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A Review of the Potts Model

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A Review of the Potts Model:

Its Connection to the Tutte Polynomial and its Application to Complex Experiments

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Abstract: This paper examines a mathematical modeling tool for complex systems with nearest neighbor interactions known as the Potts model. We begin by explaining the structure of the model and defining its Hamiltonian, probability function, and partition function. We then focus on the partition function, giving examples and showing the equivalence of two different formulations. We then introduce the Tutte polynomial, a well known graph invariant. We give details of the equivalence of the Tutte polynomial and the Potts model partition function. Since the Tutte polynomial, and hence the Potts model partition function, is computationally intractable, we explore Monte Carlo simulations of the Potts model. Finally, we discuss three applications illustrating how these simulations model real world situations.

1. INTRODUCTION

The Potts model studies long term behavior of complex systems. The model is able to investigate how the internal elements of the system react with one another based on certain characteristics that each element has. As these reactions take place macroscopic properties of the system will evolve. The Potts model has proven to be a very useful tool, with a wide variety of different applications in fields such as biology, sociology, physics, and chemistry.

The Potts model's origins date back to the mid 1900s. Two mathematicians, Julius Ashkin and Edward Teller [2], were among the first to experiment with a mathematical model which simulated behavior of various elements within a system. Intrigued by the model, Cyril Domb suggested the topic to his Ph.D. student, Renfrey B. Potts [11]. With the foundation set by Ashkin and Teller, Potts was able to construct a very useful model. In 1952 he published his doctoral thesis in which he described this particular model [11]. The form which the model takes today is known as the q-state Potts model. However, for the remainder of this paper we refer to the model as merely the Potts model for simplicity.

Scientists and mathematicians use the Potts model to study and predict stochastic outcomes of complex systems. For this reason, the Potts model has many applications in the area of statistical mechanics. Statistical mechanics combines the two subjects from which it gets its name. Statistics is used to study the numerous variables and predict outcomes, while mechanics studies how the internal particles react to certain outside forces. The Potts model is mainly used to study internal reactions within a system to predict what long term outcomes are most likely. [4]

This paper focuses on the mathematical structure and real world applications of the Potts model. We begin by giving a review of basic graph theory terminology used within the Potts model. Next we introduce the basic functions of the model by defining its Hamiltonian, probability distribution, and two different formulations of its partition function. We eventually prove that these two formulations only differ by a constant factor.

We then focus on the partition function. We show that the partition function is equivalent to the Tutte polynomial. Then we show how simulations can be used to approximate the partition function so that the model can be used to study real world phenomena. We conclude by outlining three experiments which use the Potts model to predict long term results.

2. PRELIMINARY DEFINITION AND CONCEPTS

The field of graph theory provides fundamental concepts for defining and analyzing the Potts model. A good introductory source for graph theory is [15]. We give the necessary concepts below.

Definition 2.1: A *graph* G consists of a finite set V of vertices and a set E of edges joining pairs of vertices. A *multigraph* is a graph which may have multiple edges between two vertices or vertices with loops.

Vertices will represent internal elements of an object or system, while the edges represent potential interactions between pairs of elements. An example of a generic graph is given in figure 2.1.

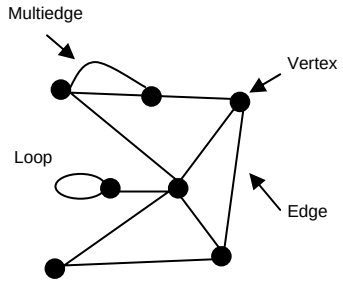


Figure 2.1: A generic graph.

For many applications it is expedient to assume that the graph has a regular structure, such as a lattice. Some common lattices are pictured below.

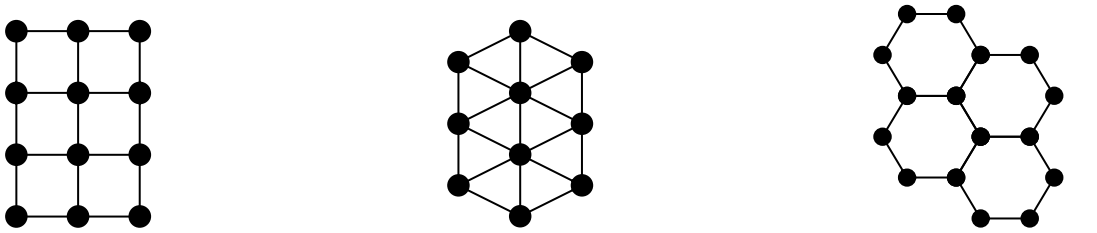


Figure 2.2: Different types of lattices.

Definition 2.2: A *complex* is highly structured object which can be modeled by a graph.

Examples of complexes include organizations of atoms, humans, fluids, and cells. All of these objects have a regular internal structure which allows for graph theoretical analysis.

Definition 2.3: We call two vertices *adjacent vertices* or *neighbors* if there exists an edge connecting them.

This concept suggests that elements can react with or influence one another based on their location in the graph.

Definition 2.4: A *connected component* of a graph, G, is the maximal subset of vertices in the graph such that there exists a path of edges between any two of the vertices.

3. THE POTTS MODEL

The Hamiltonian:

The Potts model is a mathematical modeling tool which mathematicians use to study the behavior of complexes. The structure of the Potts model allows researchers to investigate the internal elements of a complex and predict how they will interact with one another to determine the overall behavior of the complex. In other words, the model studies the microscopic internal elements and relates their interactions to the macroscopic outcome which can be observed over time. [4]

Definition 3.1: Let Q be a set of properties, and G be a graph. A *spin* at a vertex v is an assignment of an element of Q to v.

Every vertex of the graph will be assigned a spin. The combination of spin and adjacency determines which elements will interact with one another. Some common spins are temperature (hot or cold), magnetism (positive or negative), direction (up, down, or sideways), health (healthy, sick, or necrotic), and color (blue, green, red, or purple). In general we will denote the spins as $1..q$ where $q = |Q|$. When $q = 2$ the Potts model is known as the Ising model, after Ernst Ising who developed the model in the 1920's to study phase transitions. The Ising model has many important applications such as determining the critical temperature at which a magnet loses its magnetism. [6]

Definition 3.2: A *state* of a graph is a choice of spin at each vertex.

Figure 3.1: Two states of the a graph for $Q = \{\text{black, white}\}$.

Since the elements are assigned different spins and react with one another depending on their position on the lattice and their specific spins, there will be some measure of overall energy of the system. The function which measures the overall energy of a complex is the Hamiltonian. The Hamiltonian measures the energy of a particular state of a graph by assigning a value to every edge within the complex. This value will vary depending on the application. In the literature on the Potts model there are two dominant definitions for the Hamiltonian of a system. We will see in the next section that these definitions yield equivalent forms of the Potts model partition function.

Both definitions use the same notation, J is the interaction energy between adjacent elements of the system, and σ_i is the spin value assigned to vertex i in the state ω. They also use the *Kronecker delta function*,

$$\delta_{\sigma_i,\sigma_j} = \begin{cases} 1 & \text{if} \quad \sigma_i = \sigma_j \\ 0 & \text{if} \quad \sigma_i \neq \sigma_j \end{cases}.$$

Definition 3.3: The first Hamiltonian [5] is given by,

$$h_1(\omega) = -J \sum_{\{i,j\} \in E(G)} \delta_{\sigma_i,\sigma_j}$$

where ω is a state of a graph G.

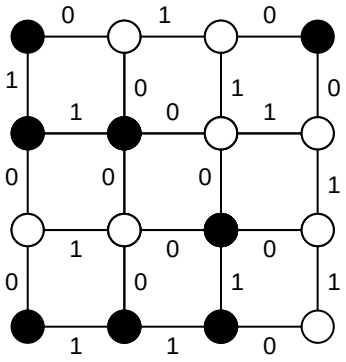
Definition 3.4: The other definition [17] for the Hamiltonian is,

$$h_2(\omega) = J \sum_{\{i,j\} \in E(G)} \left(1 - \delta_{\sigma_i,\sigma_j}\right).$$

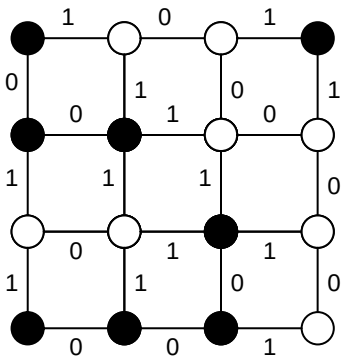
In definition 3.3 a 1 is placed on edges between neighbors with like spins and a 0 on edges with elements which have different spins. In the second definition of the Hamiltonian the opposite is true.

The following example calculates both Hamiltonians of a state ω of a 4×4 square lattice with spins of either white or black for each vertex.

Example 3.1:



In computing h_1 we place a 1 on edges between neighbors with like spins, and a 0 on edges between neighbors which have different spins. Thus $h_1(\omega) = -11J$.



In computing h_2 we place a 0 between adjacent neighbors with the same spin and a 1 between adjacent neighbors with opposite spins getting $h_2(\omega) = 13J$.

The Potts Model Partition Function:

In Example 3.1 we calculated the Hamiltonian of one state of the 4×4 lattice using both definitions. Notice that if we change one of the black elements to white, we get a completely different state with a different Hamiltonian measurement. In fact, there are q^n different states of a graph, where n is the number of vertices.

Definition 3.5: The *Potts model probability function* is the function which calculates the probability of finding the lattice in a particular state. This probability function depends on the Boltzmann distribution from statistical mechanics (for a system following the Boltzmann distribution laws the number of particles in a given energy state are exponentially distributed.)

$$\frac{\exp(-\beta h(\omega))}{\sum_{\substack{\text{all states} \\ \varpi \in \Omega}} \exp(-\beta h(\varpi))}$$

In this equation ω is the particular configuration and h may be either h_1 or h_2. We allow Ω to represent the set of all possible configurations of the lattice, therefore, ω and ϖ are elements of Ω. Also, $\beta = \frac{1}{\kappa T}$, where *T* represents the temperature of the system, and $\kappa = 1.38 \times 10^{-23}$ joules/Kelvin is the Boltzmann constant.

Definition 3.6: The *Potts model partition function* is the denominator of the Potts model probability function,

$$P_i = \sum_{\substack{\text{all states} \\ \varpi \in \Omega}} \exp(-\beta(h_i(\varpi))) .$$

[4]

The following example demonstrates how the probability function calculates the probability that a particular state ω will actually occur.

Example 3.2:

Let G be the graph in figure 3.2 and let $Q = \{\text{black, white}\}$. Compute the probability of the state ω occurring as a function of β and J.

$G =$ 

Figure 3.2: The graph G.

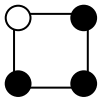
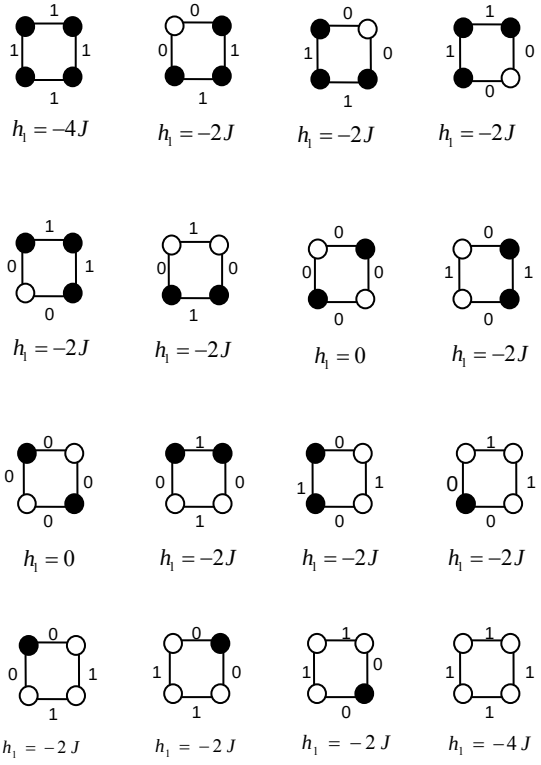
$\omega =$ 

Figure 3.3: One particular state of G .

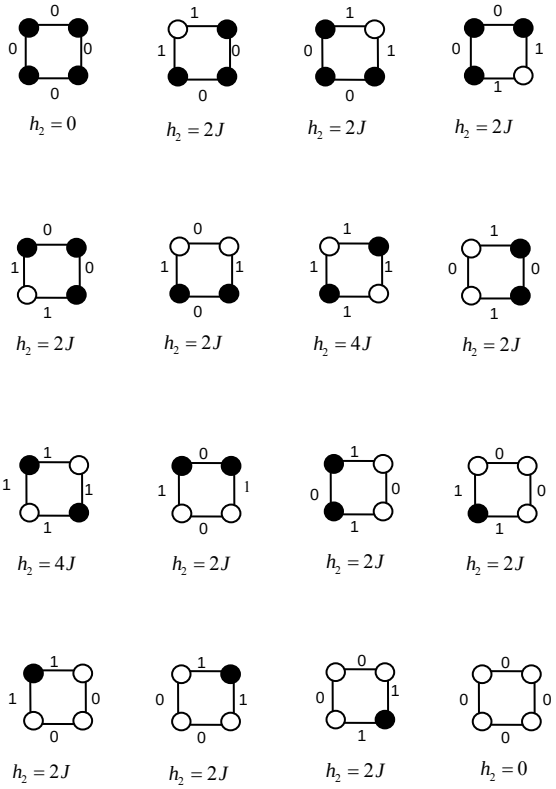
The first step is to find all the possible states and calculate their Hamiltonians. There are 16 possible configurations since the number of vertices is 4 and the number of spins is 2.



We can use these Hamiltonians in the Potts model probability function of definition 3.5 to find the probability of the state ω occurring out of all the possible states.

The probability of the state ω occurring is $P_1(\omega) = \dfrac{\exp(2\beta J)}{12\exp(2\beta J) + 2\exp(4\beta J) + 2}$.

The computation for the second Hamiltonian is similar. The Hamiltonians for the sixteen states are given below.



This time when we calculate the Potts model probability function the result is,

$$P_2(\omega) = \frac{\exp(-2J\beta)}{12\exp(-2J\beta) + 2\exp(-4J\beta) + 2}.$$

In Example 3.2 we were able to exactly compute the probability of the particular state. In fact, we can always calculate the numerator exactly. However computing the partition function is only tractable for small lattices and small values of q. In general, this function is NP-hard to compute.

Mathematicians explore properties of the Potts model partition function in a variety of ways. One way is to interpret it as an evaluation of the Tutte polynomial [17]. Another is to approximate the function using a simulation technique such as the Metropolis Algorithm [10]. This calculation is not exact, however, it allows researchers to use the Potts model to investigate complex applications.

4. AN EVALUATION OF THE TUTTE POLYNOMIAL

Basic Terminology:

The Tutte polynomial is a tool which mathematicians use to study properties of graphs. In this paper, we use the Tutte polynomial to calculate the Potts model partition function of graphical lattices in a number of special cases. Allow G to denote any general graph and e to represent an edge of G. Let, $|E(G)|$ denote the number of edges

in G, $|V(G)|$ the number of vertices, and $k(G)$ the number of connected components in G.

Tutte polynomial analysis uses two graph operations. These two operations are the deletion of an edge and the contraction of an edge. Write $G-e$ for the graph which results from deleting the edge e and G/e to for the graph which results from contracting edge e.

Figure 4.1 illustrates these two operations.

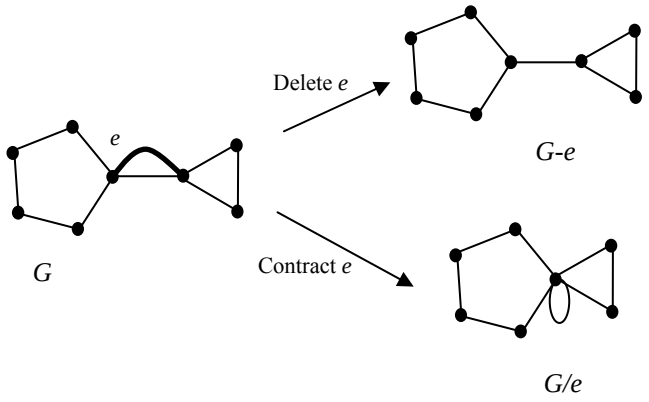


Figure 4.1: Deletion and contraction of edge *e* of a graph *G*.

Finally, we must define two important graphs. Denote the graph with two vertices and a single edge (bridge) between them by B and the graph with only one vertex and a single loop by L.

Figure 4.2: The graphs B and L

Defining the Tutte Polynomial:

Definition 4.1: The *Tutte polynomial T(G; x, y)* is defined using the following three recursive formulas.

a. $T(G;x,y)=T(G-e;x,y)+T(G/e;x,y)$ if e is not a bridge or a loop.

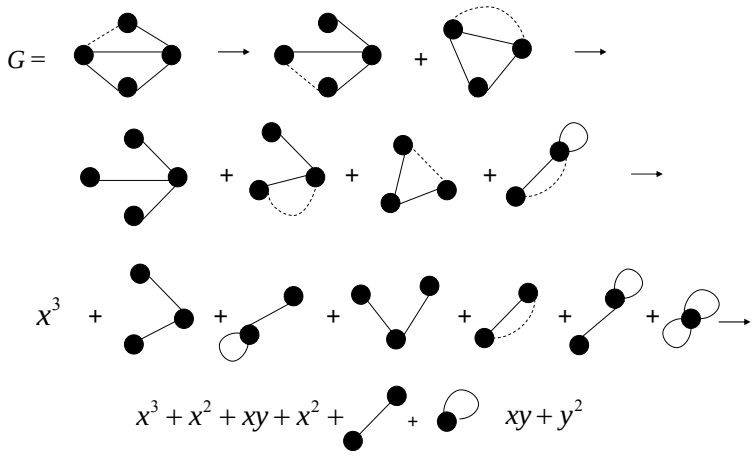
b. $T(G;x,y)=x^i y^j$ if G has only i bridges and j loops.

[15]

We give an example of computing the Tutte polynomial recursively in Example 4.1.

Example 4.1:

We use the deletion/contraction reduction of edges to reduce the graph to simply bridges and loops. The edge which we delete and contract in the following step is dotted to clarify the process. We use the deletion/contraction reduction until we are left with only bridges and loops. Bridges correspond to the variable x and loops correspond to the variable y.



Thus $T(G,x,y) = x^3 + 2x^2 + x + 2xy + y + y^2$

The Tutte polynomial is well defined; that is, one can delete and contract the edges in any order and the resulting polynomial will be the same. One proof that the Tutte polynomial is well defined involves showing by induction on the number of edges that

$$T(G;x,y) = \sum_{F \subseteq E} (x-1)^{k(F)-k(G)} (y-1)^{|F|-|V(G)|+k(F)},$$

where $k(F)$ is the number of connected components of the spanning subgraph of G induced by the edges in F. A spanning subgraph is a, not necessarily, connected subgraph of G that contains all the vertices of G. [3]

One fascinating property of the Tutte polynomial is its universality. There is a well known theorem which states that any multiplicative graph invariant which has a deletion/contraction reduction must be an evaluation of the Tutte polynomial.

Theorem 4.1 (see also [3])**:**

If $f(G)$ is a function on graphs such that

A. $f(G) = 1$ *if G consists of only one vertex and no edges,*
B. $f(G) = af(G-e) + bf(G/e)$ *whenever e is not a loop or a bridge,*

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

then f is an evaluation of the Tutte polynomial and takes the form

$$f(G) = a^s b^t T\left(G; \frac{x_0}{b}, \frac{y_0}{a}\right)$$

where

$s = |E(G)| - |V(G)| + k(G),\ t = |V(G)| - k(G)$ *and* $x_0 = f(B)$ and $y_0 = f(L)$.

The Potts Model as an Evaluation of the Tutte Polynomial:

Recall that the Potts model is only concerned with neighbors of a complex, and all complexes can be depicted as graphs. In the first definition of the Hamiltonian an edge between two neighbors on a lattice receives a value of 0 if the incident vertices (elements) do not have the same spin. Therefore, we can delete these edges. Also, if the incident elements do have the same spin the edges receive a value of 1. It makes sense, in this case, to contract these edges with some weighting factor. This is the intuitive rational for the Potts model partition function having a deletion/contraction reduction and thus being an evaluation of the Tutte polynomial.

The proof for showing that the Potts model partition function is an evaluation of, and in fact equivalent to, the Tutte polynomial involves showing that conditions A, B, and C of Theorem 4.1 hold for the form of the function. The next section outlines this proof.

Theorem 4.2 (see also [3])**:**

If

$$P(G, q, \beta) = \sum_{\substack{\text{all states} \\ \varpi}} \exp(-\beta h_1(\varpi))$$

then,

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

Proof

Recall that the Potts model partition function has the form,

$$P(G; q, \beta) = \sum_{\substack{\text{all states} \\ \varpi}} \exp(-\beta(h_1(\varpi))).$$

In order to prove that the Potts model is an evaluation of the Tutte polynomial we must show that conditions A, B, and C of Theorem 4.1 hold. We then apply the recursive

formulas from definition 4.1 to obtain the Tutte polynomial evaluation of the Potts model partition function.

First, consider two graphs G and H which are disjoint.

$$\begin{aligned} P(G\cup H;q,\beta) &= \sum_{\substack{\text{states } \omega \\ \text{of } G\cup H}} \exp\left(-\beta h_1(\omega)\right) \\ &= \sum_{\substack{\text{states } \omega_G \text{ of } G \text{ and} \\ \text{states } \omega_H \text{ of } H}} \exp\left(-\beta\left(h_1(\omega_G)+h_1(\omega_H)\right)\right) \\ &= \sum_{\text{states } \omega_G \text{ of } G} \exp\left(-\beta h_1(\omega_G)\right) \sum_{\text{states } \omega_H \text{ of } H} \exp\left(-\beta h_1(\omega_H)\right) \\ &= P(G;q,\beta)P(H;q,\beta). \end{aligned}$$

If G and H share a single vertex, then we allow $G*H$ to denote a graph in which a state of G and a state of H that have the same spin at the shared vertex r. Thus,

$$\begin{aligned} P(G*H;q,\beta) &= \sum_{\substack{\text{states } \omega \\ \text{of } G*H}} \exp\left(-\beta h_1(\omega)\right) \\ &= \sum_{\substack{\text{states } \omega_G \text{ of } G \text{ and} \\ \text{states } \omega_H \text{ of } H, \text{ with} \\ \text{the same spin at the} \\ \text{shared vertex}}} \exp\left(-\beta h_1(\omega_G)\right)\exp\left(-\beta h_1(\omega_H)\right) . \end{aligned}$$

Now, write $s(r)$ for the spin at a vertex r. We know

$$\sum_{\substack{\omega\in \text{ states of } G \\ \text{with } s(r)=a}} \exp\left(-\beta h_1(\omega)\right) = \sum_{\substack{\omega\in \text{ states of } G \\ \text{with } s(r)=b}} \exp\left(-\beta h_1(\omega)\right) ,$$

since if $s(r)=a$, simply changing all the vertices currently assigned value a to instead have value b gives a state with $s(r)=b$ and the same Hamiltonian. So,

$$\sum_{\omega\in \text{ states of } G} \exp\left(-\beta h_1(\omega)\right) = q \sum_{\substack{\omega\in \text{ states of } G \\ \text{with } s(v)=a}} \exp\left(-\beta h_1(\omega)\right) , \text{ or}$$

$$\sum_{\substack{\omega\in \text{ states of } G \\ \text{with } s(v)=a}} \exp\left(-\beta h_1(\omega)\right) = q^{-1} \sum_{\omega\in \text{ states of } G} \exp\left(-\beta h_1(\omega)\right) .$$

Thus we see that

$$\sum_{\substack{\text{states } \omega_G \text{ of } G \text{ and} \\ \text{states } \omega_H \text{ of } H, \text{ with} \\ \text{the same spin at the} \\ \text{shared vertex}}} \exp\left(-\beta h_1(\omega_G)\right)\exp\left(-\beta h_1(\omega_H)\right)$$

$$= \sum_{\omega_G \in \text{ states of } G} \left(\sum_{\substack{\omega_H \in \text{ states of } H \\ \text{with } s(v) \text{ in } \omega_H \\ \text{equal to } s(v) \text{ in } \omega_G}} \exp\left(-\beta h_1(\omega_G)\right) \exp\left(-\beta h_1(\omega_H)\right) \right)$$

$$= q^{-1} \sum_{\omega \in \text{ states of } G} \sum_{\omega \in \text{ states of } H} \exp\left(-\beta h_1(\omega_G)\right) \exp\left(-\beta h_1(\omega_H)\right)$$

$$= q^{-1} P(G;q,\beta) P(H;q,\beta).$$

We note that $G * H$ has one less component than $G \cup H$ because of the shared vertex. We define $\tilde{P}(G;q,\beta) = q^{-k(G)} P(G;q,\beta)$, where $k(G)$ is the number of connected components of G. We can now verify that Theorem 4.1 holds for $\tilde{P}(G;q,\beta)$.

Condition A:

Allow the graph G to be a single vertex. There are q possible spins at that vertex, and hence q states of G. The Hamiltonian of each state is zero since there are no edges. Thus $\tilde{P}(G;q,\beta) = q^{-1} \sum_{\omega \in \text{ state of } G} \exp(-\beta \cdot 0) = q^{-1} q = 1$.

Condition B:

Let $e = \{c,d\}$ be an edge of G which is neither a loop nor a bridge, and write $s(c)$ and $s(d)$ for the spins at c and d respectively. Then

$$\tilde{P}(G;q,\beta) = q^{-k(G)} P(G;q,\beta)$$

$$= q^{-k(G)} \sum_{\omega \in \text{ states of } G} \exp\left(-\beta h_1(\omega)\right)$$

$$= q^{-k(G)} \sum_{\substack{\omega \in \text{ states of } G \\ \text{with } s(c) \neq s(d)}} \exp\left(-\beta h(\omega)\right) + q^{-k(G)} \sum_{\substack{\omega \in \text{ states of } G \\ \text{with } s(c) = s(d)}} \exp\left(-\beta h(\omega)\right).$$

This step is possible since the spins will either be the same or different; there are no other possibilities.

Note that if $s(c) \neq s(d)$, then $h_1(\omega_G) = h_1(\omega_{G-e})$; and if $s(c) = s(d)$, then $h_1(\omega_G) = h_1(\omega_{G-e}) + J$, since there is no edge between c and d in $G - e$, but $s(c) \neq s(d)$ means that there is a contribution of 0 in the Hamiltonian for G, and $s(c) = s(d)$ gives a contribution of 1. Therefore,

$$q^{-k(G)} \sum_{\substack{\omega \in \text{ states of } G \\ \text{with } s(c) = s(d)}} \exp\left(-\beta h_1(\omega)\right) + q^{-k(G)} \sum_{\substack{\omega \in \text{ states of } G \\ \text{with } s(c) \neq s(d)}} \exp\left(-\beta h_1(\omega)\right)$$

$$= q^{-k(G)} \exp(J\beta) \sum_{\substack{\omega \in \text{ states of } G-e \\ \text{with } s(c) = s(d)}} \exp\left(-\beta h_1(\omega)\right) + q^{-k(G)} \sum_{\substack{\omega \in \text{ states of } G-e \\ \text{with } s(c) \neq s(d)}} \exp\left(-\beta h_1(\omega)\right).$$

We would like to see $\tilde{P}(G-e;q,\beta)$, and the right hand term almost gives it, since e neither a bridge nor a loop means that $k(G)=k(G-e)$, but we are missing the states of $G-e$ where $s(c)=s(d)$. So we will simply add and subtract them, getting

$$q^{-k(G-e)}\exp(J\beta)\sum_{\substack{\omega\in \text{ states of } G-e\\ \text{with } s(c)=s(d)}}\exp\left(-\beta h_{\mathrm{l}}(\omega)\right)+q^{-k(G-e)}\sum_{\substack{\omega\in \text{ states of } G-e\\ \text{with } s(c)=s(d)}}\exp\left(-\beta h_{\mathrm{l}}(\omega)\right)$$

$$-q^{-k(G-e)}\sum_{\substack{\omega\in \text{ states of } G-e\\ \text{with } s(c)=s(d)}}\exp\left(-\beta h_{\mathrm{l}}(\omega)\right)+q^{-k(G-e)}\sum_{\substack{\omega\in \text{ states of } G-e\\ \text{with } s(c)\neq s(d)}}\exp\left(-\beta h_{\mathrm{l}}(\omega)\right)$$

$$=q^{-k(G-e)}\sum_{\omega\in \text{ states of } G-e}\exp\left(-\beta h_{\mathrm{l}}(\omega)\right)+q^{-k(G-e)}\left(\exp(J\beta)-1\right)\sum_{\substack{\omega\in \text{ states of } G-e\\ \text{with } s(c)=s(d)}}\exp\left(-\beta h_{\mathrm{l}}(\omega)\right).$$

The first term is just $\tilde{P}(G-e;q,\beta)$. For the second term, note that since e is neither a bridge nor a loop, $k(G-e)=k(G/e)$. Also, the states of $G-e$ with $s(c)=s(d)$ correspond exactly to the states of G/e, and furthermore a state of $G-e$ with $s(c)=s(d)$ has the same Hamiltonian as the corresponding state of G/e. Thus, the second term becomes

$$q^{-k(G/e)}\left(\exp(J\beta)-1\right)\sum_{\omega\in \text{ states of } G/e}\exp\left(-\beta h_{\mathrm{l}}(\omega)\right)=\left(\exp(-\beta)-1\right)\tilde{P}(G/e;q,\beta).$$

This means that if e is neither a bridge nor a loop,

$$\tilde{P}(G;q,\beta)=\tilde{P}(G-e;q,\beta)+\left(\exp(J\beta)-1\right)\tilde{P}(G/e;q,\beta),$$

which satisfies Theorem 4.1, part b, with $a=1$ and $b=\exp(J\beta)-1$.

Condition C:

For part c, we use the observations we made at the beginning of this proof, that

$$P(G\cup H;q,\beta)=P(G;q,\beta)P(H;q,\beta), \text{ and}$$

$$P(G*H;q,\beta)=q^{-1}P(G;q,\beta)P(H;q,\beta).$$

Thus,

$$\tilde{P}(G\cup H;q,\beta)=q^{-k(G\cup H)}P(G\cup H;q,\beta)$$

$$=q^{-k(G)-k(H)}P(G;q,\beta)P(H;q,\beta)=\tilde{P}(G;q,\beta)\tilde{P}(H;q,\beta).$$

Similarly, recalling that $k(G*H)=k(G)+k(H)-1$, we have that

$$\tilde{P}(G*H;q,\beta)=q^{-k(G*H)}P(G*H;q,\beta)$$

$$=q^{-k(G)-k(H)+1}q^{-1}P(G;q,\beta)P(H;q,\beta)=\tilde{P}(G;q,\beta)\tilde{P}(H;q,\beta).$$

Now, $\tilde{P}(G;q,\beta)$ satisfies all the conditions of Theorem 4.1, so it only remains to find its value on a single bridge *B*, or loop *L*, in order to write it in terms of the Tutte polynomial.

For a loop, note that there are q states, and since both end points of a loop necessarily have the same value, h_{l} is always 1. Thus,

$$\tilde{P}(L;q,\beta) = q^{-1}\sum_{q \text{ states}} \exp\left(-\beta\left(-J\cdot 1\right)\right) = q^{-1}q\exp\left(J\beta\right) = \exp\left(J\beta\right).$$

For a bridge, note that there are q states where the spins on the end points are equal, each giving a Hamiltonian of 1. There are $q(q-1)$ states where the spins on the end points are different, each giving a Hamiltonian of 0. Thus,

$$\tilde{P}(B;q,\beta) = q^{-1}\left(q(q-1)\exp\left(-\beta\cdot 0\right) + q\exp\left(J\beta\right)\right) = \left(\exp\left(J\beta\right) + q - 1\right).$$

We are now ready to apply Theorem 4.1 with $a=1$, $b=\left(\exp\left(J\beta\right)-1\right)$, $y_0 = \exp\left(J\beta\right)$, and $x_0 = \left(\exp\left(-\beta\right)+q-1\right)$. If we let $\nu = \exp\left(J\beta\right)-1$. So,

$$\tilde{P}(G;q,\beta) = \left(\exp\left(J\beta\right)-1\right)^{|V(G)|-k(G)} T\left(G;\frac{q+\nu}{\nu},\exp\left(J\beta\right)\right)$$

$$= \nu^{|V(G)|-k(G)} T\left(G;\frac{q+\nu}{\nu},\exp\left(J\beta\right)\right).$$

Thus, since $\tilde{P}(G;q,\beta) = q^{-k(G)}P(G;q,\beta)$, it follows that

$$P(G;q,\beta) = q^{k(G)}\nu^{|V(G)|-k(G)} T\left(G;\frac{q+\nu}{\nu},\exp\left(J\beta\right)\right)$$

when we use h_1 for the Hamiltonian. ///
[3]

Theorem 4.3:

If

$$P_1(G;q,\beta) = \sum_{\substack{\text{all states}\\ \varpi\in\Omega}} \exp\left(-\beta h_1(\varpi)\right)$$

And

$$P_2(G,q,\beta) = \sum_{\substack{\text{all states}\\ \varpi\in\Omega}} \exp\left(-\beta h_2(\varpi)\right)$$

then $P_2(G,q,\beta) = \exp\left(-J\beta|E(G)|\right)P_1(G,q,\beta)$.

Proof

$$P_1(G;q,\beta) = \sum_{\substack{\text{all states}\\ \varpi}} \exp\left(-\beta h_1(\varpi)\right) = \sum_{\substack{\text{all states}\\ \varpi}} \exp\left(J\beta \sum_{\{i,j\}\in E(G)} \delta_{ij}\right)$$

$$P_2(G;q,\beta) = \sum_{\substack{\text{all states}\\ \varpi}} \exp\left(-\beta J \sum_{\{i,j\}\in E(G)} 1-\delta_{ij}\right)$$

$$= \sum_{\substack{\text{all states}\\ \varpi}} \exp\left(-\beta J \sum_{\{i,j\}\in E(G)} 1 + \beta J \sum_{\{i,j\}\in E(G)} \delta_{ij} \right)$$

$$= \exp\left(-\beta J \left|E(G)\right|\right) \sum_{\substack{\text{all states}\\ \varpi}} \exp\left(\beta h_1(\varpi)\right)$$

$$= \exp\left(-\beta J \left|E(G)\right|\right) P_1\left(G; q, \beta\right).$$

Thus,

$$P_2\left(G, q, \beta\right) = q^{k(G)} \exp\left(-J\beta \left|E\left(G\right)\right|\right) v^{|V(G)|-k(G)} T\left(G; \frac{q+v}{v}, \exp\left(J\beta\right)\right),$$

when we use h_2. Notice that the two forms of the Hamiltonian only differ by a factor of $\exp\left(-J\beta \left|E\left(G\right)\right|\right)$. ///

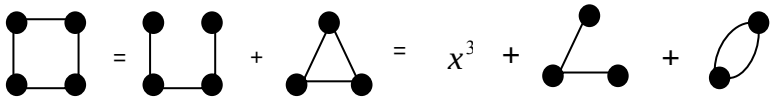
Examples of the Tutte Polynomial Evaluating the Partition Function:

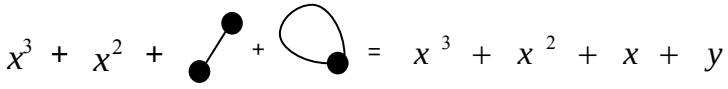
The following examples show how the Tutte polynomial is used to calculate the Potts model partition function of a simple lattice. We use an elementary lattice so that we can check our results using the actual definition of the Potts model partition function. Larger and more complicated lattices would not allow for this calculation for $q > 2$.

Example 4.2:

Recall Example 2.2 in which we calculated the Potts model probability function of a given configuration of a square. We found a partition function of $12\exp(2J\beta) + 2\exp(4J\beta) + 2$. In this example we will use the same square lattice with $q = 2$. We will show that the Potts model partition function is exactly the same as that for the Tutte polynomial definition of the partition function.

First we must calculate the Tutte polynomial of the graph.





Now we can substitute into equation (8) to get $P\left(G;\ 2,\ \beta\right) = 2^{k(G)} v^{|V(G)-k(G)|} \left[\left(\frac{q+v}{v} \right)^3 + \left(\frac{q+v}{v} \right)^2 + \left(\frac{q+v}{v} \right) + 1 + v \right]$. This evaluates to $12\exp(2J\beta) + 2\exp(4J\beta) + 2$.

We were able to obtain the same partition function using the definition involving the Tutte polynomial.

The Complexity of the Tutte Polynomial:

The Tutte polynomial does have its limitations. Evaluating the Tutte polynomial is NP-hard in general, meaning it is highly unlikely that someone will find an efficient way to compute the polynomial efficiently for all cases. However, there is a polynomial time algorithm for the Ising model when $q = 2$ and for a small number of special points. [16]

Because of the complexity of the Tutte polynomial, mathematicians were forced to come up with different ways of approximating the Potts model partition function to accommodate the numerous application of the model. Although this approach is not exact, approximations are sufficient for many important experiments involving Potts model mathematics.

5. MONTE CARLO SIMULATIONS

Potts model analysis relies heavily on probability. Since complexes are often very large with many different spin choices for their elements, the probability of a single state appearing out of the exponential number of states is nearly zero. Therefore, mathematicians are interested in what average characteristics the system is likely to exhibit in the long run.

With the aid of computer simulations mathematicians are able to predict what will happen to a complex over time depending on many different factors such as temperature, and other outside forces. The computer is given an initial state. Then it runs through the lattice to see if elements are stable in their spins or if their neighbors will influence them to change spins. At this point the computer calculates the probabilities of long run outcomes by choosing probabilistically accurate paths through the exponential number of states, depending on the stability of the internal elements. One of the most common types of simulations is known as a Metropolis Algorithm. [10]

The Metropolis Algorithm:

This method assigns probabilities to certain states by looking at the Hamiltonians and energies, and determining which states are more stable. The simulation begins with an initial state, labeled as *A*. The energy of this state is given by $\beta h_i(A)$ and can be represented as E_A. Next, the algorithm changes state *A* slightly to a new state labeled *B*, and computes its energy, $\beta h_i(B)$, which will be denoted E_B. At this point there are two possibilities for the system. If $E_B < E_A$ the probability of changing from state *A* to *B* is 1 since B has lower energy. However, if $E_B > E_A$, the probability that the lattice assumes the new state *B* is given by $p = \exp\left(-(E_B - E_A)/T\right)$ where *T* is the temperature of the

system. This temperature can be a literal temperature but it can also be any measure of the volatility of the system. [10]

This probability is calculated using relative probabilities of the two possible states. Recall the Potts model probability function. When we want to see which state is more likely we simply look at the relative probabilities of the two states by dividing one by the other. This calculation is given below.

$$\frac{\Pr(B)}{\Pr(A)} = \frac{\dfrac{\exp\left(-\beta h_i(B)\right)}{\sum_{\text{all states } \varpi} \exp\left(-\beta h_i(\varpi)\right)}}{\dfrac{\exp\left(-\beta h_i(A)\right)}{\sum_{\text{all states } \varpi} \exp\left(-\beta h_i(\varpi)\right)}} = \frac{\exp\left(-\beta h_i(B)\right)}{\exp\left(-\beta h_i(A)\right)} = \exp\left(-(E_B - E_A)/T\right)$$

As the temperature increases, this probability will also increase. However, as the system cools or becomes less volatile the system will settle into lower energy states. [10]

Once these probabilities are generated, the researcher is able to model a real world situation. Recall Example 3.2 using h_1 we found the partition function for the square lattice with 2 possible spins for its elements to be, $12\exp(2\beta J) + 2\exp(4\beta J) + 2$. The Metropolis Algorithm uses the temperature of the system to determine which states are more likely to occur over time.

Example 5.1:

In this example we determine the probability of a state with all one color occurring depending on the temperature of the lattice, by setting $J = k$.

Pr(all black, T=0.01) = .50 or 50%
Pr(all black, T=2.29) = .19 or 19%
Pr(all black, T=100,000) = .0625 or 1/16

Notice that when the temperature is very small the lattice will basically become all black or all white over time, since these are the states with the most stability and lowest energies. But, when the temperature is extremely high all 16 states seem to have an equally likely chance of occurring.

6. APPLICATIONS

Overview:

In this section we explore three unique applications of the Potts model. The first is a physical application in which the Potts model is used to simulate the behavior of foams. The second is a biological application which simulates the growth patterns of tumors. The final example is a sociological example where the Potts model is used to study human interactions.

Before we can explore these applications we must appreciate the complexity of the experiments. Recall the standard Hamiltonian $h_1 = -J\sum_{ij}\delta_{\sigma_i,\sigma_j}$. In these three applications the Hamiltonian will become a little more complex to capture external factors. These experiments use the following Hamiltonian.

$$H = -\sum_{ij} J_{ij}\delta_{\sigma_i,\sigma_j} - \sum_i f_{i\sigma_i}$$

In this case the strength of the interaction between neighboring elements J varies depending on their location on the lattice. The second sum is the addition of an outside force which also depends on the position within the lattice.

Physical Application:

The first experiment is described by Sanyal *et al* [12] in their article titled, "Viscous instabilities in flowing foams: A Cellular Potts Model." This experiment tracks a single large bubble as it flows through a foam. At first glance, foam flow may not seem to have many applications. However, "foams are of practical importance in applications as diverse as brewing, lubrication, oil recovery, and firefighting" [9]. Foams are present in many dangerous and challenging fields.

Sanyal *et al* [12] track the flow of foams to see what happens as their velocities increase. The authors begin by examining a lattice much like the one in Figure 6.1.

1	1	2	2
1	1	2	3
4	4	3	3
4	3	3	3
3	3	3	3

Figure 6.1: The lattice used to examine foams.

The elements in the experiment are not single lattice sites, but rather adjacent sites with the same spins represent a single bubble. In this case the bubble with the label 3 would be the large bubble.

The Hamiltonian for the experiment takes into account the energy of this system as well as the area of the bubbles.

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

The variable λ is the strength of the area constraint on the bubble. The unattainable value A_n is the area the bubble would assume if there were no forces acting on it, and a_n is the current area of the same bubble. The counter n is the number of bubbles.

> "The system evolves using Monte-Carlo dynamics. Our algorithm differs from the standard Metropolis Algorithm: we choose a spin at random but only reassign it if it is at a bubble wall and then only to one of its unlike neighbors. The probability of accepting the trial reassignment follows the

Boltzmann distribution (which is the standard distribution for finding probabilities using the Metropolis Algorithm)" [12].

The results of this experiment were very useful. By tracking a single large bubble through the foam the researchers were able to show that larger bubbles flow faster than smaller bubbles. They were also able to show that there is a critical velocity at which the foam starts flowing uncontrollably. These results would caution handlers to be aware of these phenomena. They may be more careful as to how much air is actually in the substance, to prevent large bubbles. They may also try to keep the flow below a certain velocity so that it stays under control.

Biological Application:

The second application involves studying a cancerous tumor. Sun *et al* [14] describe their experiment in the article titled "A Discrete Simulation of Tumor Growth Concerning Nutrient Influence." The authors use the Potts model to determine whether the amount and location of nutrients affects the growth pattern of a tumor.

The procedure begins by examining a lattice much like the one pictured below.

1	1	3	3	5	5
1	1	3	3	5	5
1	2	3	3	5	5
2	2	2	4	4	4
2	2	2	4	4	1
2	2	2	4	1	1

Figure 6.2: The lattice representing cells of human biology.

Here adjacent lattice sites with the same spin make up a single cell. For example, in figure 6.2 there are six individual cells, and two of the cells are of the same type indicated with the number 1.

The Hamiltonian used in this experiment is a bit more complicated than the previous application.

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

In this experiment $\tau(\sigma_{ij})$ gives the cell type and J varies depending on the type of cell. "If one of the grid points is not occupied by any cell, the interaction can also be modeled using a coupling constant $J_{cell-ECM}$," which measures the strength between the cell and its extracellular matrix [1] or its outer layer. The term $\lambda(\nu_{\sigma}-V_T)^2$ is the energy that growth and deformation of the cell requires. The unattainable variable V_T is the volume

which the cell would attain without any external forces. Finally, *p(i,j)* represents how much nutrient exists at the position *ij*.

There are three steps to this experiment. The first step is an evolution of a realistic cell cycle. The authors use the Metropolis Algorithm to get probabilistically accurate lattices with both healthy and malignant cells. The second step in the experiment investigates cell division. Cell division is a very intricate piece of cancer research. The authors define cell division as a function of the time since the cell last divided and the strength of cell energy. The final step is the control of the nutrient environment. In this experiment the sole nutrient source is a vein carrying iron on the left side of the tumor.

Once all three of these pieces are defined, the experiment can be performed. Monte-Carlo simulations are run to capture all of the variables and simulate how the tumor might grow.

From this experiment Sun *et al* [14] came up with two very important results. The simulation is pictured in Figure 4.3.

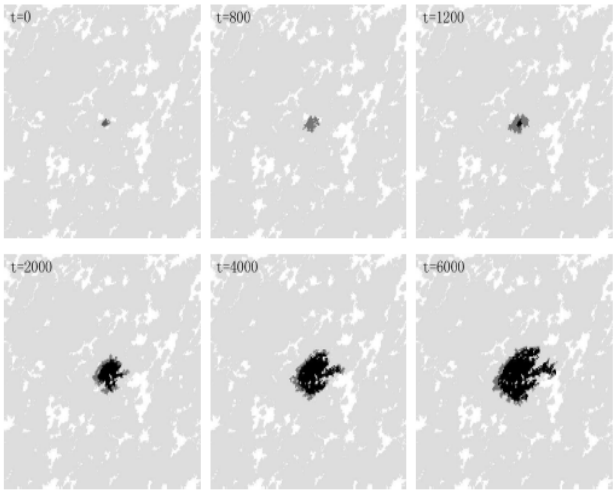


Figure 6.3: The results of the Tumor Growth experiment. [14]

The authors found that tumor growth is exponential in the beginning stages, but as additional malignant cells require more nutrients some begin to die and others can not multiply as quickly. The second result was that the tumor migrated toward the vein. If doctors can somehow use these results they may be able to make progress in the fight against cancer.

Sociological Application:

The final application studies human behavior. Although it does not use the Potts model directly, the model used in this experiment does have many of the same roots as the Potts model. The article titled, "Dynamic Models of Segregation" written by T. C. Schelling, a 2005 Nobel prize winner in Economics, describes a model very similar to the Potts model.

> "The paper examines some of the individual incentives, and perceptions of difference, that can lead collectively to segregation. The paper also examines the extent to which inferences can be drawn, from the phenomenon of collective segregation, about the preferences of individuals, the strength of those preferences, and the facilities for exercising them." [13]

The experiment begins by looking at a lattice much like the one pictured below.

x	*y*	*x*	*y*
	x	*y*	*x*
x		*y*	*y*
x	*x*	*x*	

Figure 6.4: Schelling's neighborhood

The $x's$ represent one group of people, while the $y's$ represent a different group.

Once the lattice has been constructed Schelling experiments with many different variables including the number of individuals per group, the way an individual defines their neighborhood, and the preferences of ratios within the neighborhood that people have. The experiment is conducted by looking at the overall lattice and finding all of the people who are unhappy. These people will change their position with some type of probability. Schelling defines different ways in which people can move around the lattice.

Schelling works through many different experiments to come up with some very compelling results on segregation. From this model it seems that people do consciously or subconsciously segregate themselves from people who are different than they are.

With a few slight alterations Schelling's experiment can be turned into a Potts model scenario. [7] uses a Potts-like model for a similar experiment exploring the formation of Ghettos in inner cities. This experiment is an extension of Schelling's brilliant work.

We too can imagine a Potts model for simulating human behavior in the following way. We will use a lattice to depict our neighborhood, city, business, or any other venue in which people interact with one another. This time we can use a few more groups. For example, we can have elderly people, college roommates, families with teenagers, and families with small children. To start with, members of each of these groups of people are living together in a brand new development. We label the elderly with a 1, the college roommates with a 2, the families with teenagers with a 3, and the families with small children with a 4. The beginning lattice might look something like the following.

1	2	3	4	1
2	2	1	2	3
4	1	3	4	2
3	3	2	4	4
1	3	4	2	1

Figure 6.5: Neighborhood with four different groups.

The members of these groups have preferences about who they live near. For example, the elderly do not want to live next to the college roommates because of the large parties that they tend to throw. The couples with small children might want to live next to one another so that their kids can play together without going far from home. We can develop these preferences in any way that fits reality.

The Hamiltonian for this experiment would measure overall happiness as opposed to energy. Outside forces might be the price of other houses in other neighborhoods, proximity to work, or how much people like their current house. The Metropolis Algorithm could then be run to develop higher probabilities for lattice states with higher overall happiness. Eventually, we would likely see preferences playing out in the form of segregation.

This is just a rough sketch of a Potts model scenario. Hopefully it has given the reader an appreciation for the versatility of the Potts model when it comes to real world situations.

7. CONCLUSION

The Potts model has been used to study phenomena such as foam flow, tumor growth, and human interaction. With models such as the Potts model we have been able to understand and predict long term outcomes of natural happenings. However, mathematicians still do not fully understand how to calculate the Potts model partition function for arbitrary graphs, or if it is even possible. As we develop higher and more complex mathematics, questions such as these will be answered and we will be able to better our lives with more knowledge of the world around us.

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