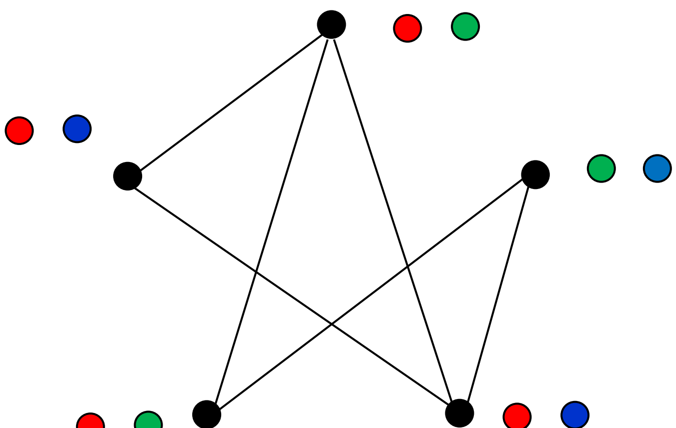
Z is the Potts model partition function in varying degrees of generality.



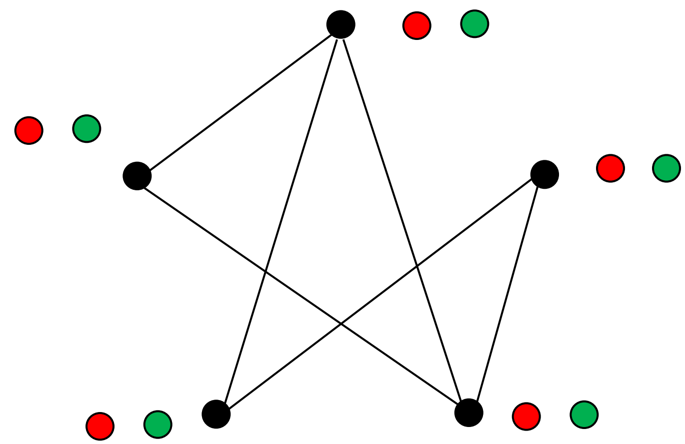
List coloring

Given a graph *G* with a list of colors for each vertex, a list coloring of *G* is a proper coloring with the color at each vertex chosen from its list.

Given *k*, generally want to know if a graph is *k-choosable*, i.e. may be list colored given *any* set of lists of size *k* at each vertex.



Can be colored from this set of lists



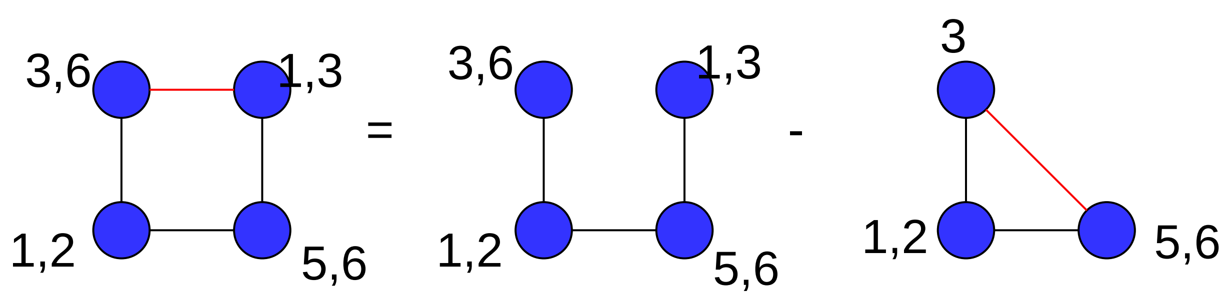
But is NOT 2-choosable. In general the choosability number is at least as big as the chromatic number.

The List Chromatic Polynomial

- Let G be a graph with lists l_i from some set L at the vertices.
- Let S be the semigroup 2^L under intersection.
- Assign edge weights of -1 to each edge

The List Chromatic Polynomial is defined by

$$C(G,\{l_i\}) := \mathbf{V}(G,\{l_i\};\mathbf{x},\mathbf{-1})$$



Basic idea is to put lists on the vertices and take the intersection when you contract.

Counts List Colorings

- The List Chromatic Polynomial counts list colorings of *G* with the given lists:

$$C(G,\{l_i\})\Big|_{x_s=|s|}$$

is the number of ways to properly color *G* from the given lists of colors at the vertices.

Straightforward to prove by induction.

Properties as a specialization of the V polynomial

Recursive:

1. If e is not a loop,
$$C(G,\{l_i\}) = C(G-e,\{l_i\}') - C(G/e,\{l_i\}'')$$

2. If e is a loop, $C(G,\{l_i\}) = 0$

3. If G is edgeless, $C(G,\{l_i\}) = \prod x_{l_i}$

State Model: $$C(G,\{l_i\}) = \sum_{A\subseteq E(G)} (-1)^{|A|} \prod_{j=1}^{k(A)} x_{c_j}$$

where c_j is the intersection of the lists on the vertices in the j^{th} component of A.

Zero-temp antiferromagnetic Potts model with an external field

- Antiferromagnetic, so $J_e < 0$ for all e.
- We also assume that all the entries of the magnetic field vectors are less than or equal to zero.

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i,\sigma_j) - \sum_{v_i\in V(G)}\sum_{\alpha=1}^{q} M_{i,\alpha}\delta(\alpha,\sigma_i)$$

(contributes $M_{i,\alpha}$ when v_i has color α in the state.)

Note: This Hamiltonian is always greater than or equal to zero

Zero temperature limit

$$Z = \sum_{\text{all states } \sigma} \exp(-\beta h(\sigma))$$

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i, \sigma_j) - \sum_{v_i \in V(G)} \sum_{\alpha=1}^{q} M_{i,\alpha}\delta(\alpha, \sigma_i)$$

As $T \to 0$, then $\beta = 1/\kappa T \to \infty$, so $\exp(-\beta h(\sigma)) = 0$,

unless $h(\sigma) = 0$, in which case $\exp(-\beta h(\sigma)) = 1$.

Thus, Z counts states where $h(\sigma) = 0$.

The correspondence

Since $J_e < 0$, and $M_{i,\alpha} \leq 0$, both terms must be zero in

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i,\sigma_j) - \sum_{v_i\in V(G)}\sum_{\alpha=1}^{q} M_{i,\alpha}\delta(\alpha,\sigma_i)$$

- The first term is zero *iff* the state is a proper coloring
- The second term is zero *iff* the colors are chosen from the following lists at the vertices: $\alpha \in l(v_i) \Leftrightarrow M_{i,\alpha} = 0$

Thus, $h(\sigma) = 0$ *iff* the state is a list coloring of G using the lists $l(v_i)$, and hence as $T \to 0$

$$Z = \sum_{\text{all states } \sigma} \exp(-\beta h(\sigma))$$ counts list colorings.

Most especially….

- We now have an external field analog for the classical relation between the chromatic polynomial and the zero-temperature antiferromagnetic Potts model.
- List coloring is a heavily studied variation of graph coloring, where a graph is properly colored using only colors from lists specified for each vertex.
- The V-polynomial specializes to the List Chromatic polynomial, like the Tutte polynomial specializes to the Chromatic polynomial.
- The List Coloring polynomial gives a graph polynomial expression for the zero-temperature antiferromagnetic Potts model with external field and boundary conditions.

Some consequences

Ground states and ground state entropy-- At zero temperature, the system settles into minimum energy states.

$$\kappa \lim_{n\to\infty} \lim_{T\to 0} \frac{1}{n} \ln(Z(G_n, J, M; q, T)) = \kappa \lim_{n\to\infty} \frac{1}{n} \ln(P(G_n; L_n)).$$

- In the zero field model this is easy: get zero energy states iff at least as many spins as the chromatic number.

- With an external field, this depends entirely on the nature of the external field contributions. If the lists are larger than the choosability number, get zero energy states. This will always happen for plane graphs if at least 5 zeros in the external field contributions (Carsten Thomassen, 1994)

- Otherwise, anything goes (contrast single spins, and cubic lattice)

- For example, let q=3, cubic lattice with diagonals, and assign the following external field contributions according to the coordinates of (-1,0,0) if $x+y=0 \bmod 3$, (0,-1,0) if $x+y=1 \bmod 3$, (0,0,-1) if $x+y=2 \bmod 3$,

This does not have a zero energy state since the lattice cannot be colored from the resulting lists.

- On the other hand, Thomassen showed that planar graphs are 5-choosable. Thus, in a planar system as long as there are at least 5 zero entries in the external field contribution at each vertex then the system will have zero energy states.

More consequences

- *Independence of preference strength*--in zero temp analyses the values of the entries in the external field contributions do not matter, just their positions.
- *Boundary conditions*--many models assume boundary conditions. The field vectors let you fix spins on boundary vertices, thus yielding polynomial and cluster expansions for these models. E.g. polynomial of J. L. Jacobsen and H. Saleur, (2008) can be recovered.
- *Computational complexity*--list coloring can be done in $O(n^{t+2})$-time where t is tree width, so ditto the number of zero energy states.

New directions for list coloring

Example:

- Classes of graphs—
  - Previous research has been on e.g. outer planar or 1-planar.
  - Physics application refocuses this on families of lattices.
- Partial list coloring--
  - Partial list coloring bounds previously focused on lower bounds for the number of vertices colored when the graph can't be list colored.
  - Application suggests that a productive direction would be estimating the minimum number of monochromatic edges when the graph can't be list colored, as this will give the energy of a minimum energy state.

For more information

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