Between combinatorics and analysis (with a little help from statistical physics)

Alan Sokal

UCL Inaugural Lecture

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e.g.

Vertices Colors Edges



Map coloring countries



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Sudoku	boxes of 9×9 grid	numbers $1, \ldots, 9$	same row, same column, same 3×3 square

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• Note that here $P_G(q)$ is a polynomial in q

Theorem (Birkhoff 1912): For every graph G, $P_G(q)$ is the restriction to positive integers q of a polynomial in q (called the chromatic polynomial of G).



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In particular, we can ask about the real or complex roots of P_G .

Conjecture: For every planar graph G, the value q = 4 is *not* a root of the chromatic polynomial P_G , i.e. $P_G(4) \neq 0$.

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Or in simpler language:

Every planar graph can be (properly) colored with four colors.

Conjecture Theorem (Appel and Haken 1976): For every planar graph G, $P_G(4) \neq 0$.

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But the real or complex roots of P_G are still of interest ...
But first, a generalization ...

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 $W_{ij} = \begin{cases} 1 & \text{if } i \text{ is colored differently from } j \\ 1 + v_{ij} & \text{if } i \text{ is colored the same as } j \end{cases}$

• Note that if we take $v_{ij} = -1$ for all edges ij, then the weight becomes

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$$Z_G^{\text{Potts}}(q, \mathbf{v}) = \sum_{\text{colorings } \sigma} W(\sigma)$$

• Note in particular that $Z_G^{\text{Potts}}(q, -1) = P_G(q)$

• Potts (1952) introduced this as a model in statistical physics:

Each atom in a crystal lattice can be in any one of *q* states.



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Fortuin–Kasteleyn representation of the Potts model

Theorem (Fortuin + Kasteleyn 1969): For every graph G, $Z_G^{\text{Potts}}(q, \mathbf{v})$ is the restriction to positive integers q of a polynomial in q (and \mathbf{v}):

$$Z_G^{\text{Potts}}(q, \mathbf{v}) = \sum_{A \subseteq E} q^{k(A)} \prod_{e \in A} v_e$$

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Corollary (Birkhoff 1912): $P_G(q) = Z_G^{\text{Potts}}(q, -1)$ is a polynomial.

PROOF. Write

$$Z_G^{\text{Potts}}(q, \mathbf{v}) = \sum_{\sigma: V \to \{1, 2, \dots, q\}} \prod_{e=ij \in E} \left[1 + v_e \delta(\sigma_i, \sigma_j) \right]$$
where $\delta(\sigma_i, \sigma_j)$ is the Kronecker delta $\delta(a, b) = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{if } a \neq b \end{cases}$

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$$Z_G^{\text{Potts}}(q, \mathbf{v}) = \sum_{A \subseteq E} q^{k(A)} \prod_{e \in A} v_e$$

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- It includes the chromatic polynomial as a special case: $P_G(q) = Z_G(q, -1)$
- Note that Z_G(q, v) is multiaffine in v,
 i.e. of degree 1 in each v_e separately.

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and is connected with the physics of phase transitions.

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- But some changes are abrupt, e.g. water boiling or freezing.
- These abrupt changes are called phase transitions.
- Mathematically, a phase transition occurs whenever some physical quantity (e.g. density) varies nonanalytically as a function of some control parameter (e.g. temperature).

("nonanalytic" = in sense of complex analysis)

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The discontinuity at h = 0 is a phase transition.

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The partition function $Z_G(q, \mathbf{v})$ is a polynomial in q and \mathbf{v} , and all physical quantities will be ratios of polynomials. That is as analytic as one can possibly get! How can such a phase transition occur in the Ising or Potts model on a finite graph G?

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MORAL: Phase transitions never occur in a physical system with finitely many degrees of freedom.

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But for all practical purposes that is a phase transition!

So it makes sense to first study phase transitions in an idealized system where the discontinuity is a true discontinuity:

namely, the Ising or Potts model on an infinite graph, such as the square lattice \mathbb{Z}^2 :



The infinite-volume limit

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Instead we need to consider a sequence $\{G_n\}$ of finite graphs converging to G (e.g. larger and larger squares in \mathbb{Z}^2) — the so-called infinite-volume limit. But $Z_G(q, \mathbf{v})$ makes no sense for an infinite graph G (e.g. \mathbb{Z}^2).

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It then turns out that $\lim_{n \to \infty} Z_{G_n}(q, \mathbf{v})$ does not exist, but $f(q, \mathbf{v}) = \lim_{n \to \infty} \frac{1}{|G_n|} \log Z_{G_n}(q, \mathbf{v})$ does.

(Physicists call *f* the free energy per unit volume.)

A fact from real analysis

How do phase transitions occur in the infinite-volume limit?

FACT: If (f_n) is a pointwise convergent sequence of real-analytic functions of a real variable, then the limiting function f need not be analytic — indeed, need not even be continuous.

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ANSWER: The domains D_n may not be uniform in n. Singularities may creep in from the complex plane and pinch the real axis as $n \to \infty$.

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ANSWER: The domains D_n may not be uniform in n. Singularities may creep in from the complex plane and pinch the real axis as $n \to \infty$.

EXAMPLE:
$$f_n(x) = \tanh(nx)$$
 has poles at $x = \pm \frac{\pi}{2n}i$.

Apply the above to
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- Promote one or more physical quantities (e.g. temperature) to complex variables.
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The Yang–Lee approach to phase transitions:

- Promote one or more physical quantities (e.g. temperature) to complex variables.
- Investigate the complex zeros of the partition function Z_{G_n} .
- The real limit points (as $n \to \infty$) of those complex zeros are the possible points of phase transitions.

The Lee–Yang theorem for the Ising model

Therefore ... If a domain $D \subset \mathbb{C}$ is free of zeros (uniformly in the volume G_n), then the intersection of D with the real axis is free of phase transitions.

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Example: Lee–Yang theorem for the ferromagnetic Ising model.

Consider a ferromagnetic Ising model with complex magnetic field h. Then the zeros of $Z_{G_n}(h)$ lie only on the imaginary axis.

Conclusion: The only possible phase-transition point is h = 0.

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P.S. The Lee–Yang theorem is actually a beautiful theorem about zeros of multiaffine polynomials in several complex variables. The result quoted above is a mere corollary.

Phase transitions, summarized ...

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This motivates studying the complex roots of the chromatic polynomial $P_G(q)$.

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But first ... some facts about the real roots ... to motivate some conjectures about the complex roots.

• $P_G(q) \neq 0$ whenever q < 0

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- $P_G(q) \neq 0$ whenever q < 0(The coefficients of $P_G(q) = \sum_{k=1}^n a_k q^k$ alternate in sign)
- For planar G, $P_G(q) > 0$ whenever $q \ge 5$ (Birkhoff + Lewis 1946)
- Birkhoff–Lewis conjecture:

For planar G, $P_G(q) > 0$ whenever $q \ge 4$

Complex roots of the chromatic polynomial

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Complex roots of the chromatic polynomial

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Complex roots of the chromatic polynomial

- Recall $P_G(q) \neq 0$ whenever q < 0
- Is this the tip of the iceberg of a Lee–Yang-type theorem?
- Conjecture (Farrell 1980): $P_G(q) \neq 0$ whenever $\operatorname{Re} q < 0$

Chromatic roots of cubic graphs on 16 vertices



Chromatic roots of cubic graphs on 16 vertices



Chromatic roots of cubic graphs on 18 vertices



Chromatic roots of cubic graphs on 18 vertices



Chromatic roots of cubic graphs on 20 vertices



Chromatic roots of cubic graphs on 20 vertices



Complex roots of the chromatic polynomial (2nd try)

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- In particular, we can make $v_{\text{eff}} = -q$, which gives a zero of $Z_G(q, \mathbf{v})$. QED
- For the chromatic polynomial (v = -1), $\left|\frac{v}{q+v}\right| < 1$ means |q-1| > 1. This is where the chromatic roots are dense.

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- But other graph-theoretic parameters can: (maximum degree, maxmaxflow, ...)
- What determines where the chromatic roots of a graph go in the complex plane?
- We know very little at present.
- The study of chromatic roots is still a very young field.

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