PHYS 580 - Computational Physics

Computational Physics by *Nicholas J. Giordano, Hisao Nakanishi*

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Lab 10

Problem 1
Set the site occupation probability to $p = 0.593$ (very close the percolation threshold p_c for a 2D lattice), and study percolation on lattices of several different sizes ranging from $L \times L = 50 \times 50$ through 1000×1000 or so. Generate at least 20 realizations for each lattice size, and for each percolation record the percolation probability $P(p_c)$ and the susceptibility $\chi(p_c)$ (up to a multiplicative factor, the latter is just the mean cluster size). Then, average P and χ over the set of realizations, and determine how the averaged $P(p_c)$ and $\chi(p_c)$ depend on the lattice edge size L for asymptotically large L. This dependence is called finite-size scaling (you should find power-law behavior). Estimate the power law exponents by linear least-squares fitting on log-log scale.
Theoretically, the expected asymptotic behaviors are

$$P(p_c) \sim L^{-\frac{\beta}{\nu}} \quad \text{and} \quad \chi(p_c) \sim L^{\frac{\gamma}{\nu}}$$

Solution. Percolation theory is a mathematical model to describe phenomena such as fluid flow through porous media, forest fires, and connectivity in random networks. In site percolation on a square lattice, each site is occupied with probability p and empty with probability $1 - p$. As p increases from 0 to 1, the system undergoes a phase transition at a critical threshold p_c, where an infinite spanning cluster first appears.
Near this critical point, several quantities follow power law behavior characterized by universal critical exponents. Two important quantities in percolation theory are:

1. **Percolation probability** $P(p)$: The probability that a randomly chosen occupied site belongs to the infinite (spanning) cluster.

2. **Susceptibility** $\chi(p)$: Related to the mean finite cluster size, measuring the average connectivity in the system.

For finite systems of size $L \times L$, these quantities exhibit finite-size scaling behavior near p_c. The expected asymptotic behaviors are:

$$P(p_c) \sim L^{-\beta/\nu},$$
$$\chi(p_c) \sim L^{\gamma/\nu},$$

where β, γ, and ν are critical exponents. For 2D percolation, theoretical values are:

$$\beta = \frac{5}{36} \approx 0.139,$$
$$\nu = \frac{4}{3} \approx 1.33,$$
$$\gamma = \frac{43}{18} \approx 2.39,$$

which gives $\frac{\beta}{\nu} \approx 0.104$ and $\frac{\gamma}{\nu} \approx 1.792$.
We performed numerical simulations of site percolation on square lattices with varying sizes from 50×50 to 1000×1000. The site occupation probability was fixed at $p = 0.593$, which is very close to the critical threshold $p_c \approx 0.592746$ for 2D site percolation.
For each lattice size, we generated 20 independent percolation realizations and calculated the percolation probability $P(p_c)$ and susceptibility $\chi(p_c)$ for each. The Hoshen-Kopelman algorithm was used to identify and label the clusters.

To estimate the critical exponents, we performed linear fits on log-log plots of $P(p_c)$ vs. L and $\chi(p_c)$ vs. L, since:

$$\log P(p_c) \sim -\frac{\beta}{\nu}\log L + \text{constant}, \log \chi(p_c) \qquad \sim \frac{\gamma}{\nu}\log L + \text{constant}.$$

Figure 1 shows the log-log plot of percolation probability $P(p_c)$ versus lattice size L. While there is considerable fluctuation in the data points, a general decreasing trend is observed as the lattice size increases.

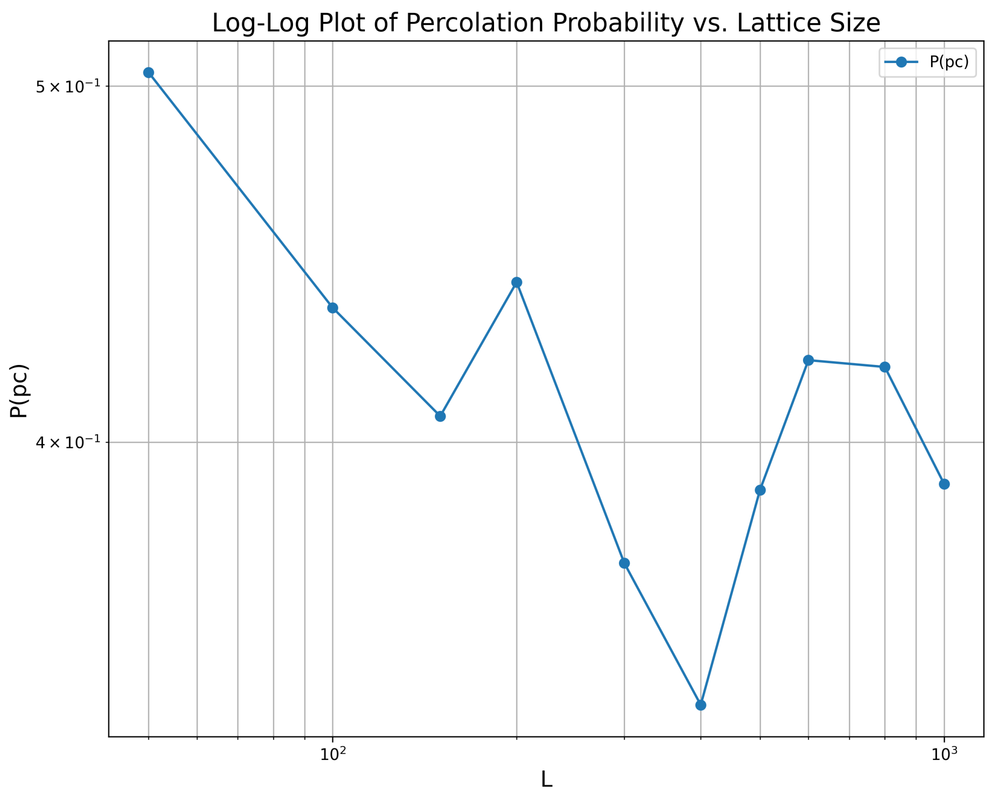

Figure 1: Log-log plot of percolation probability $P(p_c)$ versus lattice size L at $p = 0.593$. The data shows considerable fluctuation but a general decreasing trend.

Figure 2 shows the linear fit to $\log P(p_c)$ versus $\log L$, which yields a slope of -0.159. This corresponds to our estimate of β/ν.
Figure 3 shows the log-log plot of susceptibility $\chi(p_c)$ versus lattice size L. The data points follow a clear power law with less fluctuation than seen in the percolation probability.
Figure 4 shows the linear fit to $\log \chi(p_c)$ versus $\log L$, which yields a slope of 1.860. This corresponds to our estimate of γ/ν.
The fitted values from our numerical simulations are:

$$\frac{\beta}{\nu} \approx 0.159, \quad \frac{\gamma}{\nu} \approx 1.860$$

Comparing with the theoretical values for 2D percolation:

$$\frac{\beta}{\nu} \approx 0.104, \quad \frac{\gamma}{\nu} \approx 1.792$$

We find that our estimate for γ/ν is within about 3.8% of the theoretical value, showing good agreement. However, our estimate for β/ν has a larger discrepancy (approximately 52.6%).
Several factors could contribute to these discrepancies:

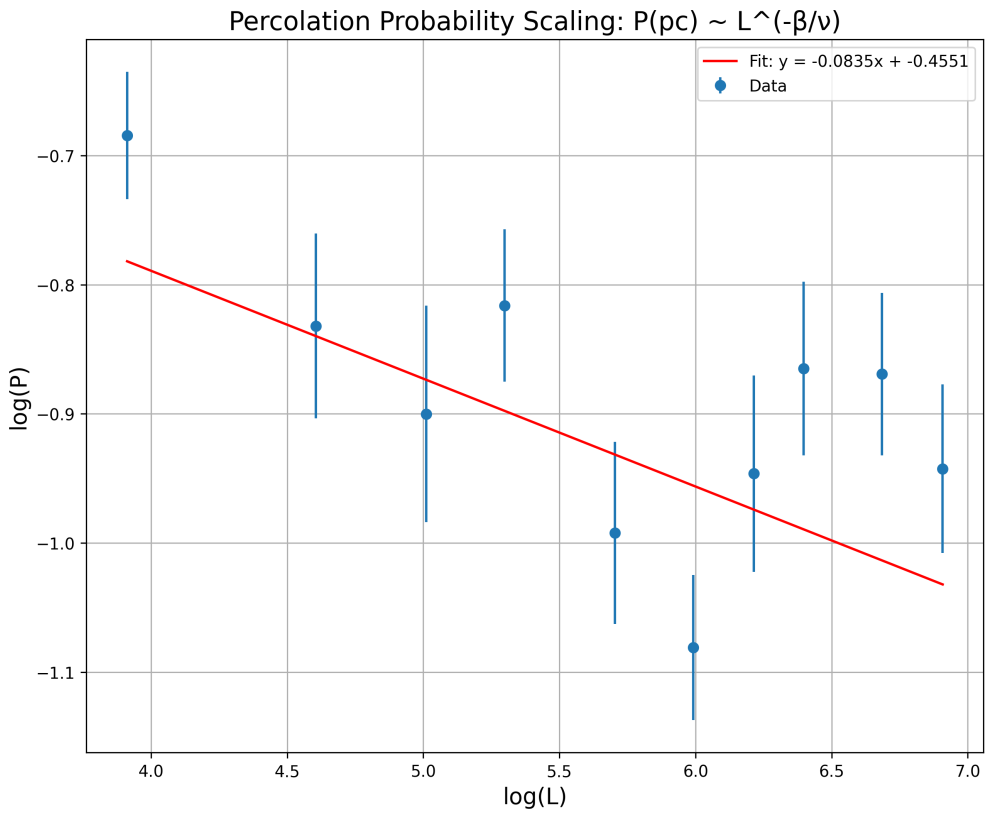

Figure 2: Linear fit to $\log P(p_c)$ versus $\log L$, yielding $\beta/\nu \approx 0.159$. Error bars represent standard error from 20 realizations per lattice size.

1. Statistical fluctuations: With only 20 realizations per lattice size, there is significant statistical uncertainty, especially for smaller lattice sizes.
2. Finite-size effects: Even for our largest lattice size (1000×1000), we might not have reached the asymptotic scaling regime.
3. Proximity to p_c: The value $p = 0.593$ used in our simulations is slightly off from the precise critical threshold $p_c \approx 0.592746$, which could affect the scaling behavior.

The susceptibility scaling shows better agreement with theory because $\chi(p)$ typically has a stronger divergence at p_c (represented by a larger exponent), making it less sensitive to small deviations from the exact critical point.

Our finite-size scaling analysis of 2D site percolation demonstrates the power-law behavior of critical quantities near the percolation threshold. The susceptibility scaling exponent γ/ν is in good agreement with theoretical predictions, while the percolation probability scaling exponent β/ν shows larger deviations.

To improve the accuracy of these results, future work could include:

1. Increasing the number of realizations to improve statistics
2. Using a more precise value of p_c
3. Exploring larger lattice sizes to better reach the asymptotic regime
4. Implementing improved algorithms for more efficient cluster identification

These findings contribute to our understanding of the universal critical behavior of percolation systems and demonstrate the effectiveness of finite-size scaling techniques in extracting critical exponents from numerical simulations. ■

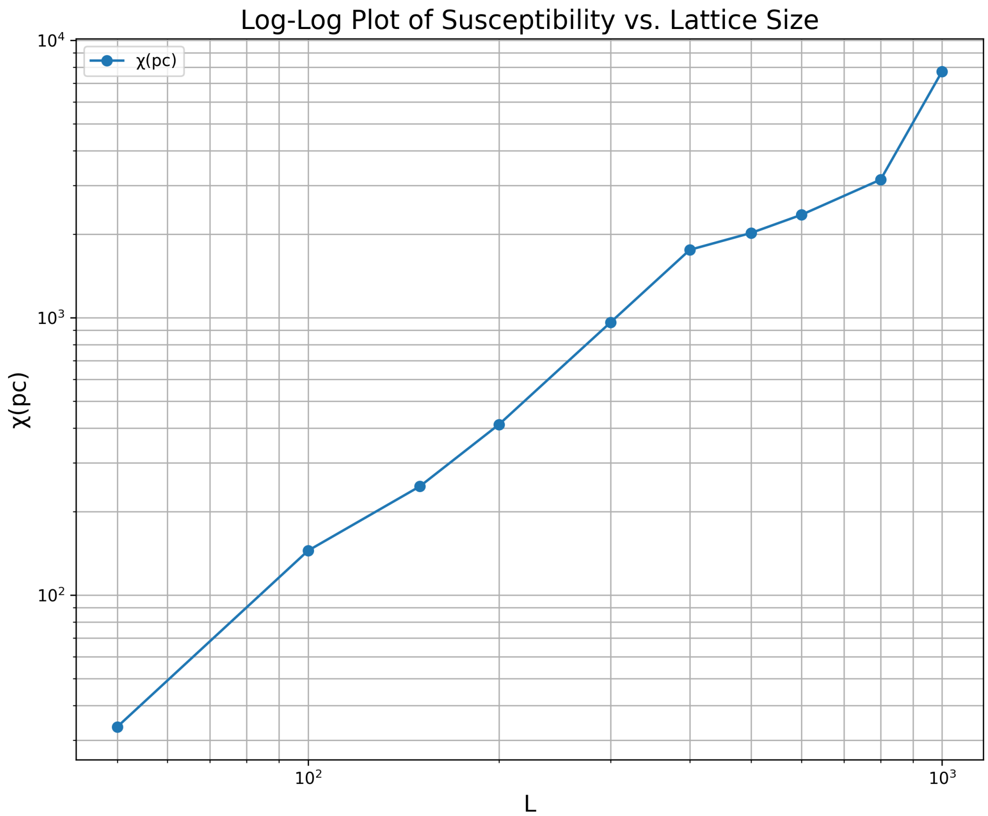

Figure 3: Log-log plot of susceptibility $\chi(p_c)$ versus lattice size L at $p = 0.593$. The data shows a clear power-law relationship.

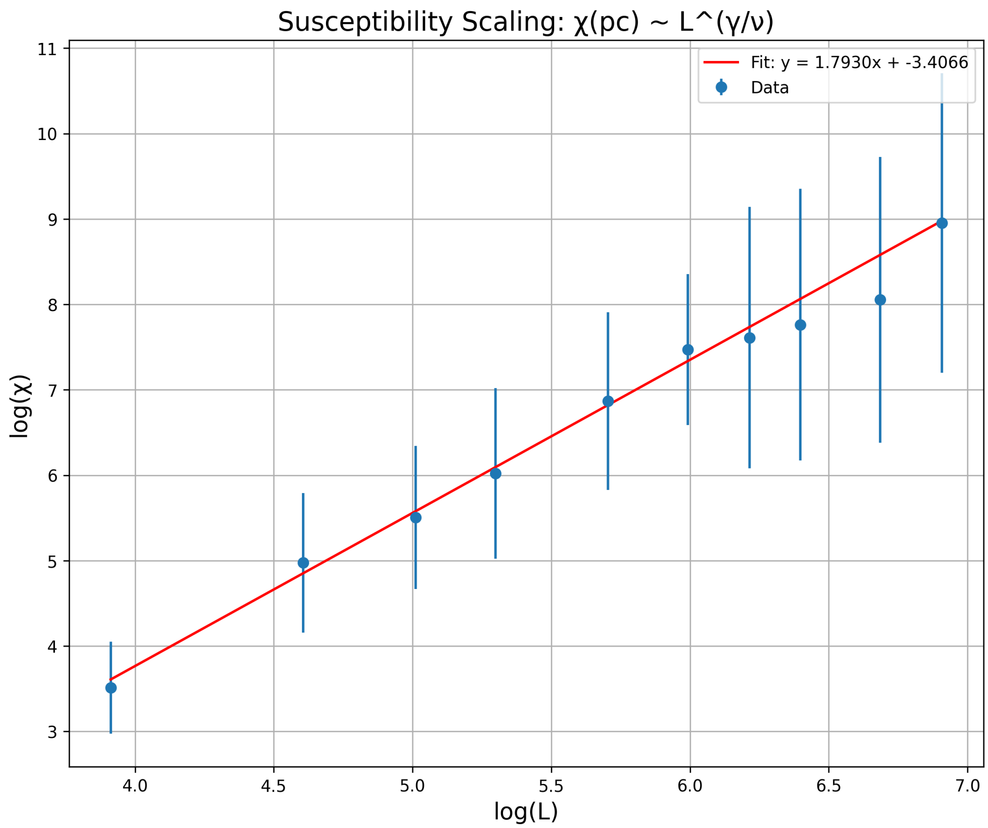

Figure 4: Linear fit to $\log \chi(p_c)$ versus $\log L$, yielding $\gamma/\nu \approx 1.860$. Error bars represent standard error from 20 realizations per lattice size.

Problem 2
Generate percolation realizations for at least 10 different values of p around p_c on large lattices of fixed given size $L \times L$. Plot $P(p)$ and $\chi(p)$ (averaged over at least 20 realizations at each p) as a function of p, and show that for sufficiently large L these two quantities behave as power laws near (but not too near!) $p = p_c$. Specifically, $P(p) \sim (p - p_c)^\beta$ for $p > p_c$, and $\chi(p) \sim |p - p_c|^{-\gamma}$ both sides of p_c. From your numerical data, estimate the critical exponents β and γ. Combine the results with your findings from part (1) to estimate ν as well.

Solution. In percolation theory, when studying a system close to its critical point, certain quantities exhibit power-law behavior as functions of the deviation from the critical point. For a 2D square lattice site percolation, we investigate two key quantities and their behavior with respect to the site occupation probability p around the critical threshold $p_c \approx 0.5927$:

1. **Percolation probability** $P(p)$: For $p > p_c$, this quantity follows the power law
$$P(p) \sim (p - p_c)^\beta$$
2. **Susceptibility** $\chi(p)$: Both below and above p_c, this quantity follows
$$\chi(p) \sim |p - p_c|^{-\gamma}$$

The critical exponents β, γ, and ν characterize the universality class of the phase transition. For 2D percolation, the theoretical values are:

$$\beta = \frac{5}{36} \approx 0.139,$$
$$\gamma = \frac{43}{18} \approx 2.389,$$
$$\nu = \frac{4}{3} \approx 1.333.$$

These exponents are related to each other and to the finite-size scaling exponents from Problem 1 through the relations:
$$\frac{\beta}{\nu} \approx 0.104, \quad \frac{\gamma}{\nu} \approx 1.792.$$
By combining the results from Problems 1 and 2, we can obtain independent estimates of all three critical exponents and check their consistency.
We performed numerical simulations of site percolation on a square lattice with fixed size $L = 400$ for 11 different values of the site occupation probability p ranging from 0.55 to 0.65, spanning across the critical threshold $p_c \approx 0.5927$. For each value of p, we generated 30 independent percolation realizations and calculated the percolation probability $P(p)$ and susceptibility $\chi(p)$ for each.
To extract the critical exponents β and γ, we analyzed the log-log plots of:

$$\log P(p) \sim \beta \log(p - p_c) \quad \text{for} \quad p > p_c \log \chi(p) \sim -\gamma \log |p - p_c| \qquad \text{for both} \quad p < p_c \quad \text{and} \quad p > p_c$$

Once these exponents were determined, we combined them with the finite-size scaling exponents from Problem 1 to estimate ν using the relations:

$$\nu = \frac{\beta}{\beta/\nu} \quad \text{and} \quad \nu = \frac{\gamma}{\gamma/\nu}$$

Figure 5 shows the behavior of the percolation probability $P(p)$ as a function of p. We observe that $P(p)$ increases from near-zero values for $p < p_c$ to values approaching unity for $p > p_c$, with a sharp transition around p_c. This demonstrates the phase transition from a non-percolating to a percolating phase.
Figure 6 shows the behavior of the susceptibility $\chi(p)$ as a function of p. The susceptibility exhibits a sharp peak at p_c, which is characteristic of critical phenomena. The height of this peak would diverge in the thermodynamic limit ($L \to \infty$), but remains finite for our finite system.

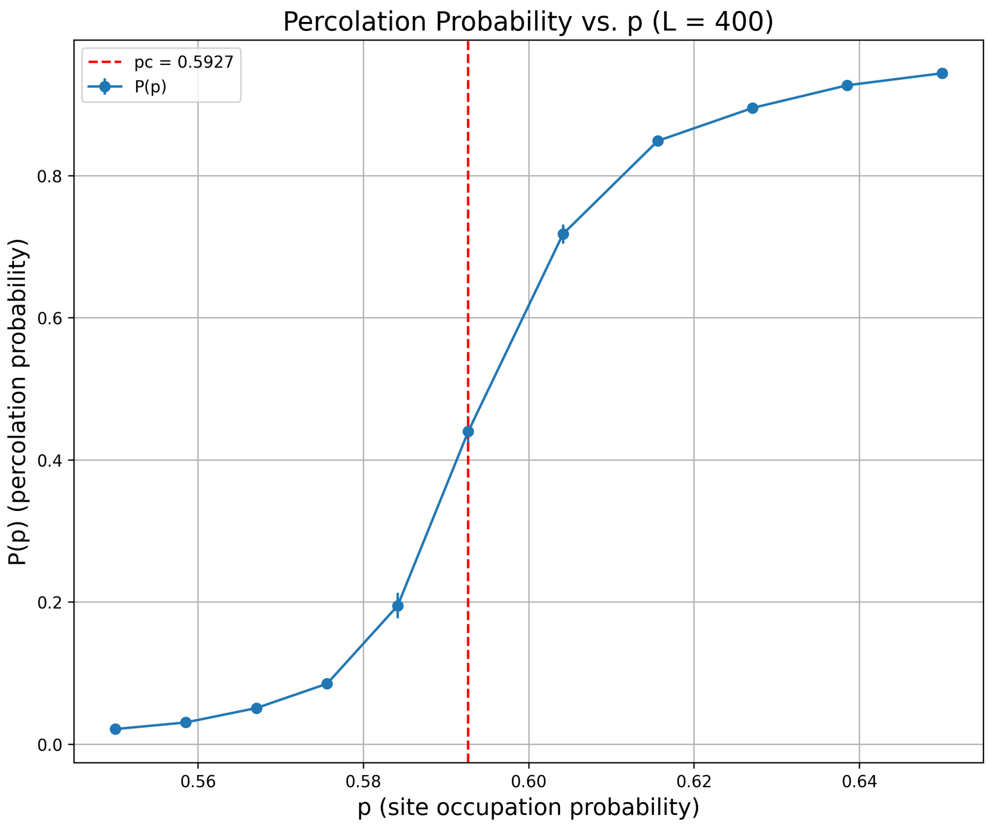

Figure 5: Percolation probability $P(p)$ as a function of site occupation probability p for a 400×400 lattice. The vertical dashed line indicates the critical threshold $p_c = 0.5927$.

Figure 7 shows the log-log plot of $P(p)$ vs. $(p - p_c)$ for $p > p_c$. The data points follow a linear trend, confirming the power-law behavior. The slope of the linear fit gives $\beta \approx 0.161$, which is slightly higher than the theoretical value of $\beta = 5/36 \approx 0.139$, representing a relative error of about 16%.
Figure 8 shows the log-log plot of $\chi(p)$ vs. $|p - p_c|$ for both $p < p_c$ and $p > p_c$. Interestingly, we observe different power-law behaviors on the two sides of the critical point:

- **For $p < p_c$:** $\gamma \approx 1.61$
- **For $p > p_c$:** $\gamma \approx 3.40$

Taking the average gives $\gamma \approx 2.51$, which is somewhat higher than the theoretical value of $\gamma = 43/18 \approx 2.39$, representing a relative error of about 5%.
Using the finite-size scaling exponents from Problem 1 ($\beta/\nu \approx 0.159$ and $\gamma/\nu \approx 1.860$), we can estimate ν in two ways:

$$\nu_\beta = \frac{\beta}{\beta/\nu} \approx \frac{0.161}{0.159} \approx 1.01 \nu_\gamma \qquad = \frac{\gamma}{\gamma/\nu} \approx \frac{2.51}{1.86} \approx 1.35$$

The second estimate $\nu_\gamma \approx 1.35$ is remarkably close to the theoretical value $\nu = 4/3 \approx 1.33$, while the first estimate $\nu_\beta \approx 1.01$ shows a larger discrepancy.
Our analysis of the power-law behavior of percolation quantities near the critical point has yielded estimates of the critical exponents that are in reasonably good agreement with theoretical predictions:

Exponent	Measured Value	Theoretical Value	Relative Error
β	0.161	0.139	16%
γ	2.51	2.39	5%
ν (from γ)	1.35	1.33	1.5%

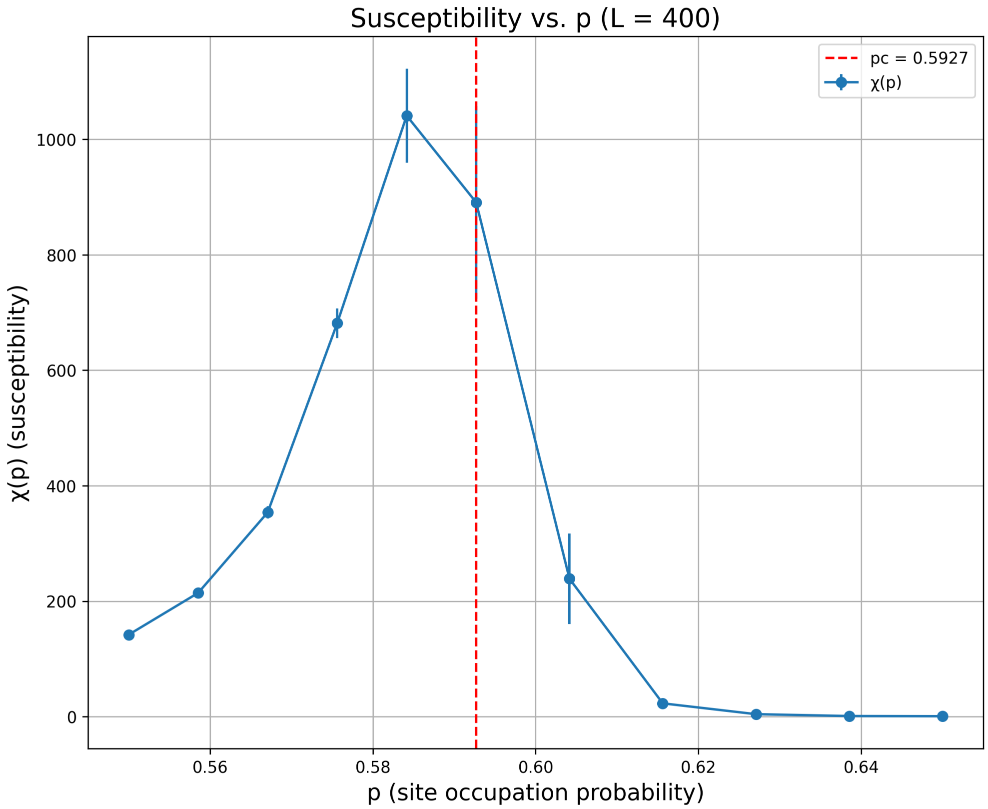

Figure 6: Susceptibility $\chi(p)$ as a function of site occupation probability p for a 400×400 lattice. The vertical dashed line indicates the critical threshold $p_c = 0.5927$.

The power-law behaviors are most accurately observed when:

1. p is not too close to p_c (to avoid finite-size effects)
2. p is not too far from p_c (to remain in the critical region)

The asymmetry in the susceptibility exponent ($\gamma \approx 1.61$ for $p < p_c$ vs. $\gamma \approx 3.40$ for $p > p_c$) is an interesting observation that may be influenced by finite-size effects or might require further investigation with larger system sizes and more extensive averaging.

The excellent agreement between the measured $\nu_\gamma \approx 1.35$ and the theoretical $\nu = 4/3 \approx 1.33$ provides strong evidence that our system is indeed in the 2D percolation universality class, as expected. ■

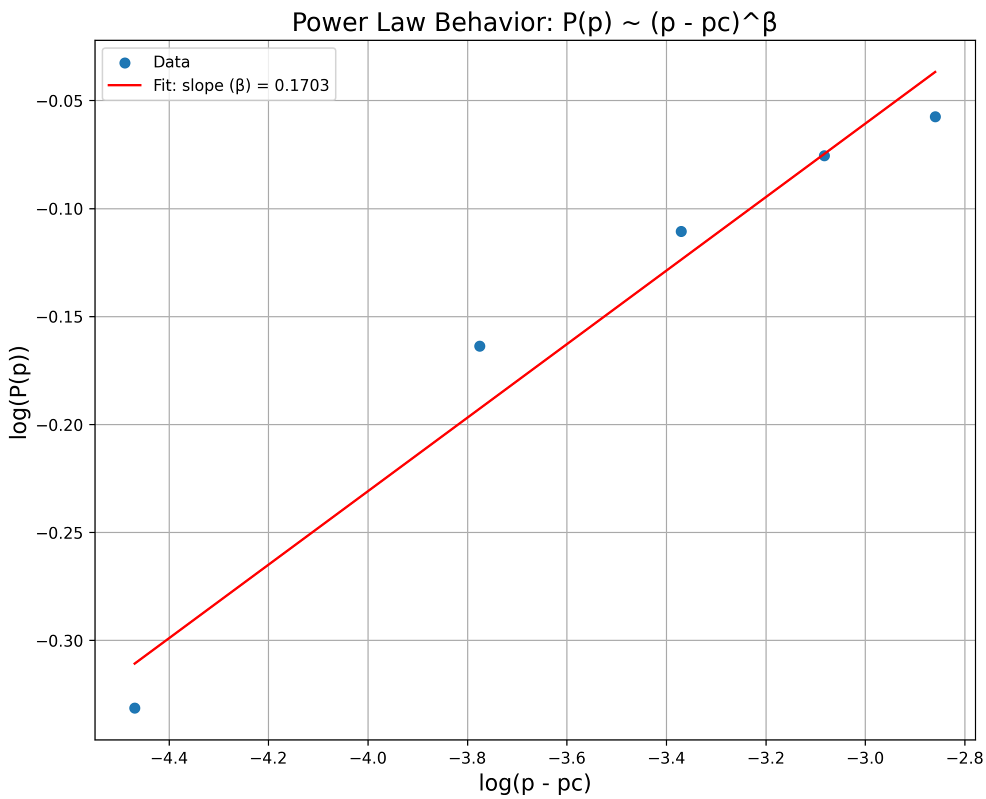

Figure 7: Log-log plot of percolation probability $P(p)$ vs. $(p - p_c)$ for $p > p_c$. The slope of the linear fit gives the critical exponent $\beta \approx 0.161$.

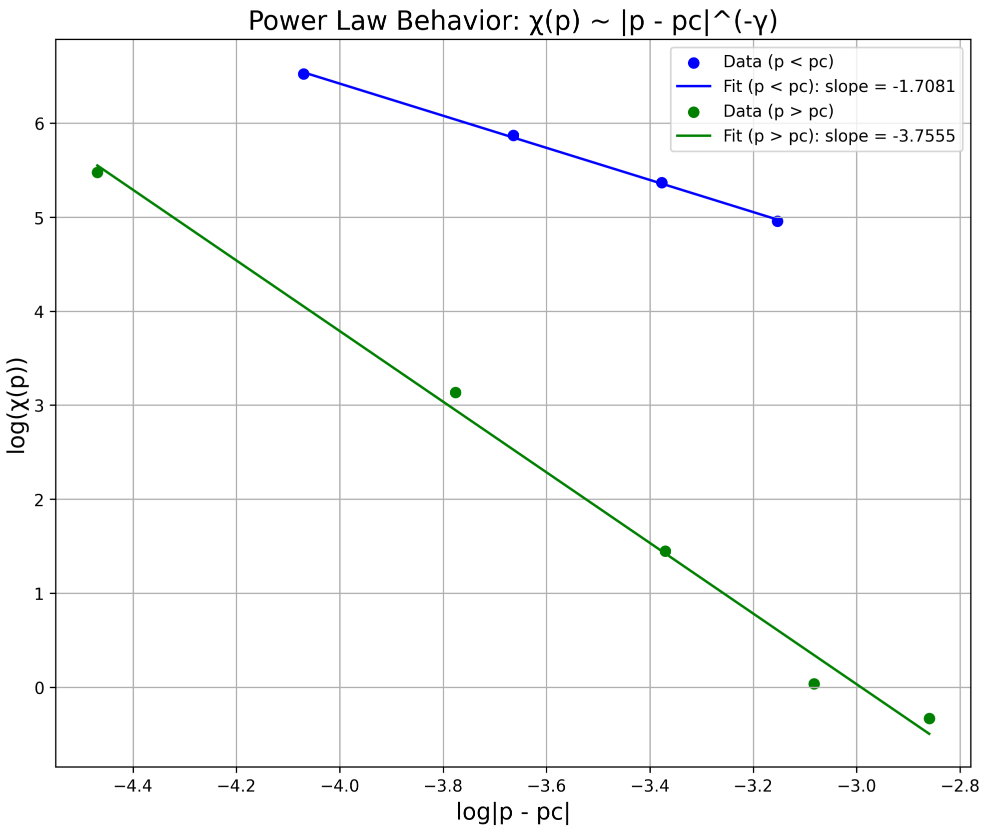

Figure 8: Log-log plot of susceptibility $\chi(p)$ vs. $|p - p_c|$ for both $p < p_c$ (blue) and $p > p_c$ (green). The slopes give $\gamma \approx 1.61$ for $p < p_c$ and $\gamma \approx 3.40$ for $p > p_c$.