Computational methods in percolation

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Oct 29, 2008

Outline

Acknowledgements

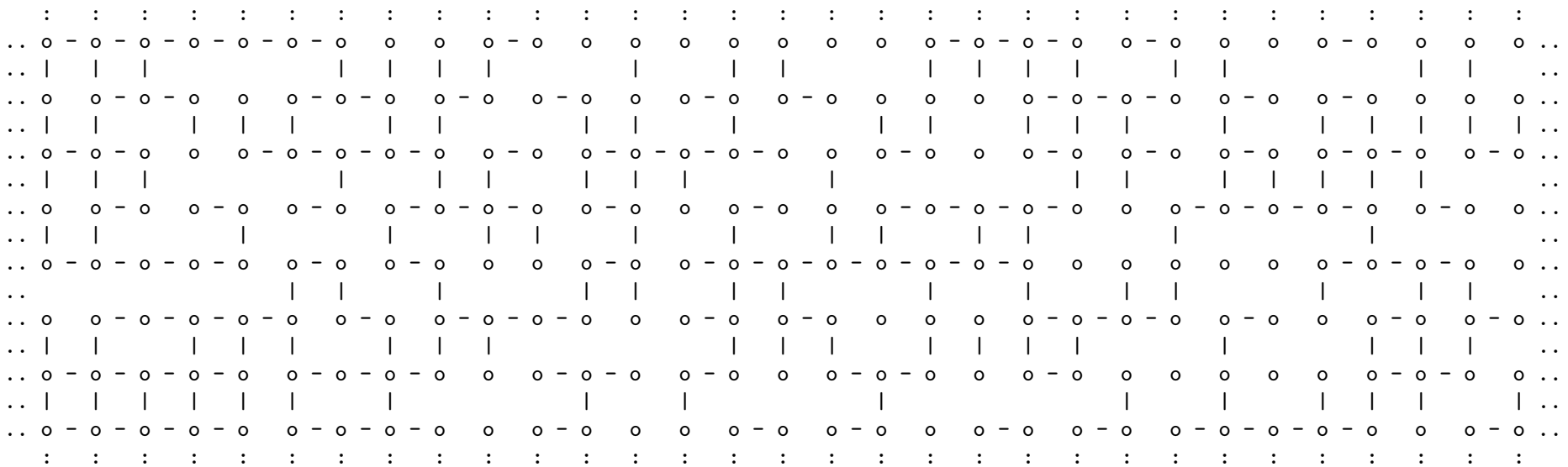
This is an excerpt from a project with Janek Wehr in spring 2008.

I would like to thank Janek Wehr, Tom Kennedy, and John LaPeyre for multiple insights.

Main questions

What is percolation?

Take a lattice of **sites** — for today, $\mathbb{Z}^2$. With fixed probablity p, the *bond density*, connect nearest-neighbor sites with a **bond**. The bonds are independent and identically distributed. Connected nearest-neighbor sites are said to share an **open bond**. Here, $p = 0.51$:



(This is called *bond percolation*, where all sites are populated and edges are populated randomly. The opposite case is called *site percolation*; I will not discuss it today.)

It is easy to construct a formal probability measure on finite lattices; for $\mathbb{Z}^2$, one uses cylinder sets to construct a measure. See Grimmett's *Percolation* for more information.

Why percolation?

Lattice percolation, along with the Ising model, is to statistical mechanics as the fruit fly is to biology: easy to produce in large numbers, not too smart or multifaceted, yet with some properties that (one hopes) shed light on more complex systems.

Percolation may be used to model filtering of fluids through porous materials, current in complex electric circuits, etc. Mathematicians have, as usual, mathematized percolation into a pure subject which is interesting in its own right.

One reason I find percolation fascinating is that it has a nice blend of theory and computation. In fact, many questions in percolation can only (at present) be handled numerically. Other questions may be reduced theoretically into problems which are simpler to handle numerically. The main purpose of this talk is to shed some light on where such numerical results come from.

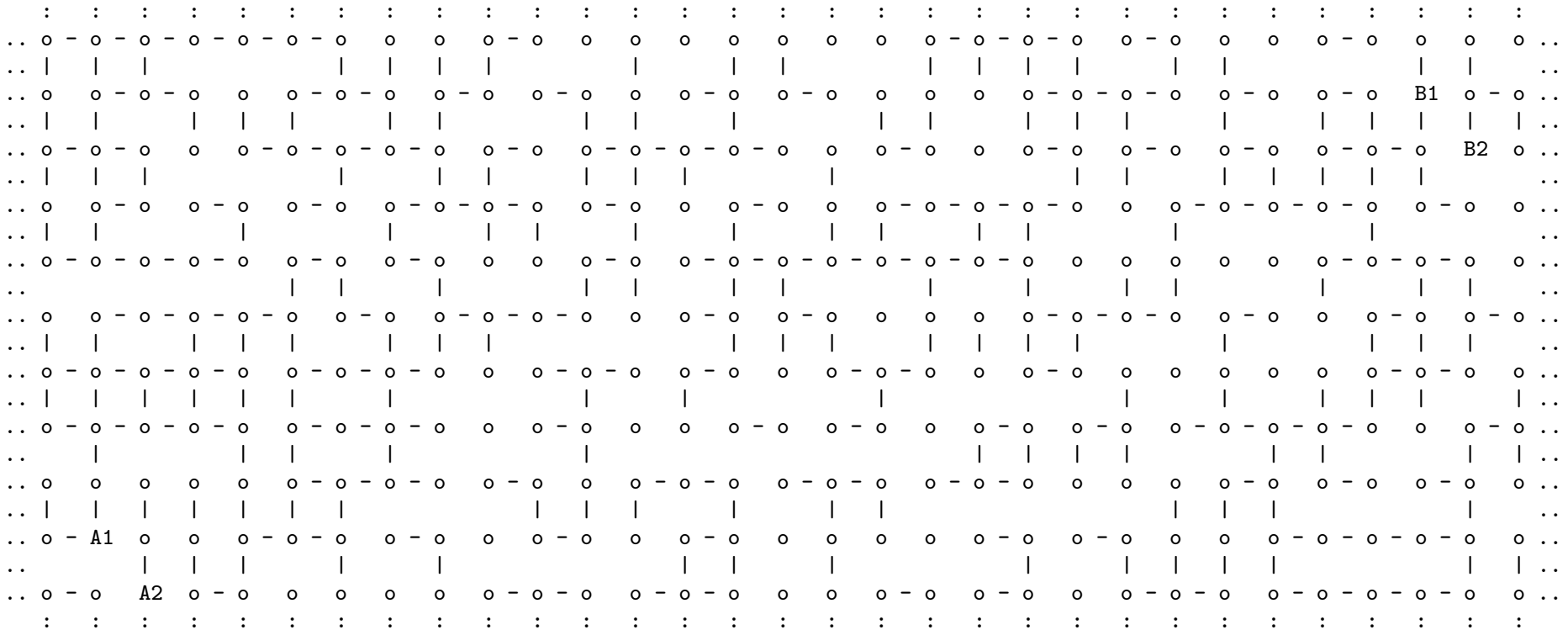
Questions

Many questions may be asked about percolation. Here are a few (some having arisen in my recent project with Janek Wehr) which I'll touch on today:

- Are there infinite clusters, and if so, with what probability? (As it turns out, the infinite cluster is unique if it exists.)
- What is the probability that a fixed site is in the infinite cluster: $\theta(p) := P(A \in \mathcal{C})$?
- What is the probability that one of a pair of adjacent sites is in the infinite cluster: $\sigma(p) := P(A_1 \in \mathcal{C} \cup A_2 \in \mathcal{C})$?
- What is the probability that there is a path between two adjacent sites: $\tau(p) := P(A_1 \circ\!\!-\!\!\circ A_2)$?
- What is the probability that there is a path between two distant sites: $P(A \circ\!\!-\!\!\circ B) = P(A, B \in \mathcal{C})$?
- What is the probability that there is at least one path between pairs of distant sites: $P(A_1, B_1 \in \mathcal{C} \text{ or } A_1, B_2 \in \mathcal{C} \text{ or } A_2, B_1 \in \mathcal{C} \text{ or } A_2, B_2 \in \mathcal{C})$?

Meaning of A_1, A_2, B_1, B_2

Throughout, I take A_1, A_2 to be on opposite corners of a square, and likewise for B_1, B_2. However, I take the A's to be very far from the B's. This is the situation that arose, for reasons outside the scope of this talk, in the project with Wehr. What does "very far" mean? Far enough that $P(A, B \in \mathcal{C}) \approx P(A)P(B)$.



Theoretical reduction

Probability concepts: independence

This talk is light on probability. However, we do need need two key concepts: independence and the inclusion/exclusion principle.

Definition: Two events X and Y are said to be *independent* if their probabilities factor, i.e. $P(X \cap Y) = P(X)P(Y)$.

For intuition, take X and Y to be getting heads from flipping each of two fair coins.

(1) In the usual setup, we have $P(X) = 1/2$ and $P(Y) = 1/2$. Getting two heads happens happens a quarter of the time, i.e. $P(X \cap Y) = 1/4 = P(X)P(Y)$. The events X and Y are independent.

(2) Now suppose the coins are welded together side by side. The left coin still comes up heads half the time, as does the right — so, $P(X) = P(Y) = 1/2$. Yet two heads and two tails each happen half the time, so $P(X \cap Y) = 1/2 \neq P(X)P(Y)$. These events X and Y are not independent.

Note that it's the *intersection*, not the union, of independent events which factors. Also note that we often write $P(X \cap Y) = P(X, Y)$.

Probability concepts: inclusion/exclusion

Theorem [inclusion/exclusion principle]: The union of n (not necessarily independent) events $A_1, \ldots, A_n$ factors as the alternating sum of intersections, as follows:

$$P(\cup_{i=1}^n A_i) = \sum_{i=1}^n P(A_i) - \sum_{i,j=1}^n P(A_i, A_j) + \sum_{i,j,k=1}^n P(A_i, A_j, A_k)$$
$$\ldots - (-1)^n P(\cap_{i=1}^n A_i).$$

Examples:

$$P(A \cup B) = P(A) + P(B) - P(A, B);$$
$$P(A \cup B \cup C) = P(A) + P(B) + P(C)$$
$$- P(A, B) - P(A, C) - P(B, C)$$
$$+ P(A, B, C).$$

There are various ways to prove this in the general case (see any good probability text). For $n = 2, 3$, it's easy to verify this with a Venn diagram, keeping track of the undercounting and overcounting of each region of the diagram.

Existence of the infinite cluster

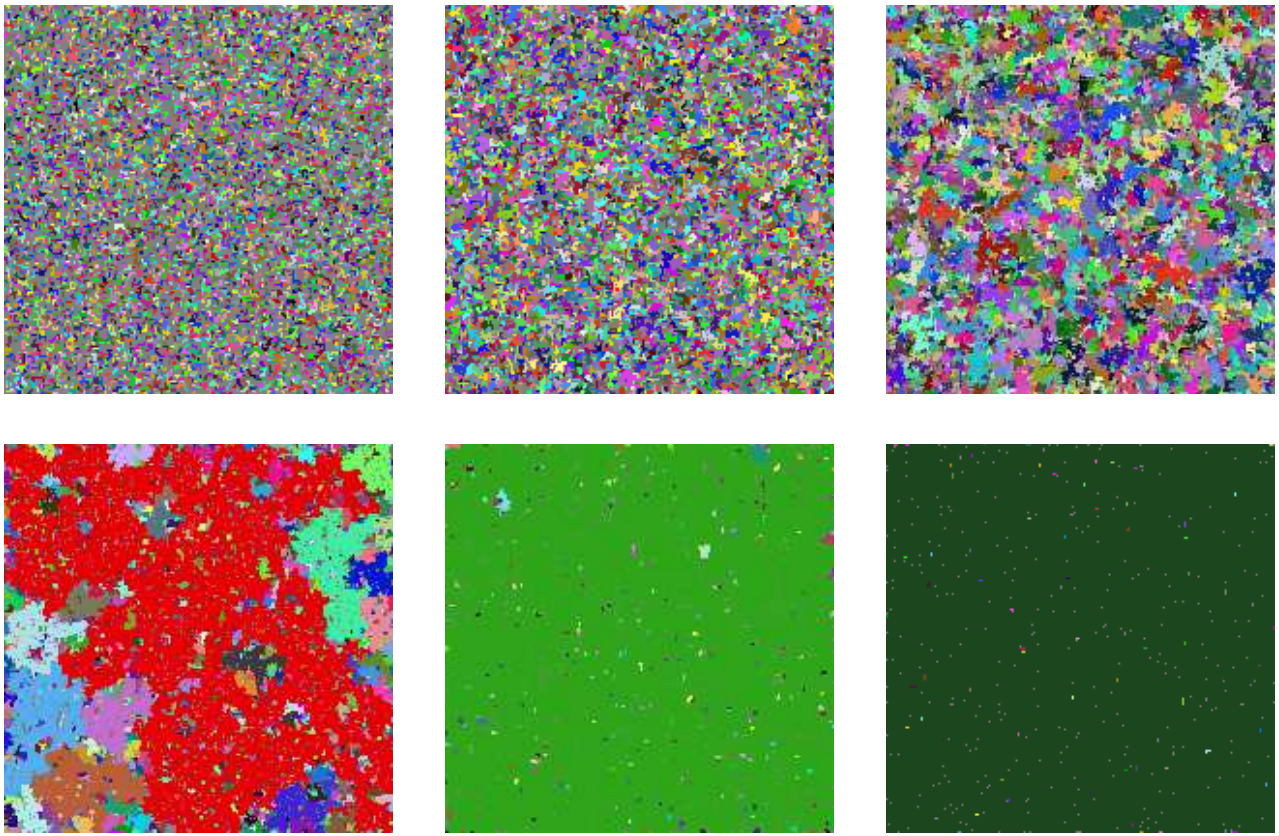
The following may be proved rigorously (see Grimmett, for example):

- There is a **critical bond density** p_c. For the 2D rectangular lattice, this is rigorously known to be $p_c = 0.5$. For the 3D rectangular lattice, this is experimentally known to be $p_c \approx 0.2488126$, to seven decimal places.
- For $p < p_c$, with probability 1 there is no infinite cluster; for $p_c < p$, with probability 1 there is a unique infinite cluster. These facts follow from Kolmogorov's zero-one law depending on whether $\theta(p) = 0$ (i.e. $p < p_c$) or $\theta(p) > 0$ (i.e. $p_c < p$).
- For $p = p_c$, it is not clear whether or not $\theta(p_c) = 0$. I believe that for $d = 2$, Kesten showed that $\theta(p_c) = 0$ so there is no infinite cluster at p_c, and that the question is open for $d > 2$. However, I as of this talk I haven't been able to find the citation.

See also the figures on the next page.

Clusters

Here are 200×200 lattices with $p = 0.2, 0.3, 0.4, 0.5, 0.6, 0.7$. Singleton clusters are marked grey; clusters of size bigger than 1 are marked with randomly selected colors.

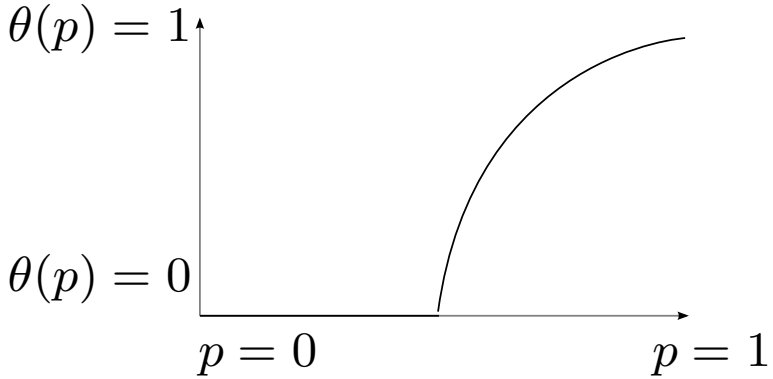


Note for later: $\xi(p)$, the *correlation length*, is the average diameter of non-infinite clusters. It diverges to infinity as p approaches p_c from either side.

$P(A \in \mathcal{C})$

Recall that $\theta(p) := P(A \in \mathcal{C})$. This may also be thought of as the fraction of lattice sites which participate in the infinite cluster. The following is known about $\theta(p)$.

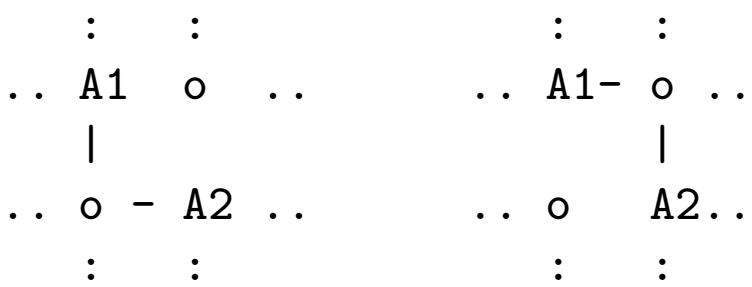
- $\theta(0) = 0$ and $\theta(1) = 1$. This is obvious: if $p = 0$ then no bonds are open; if $p = 1$ then all bonds are open and $\mathcal{C} = \mathbb{Z}^2$.
- For $p < p_c$, $\theta(p) = 0$. There is no infinite cluster, so a fixed site A can't be in it; for $p > p_c$, $\theta(p)$ is a strictly increasing function of p. (We say that there is a **phase transition** at p_c.)
- It is conjectured that for p approaching p_c from above, $\theta(p) \sim (p - p_c)^\beta$ for some **critical exponent** β. This means that, for some $0 < \beta < \infty$, $\lim_{p \searrow p_c} \frac{\log(\theta(p))}{\log(p - p_c)} = \beta$.
- $\theta(p)$ looks something like this:



$P(A_1 \circ\!\!-\!\!\circ A_2)$ and $P(A_1 \in \mathcal{C} \cup A_2 \in \mathcal{C})$

Here are two questions which may be handled numerically:

- Probability of the existence of a path between adjacent sites: $\tau(p) := P(A_1 \circ\!\!-\!\!\circ A_2)$. This is bounded below by $p^2(2-p^2)$, since the following two shortest paths (L and R for left and right, respectively) might exist:



  Note that L and R each occur with probability p^2. Then using inclusion/exclusion, $P(L \cup R) = P(L) + P(R) - P(L,R) = 2p^2 - p^4 = p^2(2-p^2)$. But there might also be less direct paths. There are combinatorial difficulties in obtaining a formula for $\tau(p)$ in terms of p.
- $\sigma(p) := P(A_1 \in \mathcal{C} \cup A_2 \in \mathcal{C})$. This shows up in another question to be discussed below. Note that the proximity of A_1 and A_2 means the events $A_1 \in \mathcal{C}$ and $A_2 \in \mathcal{C}$ are not independent.

$P(A, B \in \mathcal{C})$

If $p > p_c = 0.5$, there exists a unique infinite cluster $\mathcal{C}$ with probability 1. Successful communication from A to B requires $A, B \in \mathcal{C}$. These two events are (asymptotically) independent, so we have

$$P(A \in \mathcal{C}) = \theta(p), \qquad P(B \in \mathcal{C}) = \theta(p), \qquad P(A, B \in \mathcal{C}) = \theta^2(p).$$

This question is handled theoretically, modulo our incomplete understanding of $\theta(p)$.

Multiple paths

What is the probability that there is a path from either one of the A's to either one of the B's? Claim:

$$P(A_1, B_1 \in \mathcal{C} \text{ or } A_1, B_2 \in \mathcal{C} \text{ or } A_2, B_1 \in \mathcal{C} \text{ or } A_2, B_2 \in \mathcal{C}) = \sigma^2(p)$$

where

$$\sigma(p) = P(A_1 \in \mathcal{C} \text{ or } A_2 \in \mathcal{C}).$$

This can be proved a couple ways: using Boolean logic, and using inclusion/exclusion.

Note that the above expression reduces the question involving global events into one using local events. Then, experimental methods may be employed to attack those local questions.

Why bother — why not attack the original question numerically? In a computer, we have to do finite-size simulations; short-distance events are easier to simulate than long-distance ones.

Boolean proof

Start with

$$P\left[A_1, B_1 \in \mathcal{C} \text{ or } A_1, B_2 \in \mathcal{C} \text{ or } A_2, B_1 \in \mathcal{C} \text{ or } A_2, B_2 \in \mathcal{C}\right].$$

Gather pairs of events:

$$= P\left[(A_1, B_1 \in \mathcal{C} \text{ or } A_1, B_2 \in \mathcal{C}) \text{ or } (A_2, B_1 \in \mathcal{C} \text{ or } A_2, B_2 \in \mathcal{C})\right].$$

Boolean distributivity X and $(Y$ or $Z) = (X$ and $Y)$ or $(X$ and $Z)$:

$$= P\left[(A_1 \text{ and } (B_1 \in \mathcal{C} \text{ or } B_2 \in \mathcal{C})) \text{ or } (A_2 \text{ and } (B_1 \in \mathcal{C} \text{ or } B_2 \in \mathcal{C}))\right].$$

Boolean distributivity X or $(Y$ and $Z) = (X$ or $Y)$ and $(X$ or $Z)$:

$$= P\left[(A_1 \in \mathcal{C} \text{ or } A_2 \in \mathcal{C}) \text{ and } (B_1 \in \mathcal{C} \text{ or } B_2 \in \mathcal{C})\right].$$

Use asymptotic independence of A events and B events:

$$= P\left[A_1 \in \mathcal{C} \text{ or } A_2 \in \mathcal{C})\right] P\left[B_1 \in \mathcal{C} \text{ or } B_2 \in \mathcal{C})\right] = \sigma^2(p).$$

Inclusion/exclusion proof

Start with

$$P\left[A_1, B_1 \in \mathcal{C} \text{ or } A_1, B_2 \in \mathcal{C} \text{ or } A_2, B_1 \in \mathcal{C} \text{ or } A_2, B_2 \in \mathcal{C}\right].$$

Gather pairs of events and let E be the event $(B_1 \in \mathcal{C} \text{ or } B_2 \in \mathcal{C})$:

$$\begin{aligned}
=&P\left[(A_1, B_1 \in \mathcal{C} \text{ or } A_1, B_2 \in \mathcal{C}) \text{ or } (A_2, B_1 \in \mathcal{C} \text{ or } A_2, B_2 \in \mathcal{C})\right] \\
=&P\left[(A_1 \text{ and } (B_1 \in \mathcal{C} \text{ or } B_2 \in \mathcal{C})) \text{ or } (A_2 \text{ and } (B_1 \in \mathcal{C} \text{ or } B_2 \in \mathcal{C}))\right] \\
=&P\left[(A_1 \text{ and } E) \text{ or } (A_2 \text{ and } E)\right].
\end{aligned}$$

Apply inclusion/exclusion to the union and use asymptotic independence of A and B events, then inclusion/exclusion in reverse:

$$\begin{aligned}
=&P\left[A_1 \text{ and } E\right] + P\left[A_2 \text{ and } E\right] - P\left[A_1 \text{ and } A_2 \text{ and } E\right] \\
=&P[A_1]P[E] + P[A_2]P[E] - P[A_1 \text{ and } A_2]P[E] \\
=&\left(P[A_1] + P[A_2] - P[A_1 \text{ and } A_2]\right) P[E] \\
=&P[A_1 \in \mathcal{C} \text{ or } A_2 \in \mathcal{C}]\ P[B_1 \in \mathcal{C} \text{ or } B_2 \in \mathcal{C}] = \sigma^2(p).
\end{aligned}$$

Monte Carlo simulations

Monte Carlo simulations

Overview:

- For $M = 20, 25, 30, 35, 40, 45, \ldots$ as far as patience and CPU time hold out, and for various values of p above p_c, estimate

$$\theta_M(p) := P_M(A \in \mathcal{C})$$
$$\sigma_M(p) := P_M(A_1 \in \mathcal{C} \cup A_2 \in \mathcal{C})$$
$$\tau_M(p) := P_M(A_1 \circ\!\!-\!\!\circ A_2)$$

  for $M \times M$ lattices.

- For each fixed p, use finite-size scaling to extrapolate

$$\theta(p) = \lim_{M\to\infty} \theta_M(p), \qquad \sigma(p) = \lim_{M\to\infty} \sigma_M(p), \qquad \tau(p) = \lim_{M\to\infty} \tau_M(p).$$

Monte Carlo simulations for fixed M and p

The algorithms are simple.

To estimate a single P_M value for fixed p and M, do N trials detecting the event in question. Average these over the N trials to estimate P_M of that event. When choosing N, recall that the sample mean tends centrally toward a normal distribution and that the normal's standard deviation goes as $1/\sqrt{N}$. (I.e. to get another decimal place in the estimate of $P_M(E)$ for some event E, one needs to run 100 times as many experiments.)

For each trial:

- Populate the bonds of the lattice. Each bond is open with probability p.
- When the event is $A_1 \circ\!\!-\!\!\circ A_2$ (for $\tau_M(p)$), do a cluster walk as described below.
- When the event is $A \in \mathcal{C}$ (for $\theta_M(p)$) or $A_1 \in \mathcal{C} \cup A_2 \in \mathcal{C}$ (for $\sigma_M(p)$), mark all clusters and identify the largest one (as described below). Once the largest cluster is marked, it is easy to find if the single point A (for θ) or one of A_1 and A_2 (for σ) is in that cluster.

Cluster walking

To see if $A_1 \circ\!\!-\!\!\circ A_2$, a naive algorithm almost works:

- Start at site A_1.
- Make a list of the 0 to 4 nearest-neighbor sites which are connected to A_1 by an open bond.
- If any of those sites is A_2, then $A_1 \circ\!\!-\!\!\circ A_2$. Stop.
- Otherwise, repeat this process (by recursively calling the subroutine) for each of the neighbors.
- Once the recursions are complete with no more unmarked neighbors to visit, A_1 is not connected to A_2. Stop.

Problem: you can chase around in a circle indefinitely whenever there is a loop in the bond graph.

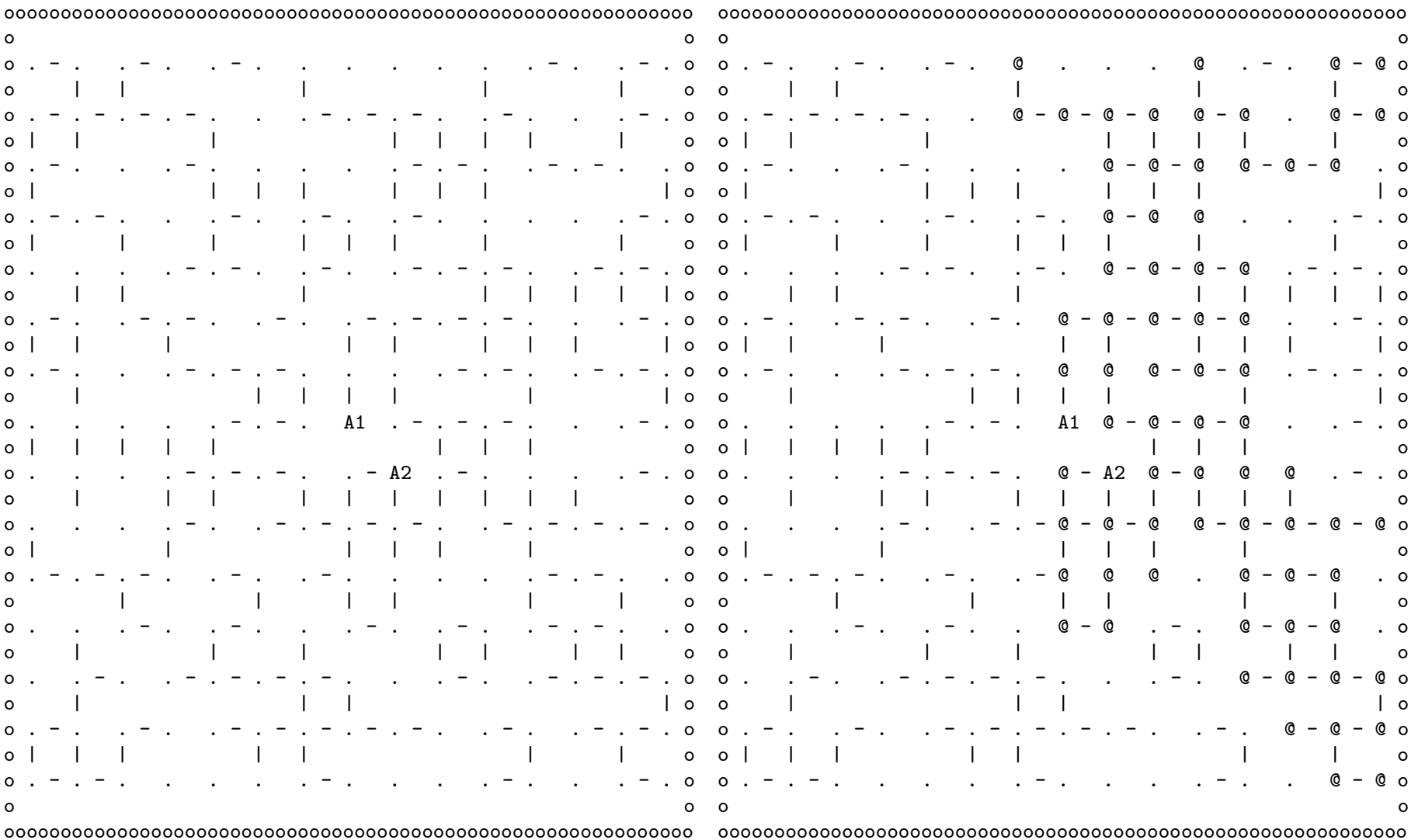
Solution: Make a matrix of site marks, all initialized to zero. Mark each site as you visit it. When recursively calling the subroutine, recurse only into non-visited sites. Infinite recursion successfully avoided.

Cluster walking

Analogy:

- To see if there's an acquaintance path between you and Jane Thomas, first ask yourself if you know Jane personally. If so, then the answer is yes and you're done.
- If not, ask everyone you know if they have an acquaintance path to Jane. If any of them have a path to her, then the answer is yes and you're done.
- Each of the people you ask might also have to ask someone else, and so on.
- Rule: they can't ask you or anyone else that's been contacted — else we get in a silly loop.
- When no one knows Jane personally, and no one has any uncontacted people left to ask, then the answer is no and you're done.
- Using this technique, you won't necessarily have found *all* acquantaince chains between yourself and Jane — you'll have found at most one chain.

Cluster walk with $M = 14$ and $p = 0.51$: before and after



Cluster marking and sizing

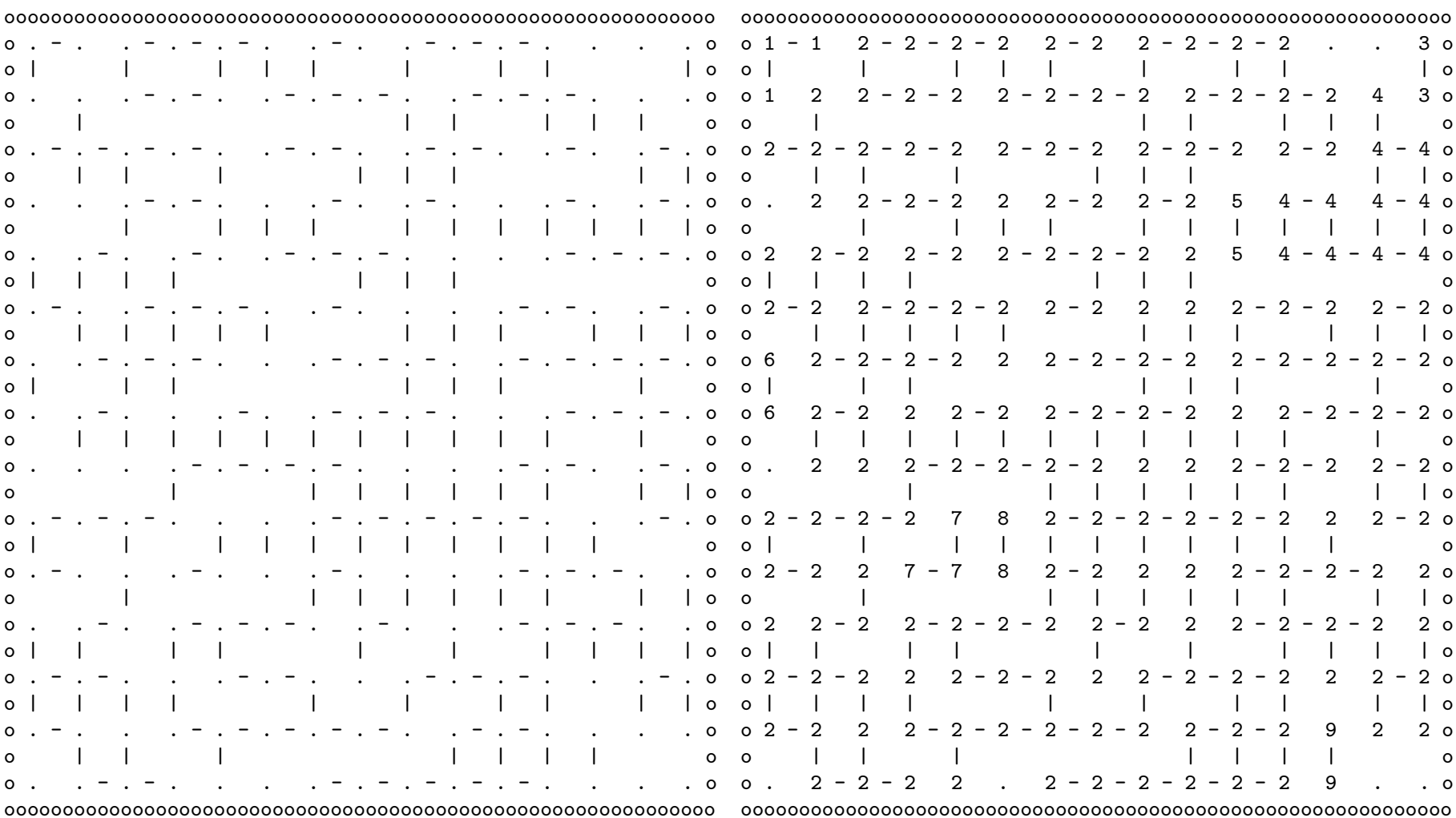
Cluster marking for the events $A \in \mathcal{C}$ and $(A_1 \in \mathcal{C} \cup A_2 \in \mathcal{C})$: we need to identify the largest cluster.

- Again keep a matrix of site marks, now serving as cluster numbers, all initially set to zero.
- Set cluster number $= 1$.
- For each site A:
  - If A's cluster number is non-zero (site A has already been visited), continue to the next site.
  - In the site-marks matrix, mark A with the current cluster number.
  - For each bonded neighbor of A, recursively call the subroutine.
  - After the recursion completes, increment the cluster number by 1.

Cluster sizing:

- Walk through the sites of the lattice, counting the size of each cluster.
- Remember the number of the largest cluster. Call this $\mathcal{C}$.

Lattice before and after cluster numbering: $M = 14, p = 0.6$



Here the largest cluster is 2.

Finite-size scaling

Finite-size scaling

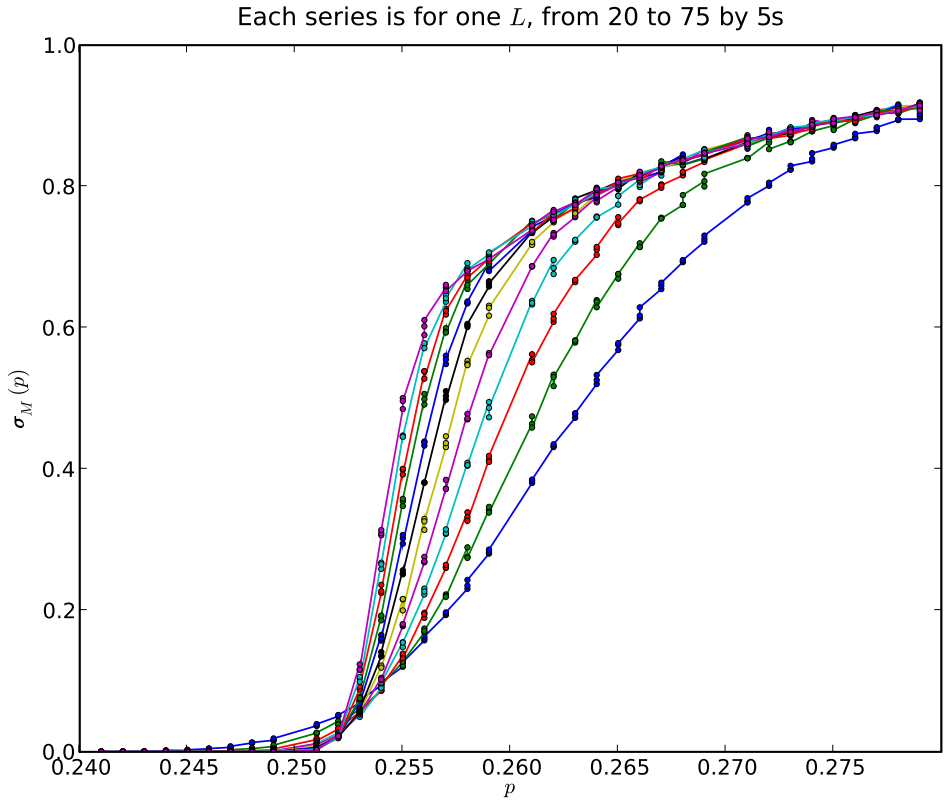
Finite-size scaling is something I'm still learning about. Thoughts gleaned from Kennedy, LaPeyre, and Wehr:

- M and ξ (correlation length) are both length scales. (For $p < p_c$, this is the average cluster diameter. For $p_c < p$, this is the average diameter of finite clusters. It diverges to infinity as $p \to p_c$ from either side.) Key point: If $M < \xi$ then the largest cluster found on the $M \times M$ lattice might not truly be a piece of the infinite cluster.
- For p comfortably above or below p_c, M passes ξ quickly and infinite values $\sigma(p)$ are obtained quickly.
- For p near p_c, one must somehow extrapolate $\sigma_M(p)$ to $\sigma(p)$.
- ξ can also be estimated numerically, if desired.
- Kennedy conjectures $\sigma_M(p) = \sigma(p)F(M/\xi)$, for some F.
- See perhaps Stauffer's text.
- Wehr: Do the comparison just for one or more p's off p_c. This is more easily achieved and might be sufficiently newsworthy.

See the next slide for some data, obtained as follows. For a range of p values: for a range of M values: for three trials: plot $\theta_M(p)$, $\sigma_M(p)$, or $\tau_M(p)$.

Finite-size scaling: $\sigma_M(p)$ vs. p (3D case)

These were actually taken from a 3D computation. (Recall $p_c \approx 0.2488126$ for $d = 3$.)
It's clear from this plot that the curve approaches some kind of limiting shape . . . .



Finite-size scaling: $\sigma_M(p)$ vs. M (3D case)

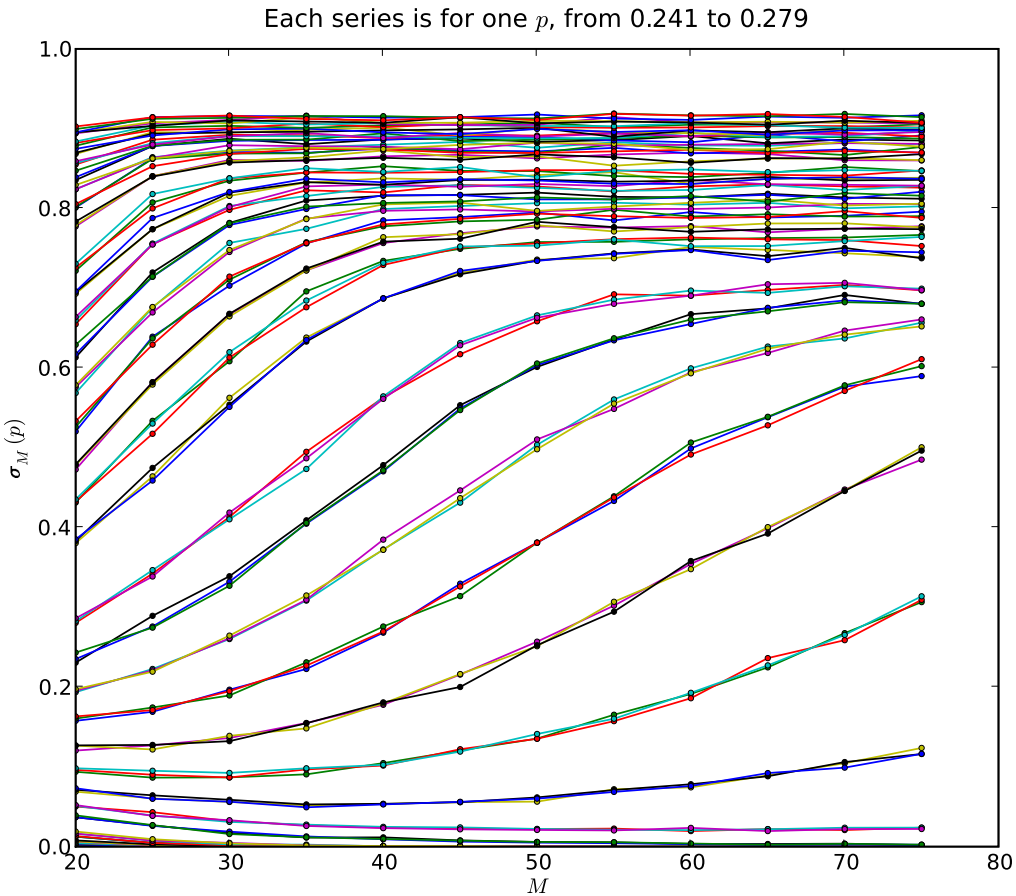
The figure on the previous slide included the following data, with each column as one data series:

	$M = 20$	$M = 25$	$M = 30$	$M = 35$	$M = 40$	$M = 45$	$M = 50$	...
...	...	...	...	...	...	...	...	
$p = 0.254$	0.0938	0.0865	0.0868	0.0906	0.1047	0.1205	0.1354	...
$p = 0.254$	0.0962	0.0901	0.0867	0.0968	0.1016	0.1221	0.1352	...
$p = 0.254$	0.0982	0.0951	0.0924	0.0982	0.1025	0.1191	0.1412	...
$p = 0.255$	0.1204	0.1269	0.1362	0.1550	0.1778	0.2157	0.2569	...
$p = 0.255$	0.1266	0.1218	0.1389	0.1482	0.1795	0.2163	0.2512	...
$p = 0.255$	0.1269	0.1275	0.1322	0.1546	0.1808	0.2001	0.2524	...
$p = 0.256$	0.1577	0.1690	0.1967	0.2227	0.2682	0.3296	0.3810	...
$p = 0.256$	0.1605	0.1744	0.1895	0.2310	0.2759	0.3140	0.3810	...
$p = 0.256$	0.1632	0.1711	0.1948	0.2269	0.2696	0.3261	0.3810	...
$p = 0.257$	0.1936	0.2227	0.2602	0.3084	0.3725	0.4312	0.5036	...
$p = 0.257$	0.1953	0.2210	0.2612	0.3094	0.3848	0.4465	0.5104	...
$p = 0.257$	0.1973	0.2193	0.2645	0.3148	0.3720	0.4368	0.4981	...
$p = 0.258$	0.2306	0.2893	0.3389	0.4090	0.4782	0.5533	0.6013	...
$p = 0.258$	0.2351	0.2759	0.3321	0.4048	0.4704	0.5491	0.6036	...
$p = 0.258$	0.2432	0.2745	0.3270	0.4057	0.4717	0.5472	0.6056	...
$p = 0.259$	0.2805	0.3422	0.4132	0.4949	0.5629	0.6172	0.6585	...
$p = 0.259$	0.2825	0.3466	0.4103	0.4734	0.5644	0.6313	0.6659	...
$p = 0.259$	0.2862	0.3386	0.4187	0.4868	0.5613	0.6284	0.6629	...
...	...	...	...	...	...	...	...	

A trick for visualizing the convergence in M is to instead plot each row as a data series.

Finite-size scaling: $\sigma_M(p)$ vs. M (3D case)

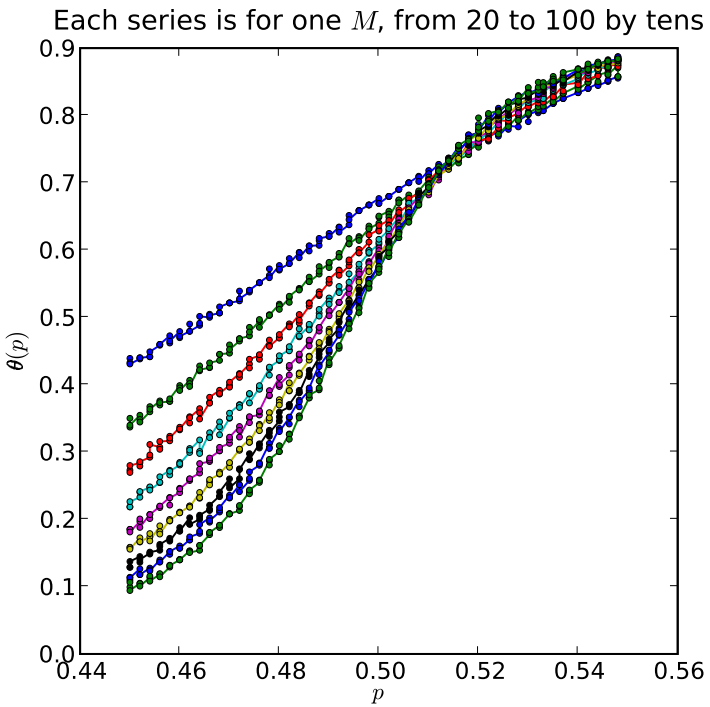
We can now clearly see *how* $\sigma_M(p)$ approaches $\sigma(p)$ as M increases. For p off p_c, σ values have stabilized. For p near p_c, they have not.

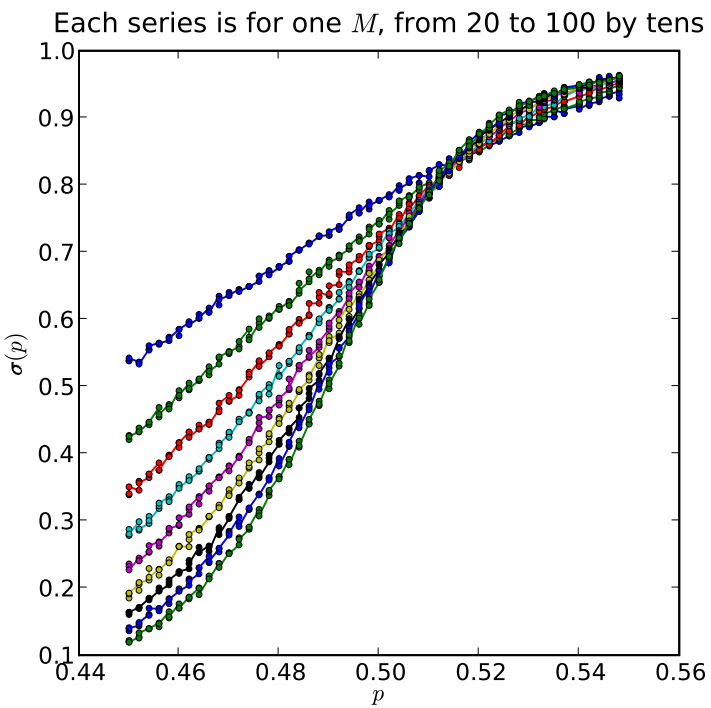


Finite-size scaling: $\theta_M(p)$ and $\sigma_M(p)$ vs. p

These are data from the 2D case. Recall that for $p < 0.5$ we already know, for theoretical reasons, $\theta(p) = 0$. So $\theta_M(p) \searrow 0$ as M increases. The fact that $\theta_M(p) \neq 0$ for specific M's is a finite-size effect.

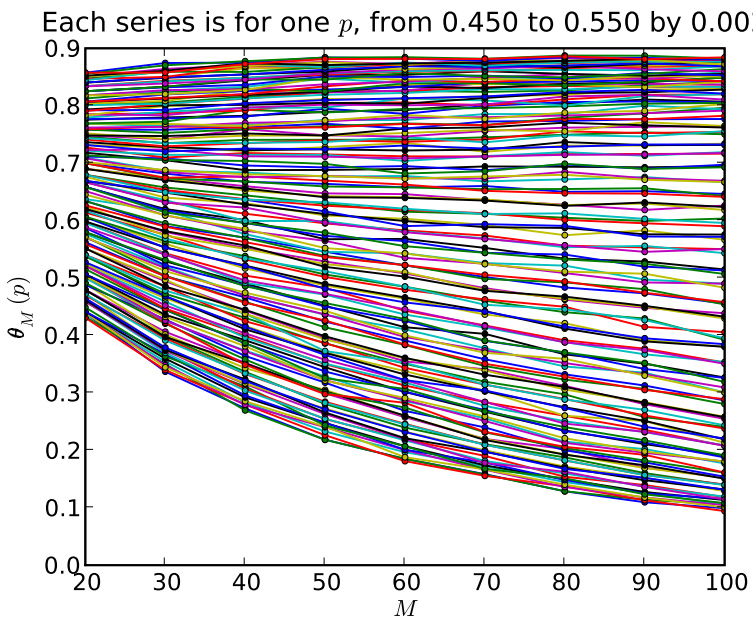
For σ, we don't have known theoretical values as we did with θ. To estimate $\sigma(p) = \lim_{M\to\infty} \sigma_M(p)$ for various p's, we need to account for finite-size effects. It's already clear that σ looks qualitatively similar to θ.

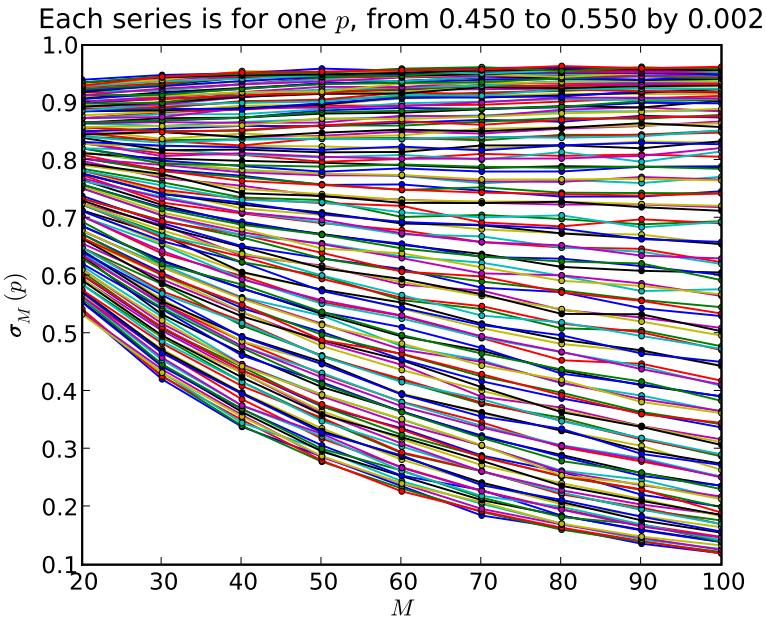




Finite-size scaling: $\theta_M(p)$ and $\sigma_M(p)$ vs. M

As in the 3D case, we can see that for many p's, the $\theta_M(p)$ and $\sigma_M(p)$ curves have already leveled out by $M = 100$. I used only a few CPU-hours to gather the data for these plots, so it would be easy to gather data for larger M's, say up to $M = 200$.

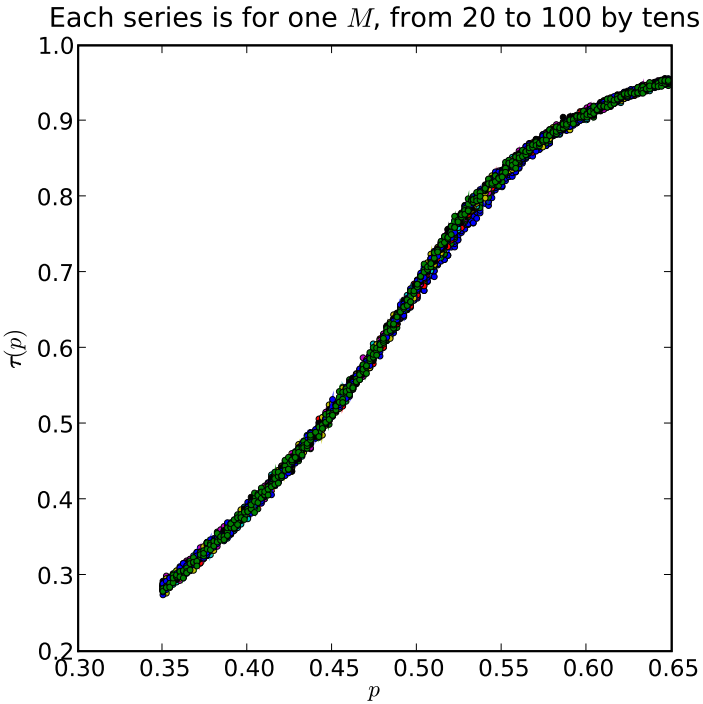


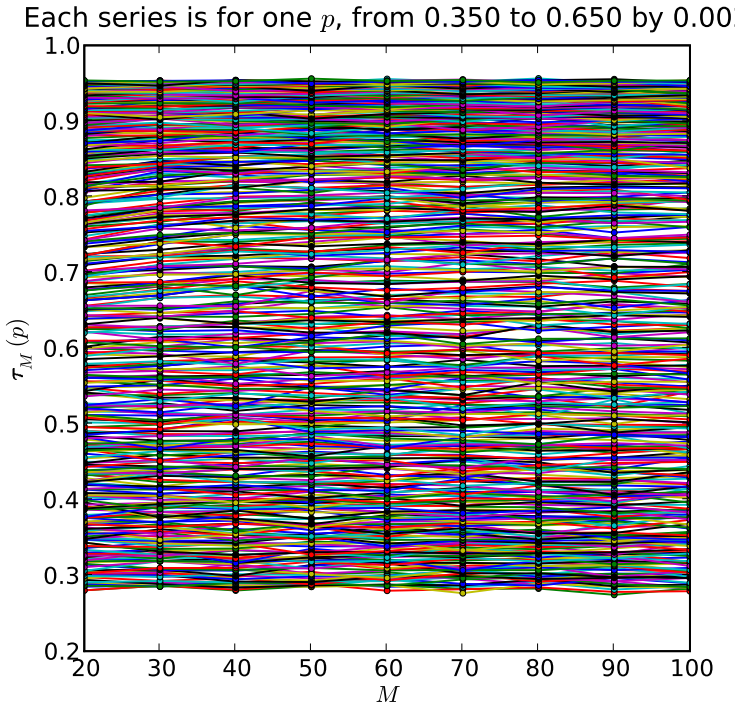


Finite-size scaling: $\tau_M(p)$ vs. p and M

Remember $\theta(p) = P(A \in \mathcal{C})$ and $\sigma(p) = P(A_1 \in \mathcal{C} \cup A_2 \in \mathcal{C})$. These are probabilities of *critical events*, since the infinite cluster $\mathcal{C}$ (whose existence is a global phenomenon) only appears for $p > p_c$.

On the other hand, $\tau(p) = P(A_1 \circ\!\!-\!\!\circ A_2)$ is a strictly local phenomenon. It is non-critical and grows smoothly in p, with negligible M dependence.





Conclusions

- All finite-lattice questions raised here are easily solved by simulation.
- Finite-size scaling is trivial for $\tau(p)$.
- For p far away from p_c, it's easy to extrapolate $\sigma(p)$ from the graph.
- For p close to p_c, one needs to either (1) be content with results for p far from p_c; (2) do simulations for larger M, hoping to surpass the correlation length $\xi(p)$ such that the curves start to level out; (3) deduce the correct formula for F.
- Thanks for attending!