From Potts to Tutte and back again…

A graph theoretical view of statistical mechanics (with applications)

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VGN INBRE

NATIONAL INSTITUTES OF HEALTH NIH

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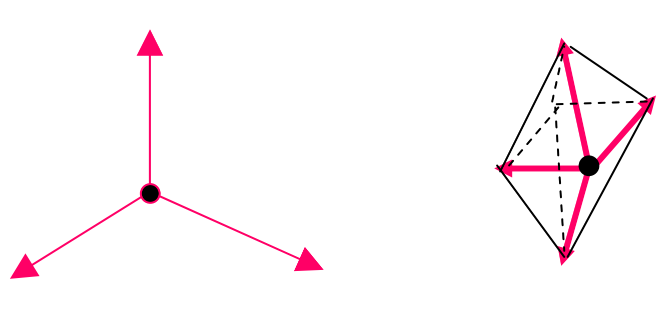
The Potts Model

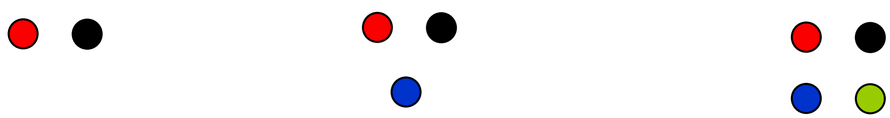
1952—(Domb)

Consider q possible states at each vertex in a network….



$q=2$ $q=3$ $q=4$

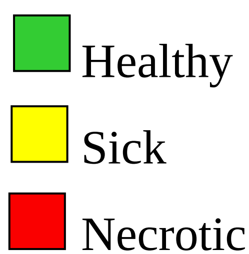
Orthogonal vectors



Colorings of the points with q colors

+

—



States pertinent to the application

The Hamiltonian

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

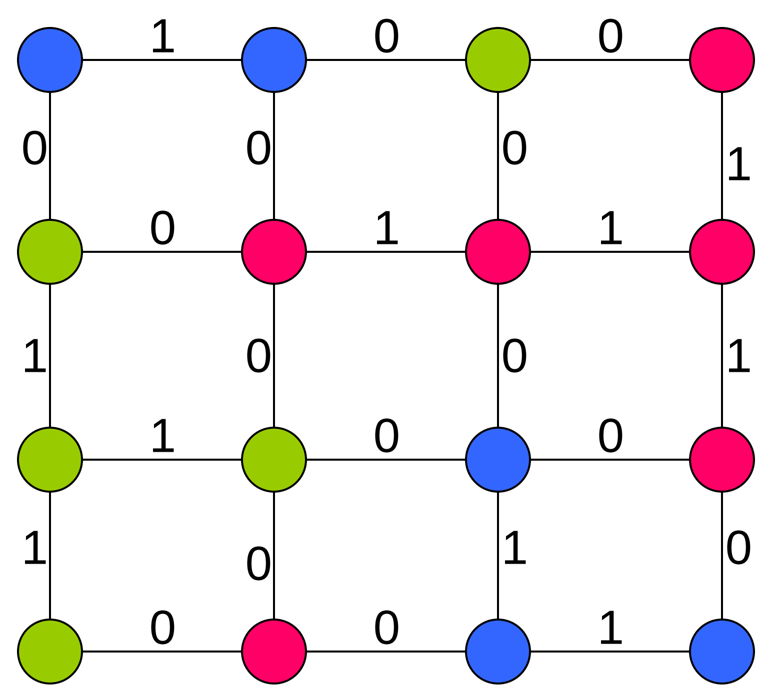
$$H(S) = \sum_{edges} -J\delta_{u,v}$$

J is the interaction energy between two adjacent points.

δ 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)

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

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

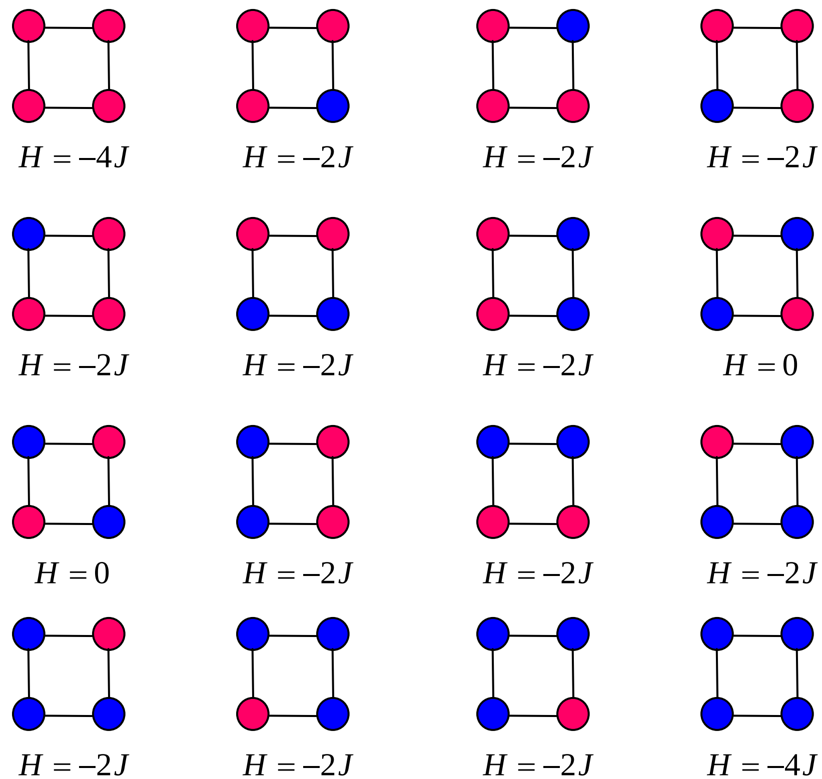
The numerator is easy. The denominator, called the *Potts Model Partition Function,* is the interesting (hard) piece.

Example

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

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

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



$$12\exp(2J\beta) + 2\exp(4J\beta) + 2$$

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)

Effect of Temperature

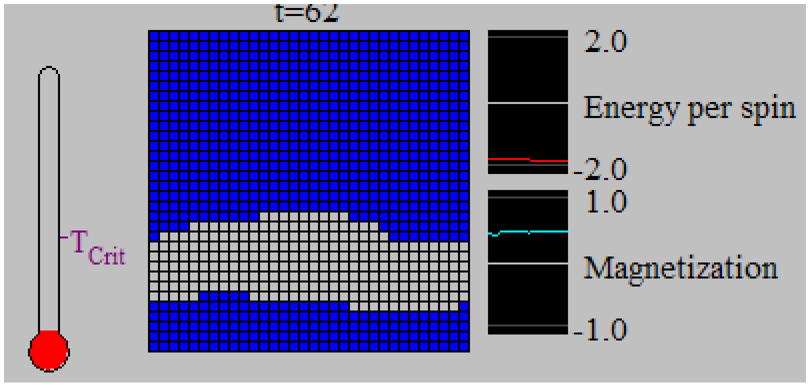
- Consider two different states **A** and **B**, with ***H*(*A*) < *H*(*B*)**. The relative probability of the system being in the two states is:

$$\frac{P(A)}{P(B)} = \frac{e^{-\beta H(A)}}{\sum_{\text{all states } \mathbf{S}} e^{-\beta H(\mathbf{S})}} \Bigg/ \frac{e^{-\beta H(B)}}{\sum_{\text{all states } \mathbf{S}} e^{-\beta H(\mathbf{S})}}$$

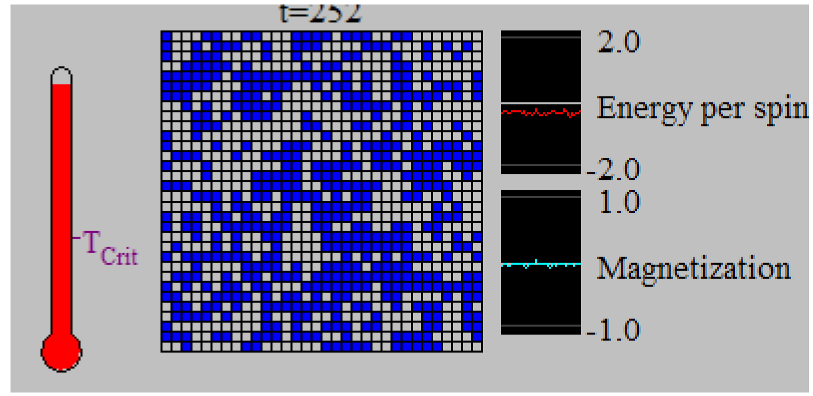
$$= \frac{e^{-\beta H(A)}}{e^{-\beta H(B)}} = e^{-\frac{D}{kT}} = e^{\frac{|D|}{kT}}, \text{ where } D = H(A) - H(B) < 0.$$

- At high temperatures (i.e., for ***kT*** much larger than the energy difference |**D**|), 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.

Ising Model at different temperatures



Cold Temperature



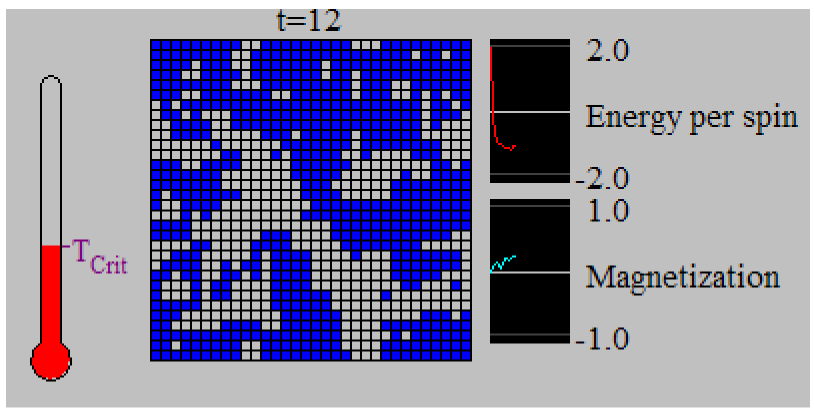
Hot Temperature

Here spins are +/- 1, and H is

$$\sum s_i s_j$$

With energy

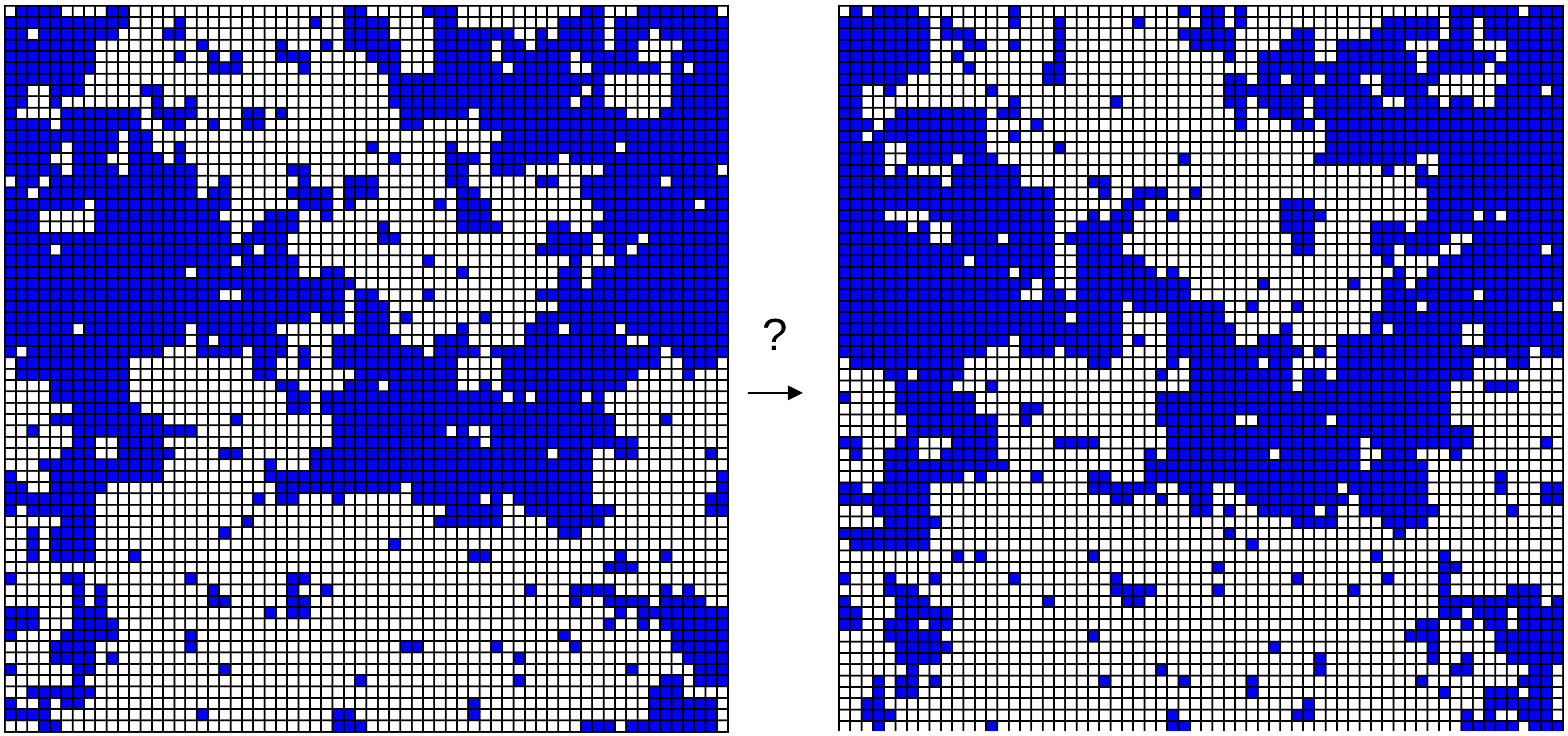
$$\frac{H}{\#\text{ of squares}}$$



Critical Temperature

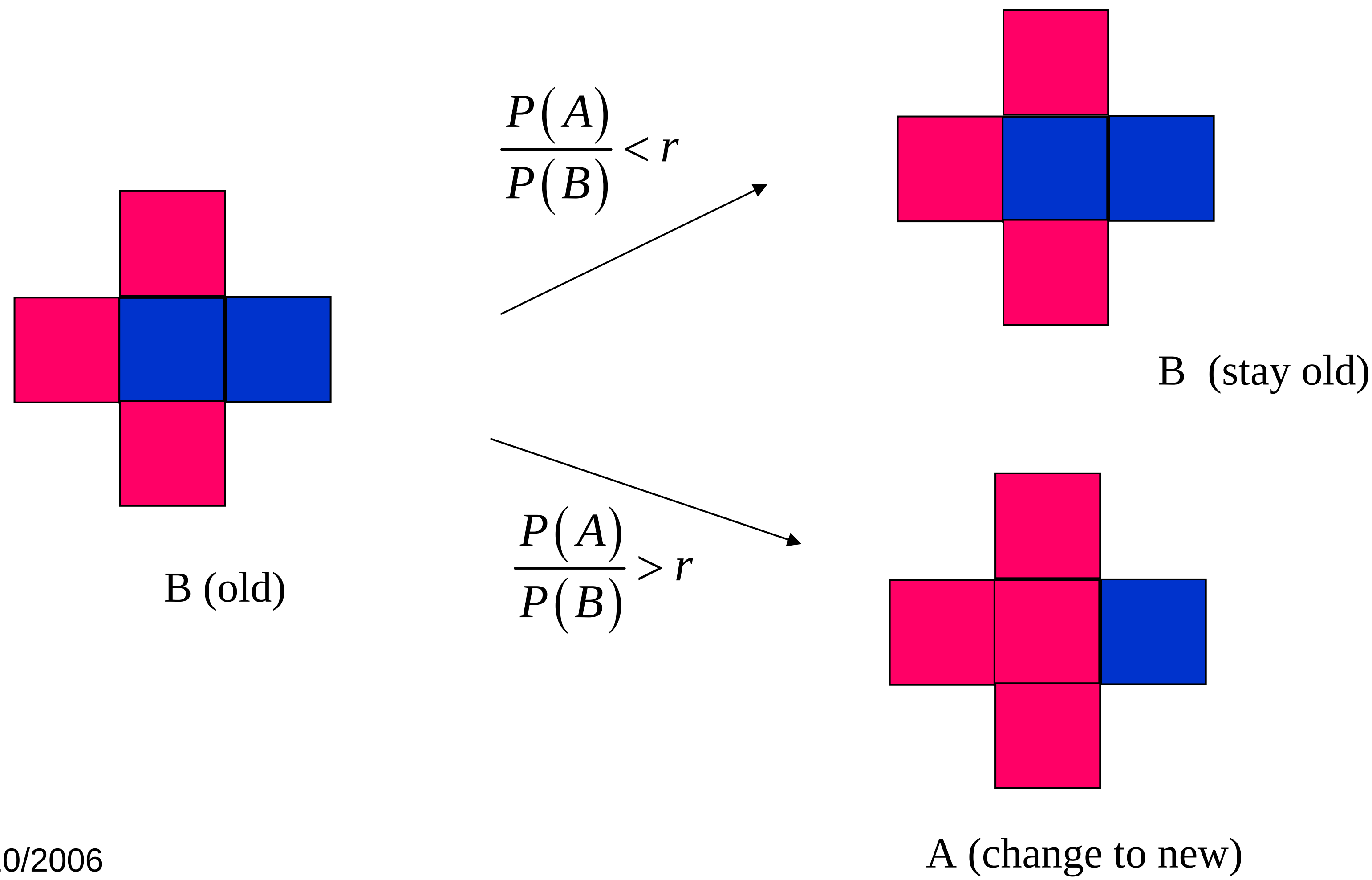
Images from http://bartok.ucsc.edu/peter/java/ising/keep/ising.html
http://bartok.ucsc.edu/peter/java/ising/isingAppletLarge.html

Monte Carlo Simulations



Monte Carlo Simulations

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



Capture effect of temperature

Given r between 0 and 1, and that $\frac{P(A)}{P(B)} = \exp\left(\frac{H(B) - H(A)}{kT}\right)$, with B the current state and A the one we are considering changing to, we have:

	High Temp	**Low Temp**
***H*(*B*) < *H*(*A*)** *B* is a lower energy state than *A*	exp('-'/*kT*) ~1	exp('-'/*kT*) ~ 0
	> *r*, so change states.	< *r*, so stay in low energy state.
***H*(*B*) > *H*(*A*)** *B* is a higher energy state than *A*	exp('+'/*kT*) ~1	exp('+'/*kT*) ~1
	> *r*, so change states.	> *r*, so change to lower energy state.

Applications of the Potts Model

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

- **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

Complex Systems with nearest neighbor interactions….

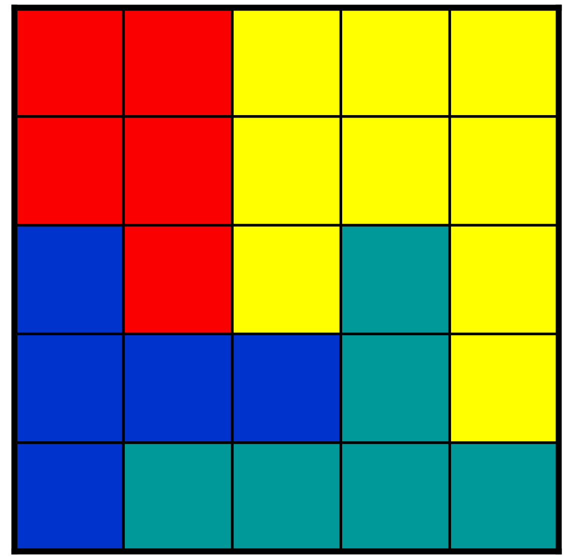
Foam Flows

A personal favorite…

Y. Jiang, J. Glazier, *Foam Drainage: Extended Large-Q Potts Model Simulation*

Studying foam drainage using the large-Q Potts model... profiles of draining beer foams, whipped cream, and egg white ...

$$H = \sum_{\{i,j\}} J(1-\delta_{\sigma_i\sigma_j}) + \lambda \sum_{n} (a_n - A_n)^2$$



The energy function is modified by the **area** of a bubble.

Results:

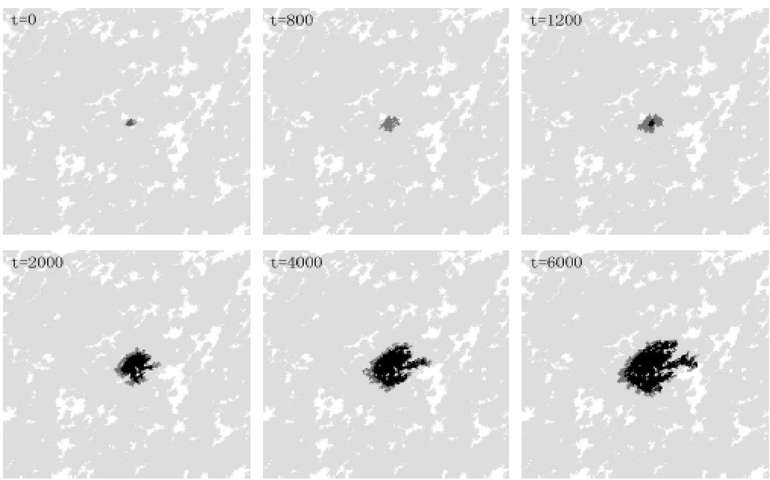
- Larger bubbles flow faster.
- There is a **critical velocity** at which the foam starts to flow uncontrollably

Biological Application

- This model was developed to see if tumor growth is influenced by the amount and location of a **nutrient**.

$$H = \sum_{ij} \sum_{ij} J_{\tau(\sigma_{ij})\tau(\sigma_{i'j'})} \left\{ 1 - \delta_{\sigma_{ij}\sigma_{i'j'}} \right\} + \sum_{\sigma} \lambda (v_\sigma - V_T)^2 + Kp(i, j)$$

- Energy function is modified by the volume of a cell and the amount of nutrients.



Results:

Tumors grow **exponentially** in the beginning.

The tumor migrated **toward** the nutrient.

Sun, L. Chang, Y. F. Cai, X. A Discrete Simulation of Tumor Growth Concerning Nutrient Influence.

Sociological Application

- The Potts model may be used to "examine some of the individual incentives, and perceptions of difference, that can lead collectively to segregation …".
- (T. C. Schelling won the 2005 Nobel prize in economics for this work)

Variables:

Preferences of individuals

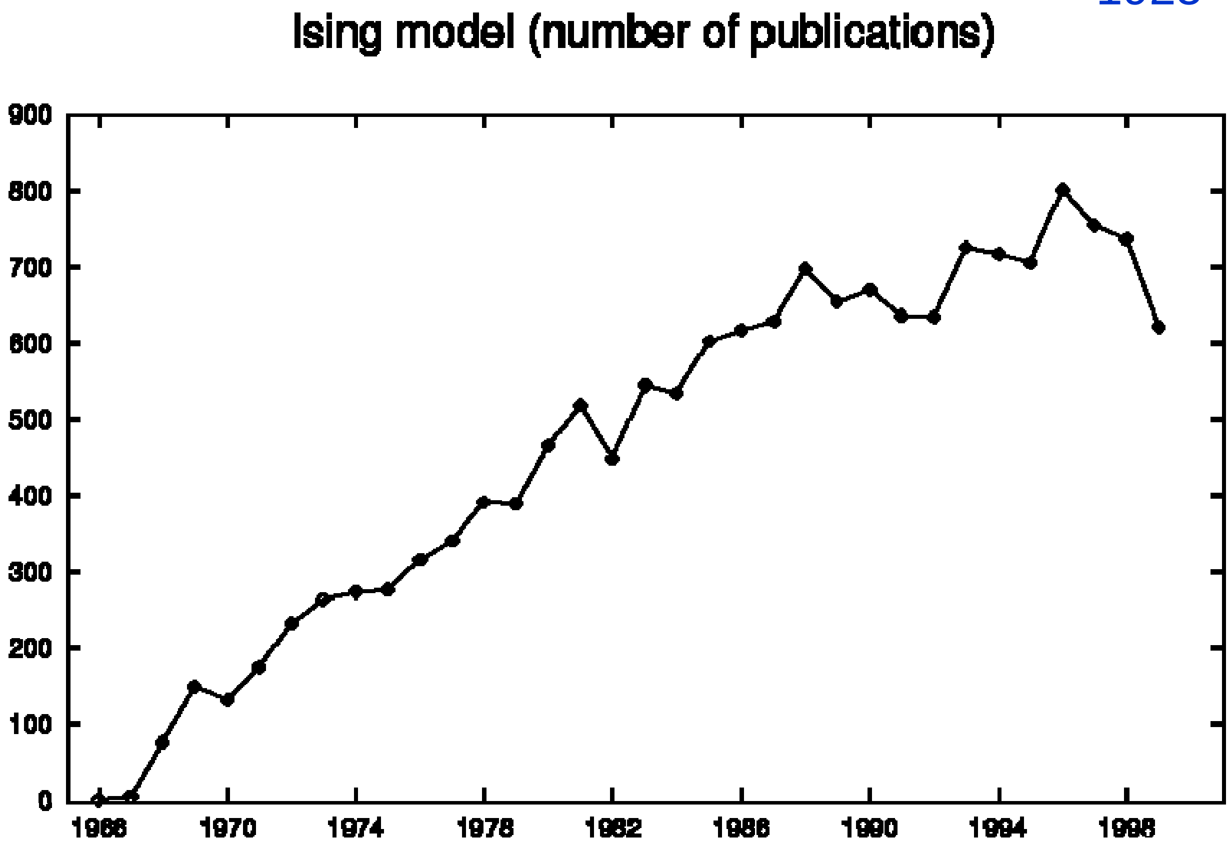
Size of the neighborhoods

Number of individuals

Schelling, Thomas C. *Dynamic Models of Segregation*. Journal of Mathematical Sociology

Ernst Ising 1900–1998

1925—(Lenz)

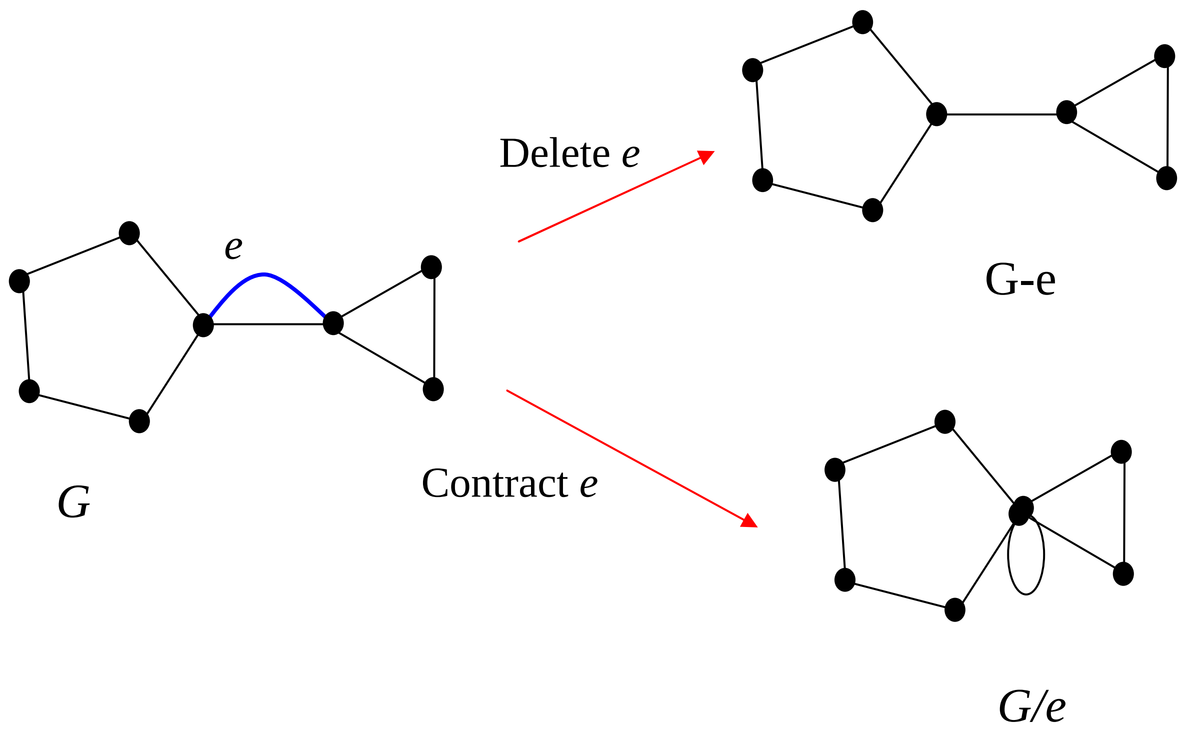


http://www.physik.tu-dresden.de/itp/members/kobe/isingconf.html

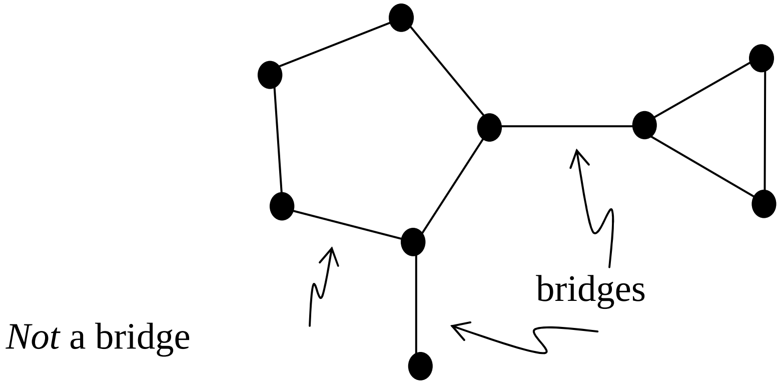
And now to Tutte…

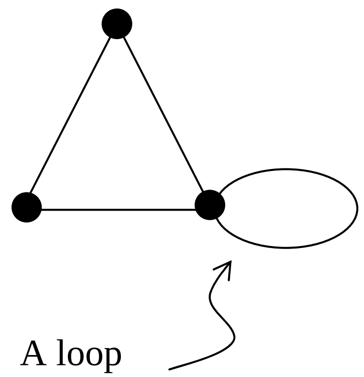
(with some preliminaries first)

Deletion and Contraction



Bridges and Loops





A *bridge* is an edge whose deletion separates the graph

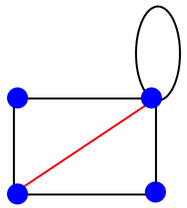
A *loop* is an edge with both ends incident to the same vertex

Tutte Polynomial

(Shaun Wylie.
161 Tutte titles)

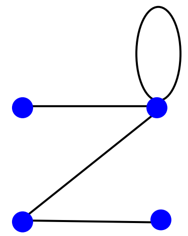
Let *e* be an edge of *G* that is neither a bridge nor a loop. Then,

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



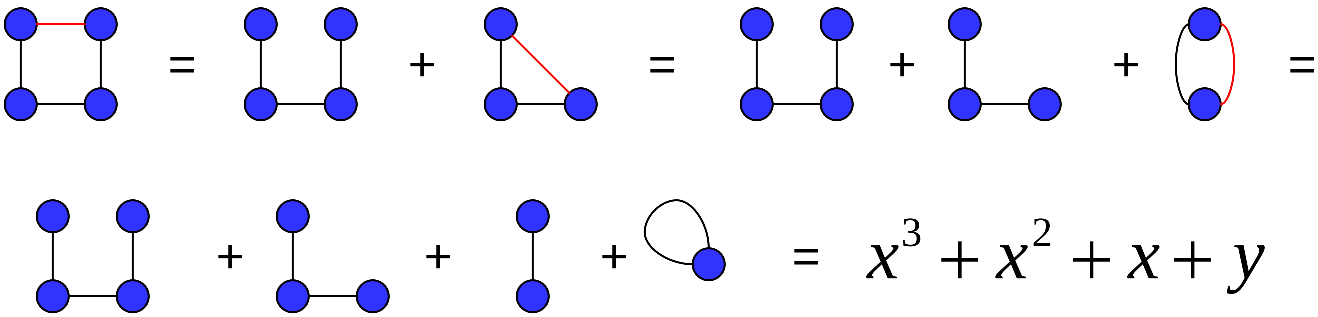
And if *G* consists of *i* bridges and *j* loops, then

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



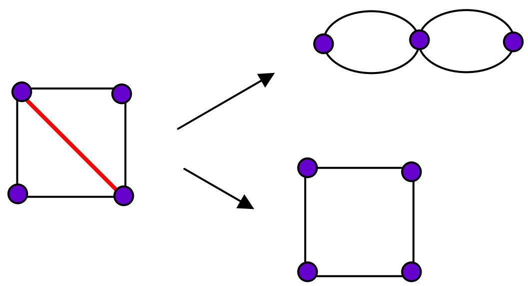
Example

The Tutte polynomial of a cycle on 4 vertices…

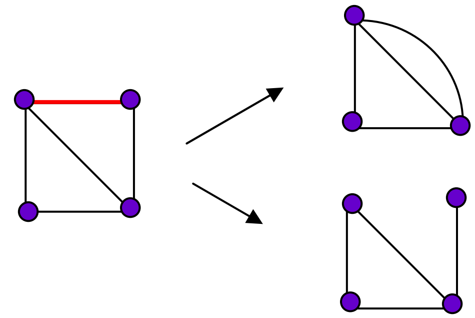


$= x^3 + x^2 + x + y$

Does the order of contraction/deletion matter?



vs.



The Dichromatic Polynomial:

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

Can show (by induction on the number of edges) that

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

TheTutte polynomial is independent of the order in which the edges are deleted and contracted!

Universality

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

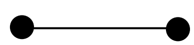
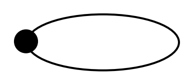
a) $f(G) = a\, f(G\text{-}e) + b\, f(G/e)$ whenever e is not a loop or an isthmus, and

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.

And back again….

The q-state Potts Model Partition Function is an evaluation of the Tutte Polynomial!

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

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

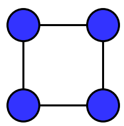
And in fact, $P(G;q,v) = Z(G;q,v) = \sum_{A \subseteq E(G)} q^{k(A)} v^{|A|}$

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

Fortuin and Kasteleyn, 1972

Example

Recall the Tutte polynomial of a 4-cycle:



$$\longrightarrow \quad x^3 + x^2 + x + y$$

Compute Potts from the Universality Theorem result:

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

Let $q = 2$ and $v = e^{\beta J} - 1$

$$2^1 \left(e^{J\beta} - 1\right)^3 \left[\left(\frac{e^{J\beta}+1}{e^{J\beta}-1}\right)^3 + \left(\frac{e^{J\beta}+1}{e^{J\beta}-1}\right)^2 + \left(\frac{e^{J\beta}+1}{e^{J\beta}-1}\right) + e^{J\beta}\right]$$

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

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.

Another reason to believe…

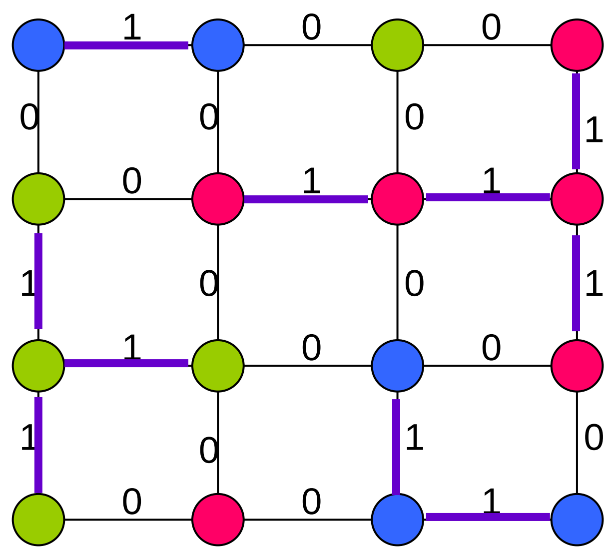
If $v = \left(1 - e^{\beta J}\right)$, then $\sum_{\text{states}} e^{-\beta H(w)} = \sum_{\text{states}} \prod_{edges} \left(v\delta(a,b)+1\right)$

$$= \sum_{A \subseteq E} q^{k(A)} v^{|A|}$$

What might we be counting here?

Inspiration: A is the set of edges labeled with 1, so these are exactly the number of edges contributing to the Hamiltonian, so give the exponent of v.

However, this then means that all the vertices in a component of A must have the same spin, so $q^{\#\ components}$ ways to assign the spins (sort of…).



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:

(1,1), (-1,-1), (j, j^2), (j^2, j), where $j = e^{\frac{2\pi i}{3}}$

But elsewhere the Tutte polynomial is NP hard to compute (Jaeger, Vertigan, Welsh, Provan—1990's).

Thus the q-state Potts Model Partition Function is likewise computationally intractable.

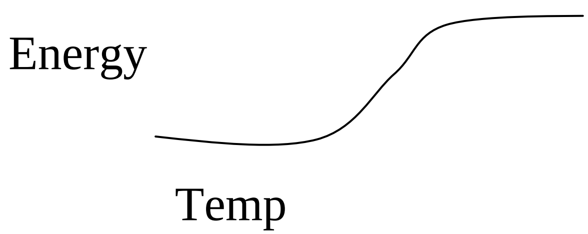
Phase Transitions and the Chromatic Polynomial

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

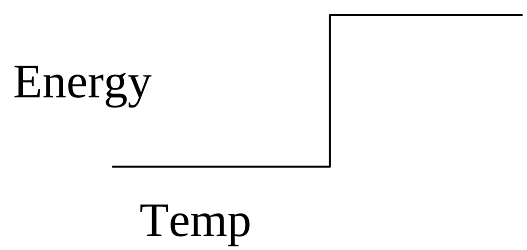
The (limiting) free energy per unit volume is:

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

Phase transitions (failure of analyticity) arise in the infinite volume limit.



$$n \to \infty$$

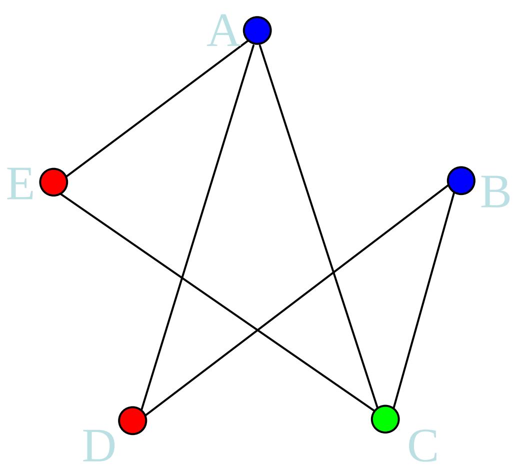


Consider antiferromagnetic model at zero temperature

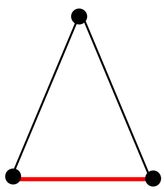
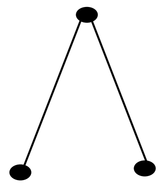
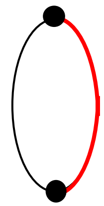
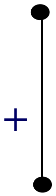
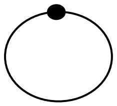
Now low energy ↔lots of edges with *different* spins on endpoints.

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:



Example

 =  -  = $n(n-1)^2$ +  + 

$$= n(n-1)^2 + n(n-1) + 0 = n^2 (n-1)$$

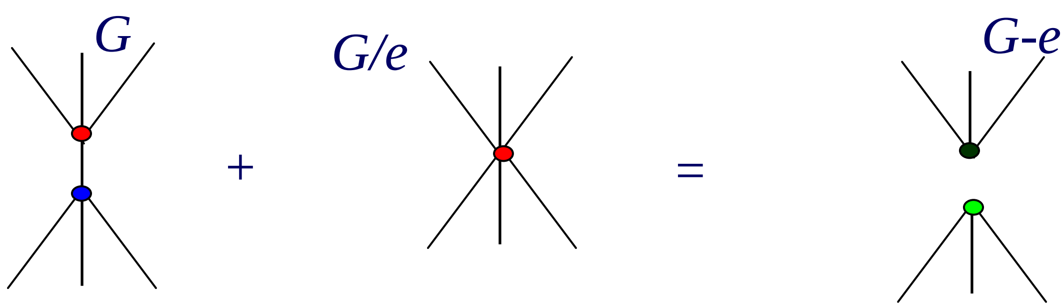
Since a contraction-deletion invariant, the chromatic polynomial

is an evaluation of the Tutte polynomial:

$$C(G;x) = (-1)^{|V|-k(G)} x^{k(G)} T(G;1-x,0)$$

Chromatic polynomial

The Chromatic Polynomial counts the ways to vertex color a graph: C(G, n) = # proper vertex colorings of G in n colors.



Recursively: Let e be an edge of G . Then,

$$C(G;n) = C(G-e;n) - C(G/e;n)$$

$$C(\bullet;n) = n$$

Zeros of the chromatic polynomial

- phase transitions correspond to the accumulation points of roots of the chromatic polynomial in the infinite volume limit

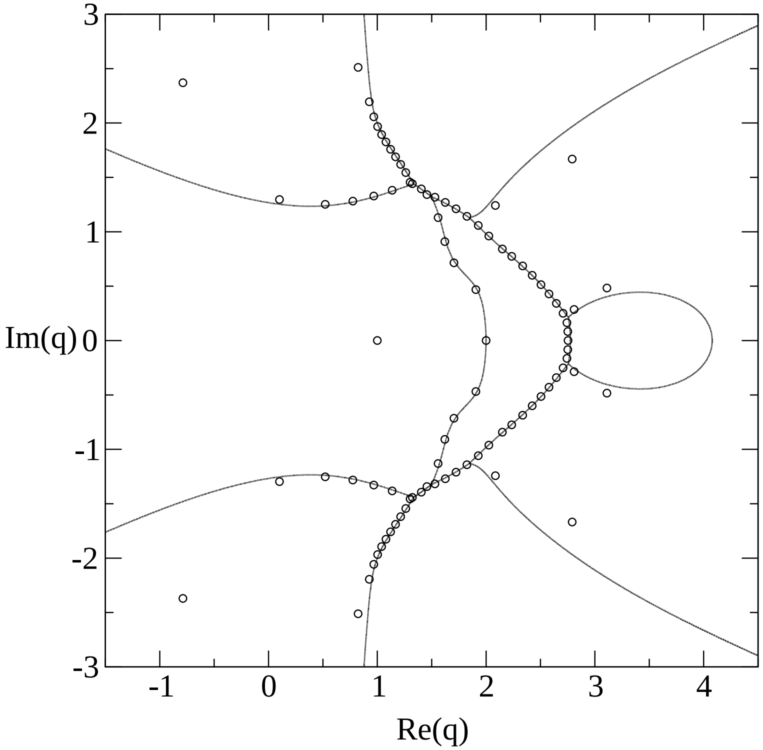
Locations of Zeros

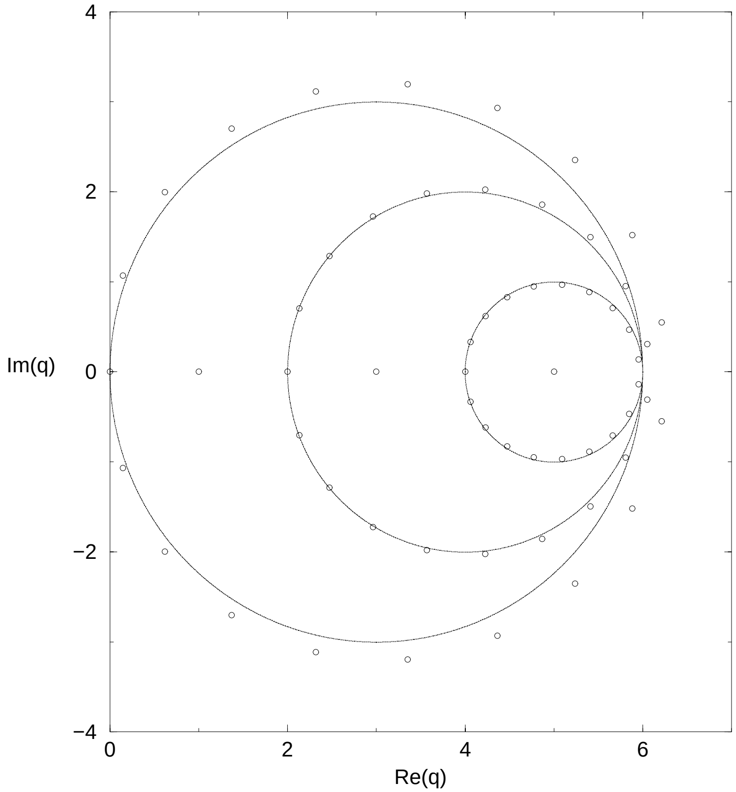
Mathematicians originally focused on the real zeros of the chromatic polynomial (the quest for a proof of the 4-color theorem…)

Physicists have changed the focus to the locations of complex zeros, because these can approach the real axis in the infinite limit.

Now an emphasis on ‘clearing’ areas of the complex plane of zeros.

Some zeros





(Robert Shrock)

What happens if….

- Interaction energy depends on the edge?
- Depends on whether the edge is contracted or deleted?
- Depends on whether the edge is a bridge or a loop?
- What if no longer multiplicative? (!)

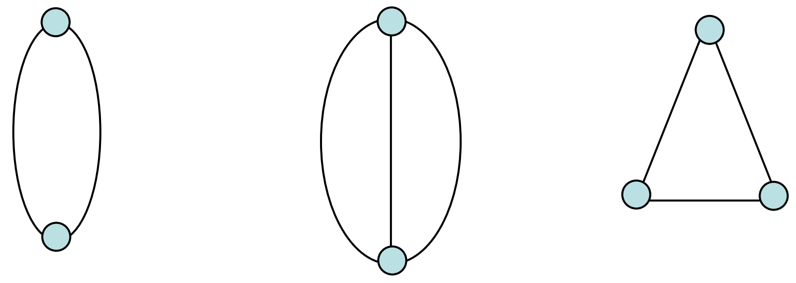
Fortuin and Kasteleyn, Traldi, Zaslavsky, Bollobas and Riordan, Sokal, E-M and Traldi, E-M and Zaslavsky….

Life gets interesting…

- 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….

- Essential characteristics encoded 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).

Thank you for your attention!

- Questions?

A very cool $q > 2$ Potts Model simulation

http://www.pha.jhu.edu/~javalab/potts/potts.html