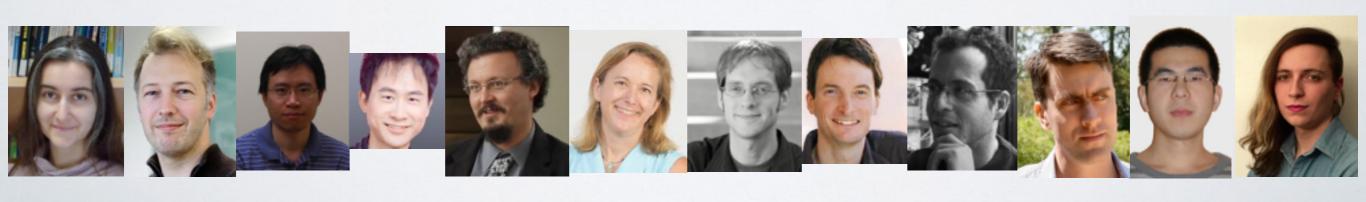
Phase Transitions in Community Detection and Clustering

Cristopher Moore, Santa Fe Institute

joint work over the years with Aurelien Decelle, Lenka Zdeborová, Florent Krzakala, Xiaoran Yan, Yaojia Zhu, Cosma Shalizi, Lise Getoor, Aaron Clauset, Mark Newman, Elchanan Mossel, Allan Sly, Pan Zhang, and Jess Banks





How can we find patterns in data?

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Fundamental limits

Phase transitions

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Optimal algorithms

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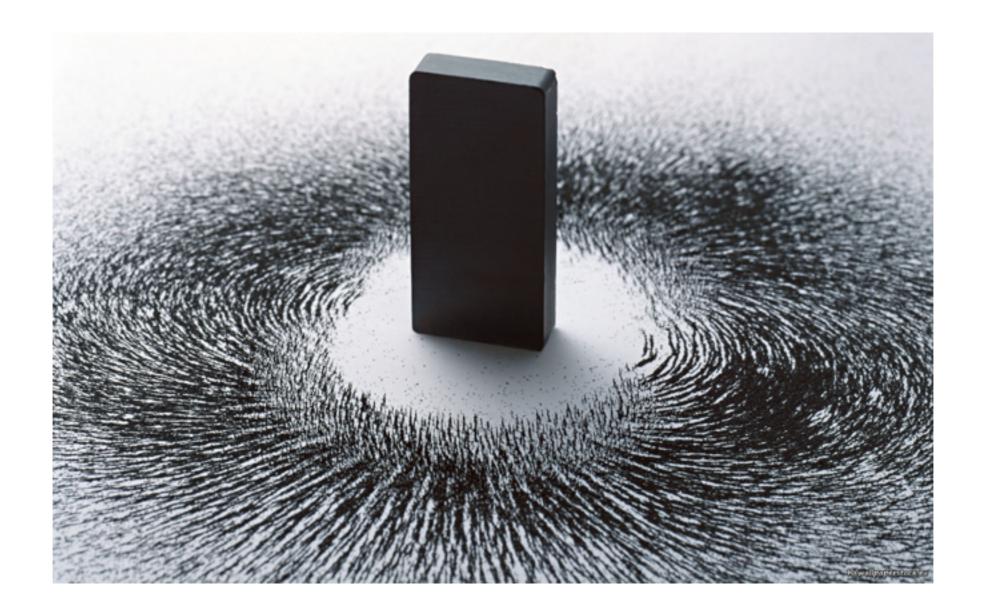
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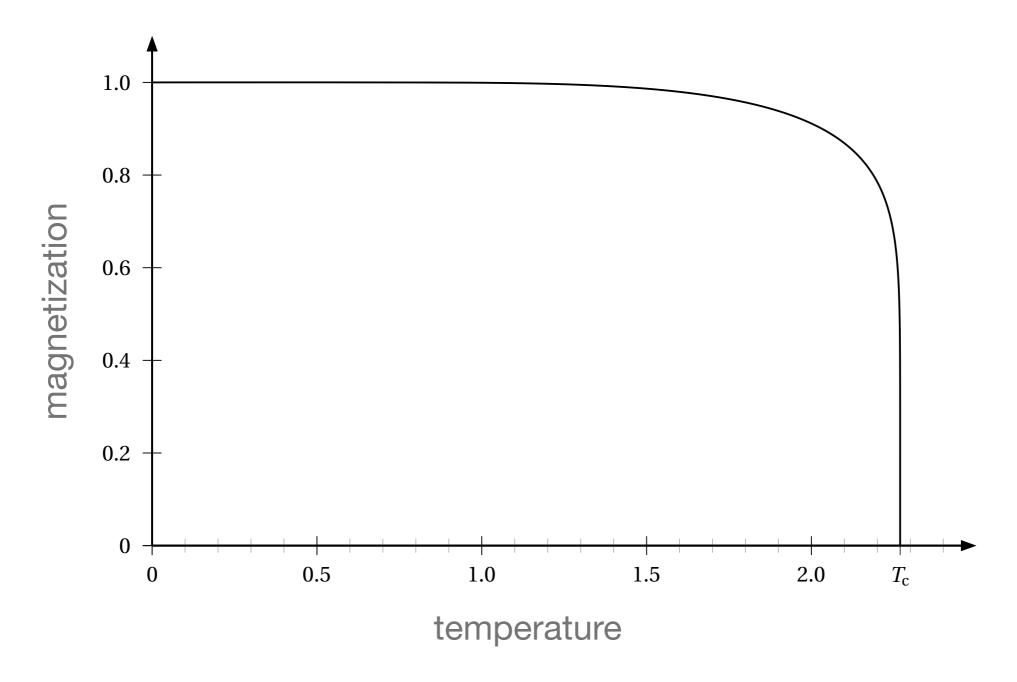
Statistical inference ⇔ statistical physics

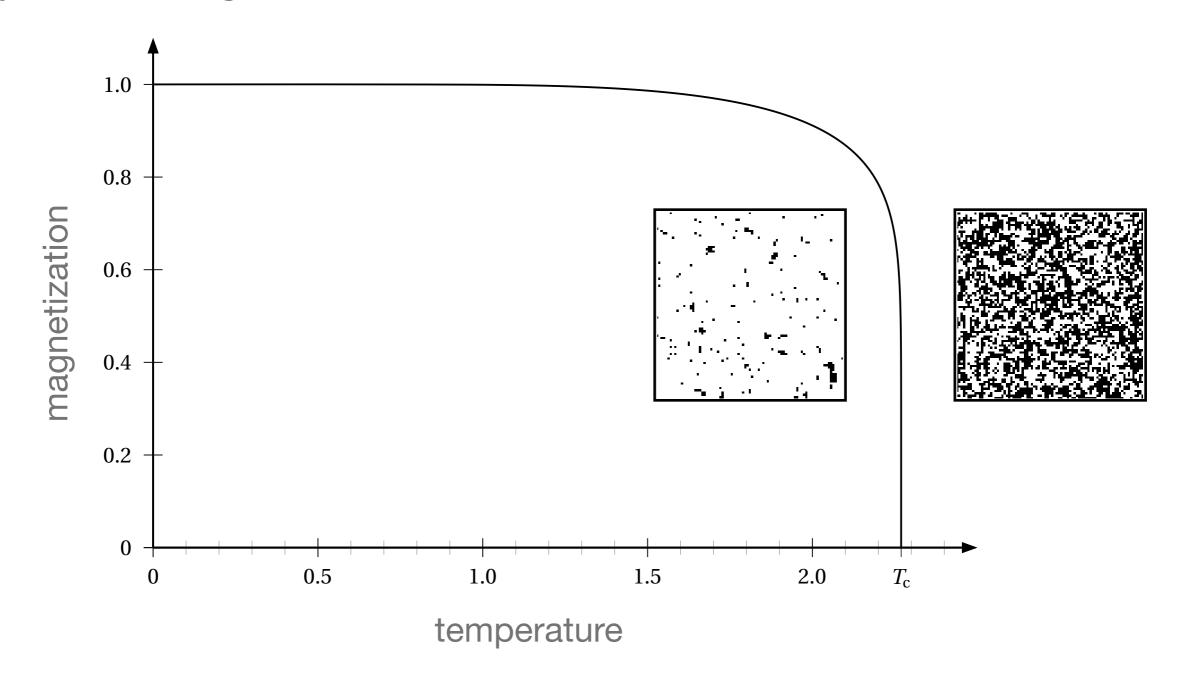


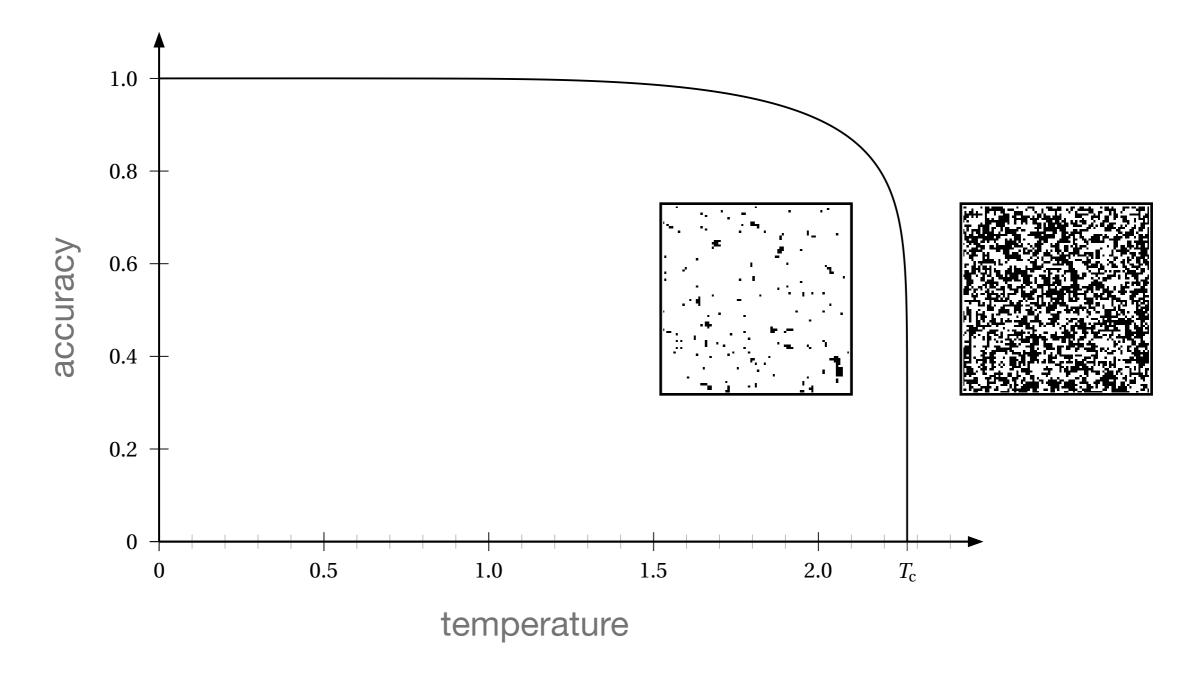


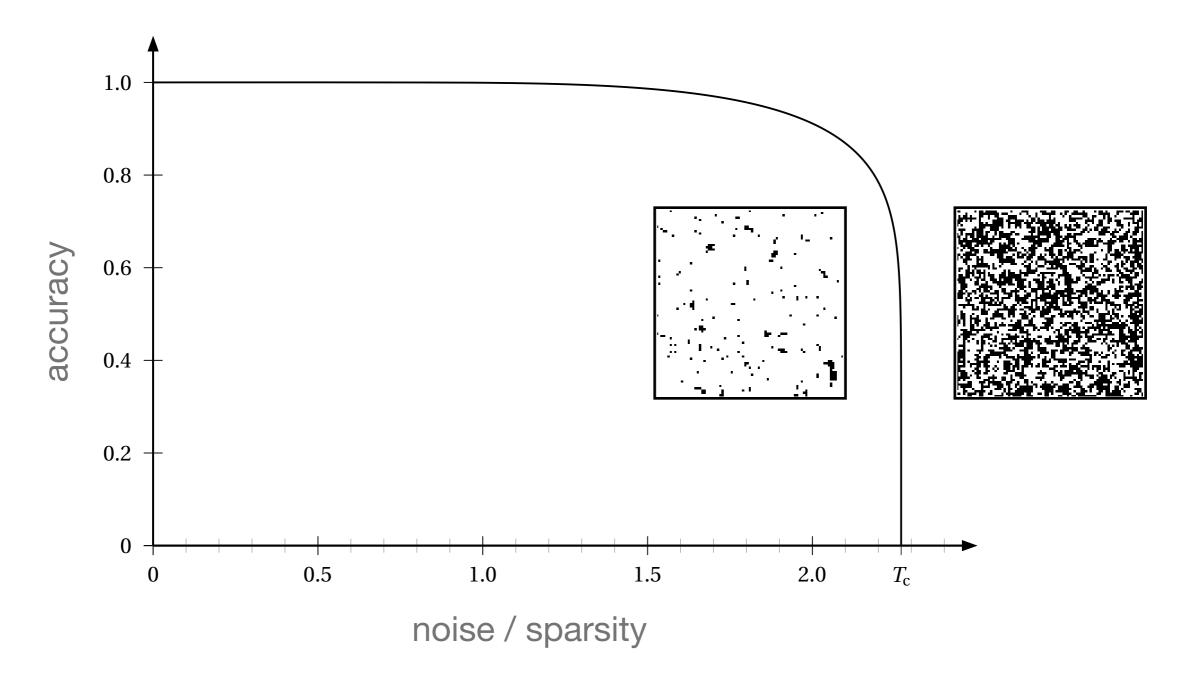
when these interactions are strong enough, and the temperature is low enough, they line up and form a magnetic field











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where are these phase transitions?

are there algorithms that succeed all the way up to these transitions?

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 $k \times k$ matrix p of connection probabilities

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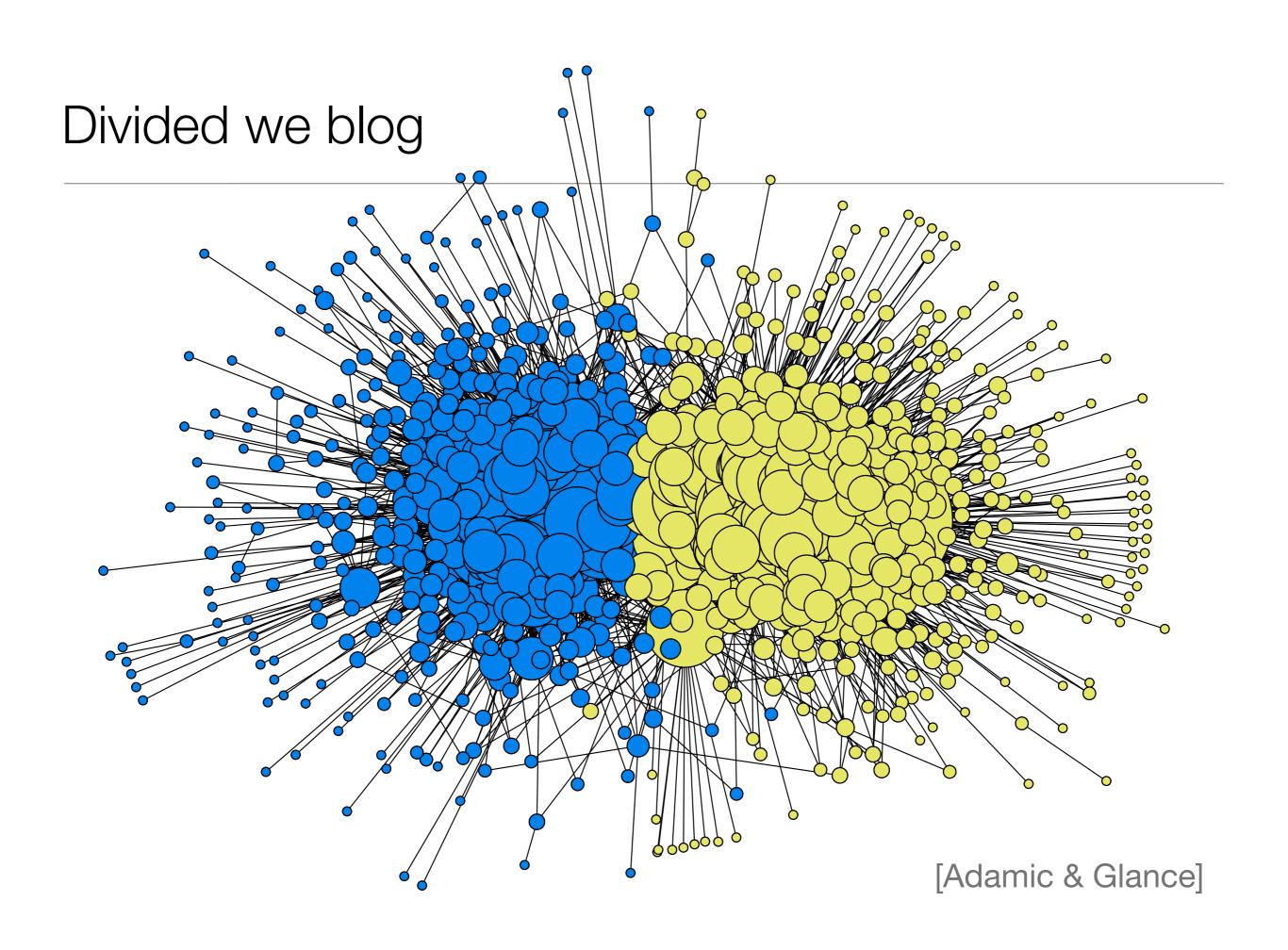
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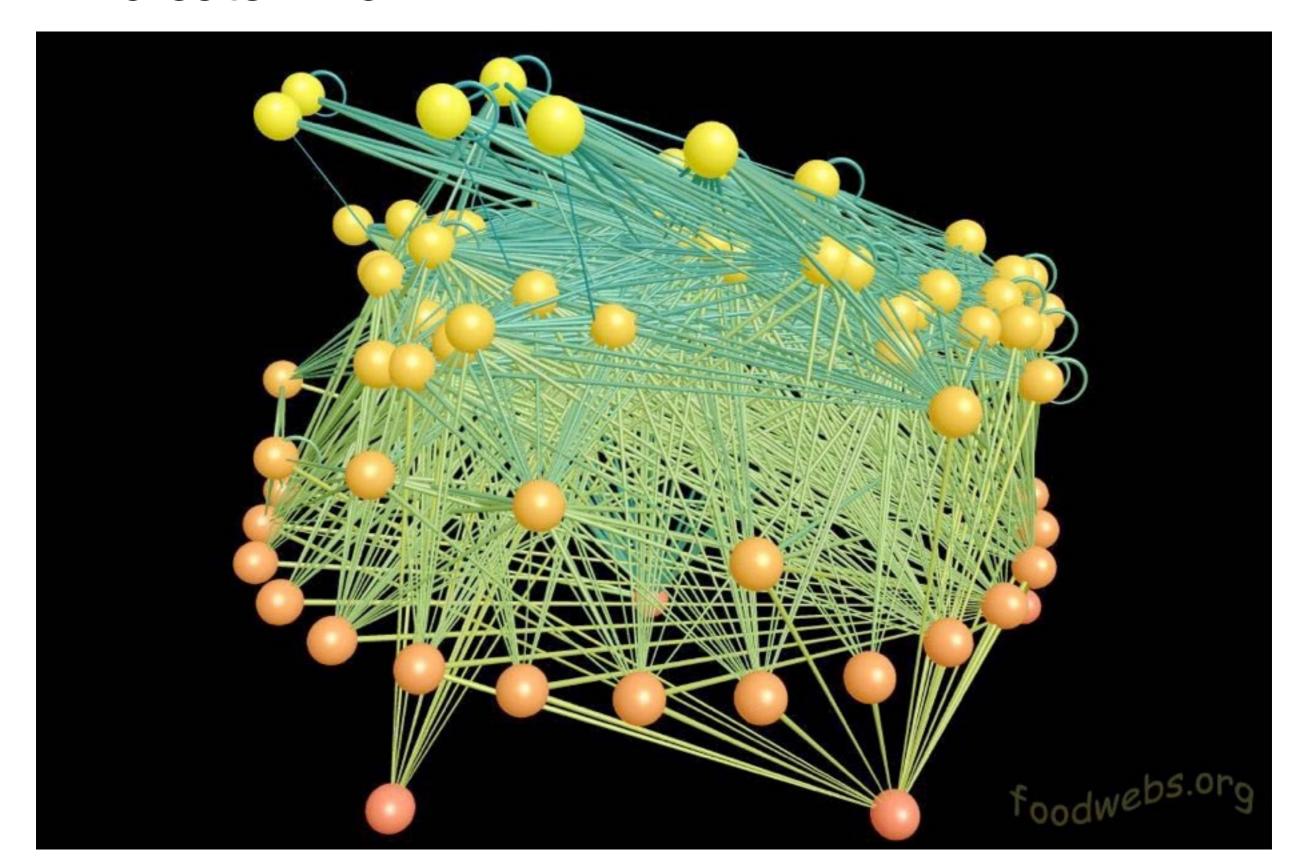
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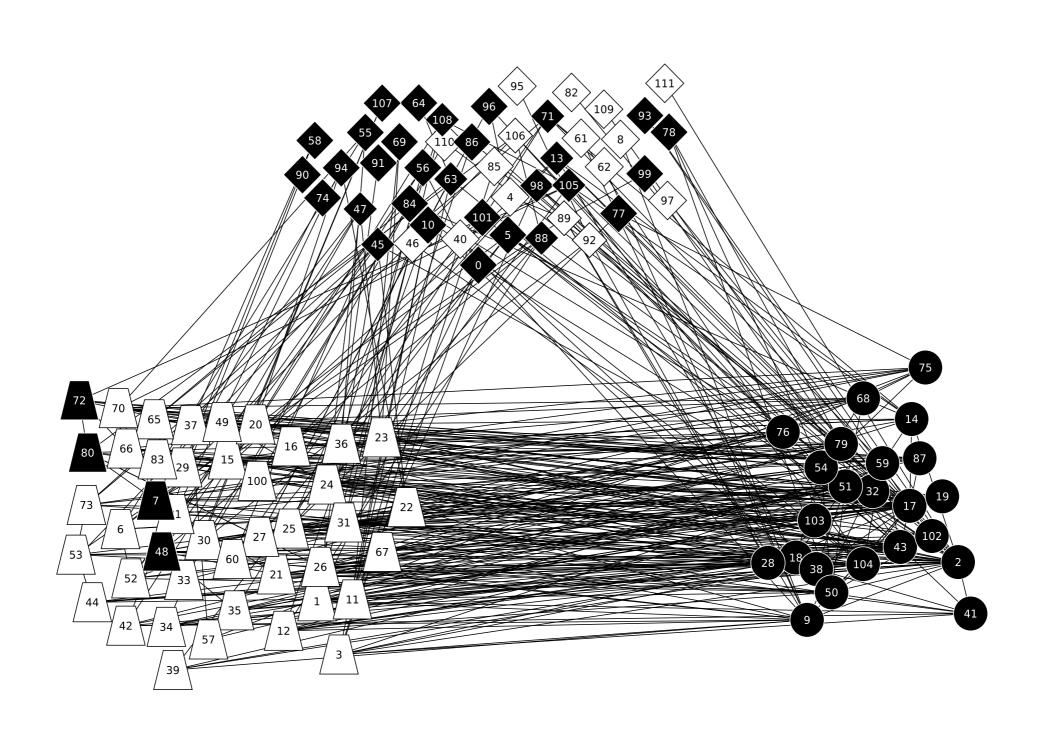
this talk: given the graph G, find the labels!



Who eats whom



I record that I was born on a Friday



Some cases of interest

$$p = \frac{1}{n} \begin{pmatrix} c_{\rm in} & c_{\rm out} \\ c_{\rm out} & c_{\rm in} \end{pmatrix}$$

$$p = \frac{1}{n} \begin{pmatrix} a & b \\ b & c \end{pmatrix}$$

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planted partitioning: $c_{in} > c_{out}$ assortative $c_{in} < c_{out}$ disassortative

core-periphery:
$$a > b > c$$

planted graph coloring: k colors, average degree c

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belief propagation (BP) lets us build analogies with statistical physics, gives natural measures of statistical significance and model selection, and reveals phase transitions in the detectability of community structure

the probability of *G* given the types *t* is a product over edges and non-edges:

$$P(G | t) = \prod_{(i,j) \in E} p_{t_i,t_j} \prod_{(i,j) \notin E} (1 - p_{t_i,t_j})$$

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using $P \sim e^{-\beta E}$ where $\beta = 1/T$ (Boltzmann) and E is the energy,

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like Ising model, but with interactions on both edges and non-edges in the sparse case p=O(1/n), interactions on non-edges are weak

probability of G given t

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 $e^{-\beta E(t)}$

 $(\beta=1 \text{ for now})$

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$$\sum_{t\in\{1,\dots,k\}^n} P(G,t)$$

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	$-\log \sum P(G \mid t)$	$F = -\log Z$	free energy

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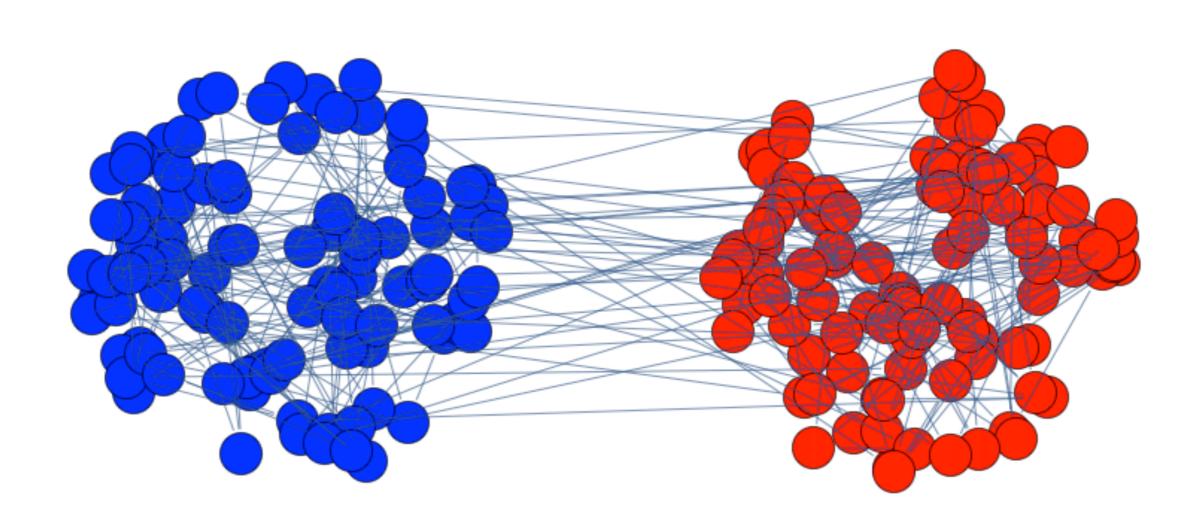
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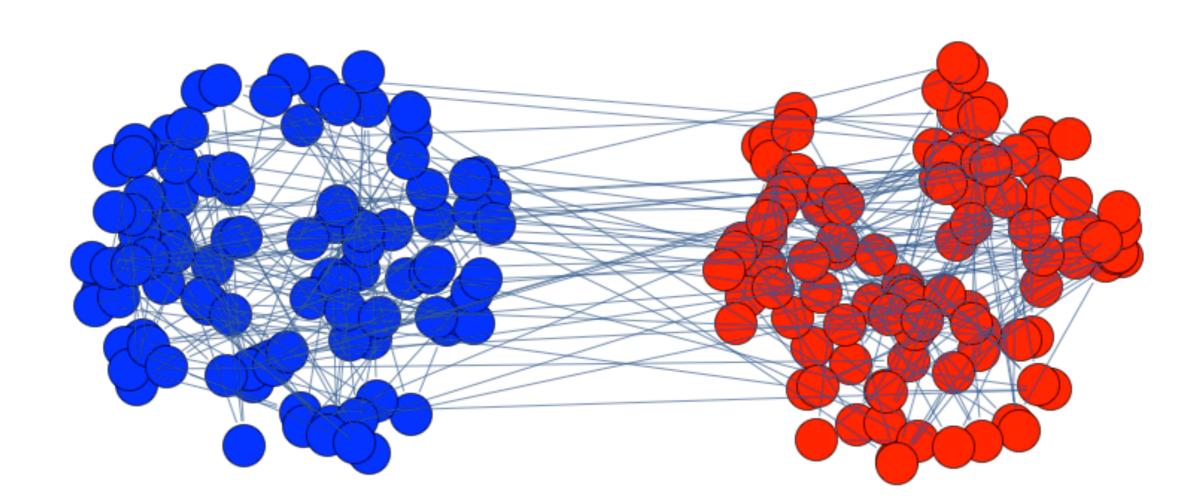
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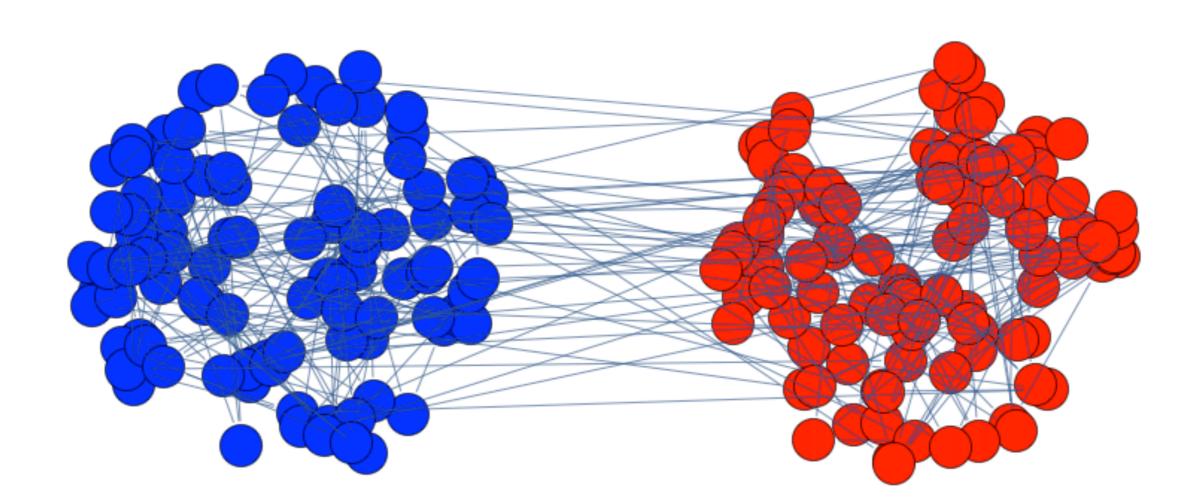


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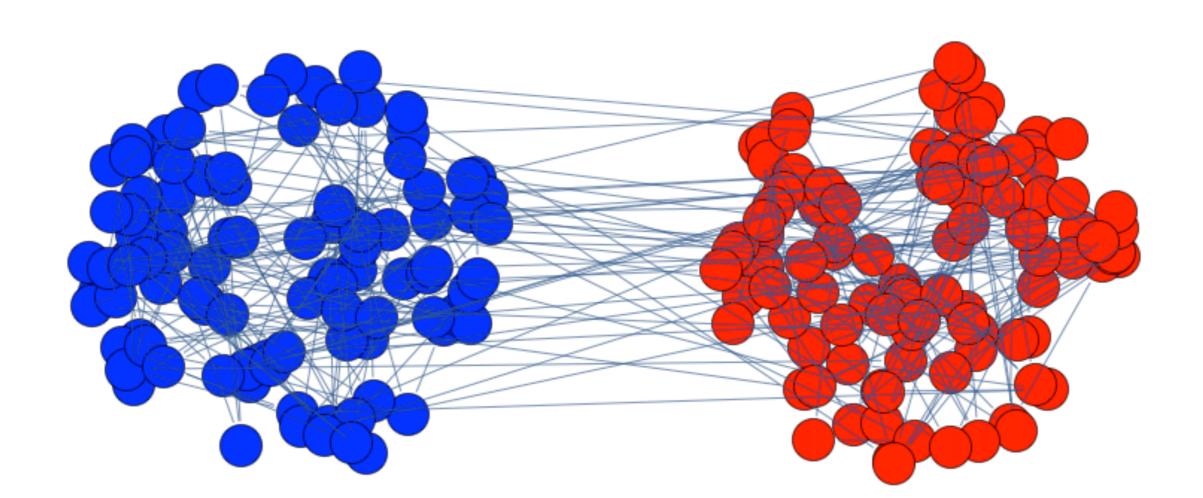
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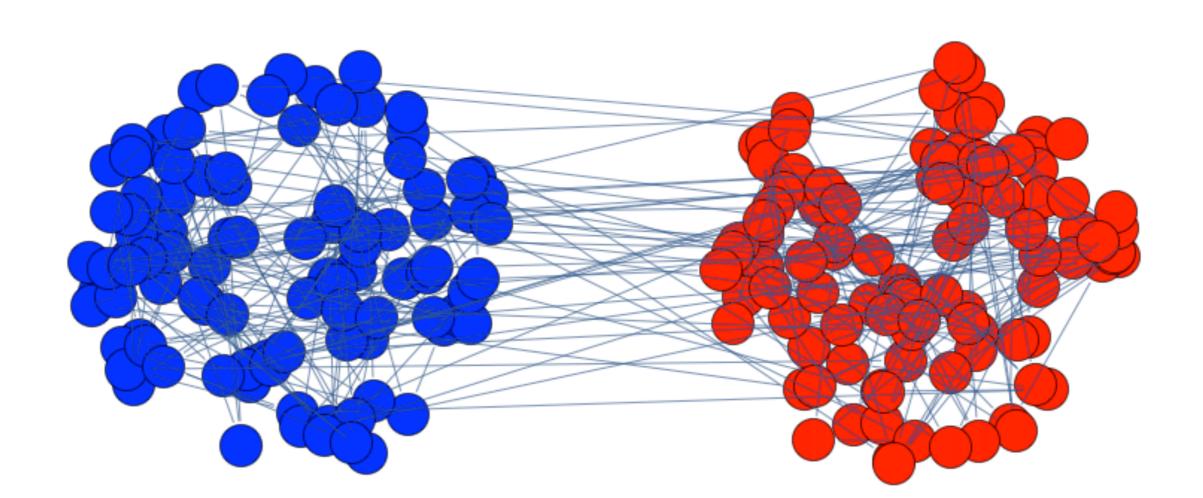
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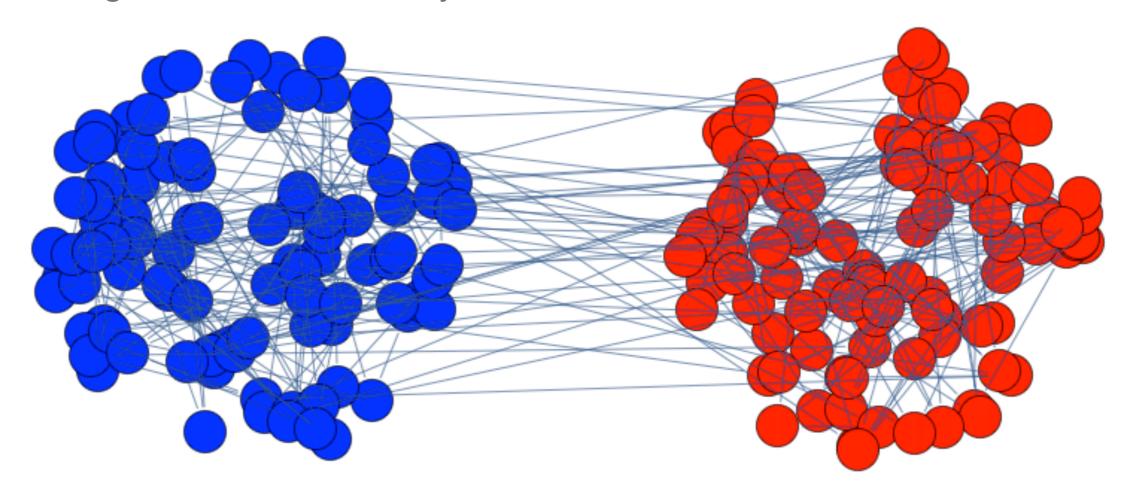
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many labelings, about as good as each other, with nothing in common! this is a sign there aren't actually communities at all...



Statistical significance vs. overfitting

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we don't just want the best fit!

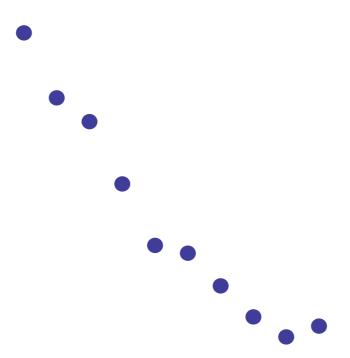
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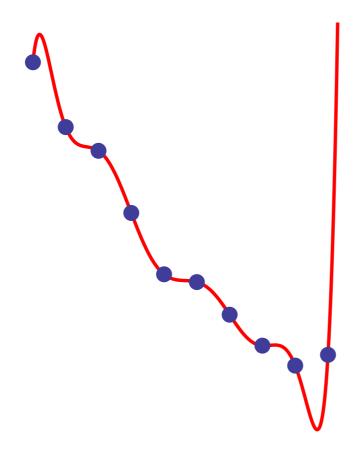
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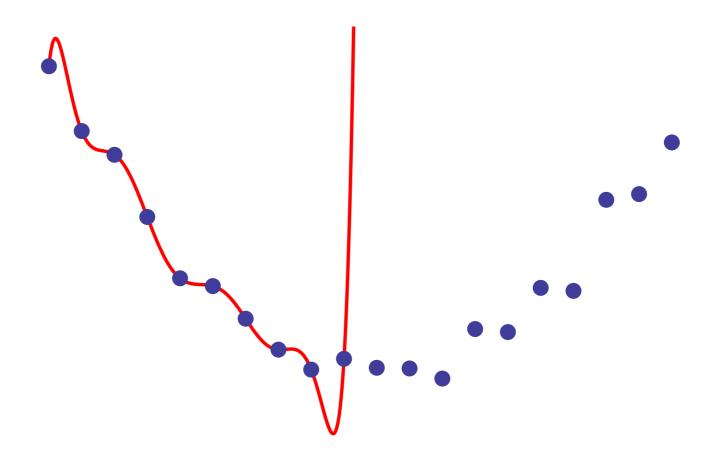
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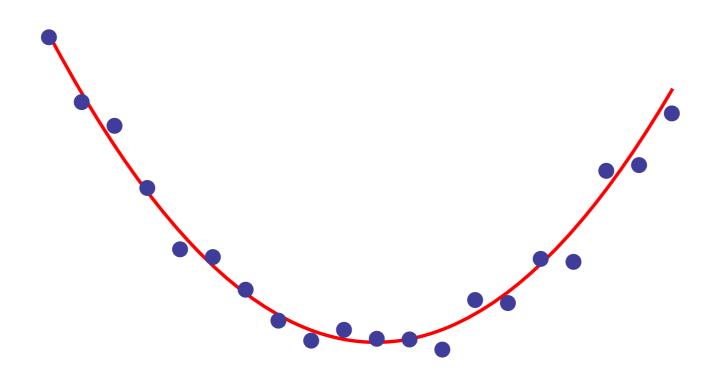
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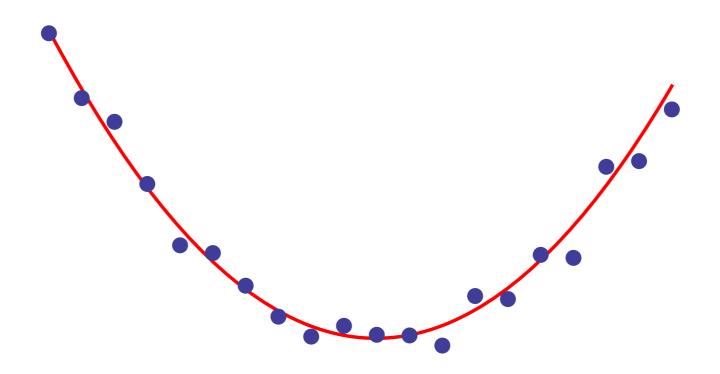


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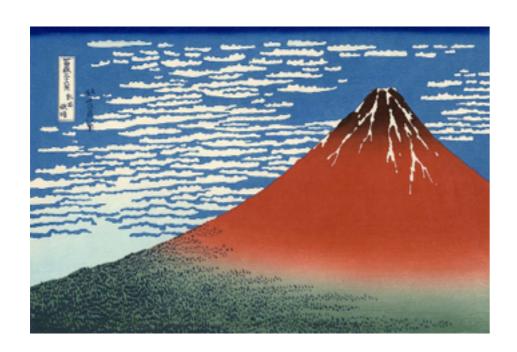
random graphs have illusory communities, that only exist because of noise sometimes the patterns we find aren't really there:



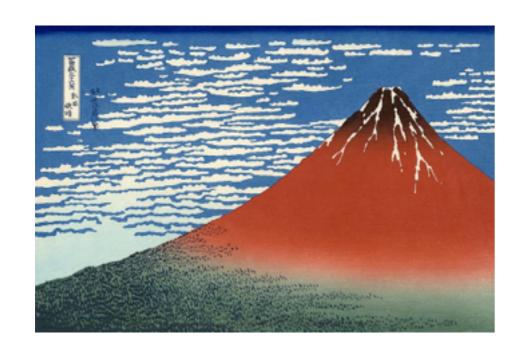
we want to understand the coin, not the coin flips



explore the landscape of models, not just the best one



explore the landscape of models, not just the best one if there is real structure in the data, there is a robust optimum

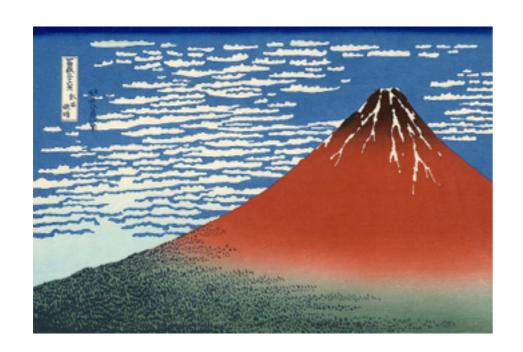




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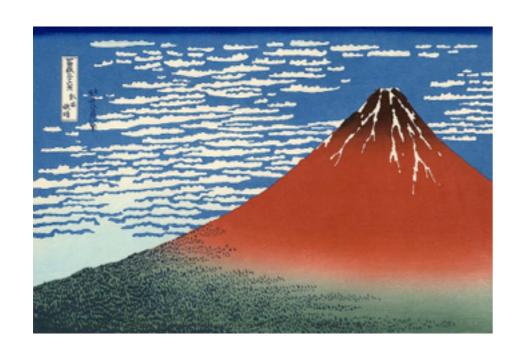
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even if you could find the optimum, why would you care?





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if there is real structure in the data, there is a robust optimum
but the landscape can be "glassy": many local optima with nothing in common
even if you could find the optimum, why would you care?
instead, sample from the entire landscape, and look for agreement

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the consensus of many likely solutions is better than the most-likely one

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best model: maximize *total* probability of *G*, summed over all possible labelings:

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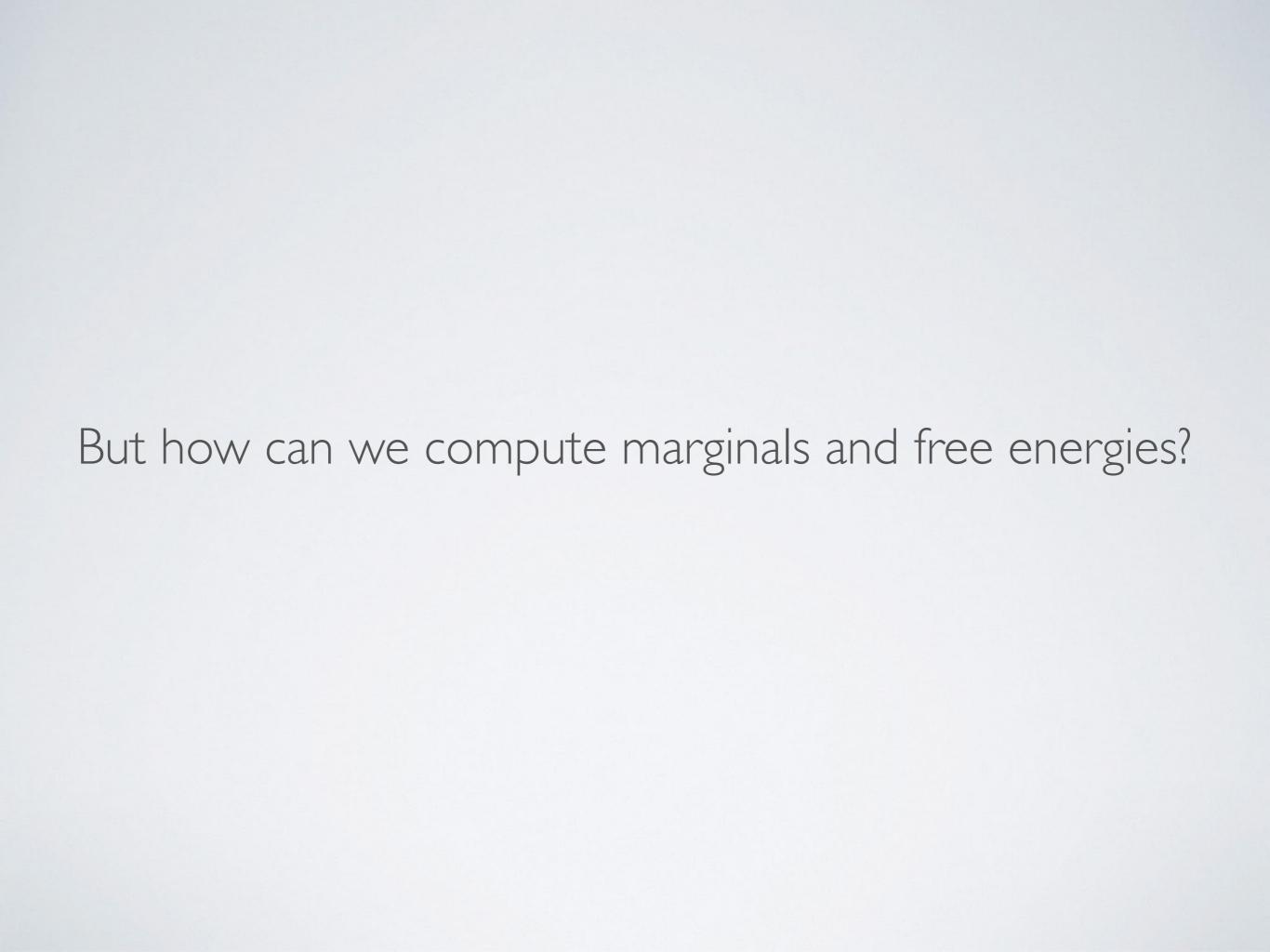
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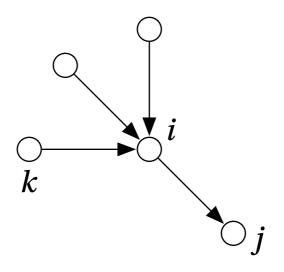
a good model fits the data robustly, with many values of the hidden variables

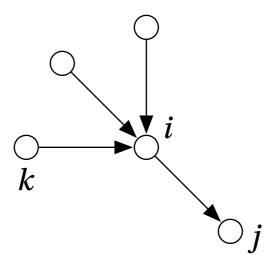




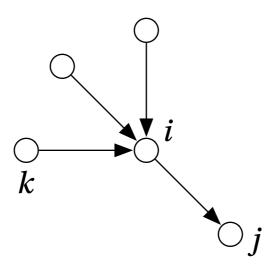
But how can we compute marginals and free energies?

Monte Carlo is too slow!



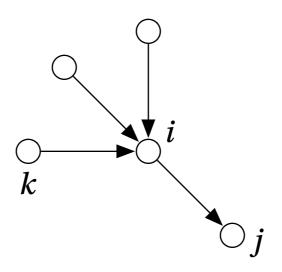


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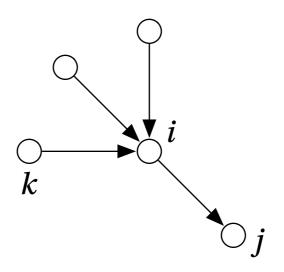
avoids an "echo chamber" between pairs of nodes



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update until we reach a fixed point (how many iterations? does it converge?)



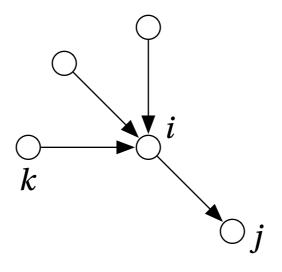
each node *i* sends a "message" to each of its neighbors *j*, giving *i*'s marginal distribution based on its other neighbors *k*

avoids an "echo chamber" between pairs of nodes

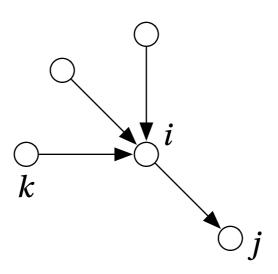
update until we reach a fixed point (how many iterations? does it converge?)

fixed point returns estimated marginals and the Bethe free energy

Updating the beliefs

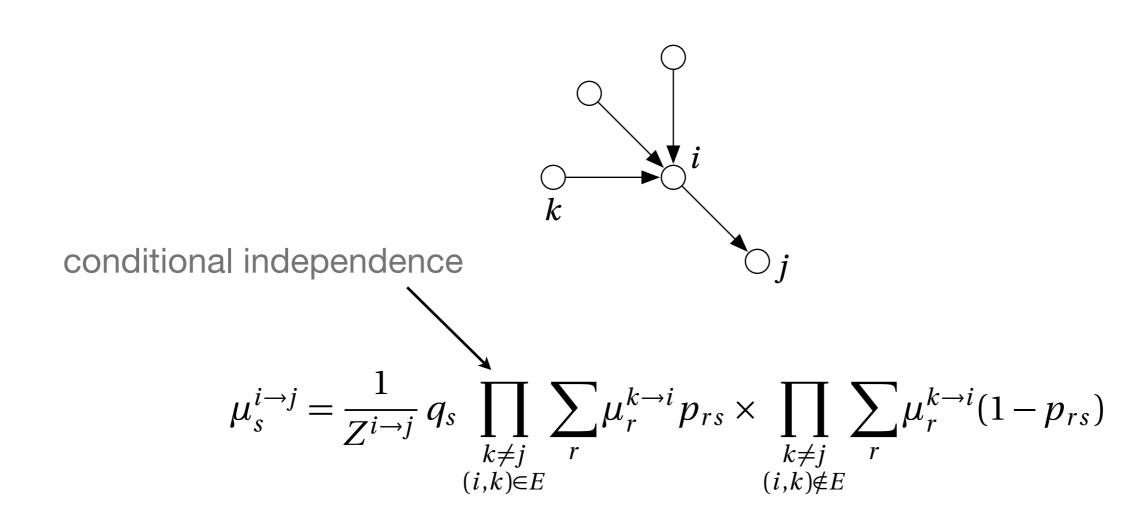


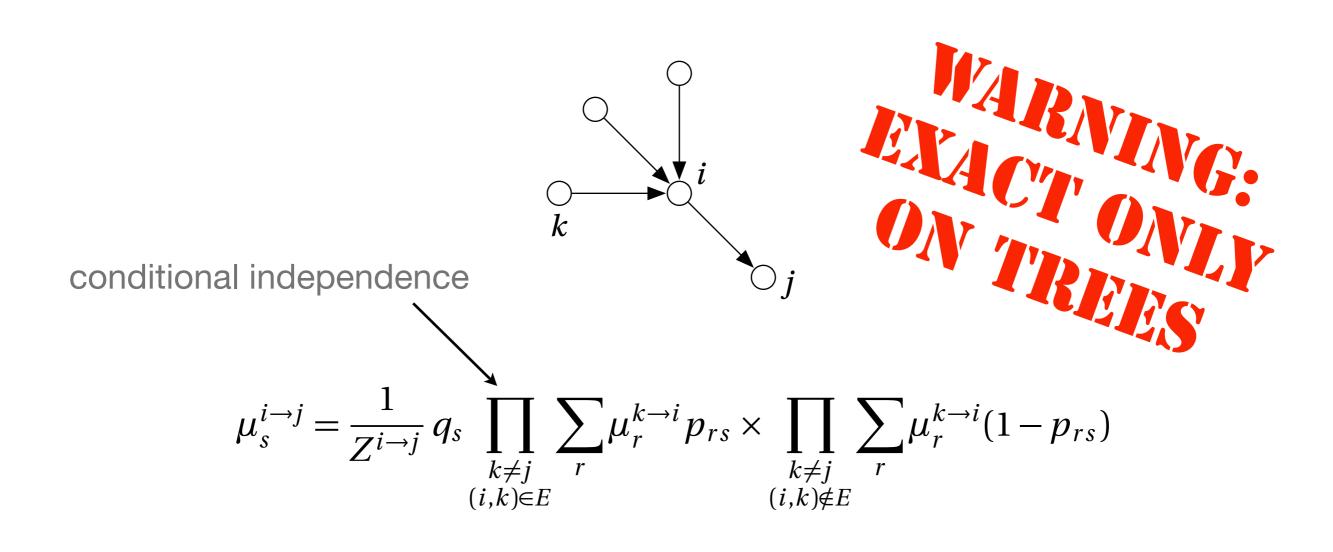
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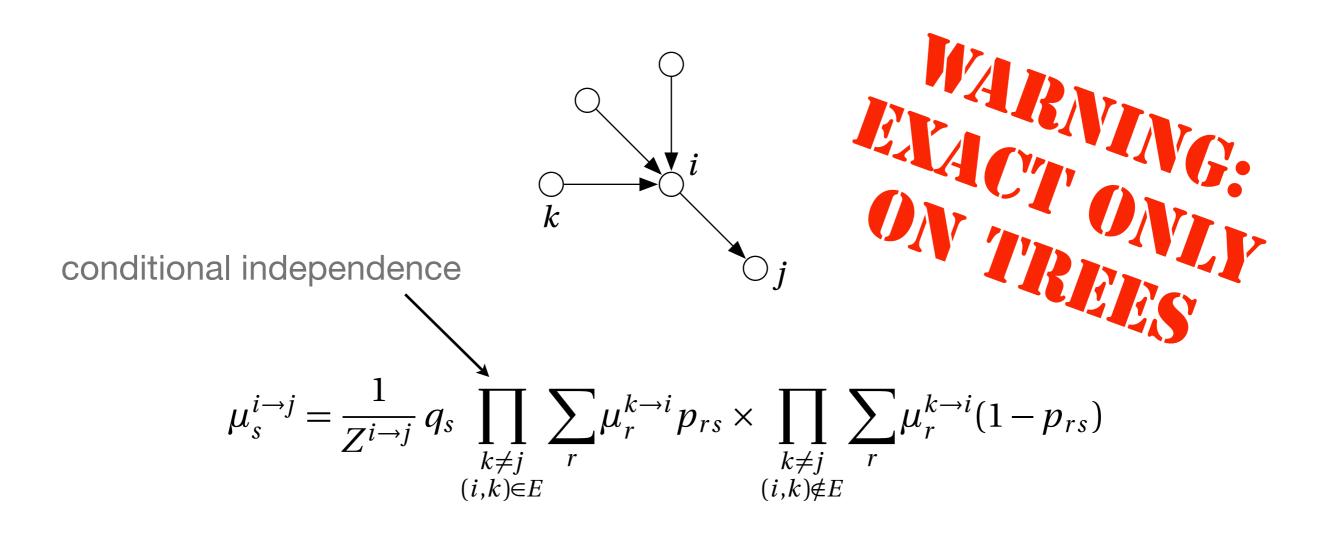


$$\mu_s^{i \to j} = \frac{1}{Z^{i \to j}} q_s \prod_{\substack{k \neq j \\ (i,k) \in E}} \sum_r \mu_r^{k \to i} p_{rs} \times \prod_{\substack{k \neq j \\ (i,k) \notin E}} \sum_r \mu_r^{k \to i} (1 - p_{rs})$$

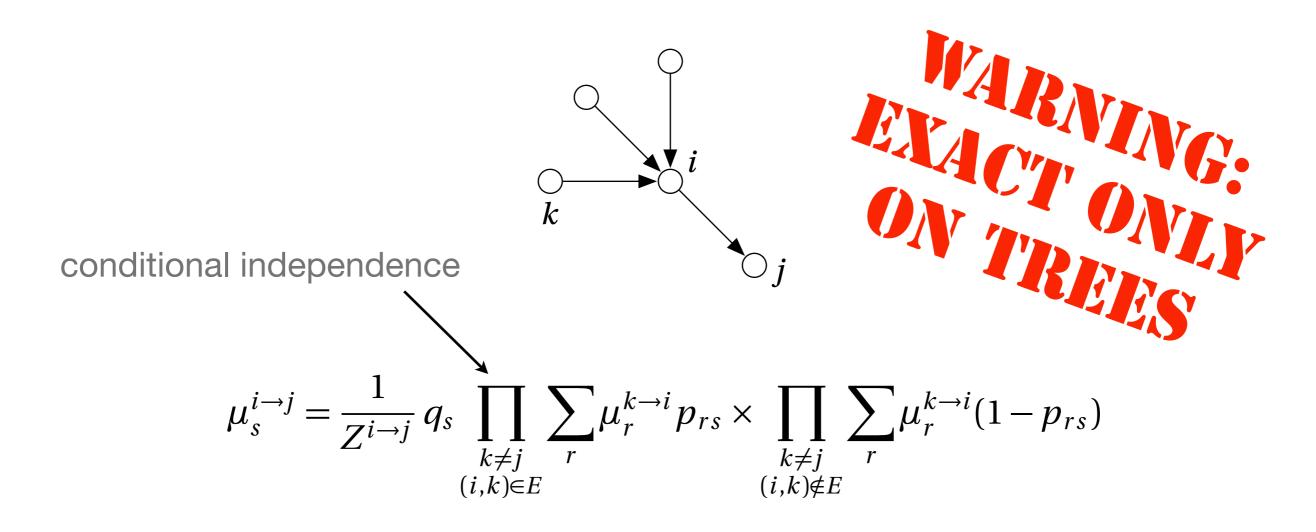
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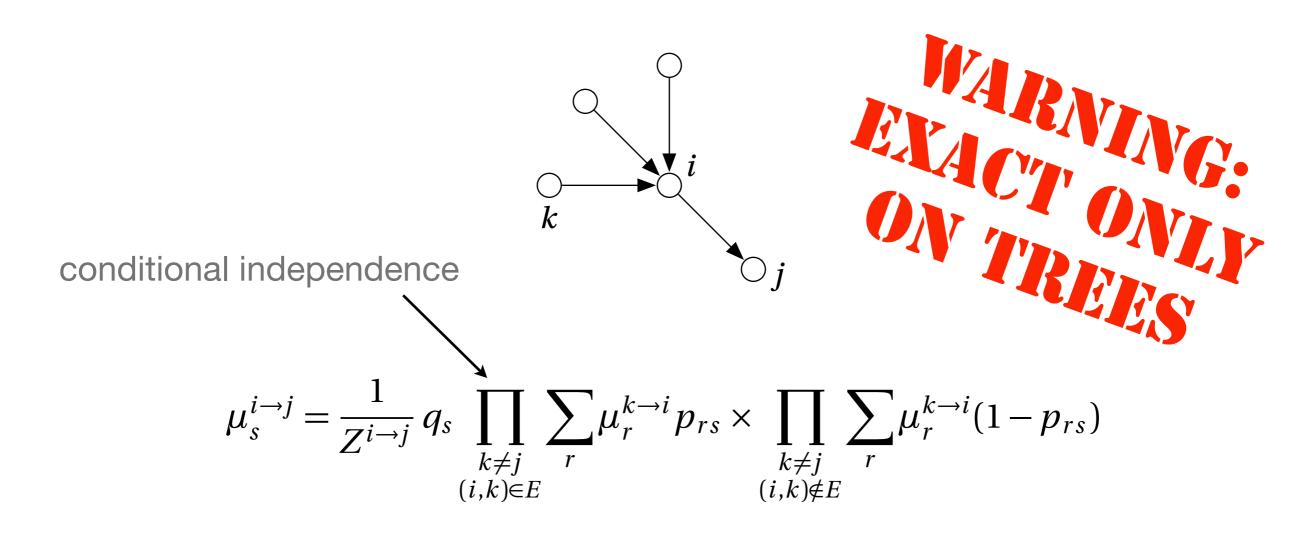




a complete graph of messages: takes $O(n^2)$ time to update. Not scalable!

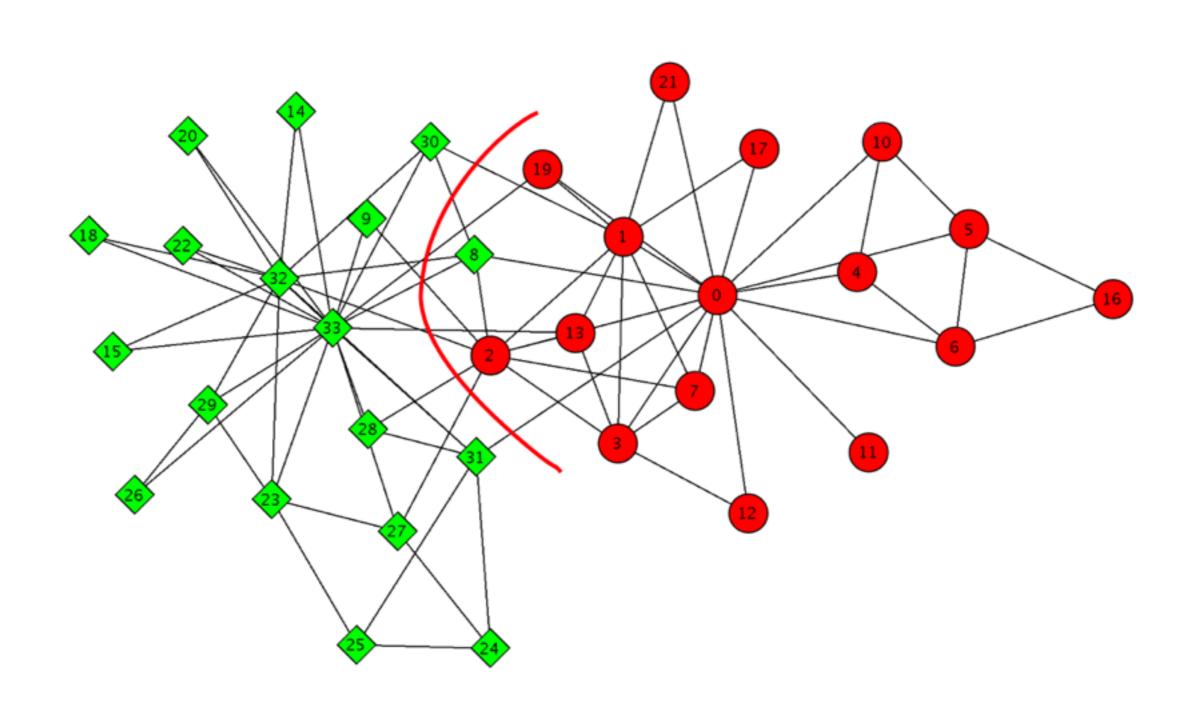


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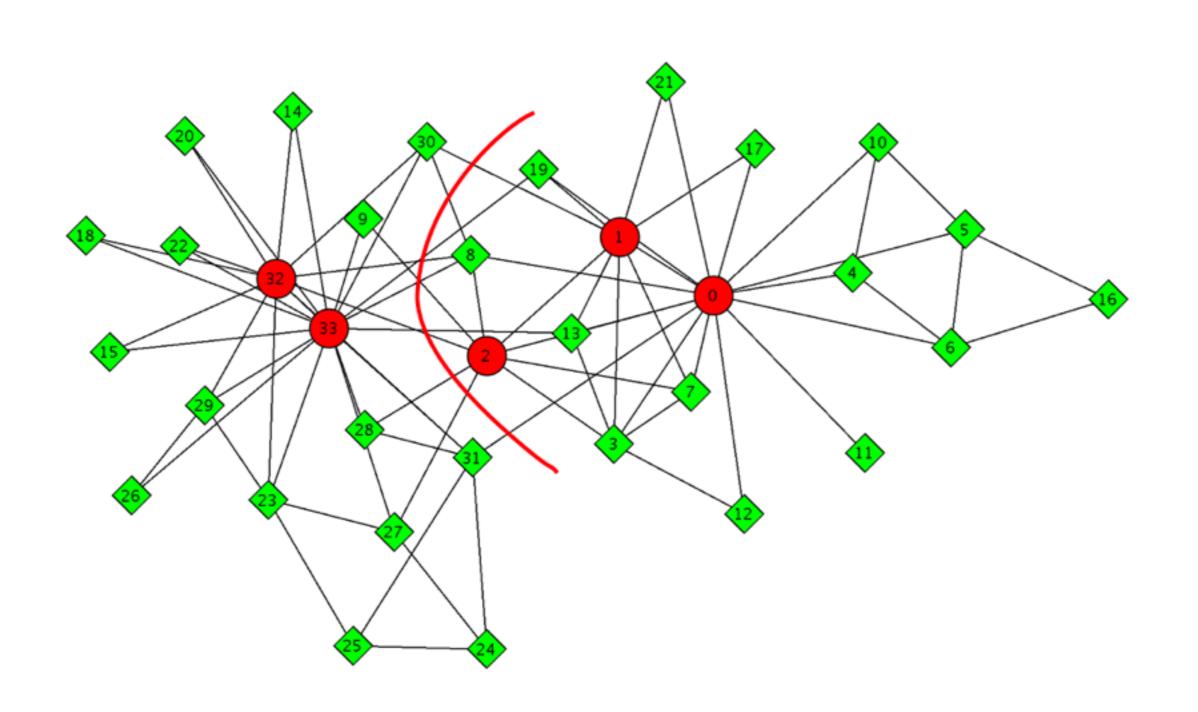


a complete graph of messages: takes $O(n^2)$ time to update. Not scalable! sparse case: can simplify by assuming that $\mu_r^{k\to i} = \mu_r^k$ for all non-neighbors i then update takes O(n+m) time: scalable!

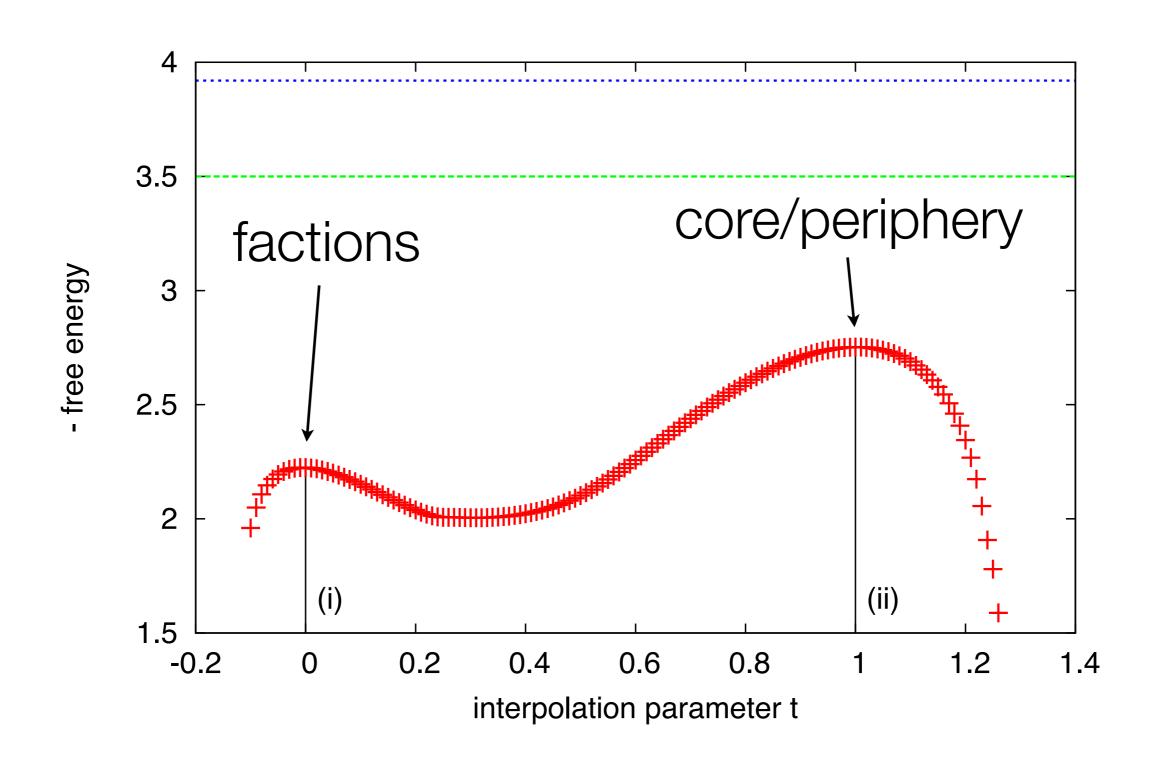
Zachary's Karate Club: Two factions

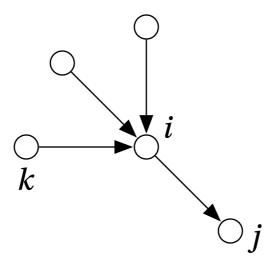


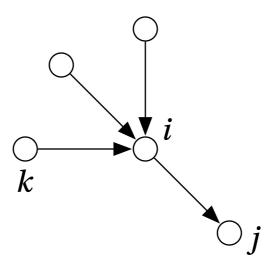
Zachary's Karate Club: Core-periphery



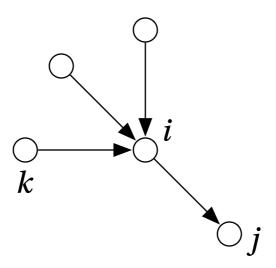
Two local optima in free energy





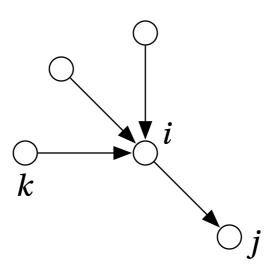


BP is a fast algorithm we can run on real networks...



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but it's also a framework for analytic calculations on ensembles of graphs (e.g. the stochastic block model) in the large-*n* limit

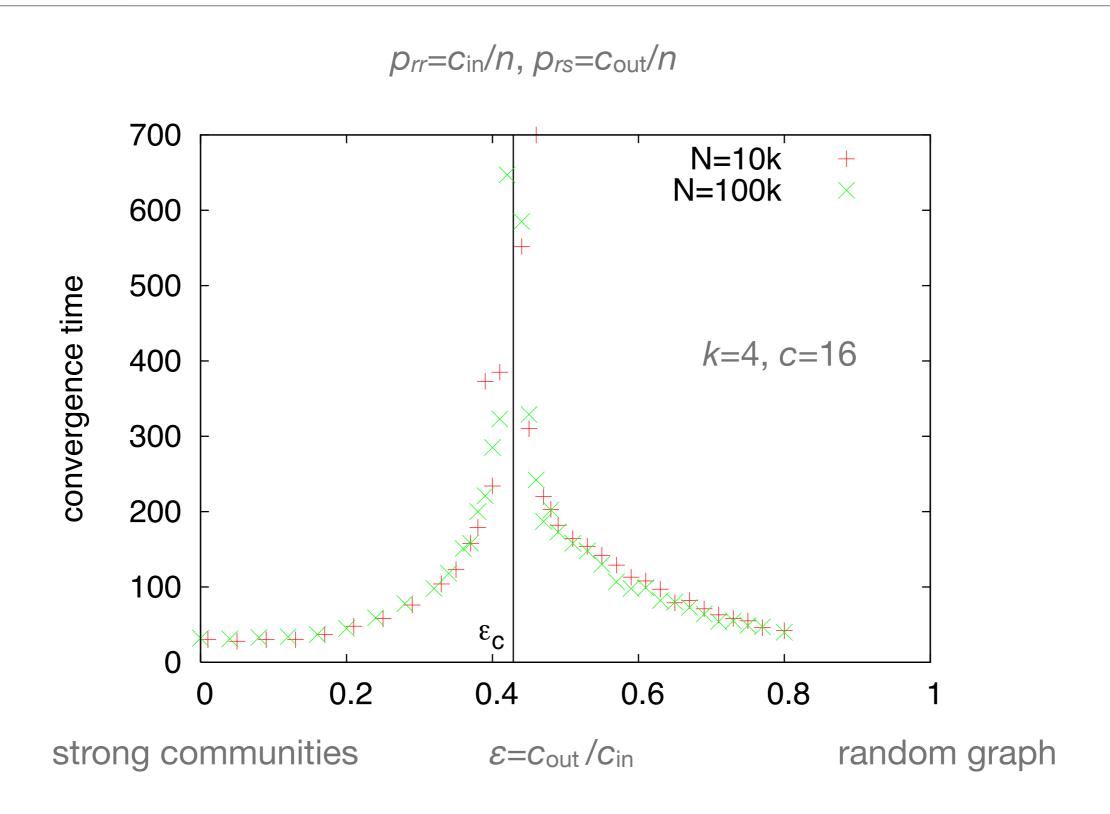


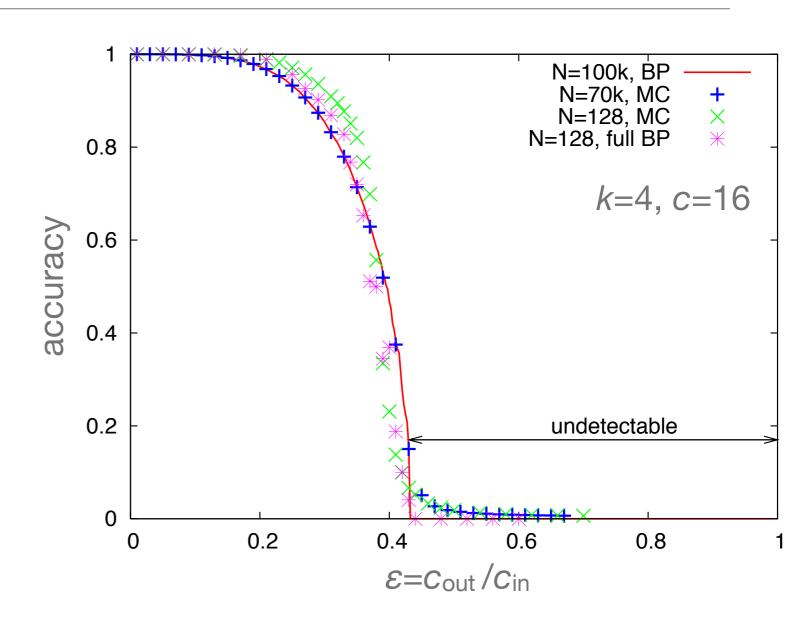
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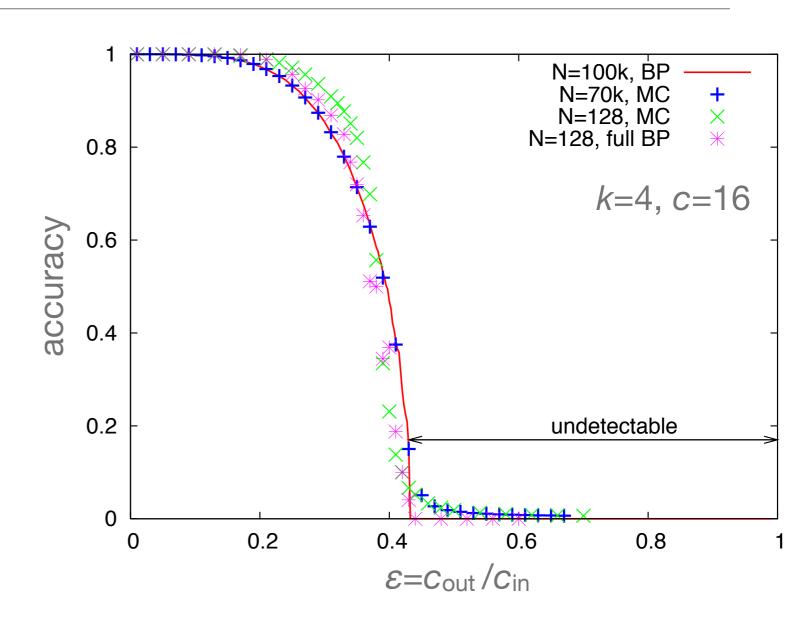
analyze fixed points of the messages, their basins of attraction, their stability

BP convergence time: nearly size-independent, but with critical slowing down at a phase transition



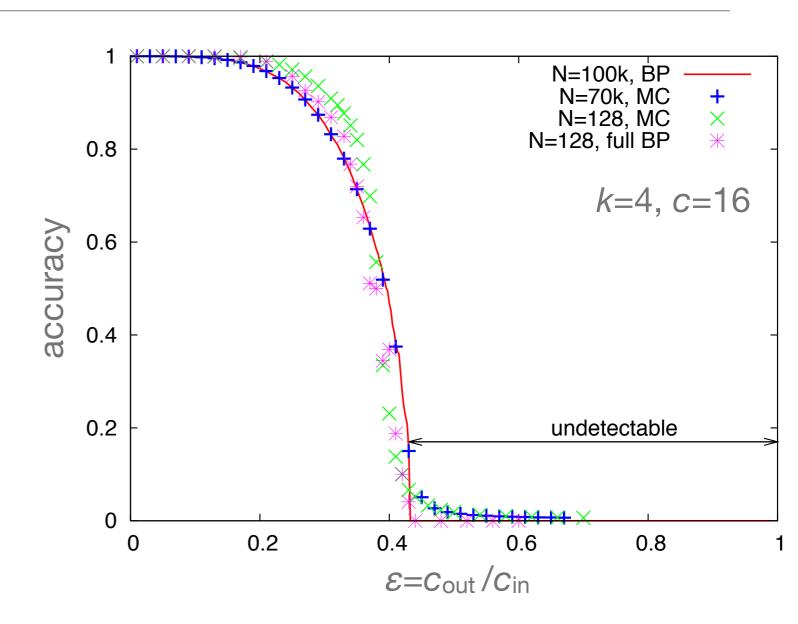


when $c_{\text{out}}/c_{\text{in}}$ is small enough, BP can find the communities



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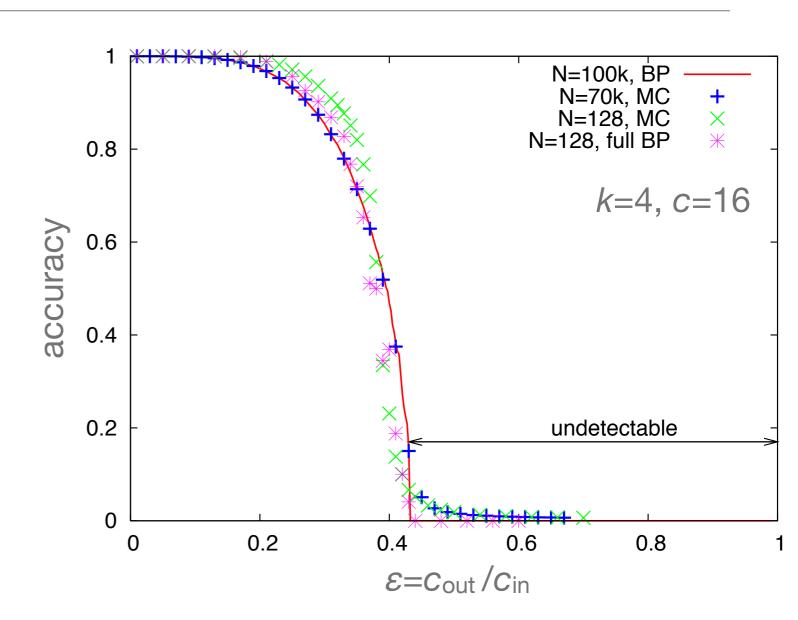


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for 2 groups, the threshold is at

$$|c_{\rm in}-c_{\rm out}|=2\sqrt{c}$$



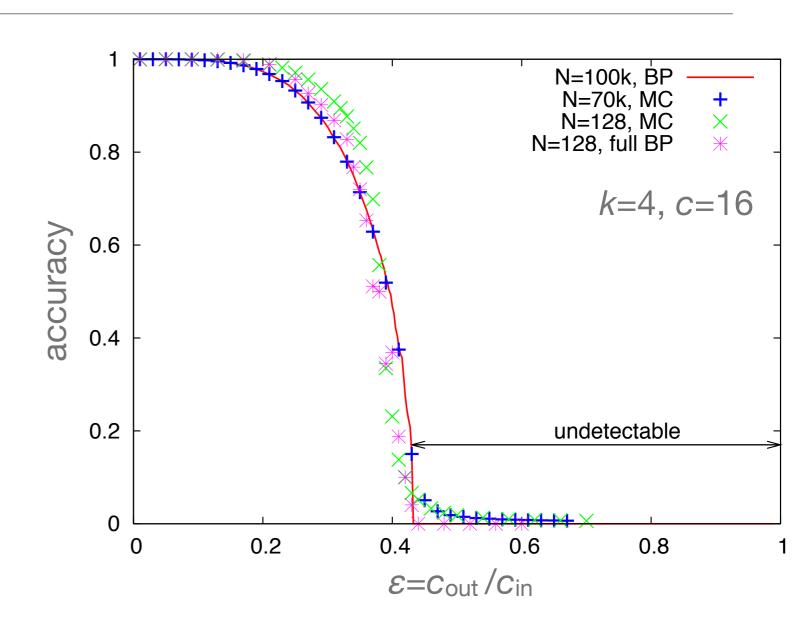
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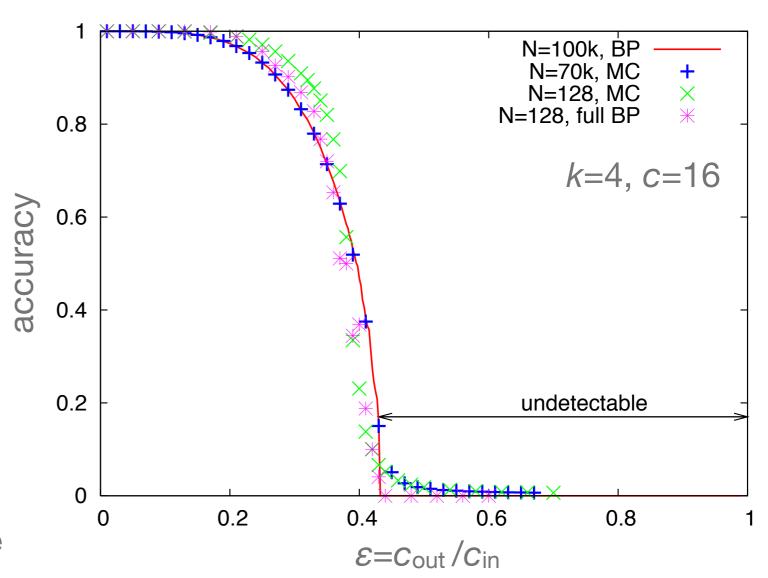
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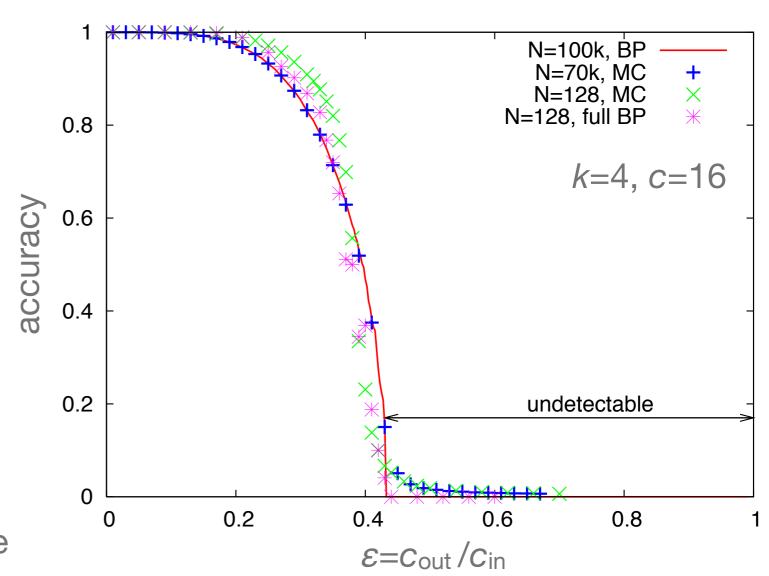
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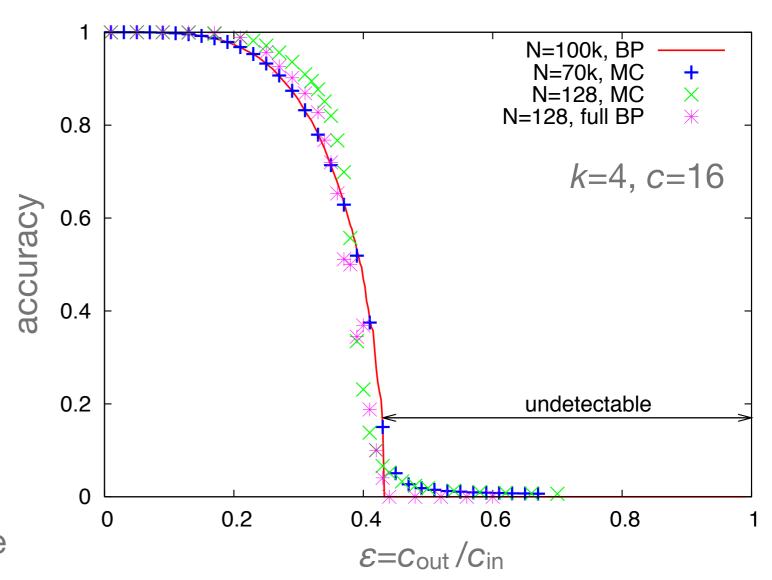
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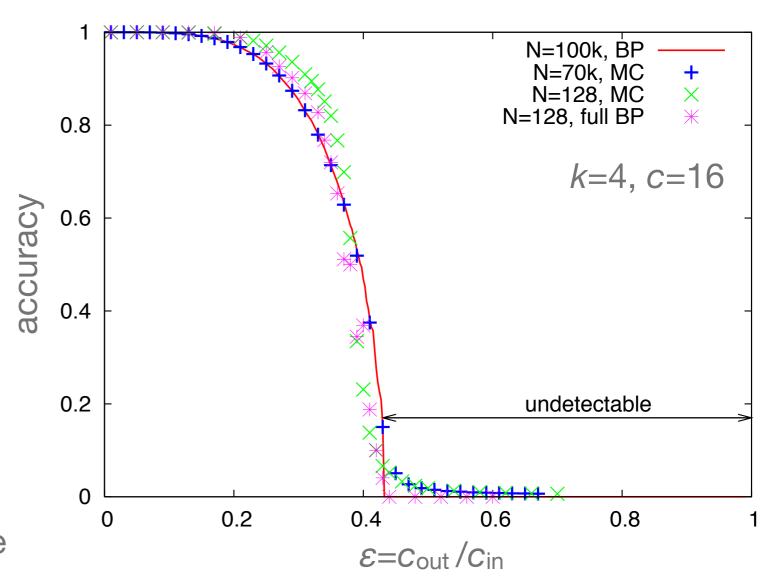
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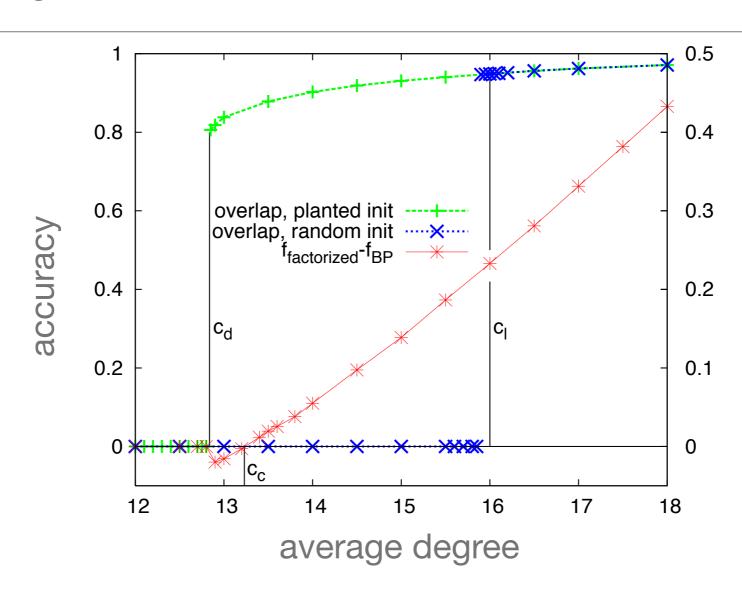
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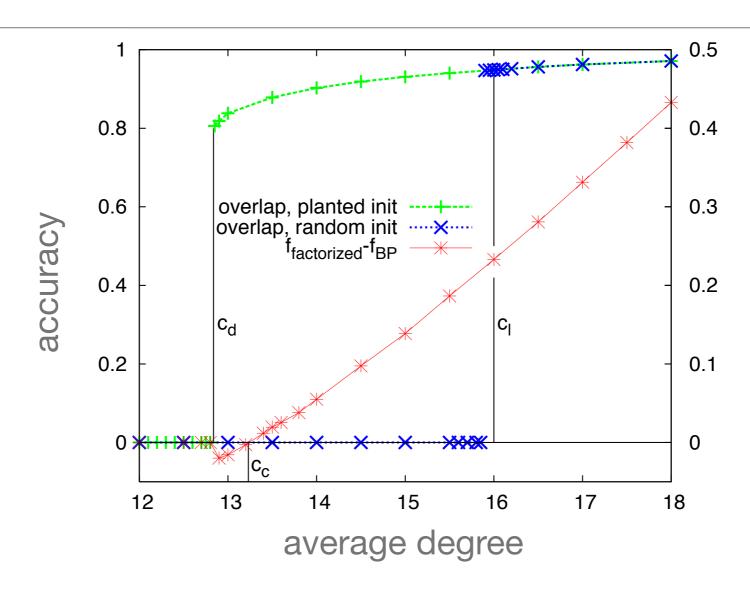
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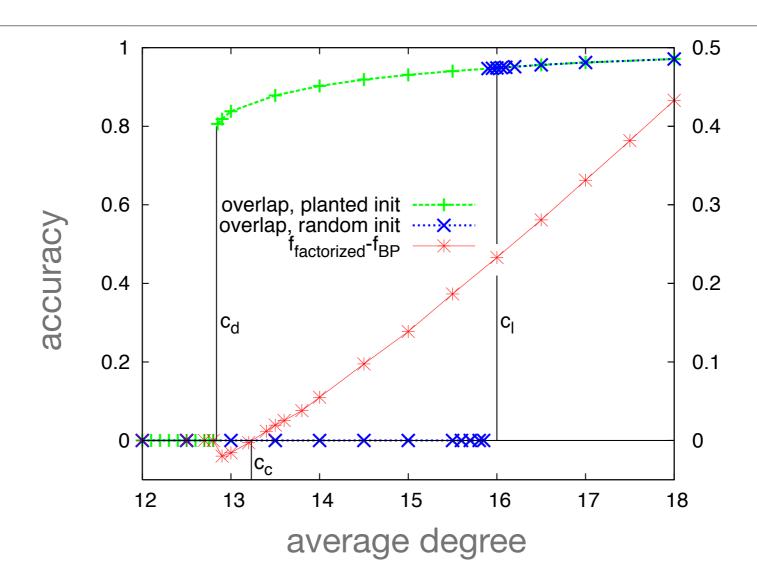


conjectured by [Decelle, Krzakala, Moore, Zdeborová, '11] proved by [Mossel, Neeman, Sly, `13; Massoulié '13] for k > 2 groups, much less is known rigorously...

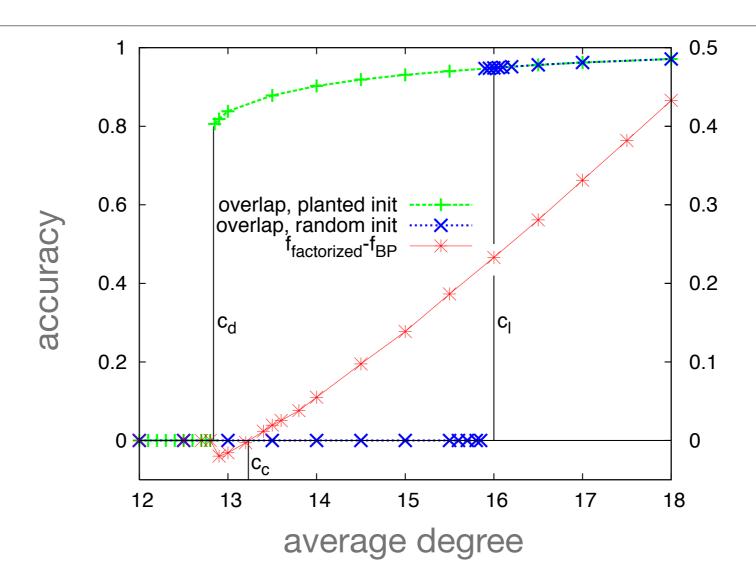




BP has two fixed points, but the accurate one has a small basin of attraction



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BP has two fixed points, but the accurate one has a small basin of attraction a free energy barrier between "paramagnetic" and "ferromagnetic" phases detection is information-theoretically possible below the Kesten-Stigum bound [Abbe+Sandon, Banks+Moore] but we believe it's computationally hard

suppose we are given the correct labels for αn nodes for free

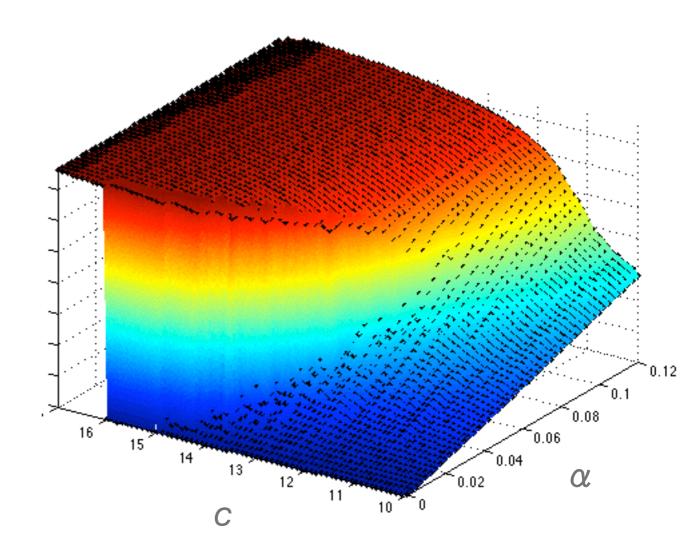
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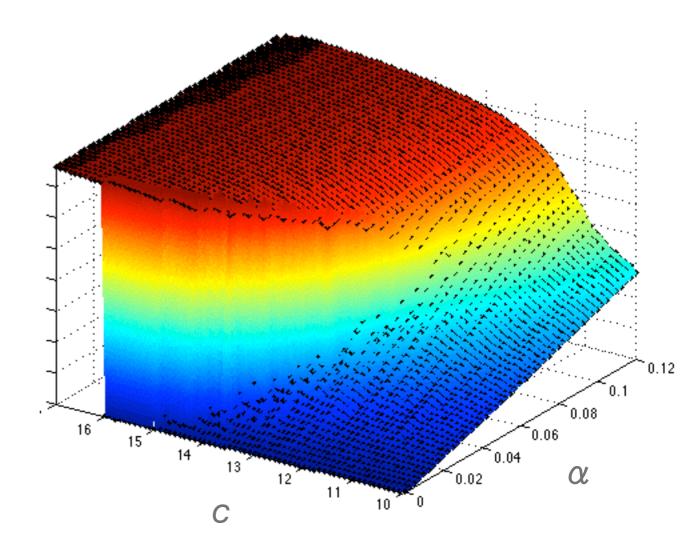
[Zhang, Moore, Zdeborová '14]

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a line of discontinuities in the (c,α) plane, ending at a critical point



[Zhang, Moore, Zdeborová '14]

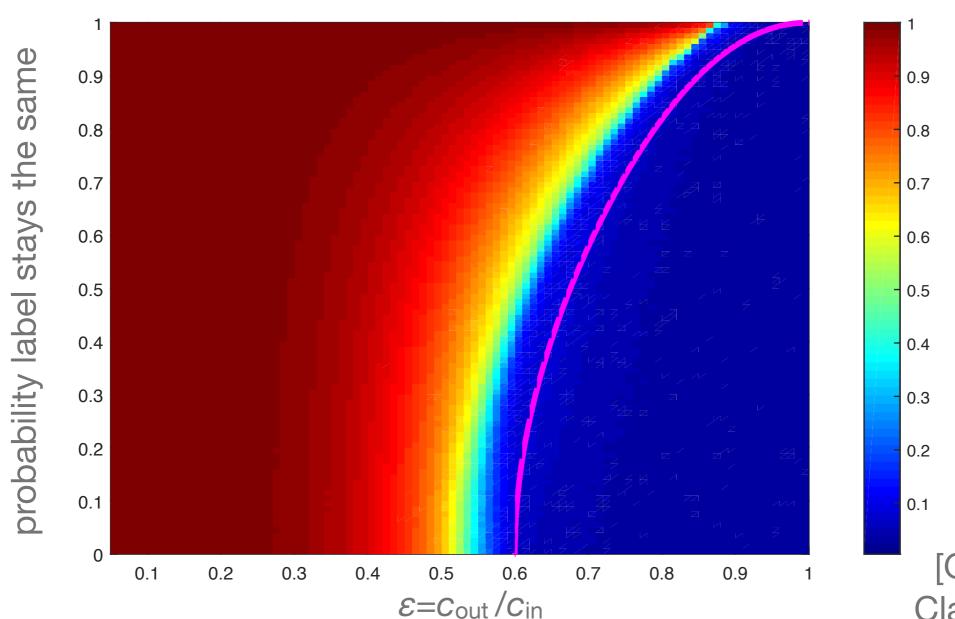
Dynamic networks

Dynamic networks

what if nodes change their label, moving from group to group over time?

Dynamic networks

what if nodes change their label, moving from group to group over time? tradeoff between persistence of labels and the strength of the communities



[Ghasemian, Zhang, Clauset, Moore, Peel]

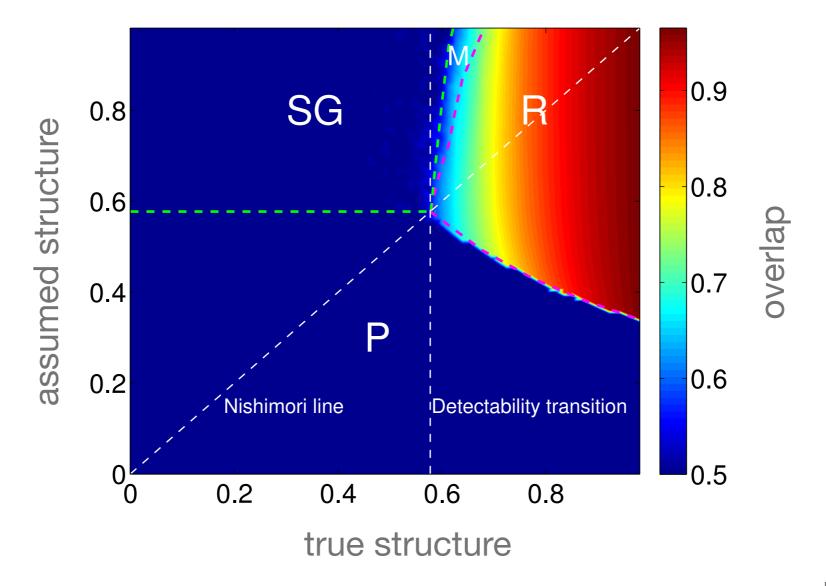
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lower temperature = greedier algorithm = assume stronger structure

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lower temperature = greedier algorithm = assume stronger structure if we get too greedy, we enter a "spin glass" where BP fails to converge



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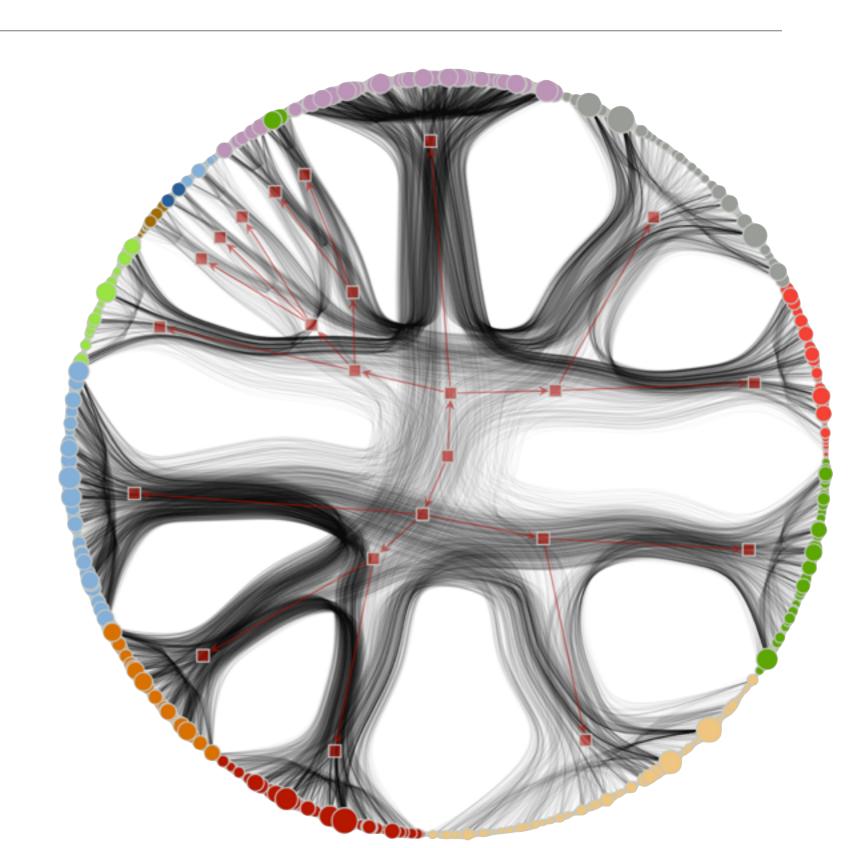
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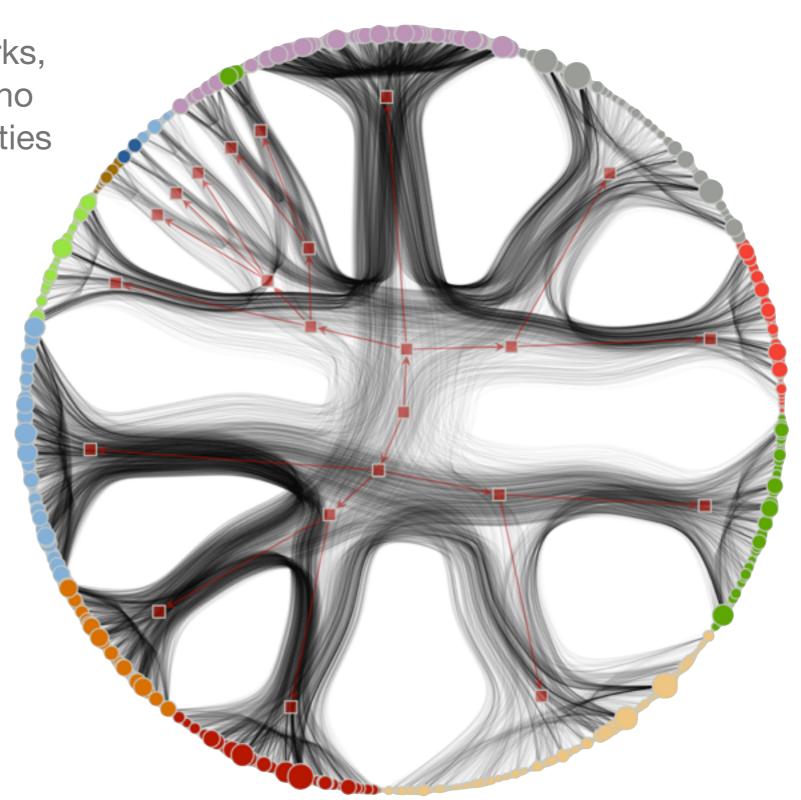
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using both text and links does better than either one alone



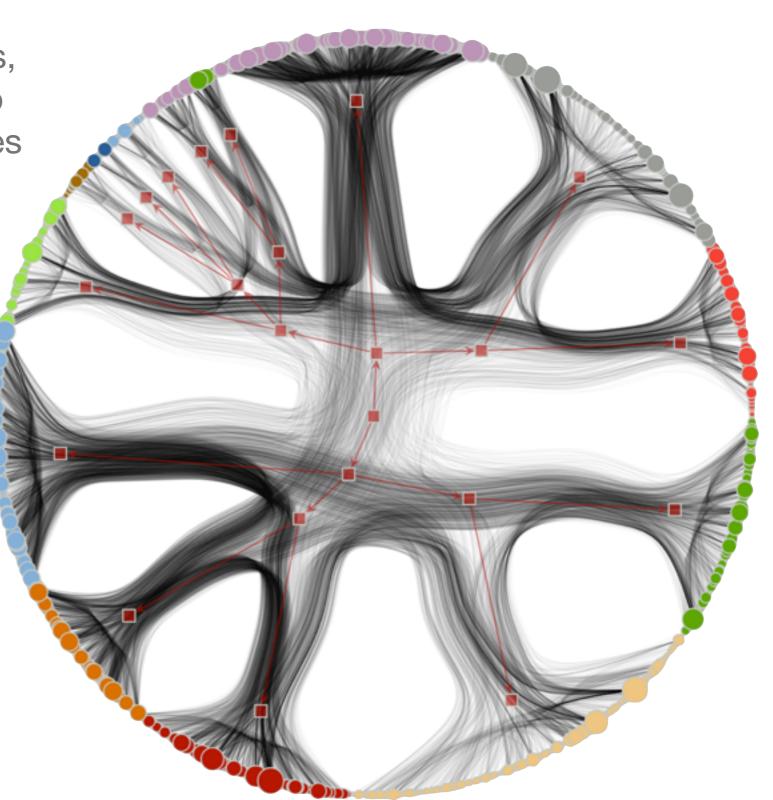
divide a network into subnetworks, until the remaining pieces have no statistically significant communities



divide a network into subnetworks, until the remaining pieces have no statistically significant communities

reveals substructure in network of

political blogs



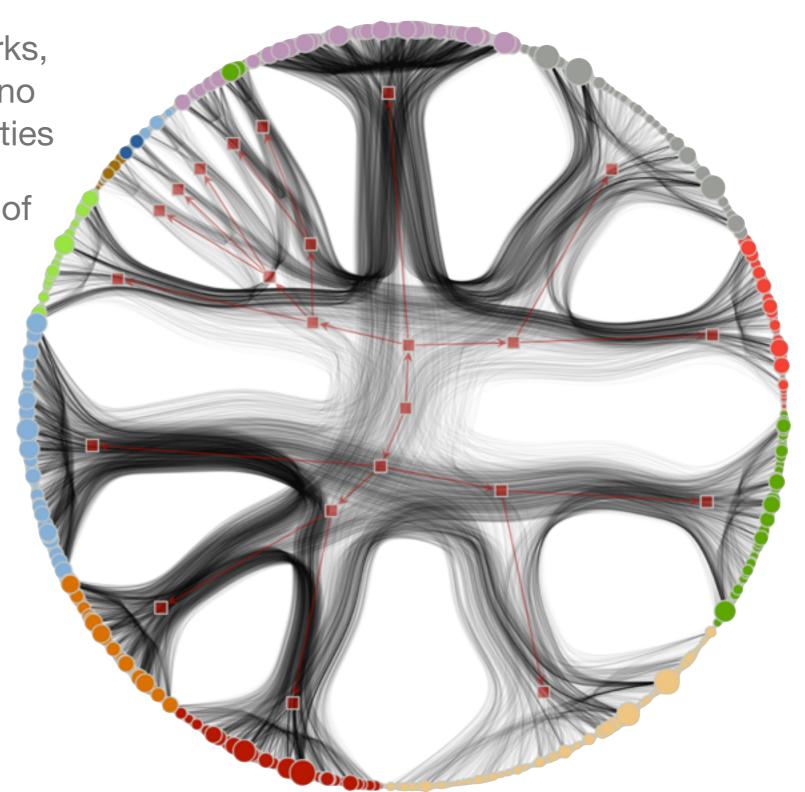
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the consensus of many high-modularity structures is better than the "best" one



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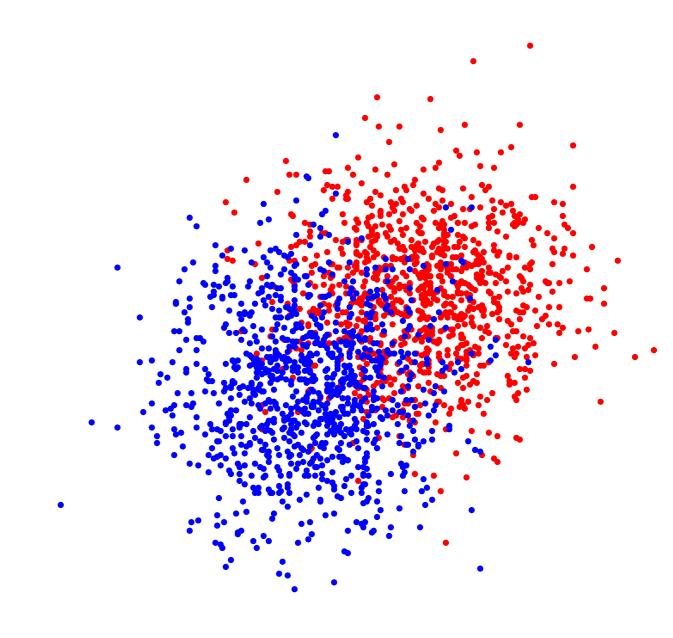
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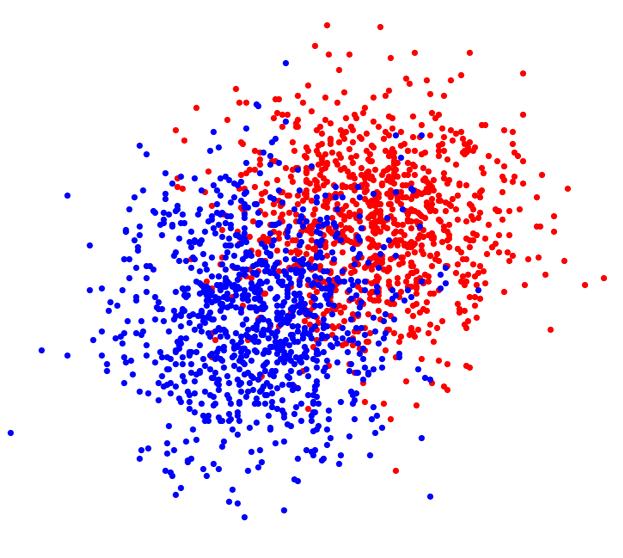
14]
coto

[Zhang and Moore, *PNAS* 2014] image by Tiago de Paula Peixoto

Clustering high-dimensional data

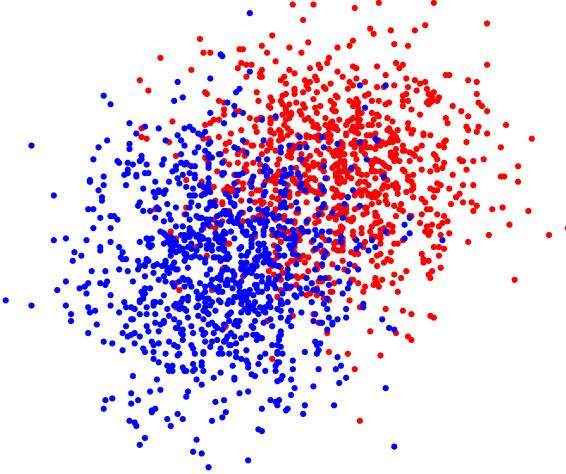


m points in n-dimensional space, where m=O(n)



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m points in *n*-dimensional space, where m=O(n)two clusters centered at ±v for some unknown vector v each point has a Gaussian noise vector *u_i*

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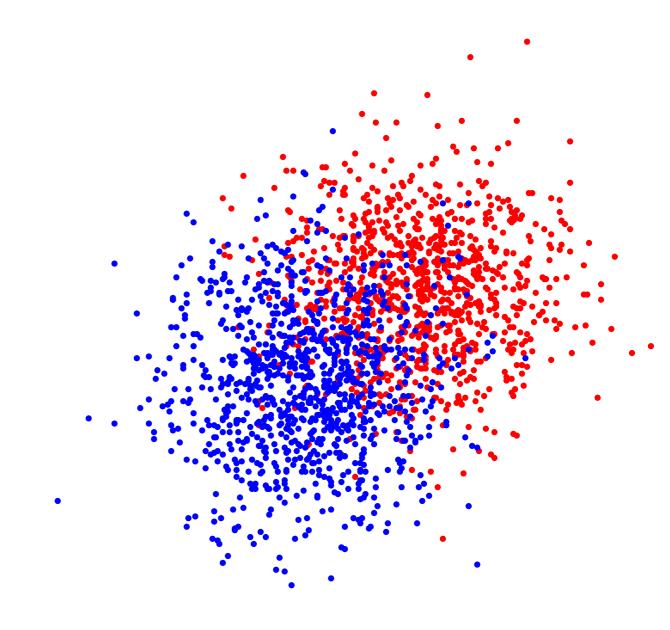
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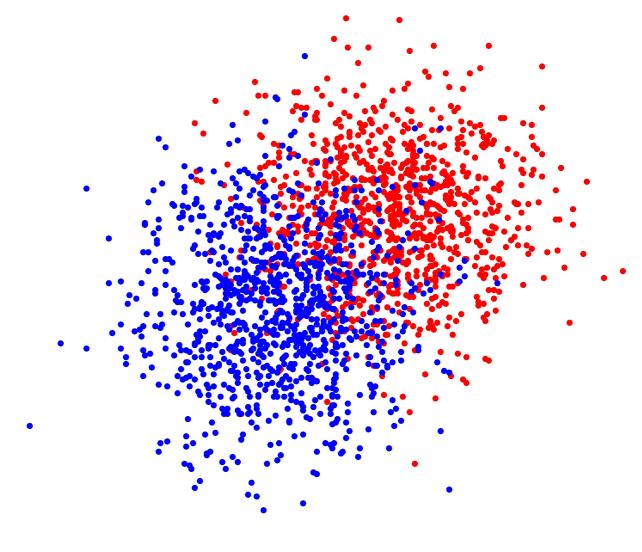
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are there phase transitions as a function of |v| vs. |u| and m/n?

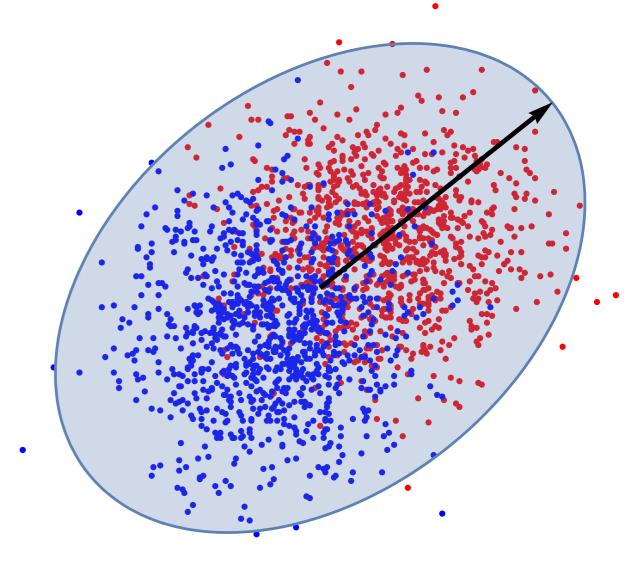
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find the direction along which the points have the largest variance



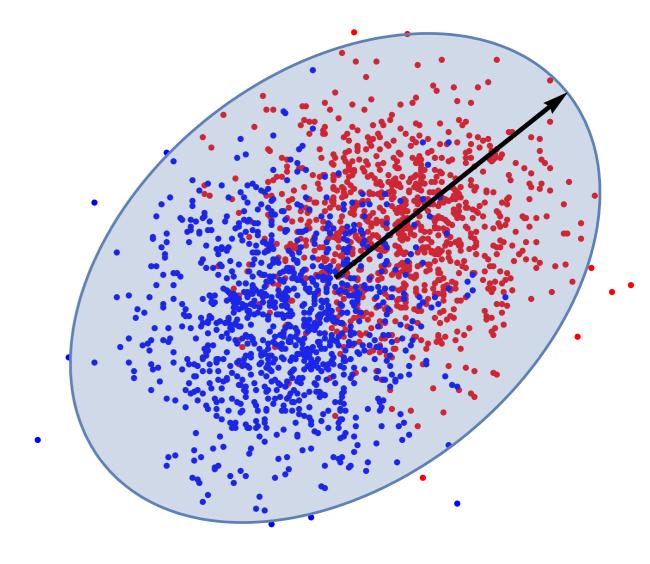
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first eigenvector of the matrix

$$\frac{1}{m} \sum_{i=1}^{m} x_i \otimes x_i$$



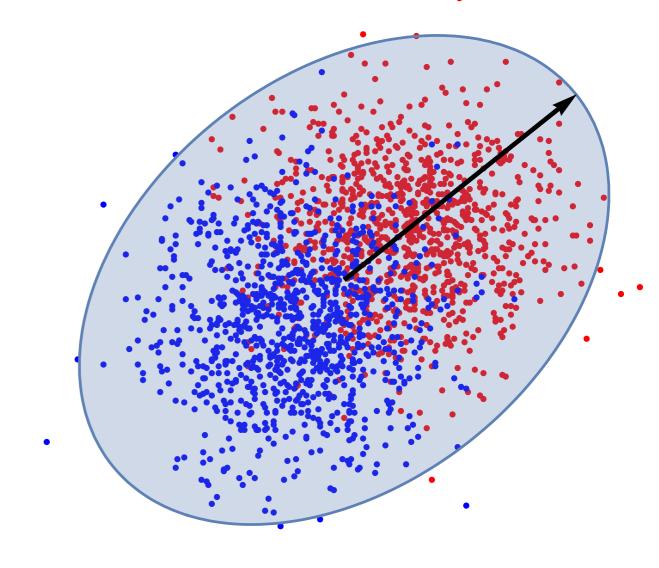
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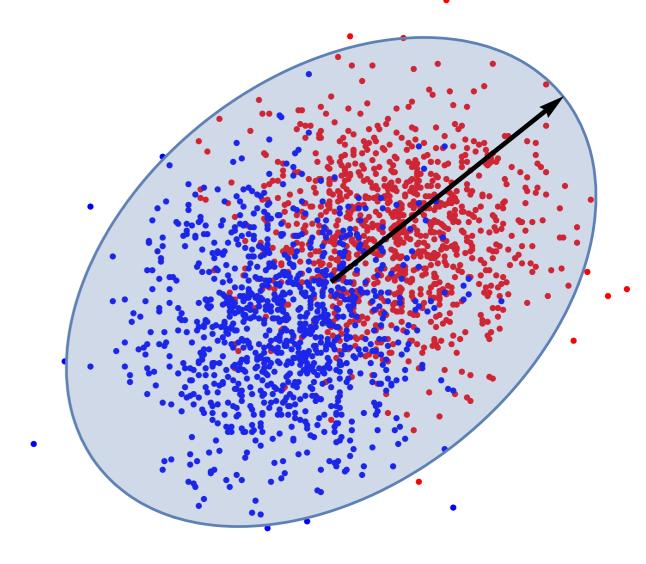
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plus a rank-1 perturbation

$$(v+\bar{u})\otimes(v+\bar{u})$$



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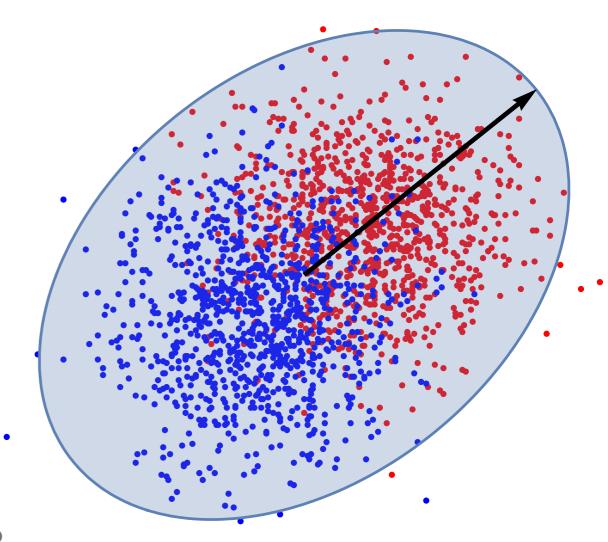
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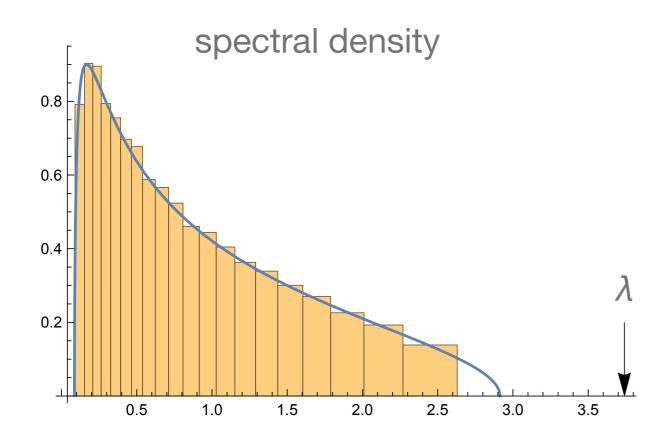
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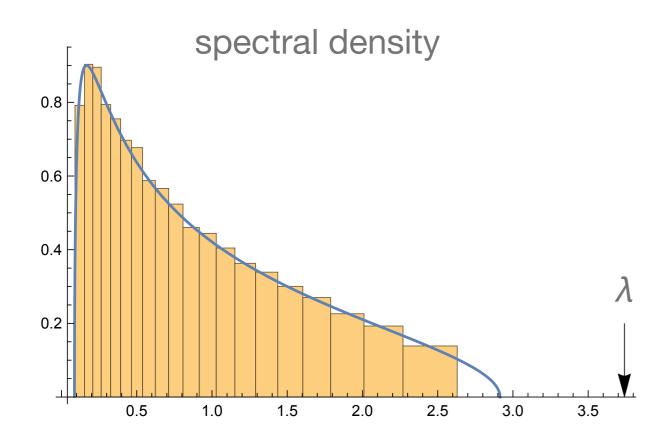
when does PCA work? and how accurately?



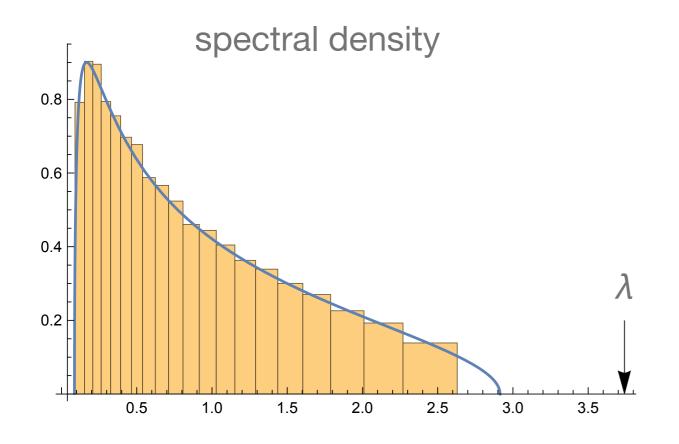
when does this perturbation rise above the "bulk" of random eigenvectors?

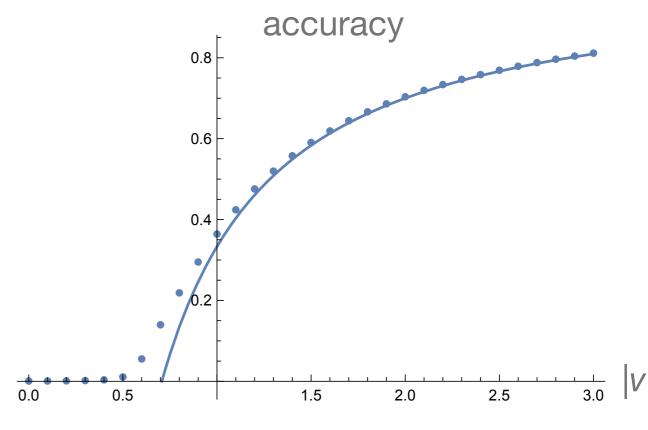


when does this perturbation rise above the "bulk" of random eigenvectors? when it does, how accurately does the leading eigenvector point to *v*?

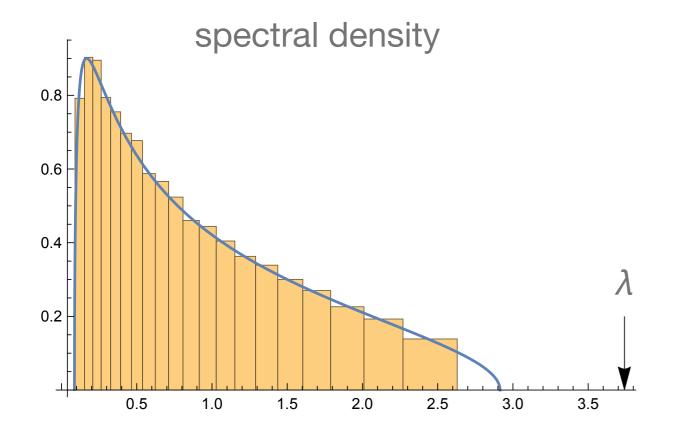


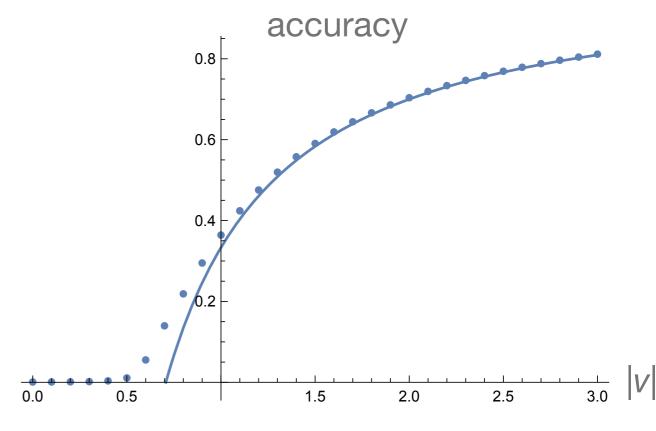
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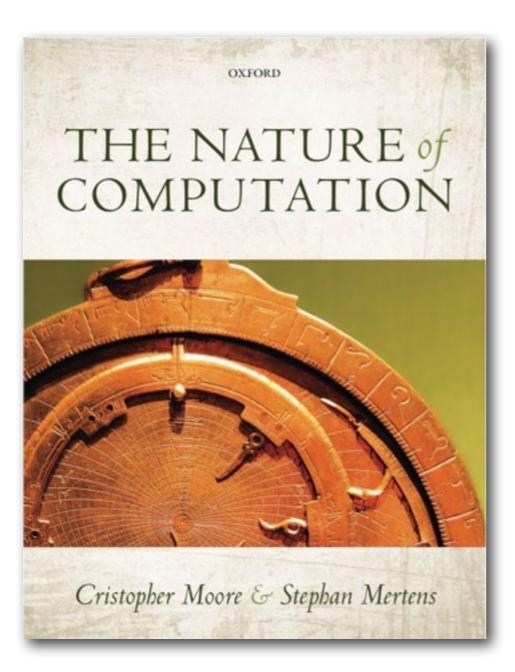
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"as simple as possible, but no simpler"

Shameless Plug



To put it bluntly: this book rocks! It somehow manages to combine the fun of a popular book with the intellectual heft of a textbook.

Scott Aaronson, MIT

This is, simply put, the best-written book on the theory of computation I have ever read; one of the best-written mathematical books I have ever read, period.

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