Computational Physics (PHYS6350)

Lecture 20: Problems in statistical physics part II

- Simulated annealing
- Percolation simulation

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Course materials: https://github.com/vlvovch/PHYS6350-ComputationalPhysics/tree/spring2025

Finding the ground state

Recall how in the Metropolis algorithm we move between states

For a move from state i to state j

- If $E_j < E_i$, the move is unconditionally accepted.
- If $E_j > E_i$, the move is accepted with a probability

$$P_a = e^{-\beta(E_j - E_i)} \qquad \beta = \frac{1}{T}$$

At $T = 0$ only the single ground state $E_i = 0$ contributes to the partition function, however, finding this state directly may be challenging (too long equilibration, have to probe a lot of states, can end up in a local minimum)

Alternative approach:

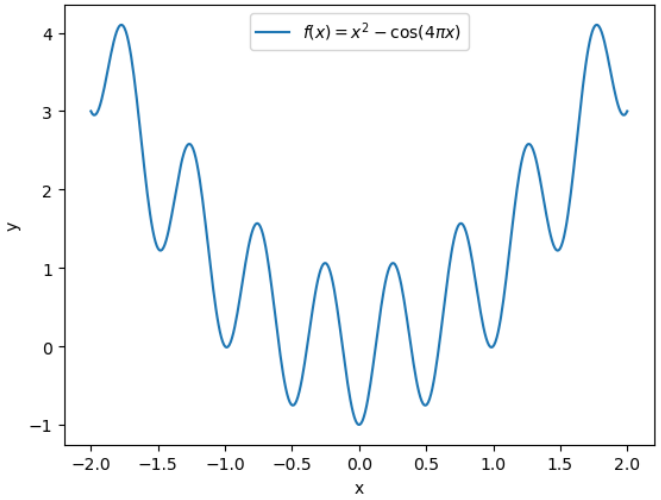
- Start at some finite T
- Run the Metropolis algorithm to reach equilibrium
- Lower the temperature a bit and run the Metropolis algorithm to reach new equilibrium
- Repeat until $T = 0$ where we will reach the ground state

Simulated annealing

Apply this logic to find the global minimum of a function f(x)

Helps avoid getting stuck in a local minimum

Example: $f(x) = x^2 - \cos(4\pi x)$



- Each step consider a move $x \to x + \Delta x$ where Δx is drawn e.g. from the *normal distribution*
- Accept the move with *acceptance probability* a la Metropolis

$$p_a = e^{-[f(x_{\text{cand}}) - f(x)]/T}$$

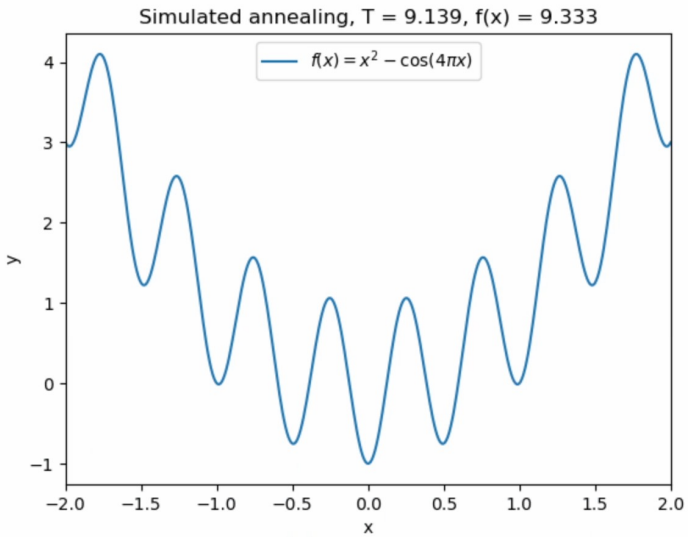
- Lower the temperature T in the next step via a *cooling schedule*
  For example exponential schedule giving at step n:

$$T_n = T_{\max} e^{-n/\tau}$$

- Stop the process once T goes below a certain threshold $T < T_{\min}$

Simulated annealing

```python
# A single step of the simulated annealing process at temperature T
# for finding the minimum of a function f(x)
# The candidate move xcand is sampled from a Gaussian distribution
# around the present value of x, with a condition xmin <= xcand <= xmax
# The move is accepted with the Metropolis based probability
def simulated_annealing_step(f, T, x, sigma, xmin = -1e9, xmax = 1e9):
    fnow = f(x)
    xcand = np.random.normal(x,sigma)
    while (xcand < xmin or xcand > xmax):
        xcand = np.random.normal(x,sigma)
    fcand = f(xcand)
    if (fcand < fnow or (T>0 and np.random.rand() < np.exp(-(fcand-fnow)/T))):
        return xcand
    else:
        return x
```



Apply it to our function

```python
x = 2
sigma = 1.
Tmin = 1.e-3
Tmax = 10.
T = Tmax
t = 0
tau = 100.

while (T > Tmin):
    T = Tmax * np.exp(-t/tau)
    x = simulated_annealing_step(f, T, x, sigma)
    t += 1
```

Simulated annealing

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    fcand = f(xcand)
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        return xcand
    else:
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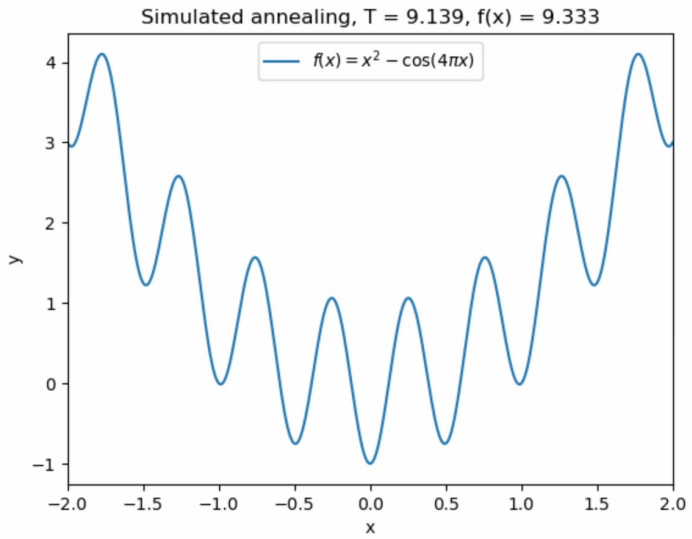

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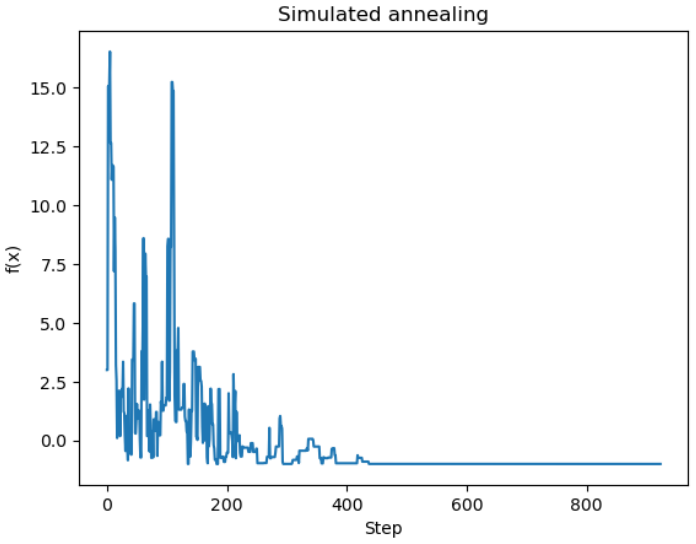
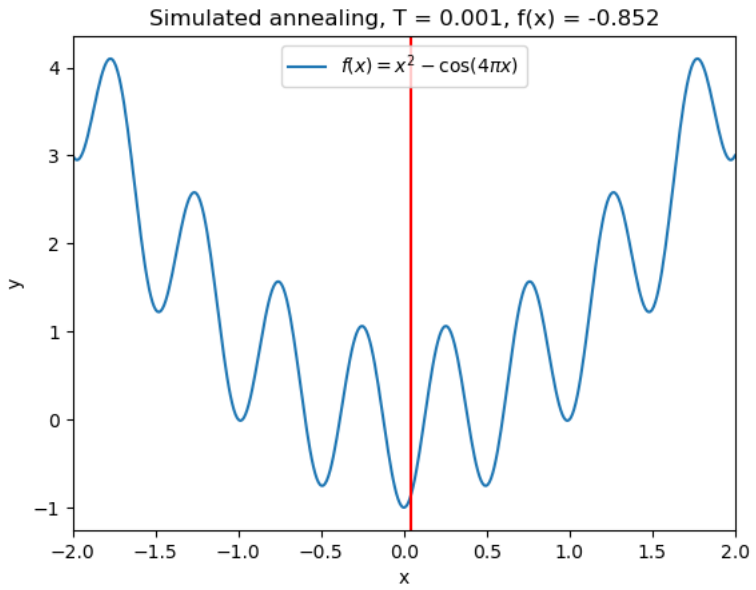


Simulated annealing

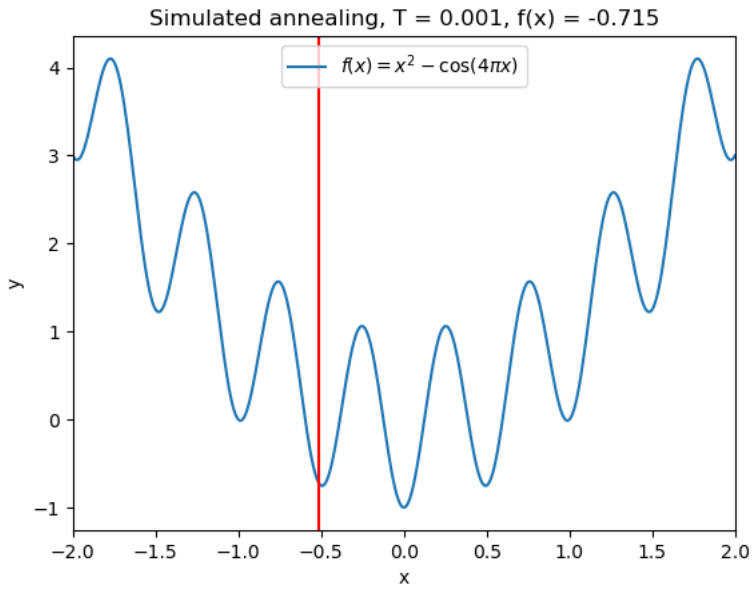
The solution is approximate and not guaranteed to give the global minimum, especially if cooling is too fast

E.g. $\tau = 100 \rightarrow 10$

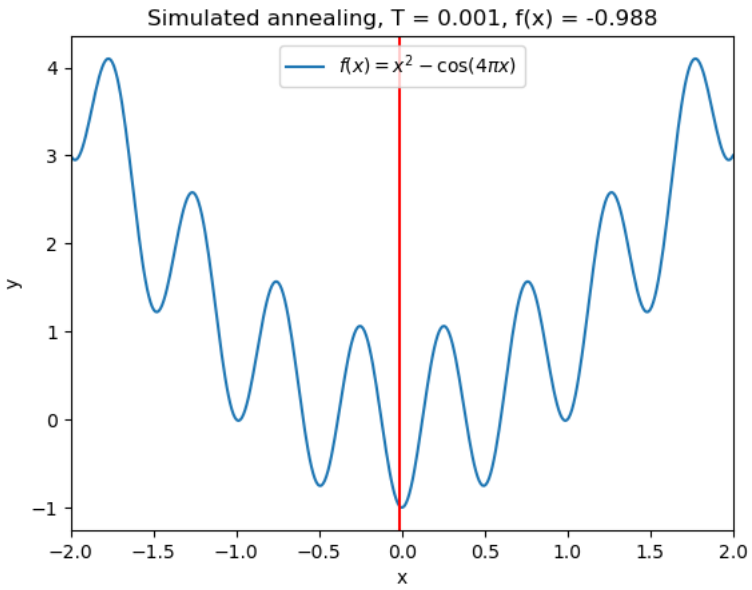
Run 1



Run 2



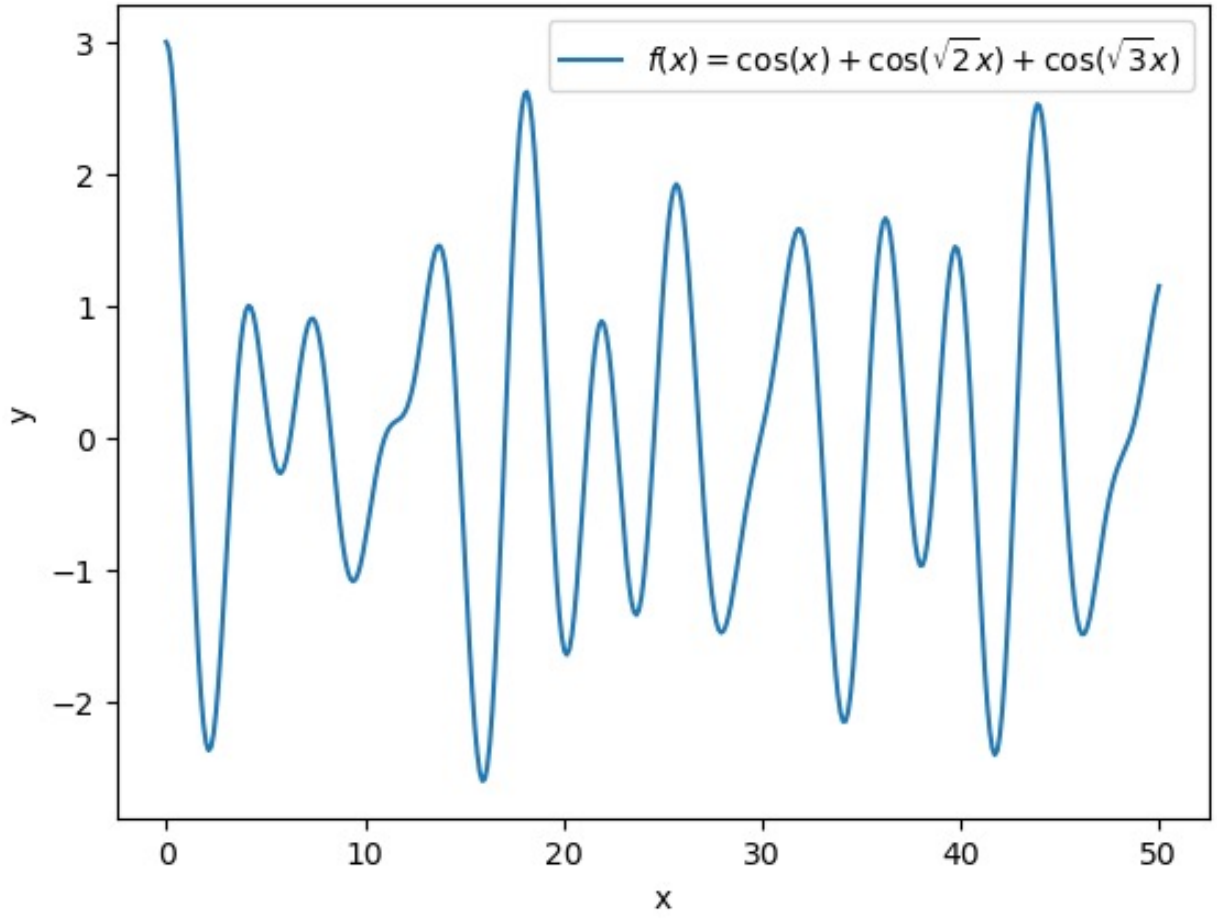
Run 3



The choice of possible moves, acceptance probabilities, and cooling schedule should be varied and tailored for the problem at hand. It is also advisable to keep track of the global minimum value achieved so far.

Simulated annealing

A more involved example $f(x) = \cos(x) + \cos(\sqrt{2}x) + \cos(\sqrt{3}x)$



Simulated annealing

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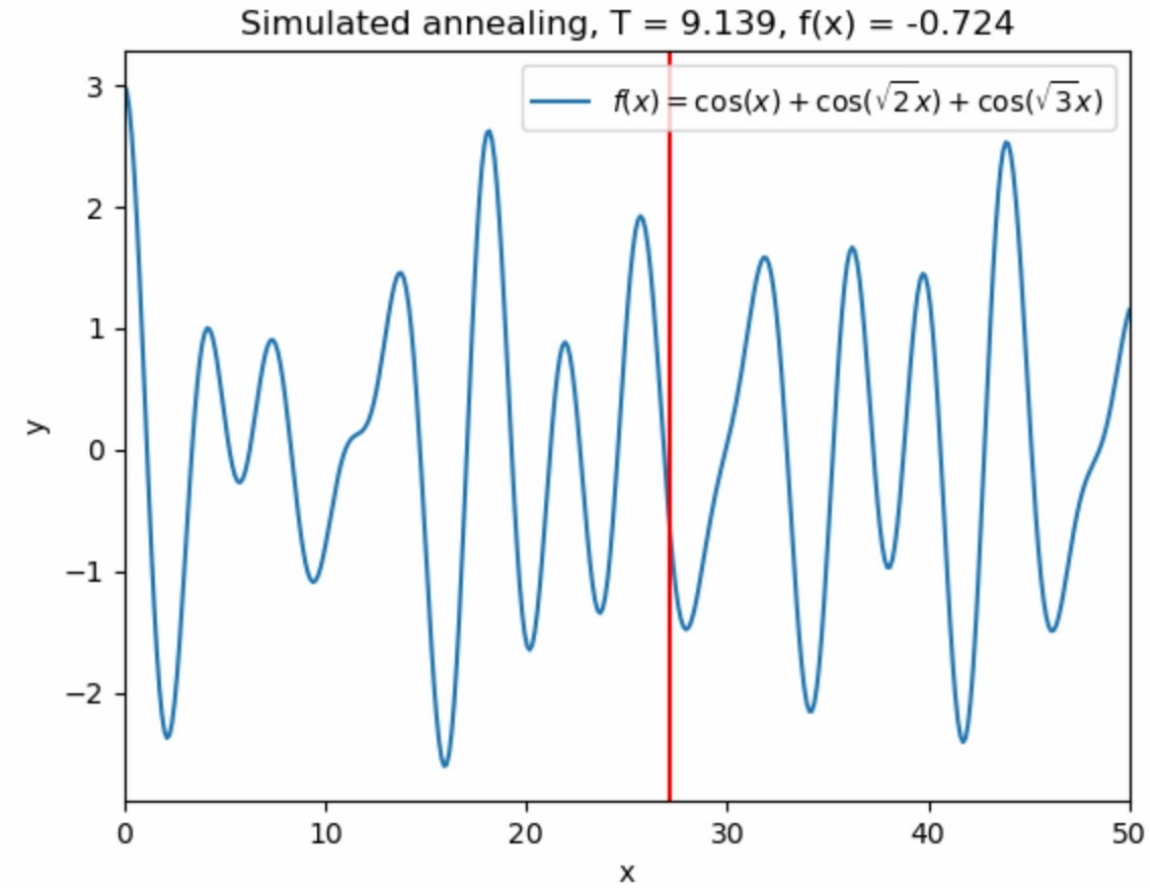
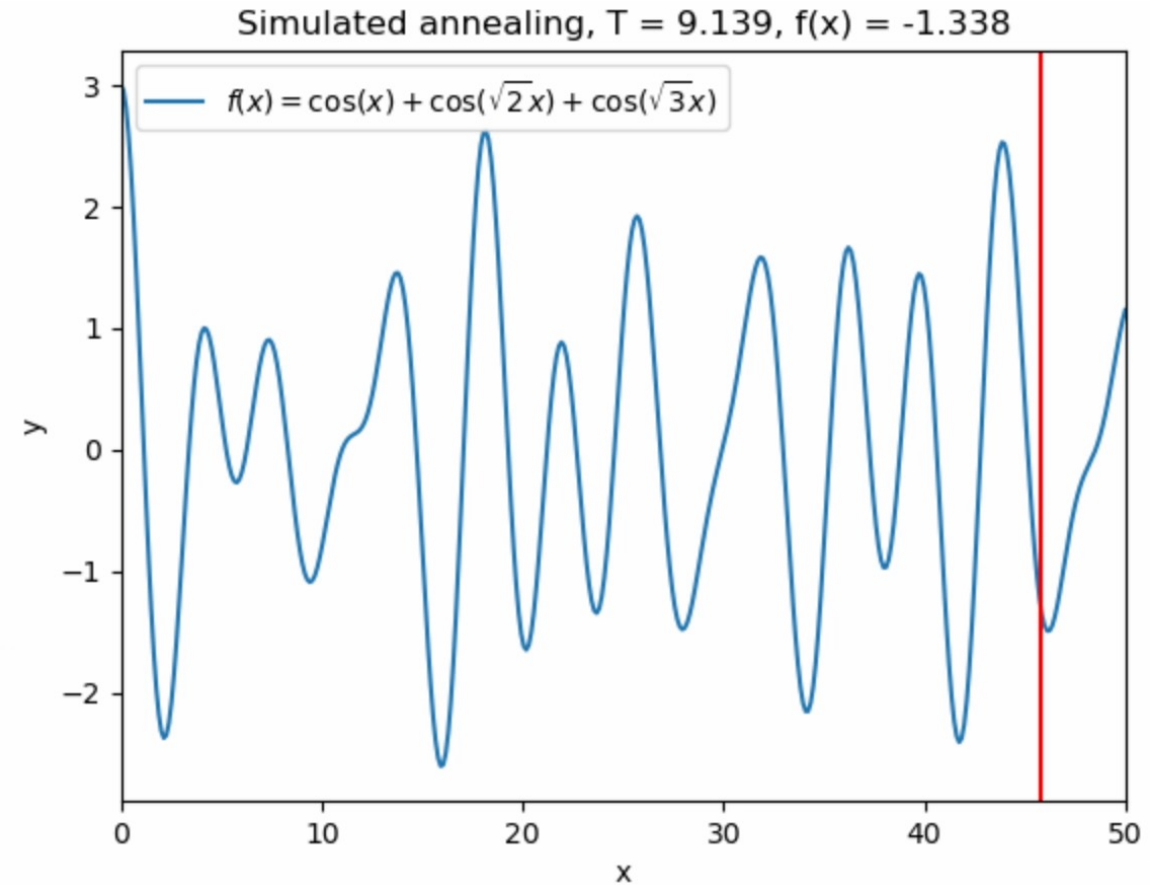
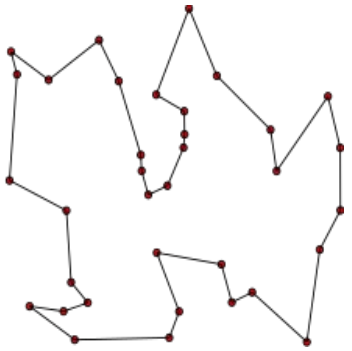




Simulated annealing and the traveling salesman problem

Traveling salesman problem (TSP):
You have N cities where each pair of cities is connected by roads.
You need to visit all cities exactly once starting ending the trip in the starting city.
The goal is to find a path with the shortest total distance to travel.



Credit: Wikipedia

The traveling salesman problem in **NP-hard**
Known exact solutions are exponential in N

Brute-force: O(N!)
Held-Karp algorithm: $O(N^2 2^N)$

Approximate solution with **simulated annealing:**

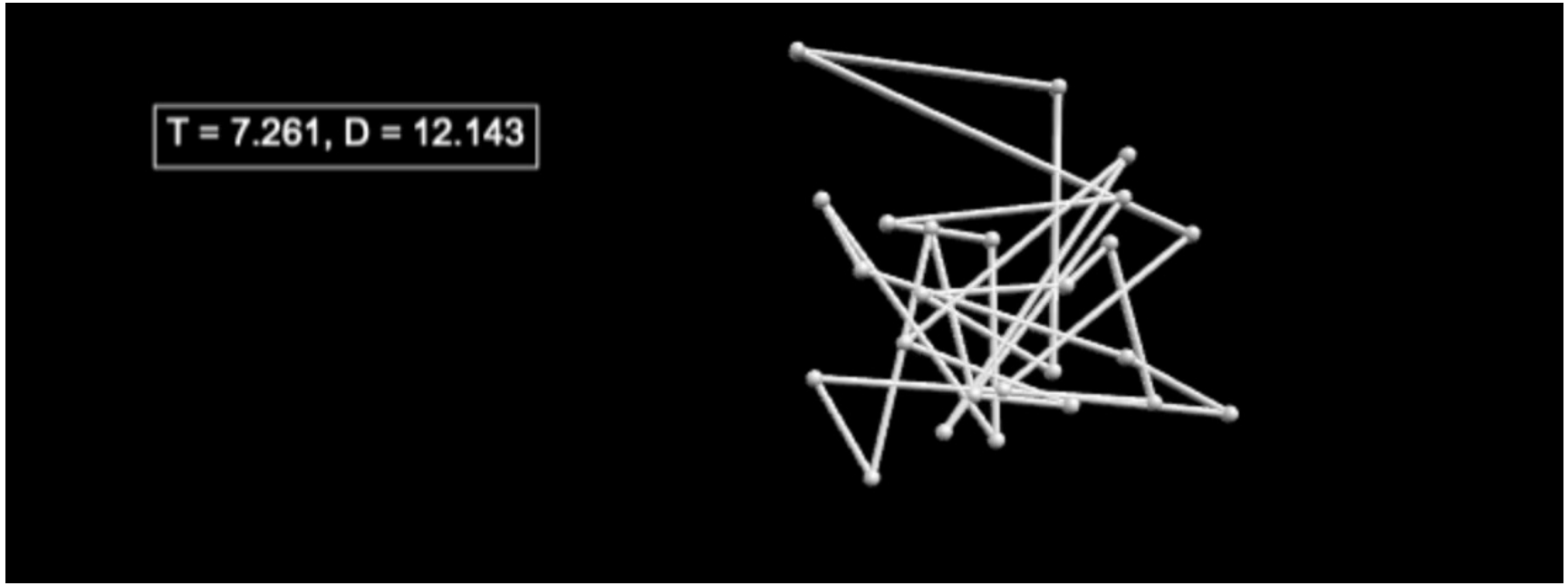
- Start with random path
- At each step swap two cities from the path and compute the total distance change ΔD
- Accept the new path with probability

$$P_a = \exp(-\Delta D/T)$$

- Decrease T in next step in accordance with annealing schedule

Simulated annealing and the traveling salesman problem

Code adapted from Example 10.4 from M. Newman, *Computational Physics*, *http://www-personal.umich.edu/~mejn/cp/programs/salesman.py*



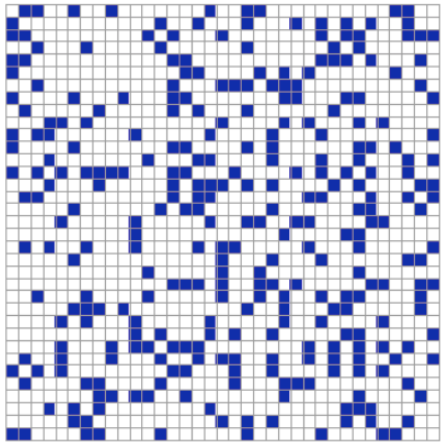
Percolation threshold

Percolation theory studies the formation of long-range connectivity in random systems.
Usually, one can imagine a geometric configuration where certain "*conducting*" objects occupy a fraction of space

Example: square lattice

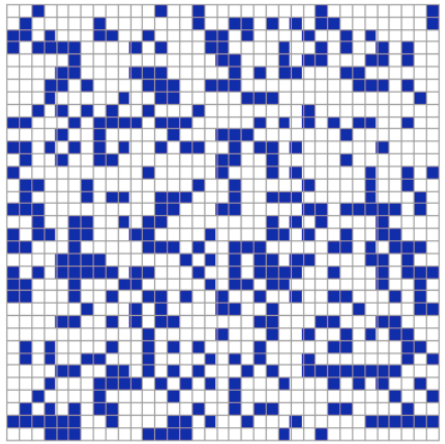
- Some fraction p of sites is occupied
- Occupied sites form clusters through connection to its four neighbors
- Above certain p_c, and long-range, "infinite" cluster forms

insulator



Site percolation with p = 0.25

insulator



Site percolation with p = 0.35

conductor

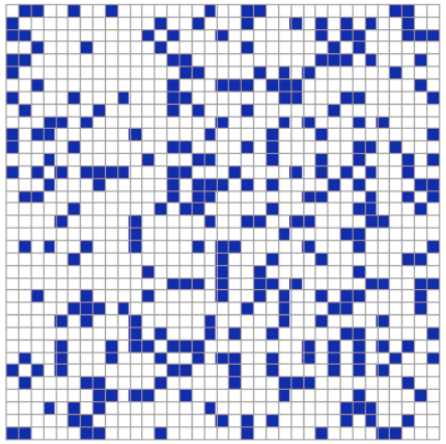
Site percolation with p = 0.65

Images from https://faculty.math.illinois.edu/~kkirkpat/percolation.html

Percolation threshold

Example: square lattice

insulator



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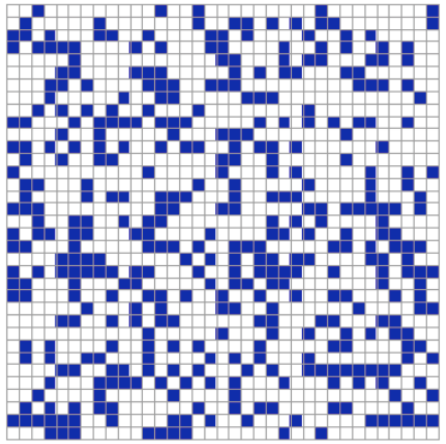

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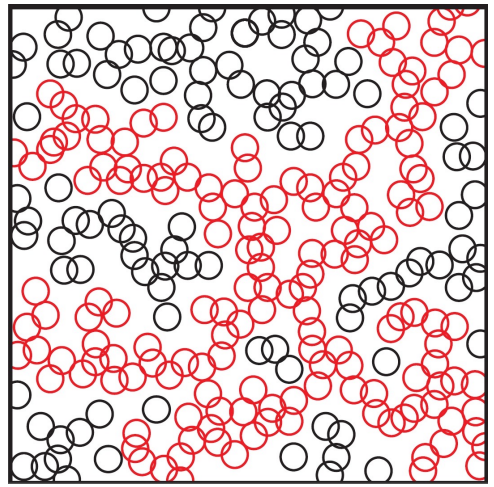
Another example:
disk percolation



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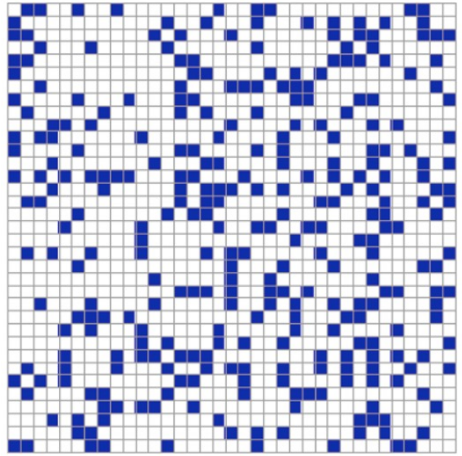
Above a **percolation threshold** p_c connectivity across the whole grid forms, insulator -> conductor

How to find p_c?

Percolation threshold simulation

Simulate percolation threshold with Monte Carlo methods



Strategy 1:

- For a given value of *p* mark each site as occupied with a probability *p*
- Find all clusters (e.g. with union-find data structure)
- Check if a conducting cluster from bottom to top edge exists
- We expect the cluster to exists for $p>p_c$ and not exist for $p<p_c$

Strategy 2:

- Start with zero occupied site
- Mark a random unoccupied site as occupied and check if it forms a new cluster
- Repeat the process until a conducting cluster is formed
- The ratio of occupied to total sites is the estimate for p_c

Caveats: finite-size effects

Percolation threshold: union-find data structure

For finding clusters we can utilize the union-find data structure

```python
# Class implementing the union-find structure with a 2D (x,y) index
# This will also store the minimum and maximum y (vertical) coordinate of each set
class UnionFind:
    def __init__(self, N):
        self.N = N
        self.parent = list(range(N**2))
        self.rank = [0] * N**2
        self.maxy = [0] * N**2
        self.miny = [0] * N**2
        for x in range(N):
            for y in range (N):
                ind = self.index(x,y)
                self.maxy[ind] = y
                self.miny[ind] = y

    def index(self, x, y):
        return self.N * x + y

    def findxy(self, x, y):
        return self.find(self.index(x,y))

    def find(self, ind):
        if self.parent[ind] != ind:
            self.parent[ind] = self.find(self.parent[ind])
        return self.parent[ind]
```

```python
    def unionxy(self, x1, y1, x2, y2):
        self.union(self.index(x1,y1), self.index(x2,y2))

    def union(self, ind1, ind2):
        root_1 = self.find(ind1)
        root_2 = self.find(ind2)

        if root_1 == root_2:
            return

        if self.rank[root_1] > self.rank[root_2]:
            self.maxy[root_1] = max(self.maxy[root_1], self.maxy[root_2])
            self.miny[root_1] = min(self.miny[root_1], self.miny[root_2])
            self.parent[root_2] = root_1
        else:
            self.maxy[root_2] = max(self.maxy[root_1], self.maxy[root_2])
            self.miny[root_2] = min(self.miny[root_1], self.miny[root_2])
            self.parent[root_1] = root_2
            if self.rank[root_1] == self.rank[root_2]:
                self.rank[root_2] += 1
```

Here implemented for a 2D grid, and keeps track of max and min y coordinate

Percolation threshold: implementing strategy 2

```
## Simulate percolation threshold on a square in 2D
## Return the fraction of occupied cells at percolation
def simulateSquarePercolation(N):
    cells = np.zeros([N,N])
    occupied = 0
    uf = UnionFind(N)
    while True:
        # Choose unoccupied cell to occupy
        while True:
            ind = np.random.randint(N**2)
            x = ind // N
            y = ind % N
            if (cells[x][y] == 0):
                break
        cells[x][y] = 1
        occupied += 1

        # Add the new cell to existing clusters
        if (x > 0 and cells[x-1][y] == 1):
            uf.unionxy(x,y,x-1,y)
        if (x < N - 1 and cells[x+1][y] == 1):
            uf.unionxy(x,y,x+1,y)
        if (y > 0 and cells[x][y-1] == 1):
            uf.unionxy(x,y,x,y-1)
        if (y < N - 1 and cells[x][y+1] == 1):
            uf.unionxy(x,y,x,y+1)

        ymin = uf.miny[uf.find(ind)]
        ymax = uf.maxy[uf.find(ind)]
        # Check if percolating cluster is found
        if (ymin == 0 and ymax == N-1):
            return occupied / N**2
```

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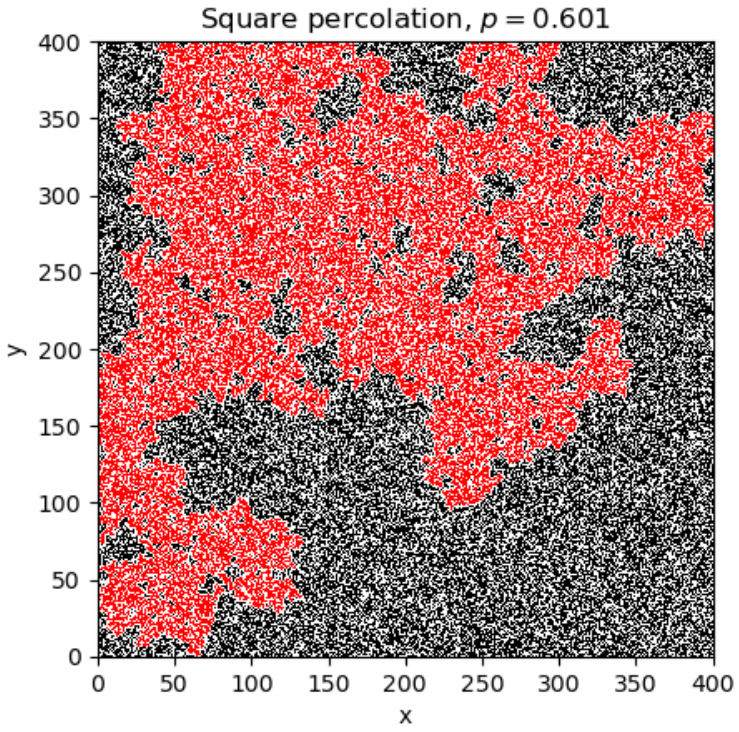
```

N = 400:



Percolation threshold: implementing strategy 2

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        cells[x][y] = 1
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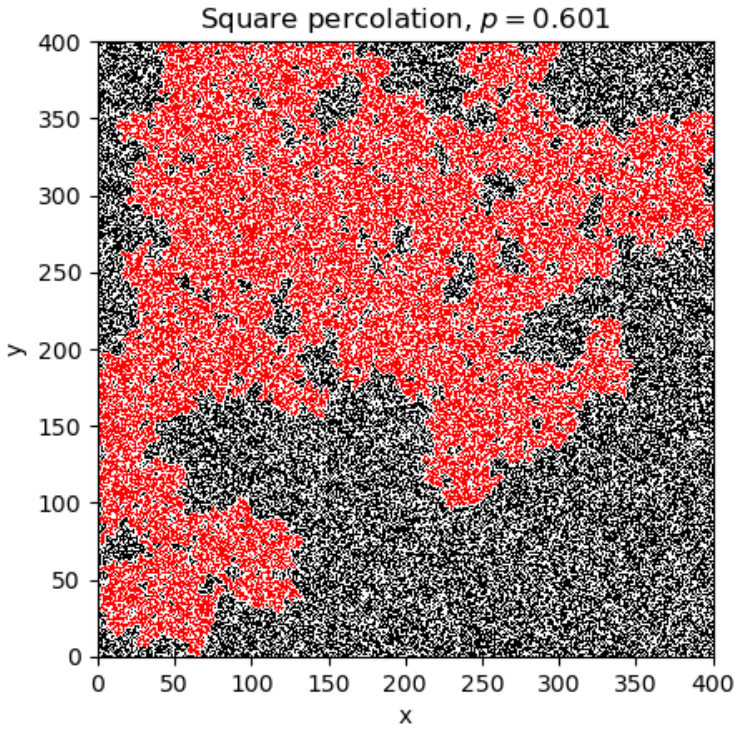

10000 runs with N = 10:

```
Simulating square percolation
NxN =  10 x 10  with M = 10000 samples
p_c =  0.5905830000000054 +- 0.023061418236939468
```

Literature value:

$p_c = 0.592746$