# A little statistical mechanics for the graph theorist

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With a lot of help from my friends….

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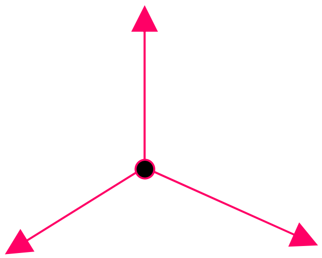
# The Potts Model

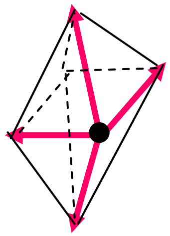
(Lenz, Ising, Domb, Potts)

Consider $q$ possible spins at each vertex in a network….

$q = 2$

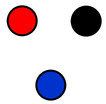


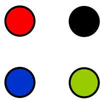
$q = 3$



$q = 4$

Orthogonal vectors

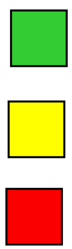




Colorings of the points with $q$ colors

+

—



Healthy

Sick

Necrotic

Values pertinent to the application

# The Hamiltonian

- The **Hamiltonian** measures the overall energy of the a state $S$ of a system.

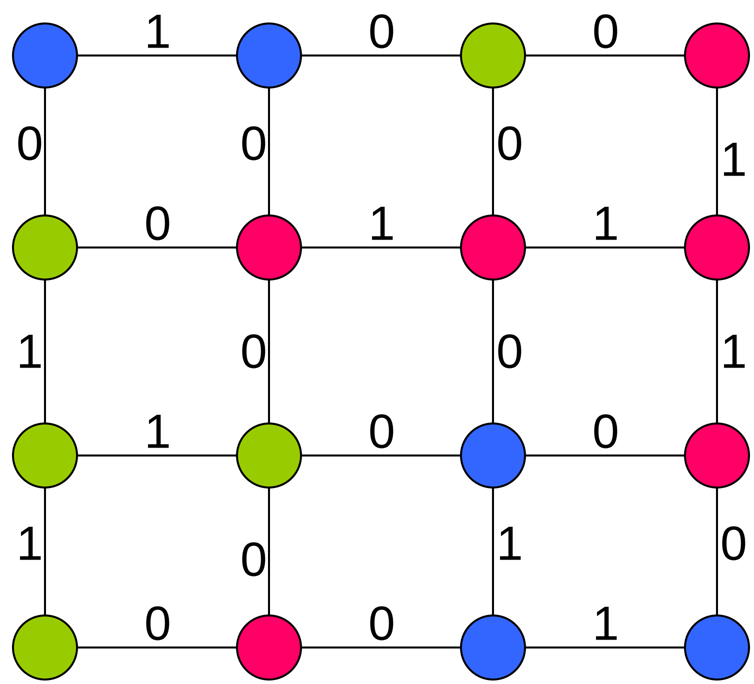
$$H(S) = \sum_{edges} -J\delta_{u,v}$$

$J$ is the interaction energy between two adjacent points.

$\delta$ is the usual Kronecker delta, and $u,v$ are the spins on the endpoints of an edge.

**Note that, if $J$ is positive (*ferromagnetic*), the more 1's, the *lower* the energy of the state.**

The Hamiltonian of a state of a 4X4 lattice with 3 choices of spins (colors) for each point




$$H = -10J$$

# 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)

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

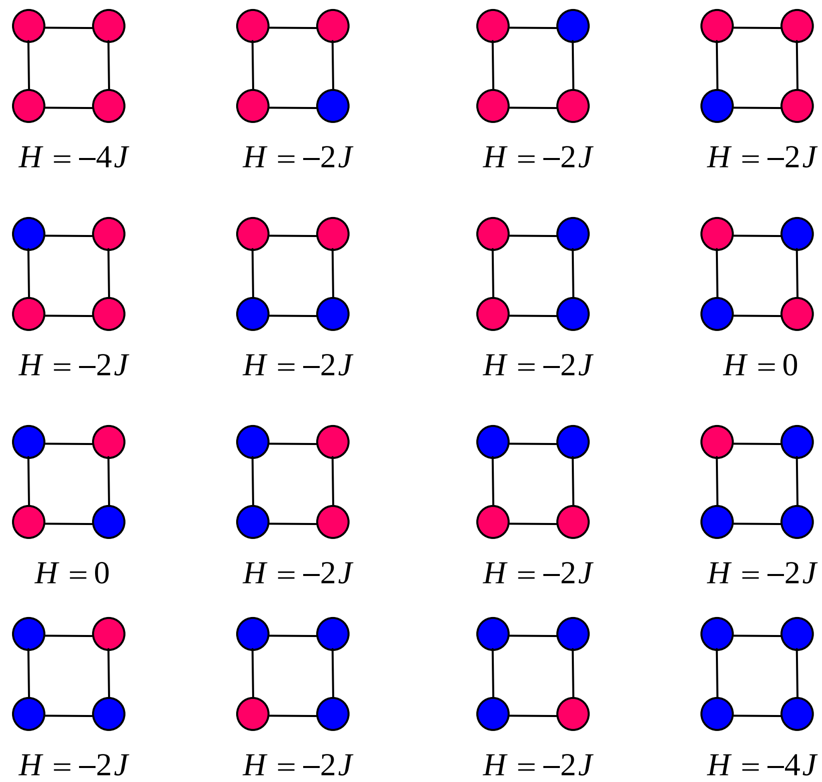
$\beta = \frac{1}{kT}$ where $k = 1.38 \times 10^{-23}$ joules/Kelvin and $T$ is the temperature of the system.

The numerator is easy. The denominator, called the *Potts Model Partition Function,* is the interesting (hard) piece.

# Example

The Potts model partition function of a square lattice with two possible spins on each element.

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




$$P(\text{all red}) = \frac{\exp(4\beta J)}{12\exp(2\beta J) + 2\exp(4\beta J) + 2}$$

$$\boxed{12\exp(2J\beta) + 2\exp(4J\beta) + 2}$$

# Probability of a state occurring depends on the temperature

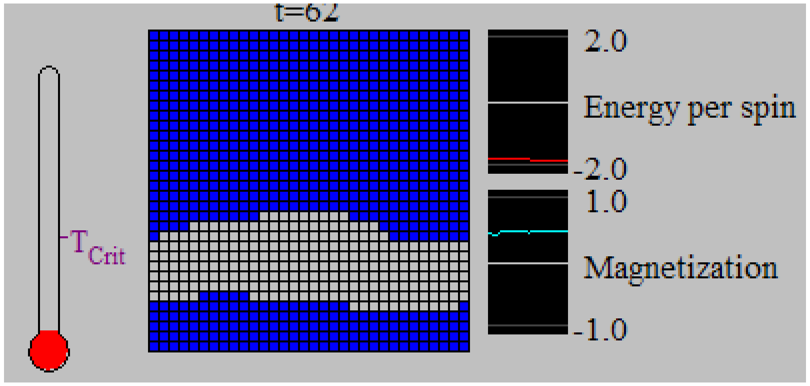
P(all red, T=0.01) = .50 or 50%

P(all red, T=2.29) = 0.19 or 19%

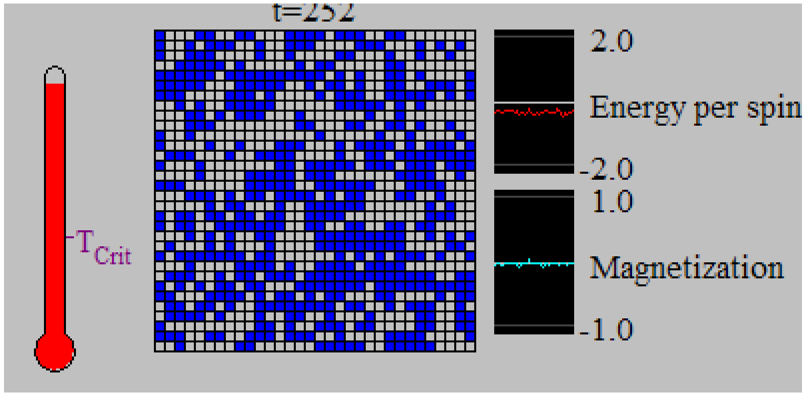
P(all red, T = 100, 000) = 0.0625 = 1/16

(Setting $J = k$ for convenience)

# Monte Carlo Simulations




Cold Temperature



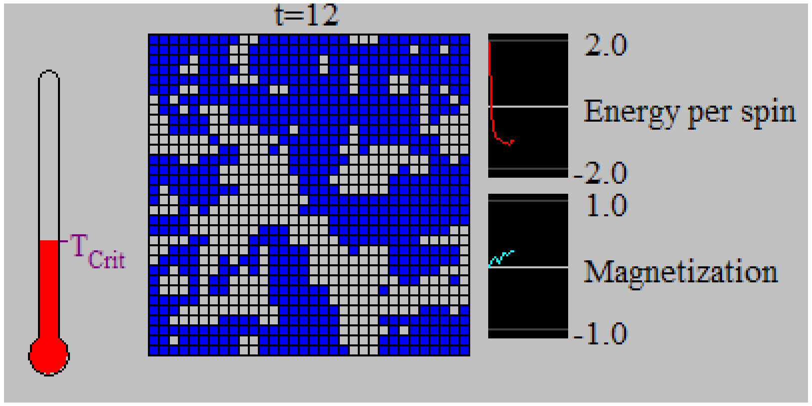

Hot Temperature

Here spins are +/- 1, and $H$ is

$$\sum s_i s_j$$

With energy

$$\frac{H}{\#\text{ of squares}}$$



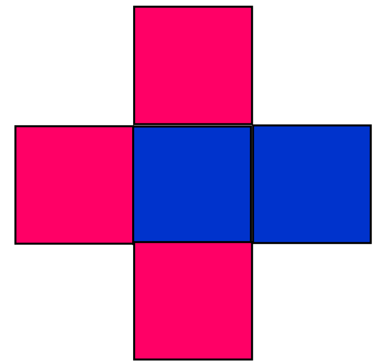

Critical Temperature

Images from http://bartok.ucsc.edu/peter/java/ising/keep/ising.html
http://bartok.ucsc.edu/peter/java/ising/isingAppletLarge.html

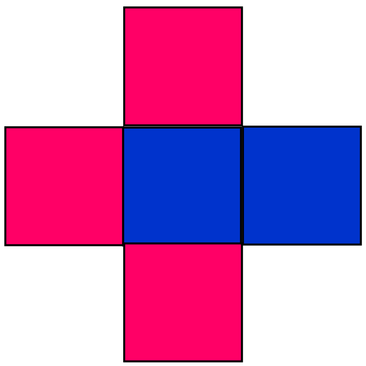
# Moving from state to state

Generate a random number $r$ between 0 and 1.

$$\frac{P(A)}{P(B)} = \exp\left(\frac{H(B)-H(A)}{kT}\right) < r$$

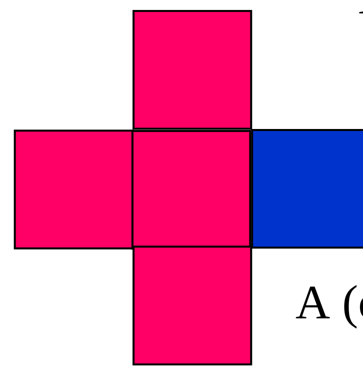


B (stay old)



B (old)

$$\frac{P(A)}{P(B)} = \exp\left(\frac{H(B)-H(A)}{kT}\right) > r$$



A (change to new)

At high temperatures (i.e., for ***kT*** much larger than the energy difference), the system becomes equally likely to be in either of the states **A** or **B -** that is, randomness and entropy "win". On the other hand, if the energy difference is much larger than ***kT***, the system is far more likely to be in the lower energy state.

# Applications of the Potts Model

(about 1,000,000 Google hits in 2005,
1,650,000 in 2006…)

Complex Systems with nearest neighbor interactions….

- **Liquid-gas transitions**
- **Foam behaviors**
- **Protein Folds**
- **Biological Membranes**
- **Social Behavior**
- **Separation in binary alloys**
- **Spin glasses**
- **Neural Networks**
- **Flocking birds**
- **Beating heart cells**

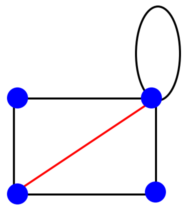
http://www.lactamme.polytechnique.fr/Mosaic/images/ISIN.41.16.D/display.html

T. C. Schelling won the 2005 Nobel prize in economics for his work using these principals with *literal* neighbors—social demographics in transitioning neighborhoods.

# Tutte Polynomial

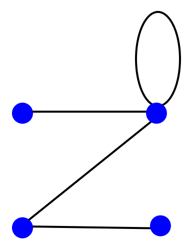
Let $e$ be an edge of $G$ that is neither a bridge nor a loop. Then,

$$T\left(G;x,y\right)=T(G-e;x,y)+T\left(G/e;x,y\right)$$



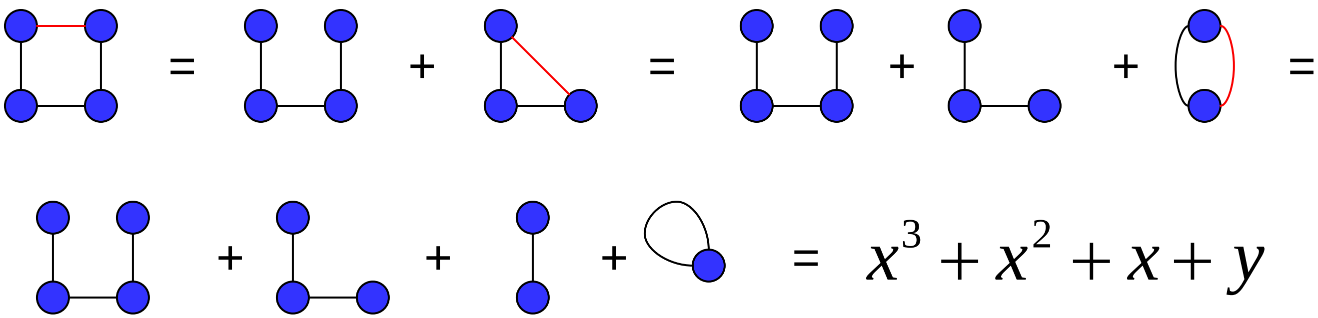
And if $G$ consists of $i$ bridges and $j$ loops, then

$$T\left(G;x,y\right)=x^{i}y^{j}$$



# Example

**The Tutte polynomial of a cycle on 4 vertices…**



$$= x^3 + x^2 + x + y$$

# Universality

THEOREM: (various forms—Brylawsky, Welsh, Oxley, etc.)
If $f$ is a function of graphs such that

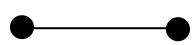
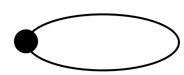
*a)* $f(G) = a\, f(G\text{-}e) + b\, f(G/e)$ whenever $e$ is not a loop or an isthmus, and

*b)* $f(GH) = f(G)f(H)$ where $GH$ is either the disjoint union of $G$ and $H$ or where $G$ and $H$ share at most one vertex.

Then,

$$f(G) = a^{|E|-|V|+k(G)}\, b^{|V|-k(G)}\; T\left(G; \frac{x_0}{b}, \frac{y_0}{a}\right),$$ where $|E|$, $|V|$, and $k(G)$

are the number of edges, vertices, and components of $G$, respectively, and where

$f($  $) = x_0$, and $f($  $) = y_0$.

**Thus *any* graph invariant that reduces with a) and b) is an evaluation of the Tutte polynomial.**

*Proof:* By induction on the number of edges.

# A reason to believe that the Potts model partition function is an evalution of the Tutte polynomial…

Note that if an edge has end points with different spins, it contributes nothing to the Hamiltonian, so in some sense we might as well delete it.

On the other hand, if the spins are the same, the edge contributes something, but the action is local, so the end points might be coalesced, i.e., the edge contracted, with perhaps some weighting factor.

Thus, the Potts Model Partition Function has a deletion-contraction reduction, and hence by the universality property, must be an evaluation of the Tutte polynomial.

# Amazing but true…

*The q-state Potts Model Partition Function is equivalent to the Tutte Polynomial!*

If we let $v = e^{\beta J} - 1$, then:

$$P(G;q,v) = q^{k(G)}\left(v\right)^{|V(G)|-k(G)} T\left(G;\frac{q+v}{v},1+v\right)$$

And in fact, $P(G;q,v) = Z\left(G;q,v\right) = \sum_{A\subseteq E(G)} q^{k(A)} v^{|A|}$

*The Potts Model Partition Function is a polynomial in q!!!*

Fortuin and Kasteleyn, 1972

(Texts by Bollobas or Welsh for good exposition)

# Computational Complexity

If we write $x = \frac{q+v}{v} = \frac{q}{v} + 1$ and $y = 1 + v$, then the Potts Model Partition Function is the Tutte polynomial evaluated on the hyperbola

$$(x-1)(y-1) = q$$

The Tutte polynomial is polynomial time to compute for planar graphs when $q$ = 2 (Ising model).

The Tutte polynomial is also polynomial time to compute for all graphs on the curve $(x-1)(y-1)=1$ and 6 isolated points. But elsewhere the Tutte polynomial is NP hard to compute (Jaeger, Oxley, Provan, Vertigan, Welsh—1990's).

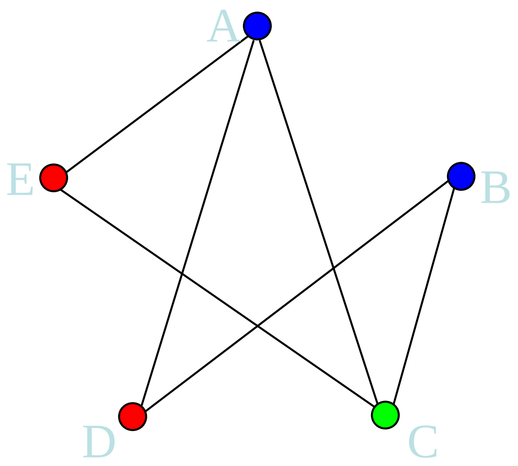
Thus the $q$-state Potts Model Partition Function is likewise computationally intractable. However, new computability results for the Tutte polynomial (bounded tree/clique width, e.g.) now hold for the Potts Model. (e.g. Oum & Seymour and Makowsky, Rotics, Averbouch, & Godlin

# Consider antiferromagnetic model at zero temperature

Now low energy $\leftrightarrow$lots of edges with *different* spins on endpoints.

At zero temperature, low energy states prevail, i.e. we really need to consider states where the endpoints on *every* edge are different.

Such a state corresponds to a *proper coloring* of a graph:



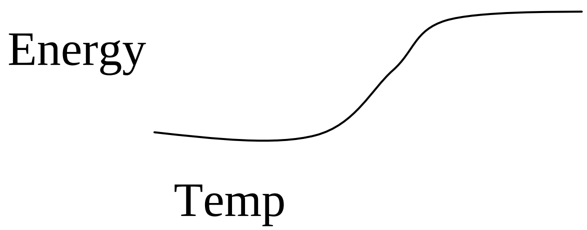
# Zeros of the chromatic polynomial

Let $\{G\}$ be an increasing sequence of finite graphs (e.g. lattices).

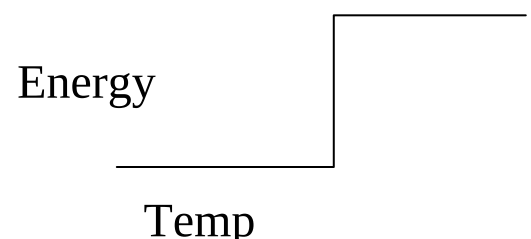
The (limiting) free energy per unit volume is:

$$f_{G_\infty}(q,v) = \lim_{n\to\infty} |V_n|^{-1} \log P(G_n; q, v)$$

Phase transitions (failure of analyticity) arise in the infinite volume limit, and correspond to the accumulation points of roots of the chromatic polynomial.




$$n \to \infty$$




This has changed the focus from real zeros (4-color theorem) to the locations of complex zeros, which can approach the real axis in the infinite limit. Now an emphasis on ‘clearing’ areas of the complex plane of zeros. (Choe, Oxley, Sokal & Wagner; Branden)

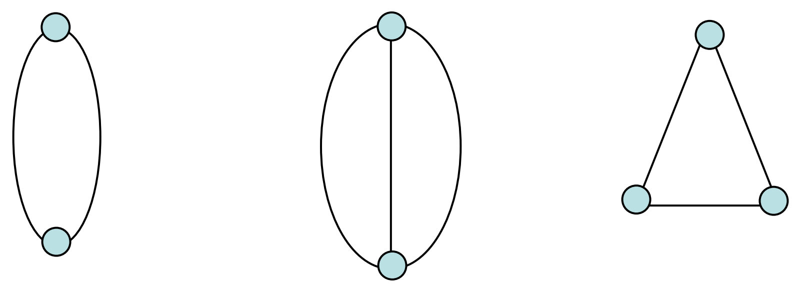
# Life gets interesting when interaction energies depend on the edge…

(Fortuin & Kastelin, Traldi, Zaslavsky, Bollobas & Riordan, Sokal, E-M & Traldi…)

No longer necessarily get a well-defined function.

*There are necessary and sufficient conditions on the relations among the edge-weights to guarantee this.*

These conditions essentially live on three small graphs:



# Can lose mulitiplicativity and invariance….

E-M & Zaslavsky

- Essential characteristics are captured by contraction/deletion
- Still need relations to assure well-defined BUT…*Retain universality properties and that a function is determined by action on 'smallest' objects (all discrete matroids not just a single bridge/loop).*
- AND…

$$\frac{Z[p]\mathcal{D}}{\Delta} \simeq \frac{Z[p]\mathcal{M}}{\Gamma}$$

that is:

$$\frac{\text{discrete matroids}}{\text{relations on little guys } \oplus \text{discretes}} \simeq \frac{\text{All matroids}}{\text{well-definedness relations}}$$