Computational Physics
Problem Set 3

Saleh Shamloo Ahmadi
Student Number: 98100872

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1 Percolation

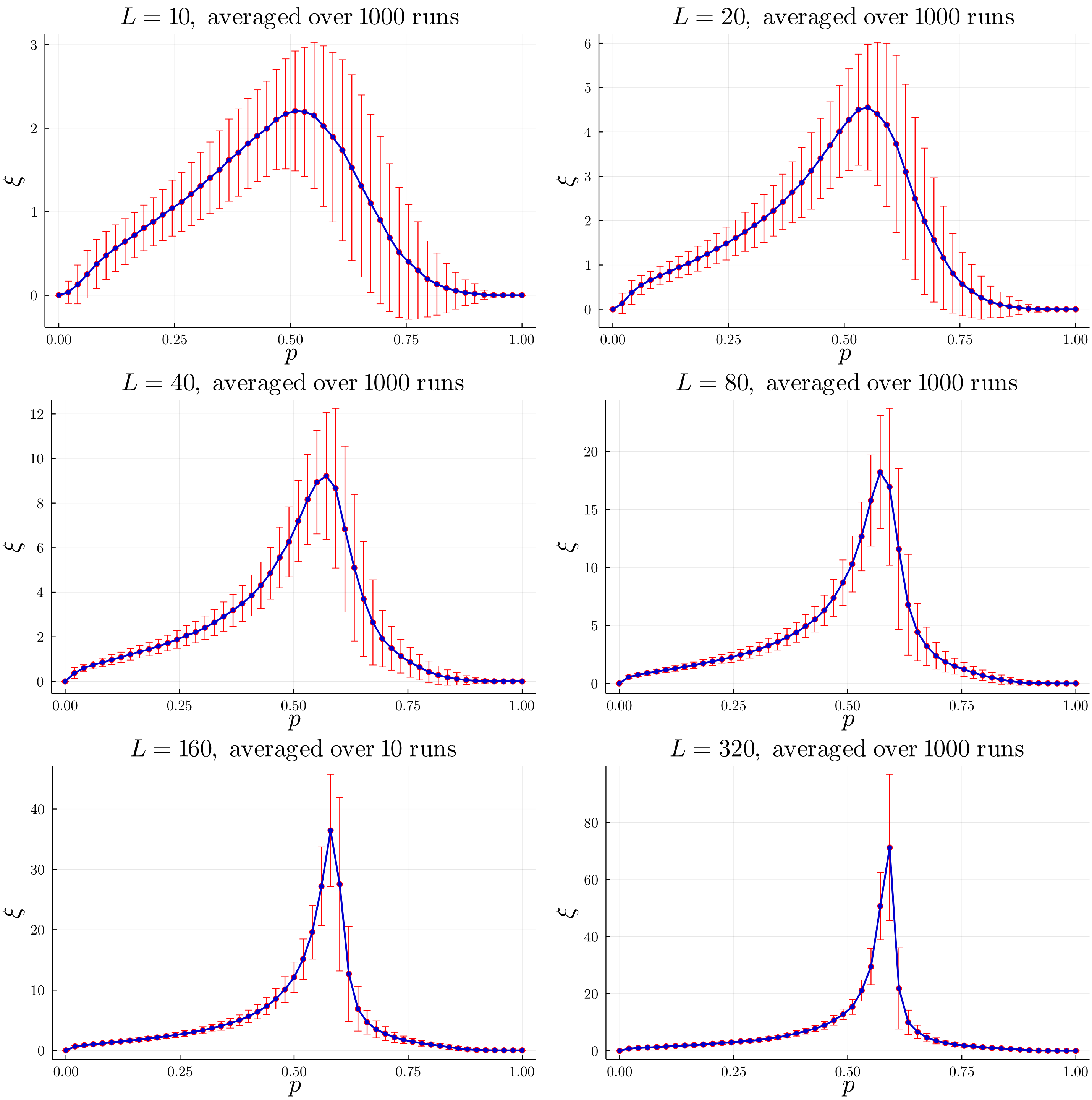
Note: we simulate *site percolation*.

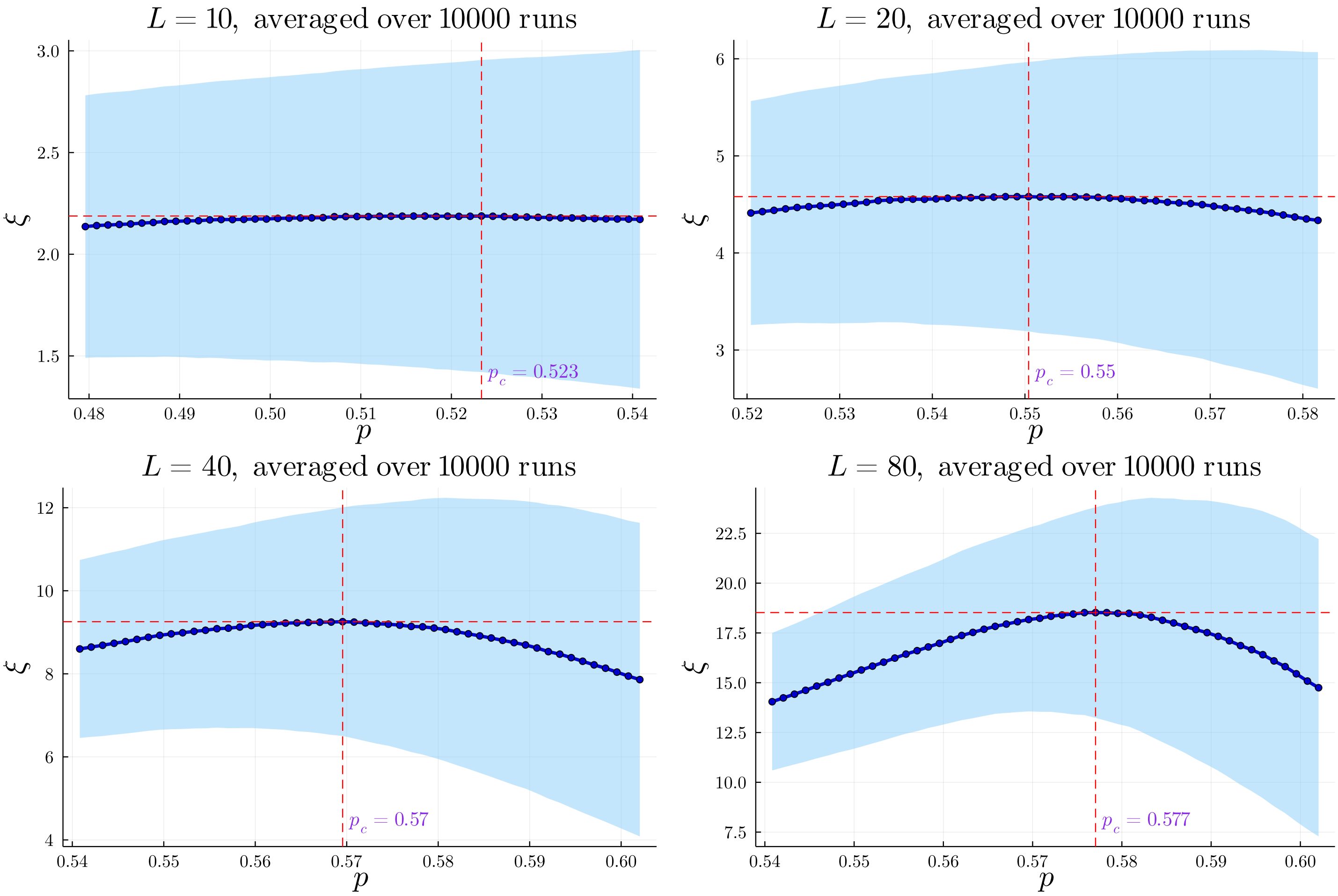
1.1 Correlation Length

The correlation length ξ is a measure of the radius of the maximum closed (non-infinite) cluster; This shows the maximum length of interactions before phase transition occures and the lattice either becomes homogenous or clusters are broken off.

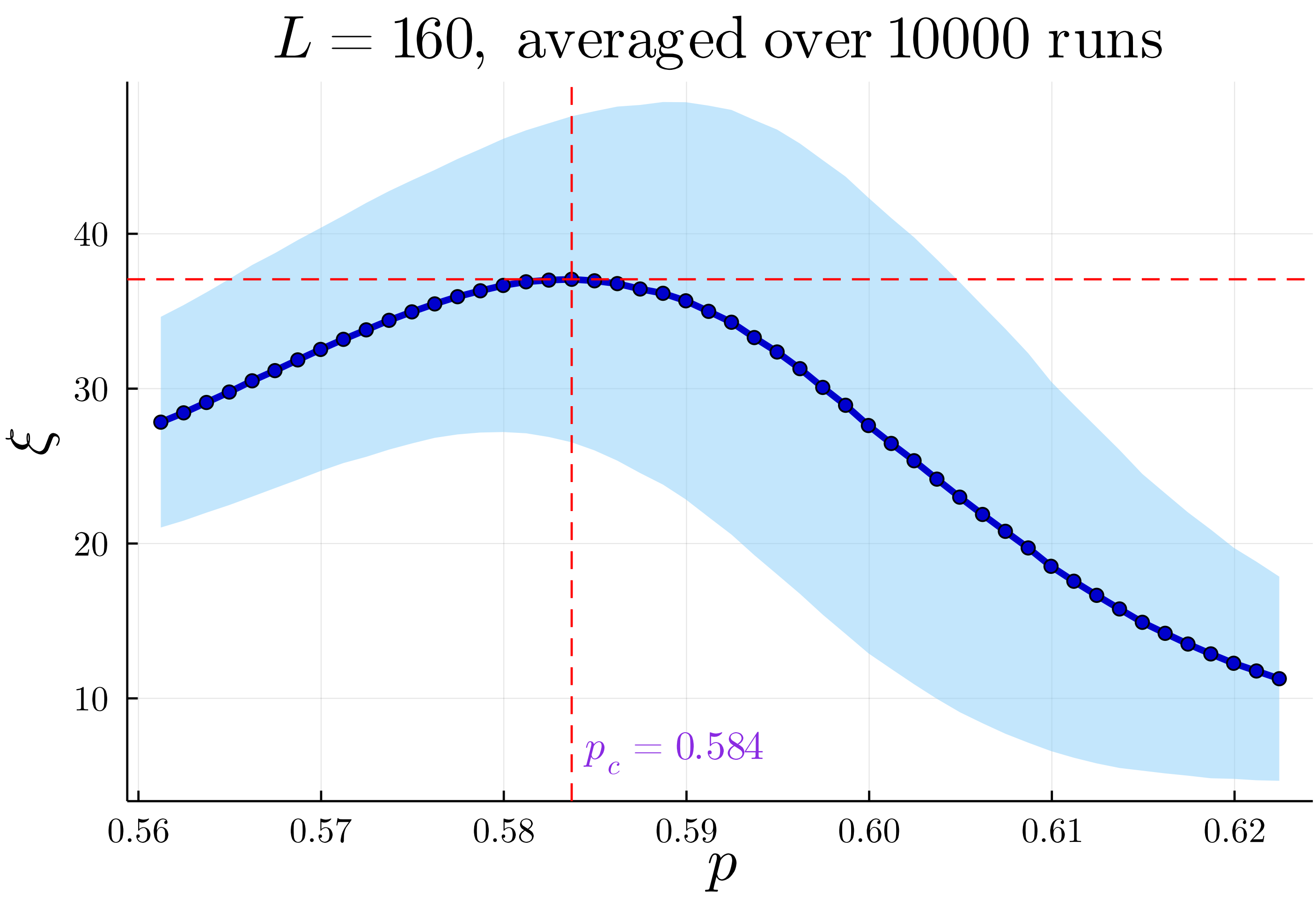
In our analysis, we use the maximum radius of gyration of closed clusters to measure the correlation length (any similar measure is valid).

The correlation length diverges (or peaks, for a finite lattice) at the critical probability p_c of forming sites in the lattice; This is because at higher probabilities, percolation happens frequently and there are less clusters and at lower probabilites, clusters break off more at smaller length scales.

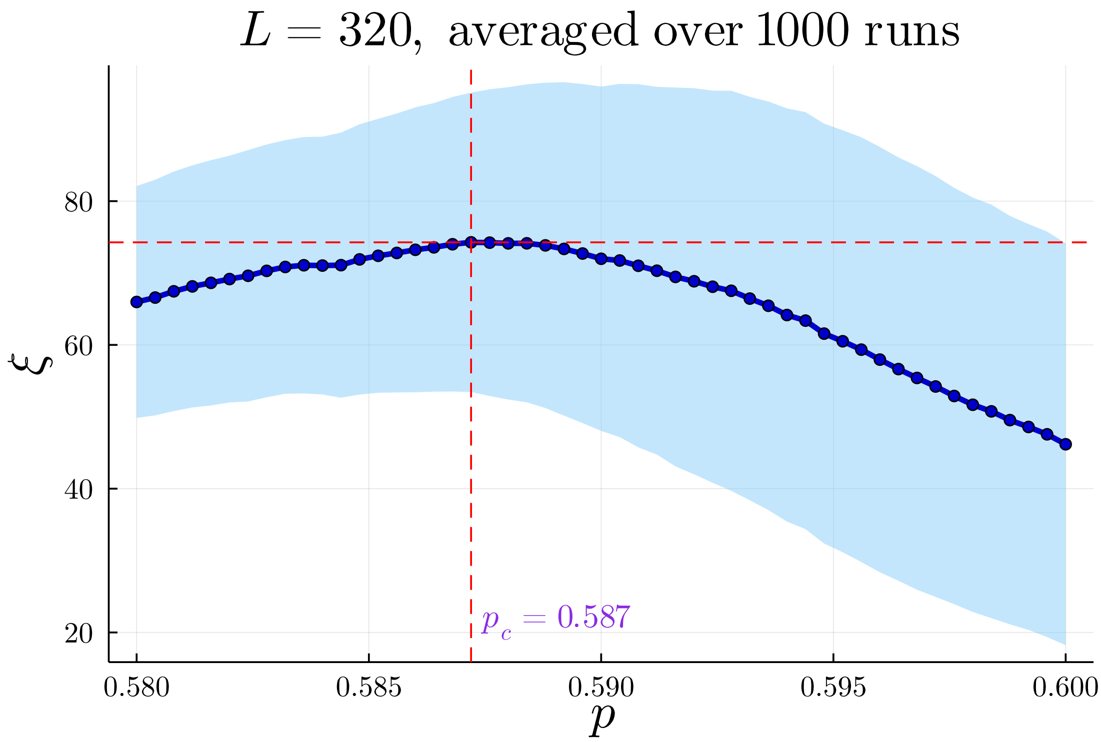

$L = 10$, averaged over 1000 runs
$L = 20$, averaged over 1000 runs
$L = 40$, averaged over 1000 runs
$L = 80$, averaged over 1000 runs
$L = 160$, averaged over 10 runs
$L = 320$, averaged over 1000 runs
ξ
p



$L = 10,$ averaged over 10000 runs
$p_c = 0.523$
$L = 20,$ averaged over 10000 runs
$p_c = 0.55$
$L = 40,$ averaged over 10000 runs
$p_c = 0.57$
$L = 80,$ averaged over 10000 runs
$p_c = 0.577$
ξ
p



$L = 160,$ averaged over 10000 runs
$p_c = 0.584$
ξ
p



Close to the critical probability p_c, the following relation holds:

$$\xi \sim |p - p_c|^{-\nu} \tag{1}$$

ν is called the *critical exponent* for the correlation length ξ. In finite lattices, because the correlation length is bounded by the lattice length, this relation breaks down at probabilites very close to p_c. We can find the valuse of ν with two methods: direct calculation from finite lattices or extrapolation.

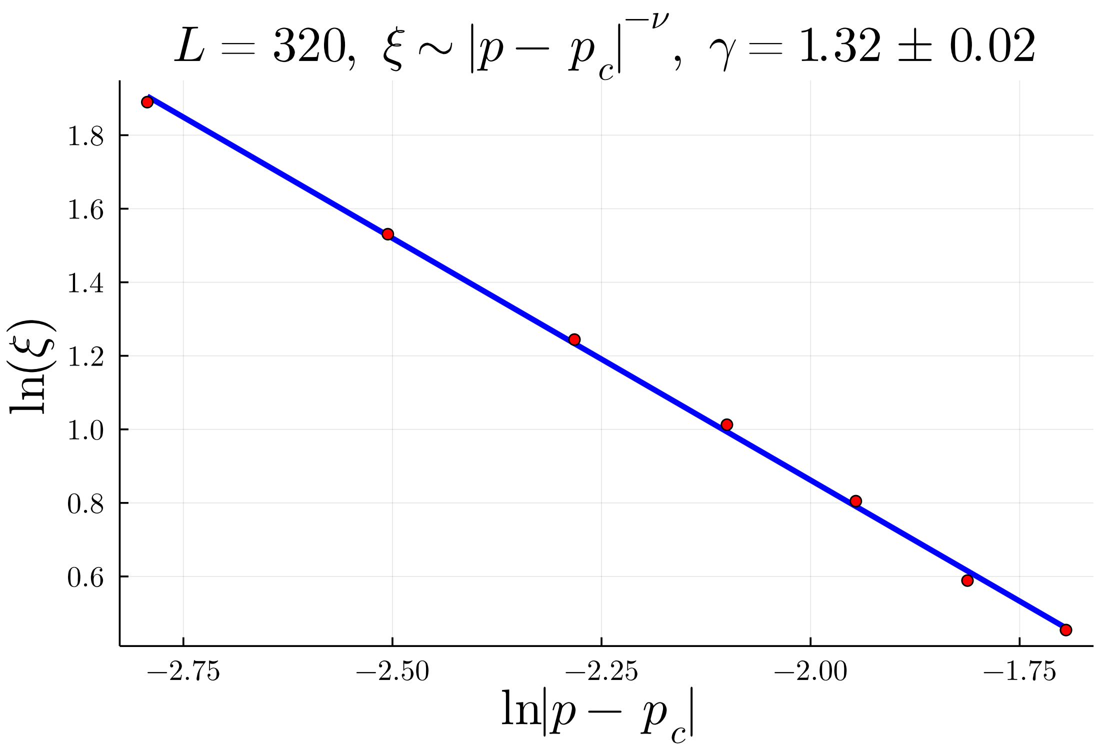
In direct calculation, we can use linear regression for the relation

$$\log \xi = -\nu \log(p - p_c) + C. \tag{2}$$

This is not especially accurate, because it is based on limited lattices that do not accurately represent unbounded trends; The edges of these lattices cut off emerging clusters.

The extrapolation method is as follows. in finite lattices, the maximum correlation length is proportional to the lattice size, since the correlation length at p_c is unbounded for infinite lattices, and is only bounded by the edges of the lattice in finite lattices. So, we can approximate the behavior of an infinite lattice by the relation

$$|p_c(\infty) - p_c(L)|^{-\nu} = L, \tag{3}$$



where $p_c(\infty)$ is the infinite lattice's critical probablity and L is the size of a finite lattice. Extrapolating $p_c(\infty)$ and ν with a non-linear curve fit, we get

$$p_c(\infty) = 0.5925, \qquad \nu = 1.346. \tag{4}$$

It can be proved that the exact value of ν is $4/3$ and larges simulations have shown that $p_c(\infty)$ for site percolation is 0.5927, so the accuracy of the extrapolated values are quite good, considering the limited sample size.

1.2 Fractal Dimension

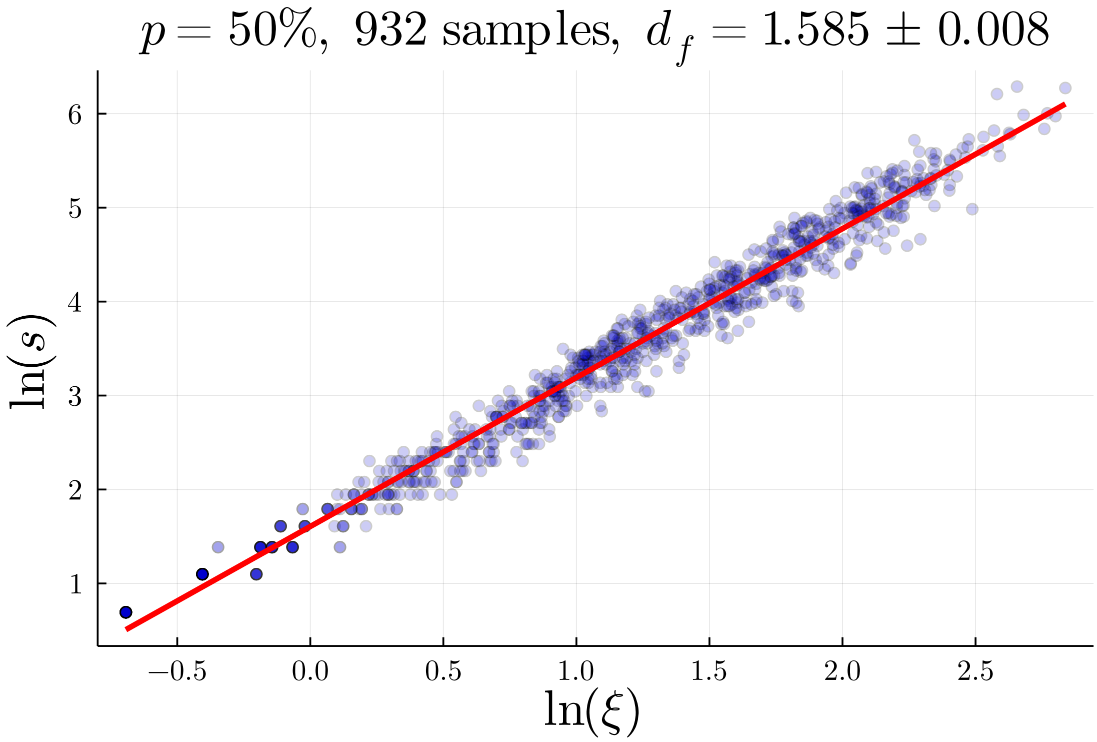
The percolation clusters exhibit fractal self-similar behavior. Using a simple breadth-frist search algorithm, we can generate clusters in a lattice and calculate their size and radius of gyration to find their fractal dimension; If s is the size of the cluster and d_f is the fractal dimension

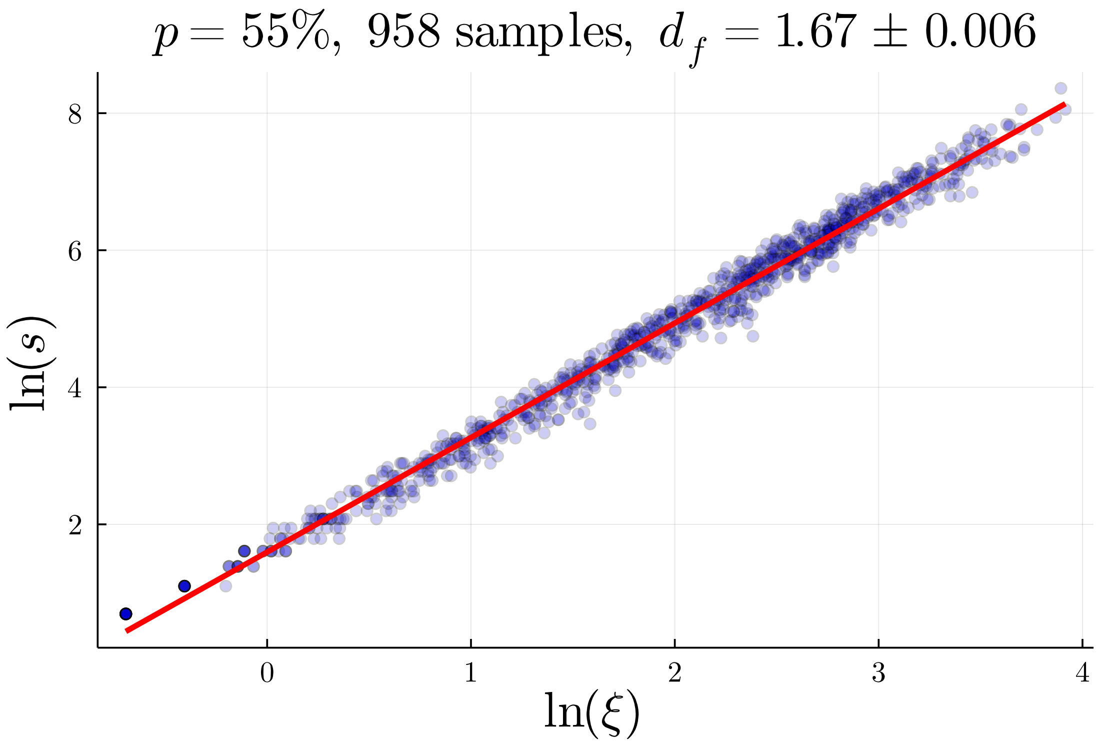
$$s \sim \xi^{d_f}, \tag{5}$$

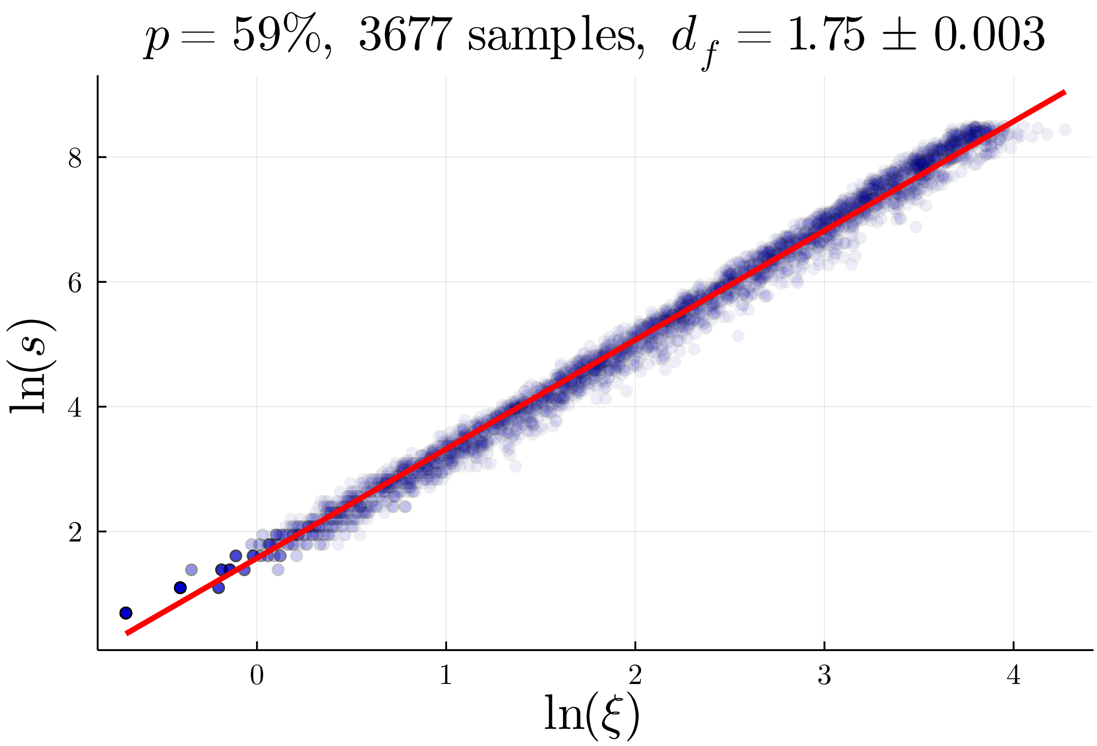
so, by using linear regression for the relation

$$\log s = d_f \log \xi + C \tag{6}$$

we can calculate the fractal dimension d_f.


$p = 50\%,\ 932$ samples, $d_f = 1.585 \pm 0.008$
6
5
4
3
2
1
ln(s)
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
ln(ξ)


$p = 55\%,\ 958$ samples, $d_f = 1.67 \pm 0.006$
8
6
4
2
ln(s)
0
1
2
3
4
ln(ξ)



2 Random Walk

2.1 Variance

We can use the recurrence relation

$$x(t) = x(t-\tau) + al, \tag{7}$$

where a is $+1$ with probability p and -1 with probability q, to find the variance. The calculation is as follows:

$$\begin{aligned}
\left\langle x^2(t) \right\rangle &= \left\langle x^2(t-\tau) \right\rangle + 2l \left\langle ax(t-\tau) \right\rangle + \left\langle a^2 \right\rangle l^2 && (8)\\
&= \left\langle x^2(t-\tau) \right\rangle + l^2 + 2l(p-q) \left\langle x(t-\tau) \right\rangle && (9)\\
&= \left\langle x^2(t-\tau) \right\rangle + l^2 + 2l^2 \left(\frac{t}{\tau} - 1 \right) (p-q)^2 && (10)
\end{aligned}$$

(Note that a^2 is always 1, and since a is dependant from x, $\langle ax \rangle = \langle a \rangle \langle x \rangle$. Also, I used $\langle x(t) \rangle = \frac{l}{\tau}(p-q)t$, which has already been proven in the lecture notes)

Repeating the recurrence relation until it reaches $x(0) = 0$

$$\left\langle x^2(t) \right\rangle = \frac{tl^2}{\tau} + \frac{2l^2}{\tau}(p-q)^2 \sum_{n=1}^{t/\tau-1} n\tau \tag{11}$$

$$= \frac{tl^2}{\tau}\left[1 + \left(\frac{t}{\tau} - 1\right)(p-q)^2\right]. \tag{12}$$

Substituting into the variance,

$$\sigma^2(t) = \left\langle x^2(t) \right\rangle - \langle x(t) \rangle^2 \tag{13}$$

$$= \frac{tl^2}{\tau}\left[1 + \left(\frac{t}{\tau} - 1\right)(p-q)^2\right] - \frac{t^2 l^2}{\tau^2}(p-q)^2 \tag{14}$$

$$= \frac{tl^2}{\tau}\left[1 - (p-q)^2\right]. \tag{15}$$

But

$$p + q = 1 \implies (p+q)^2 = 1 \implies p^2 + q^2 = 1 - 2pq, \tag{16}$$

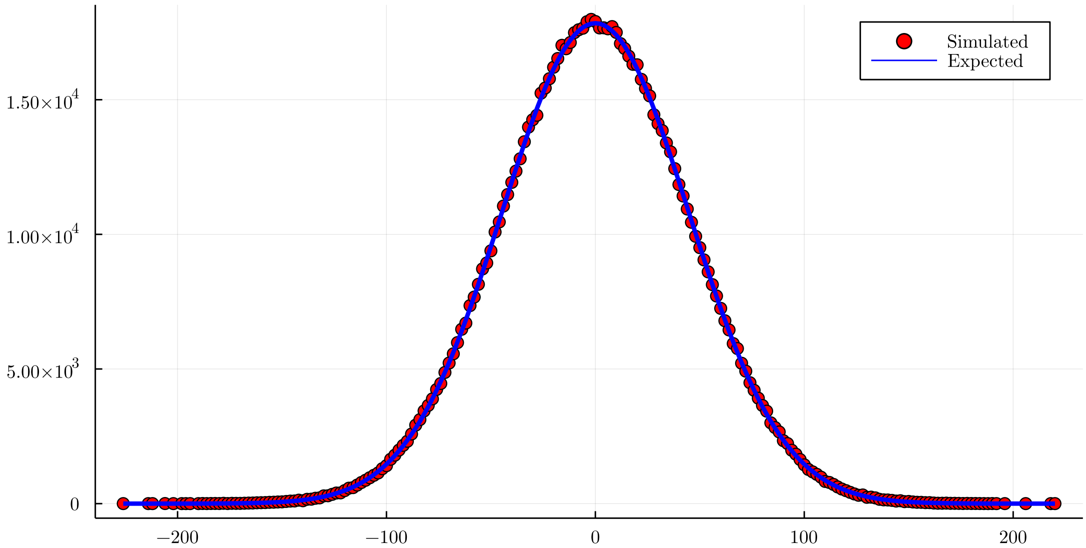
and using this to simplify the expression

$$\sigma^2(t) = \frac{tl^2}{\tau}\left[1 - (p^2 + q^2) + 2pq\right] = \frac{tl^2}{\tau}[1 - 1 + 2pq + 2pq] \tag{17}$$

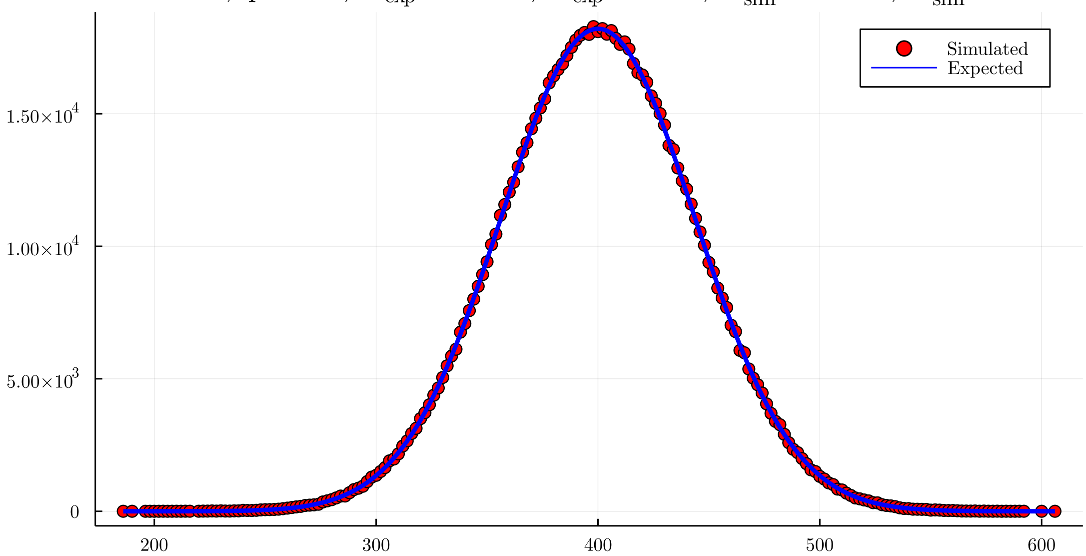
$$\boxed{\sigma^2(t) = \frac{4l^2}{\tau} pqt} \tag{18}$$

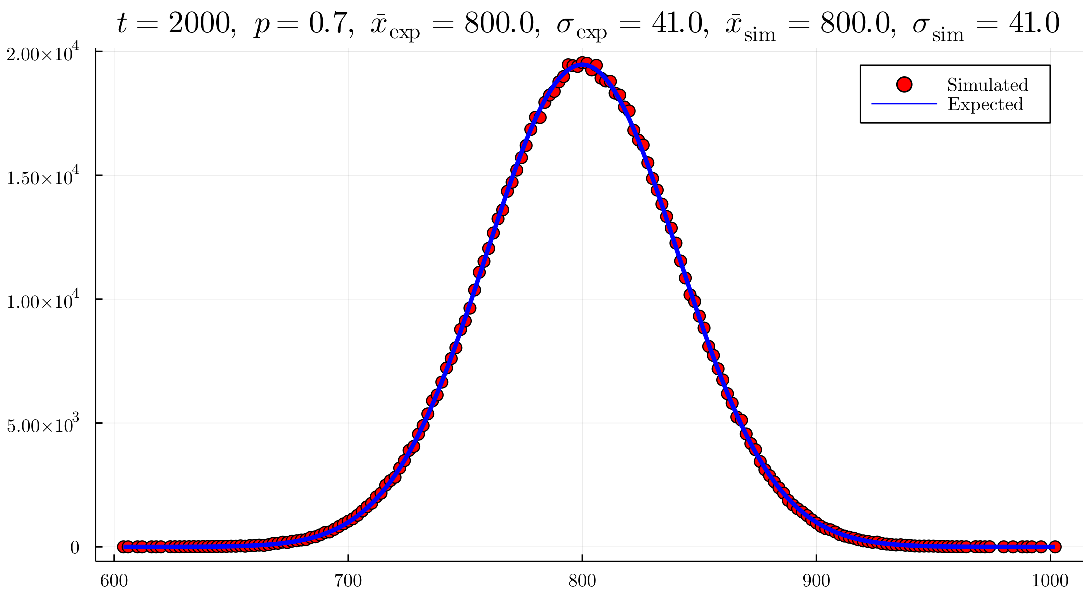
2.2 Simulation

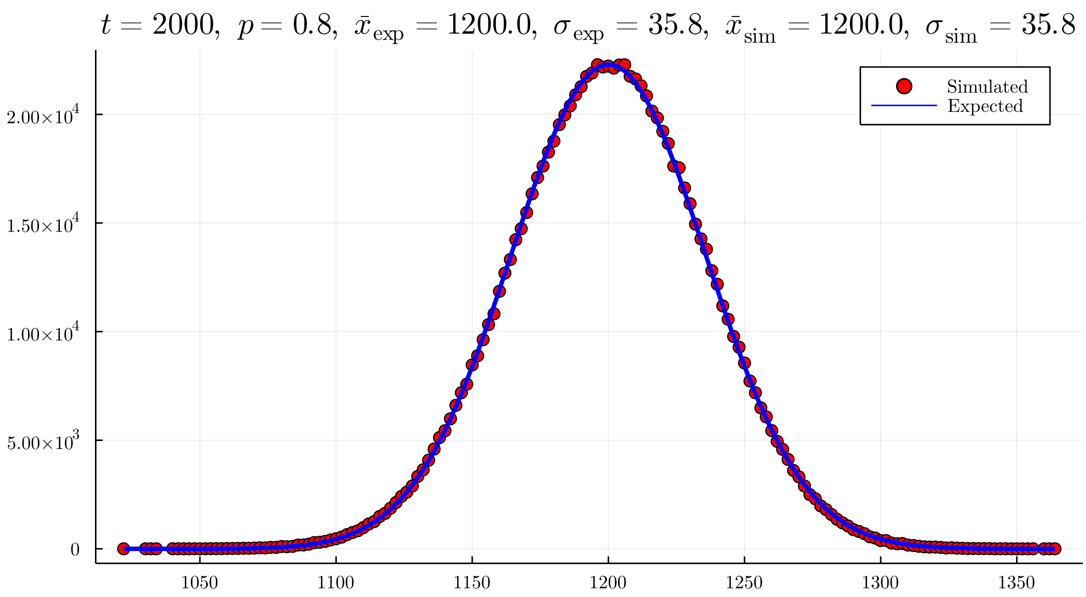
$t = 2000,\ p = 0.5,\ \bar{x}_{\mathrm{exp}} = 0.0,\ \sigma_{\mathrm{exp}} = 44.7,\ \bar{x}_{\mathrm{sim}} = 0.0,\ \sigma_{\mathrm{sim}} = 44.7$



$t = 2000,\ p = 0.6,\ \bar{x}_{\mathrm{exp}} = 400.0,\ \sigma_{\mathrm{exp}} = 43.8,\ \bar{x}_{\mathrm{sim}} = 400.0,\ \sigma_{\mathrm{sim}} = 43.8$




$t = 2000,\ p = 0.7,\ \bar{x}_{\text{exp}} = 800.0,\ \sigma_{\text{exp}} = 41.0,\ \bar{x}_{\text{sim}} = 800.0,\ \sigma_{\text{sim}} = 41.0$
Simulated
Expected
2.00×10^4
1.50×10^4
1.00×10^4
5.00×10^3
0
600
700
800
900
1000


$t = 2000,\ p = 0.8,\ \bar{x}_{\text{exp}} = 1200.0,\ \sigma_{\text{exp}} = 35.8,\ \bar{x}_{\text{sim}} = 1200.0,\ \sigma_{\text{sim}} = 35.8$
Simulated
Expected
2.00×10^4
1.50×10^4
1.00×10^4
5.00×10^3
0
1050
1100
1150
1200
1250
1300
1350