PHY604 Lecture 22

November 11, 2025

Today's lecture:
Stochastic methods

- Monte Carlo simulation in Stat Mech: The Ising model
- Simulated Annealing: Travelling salesman problem
- Genetic algorithms
- Quantum Monte Carlo

Example: The Ising model

- The Ising model is a classic model in statistical physics for describing magnetic systems

- Describe a magnetic material as classical spins on a lattice
  - Spins can only point up or down
  - Energy is given by:

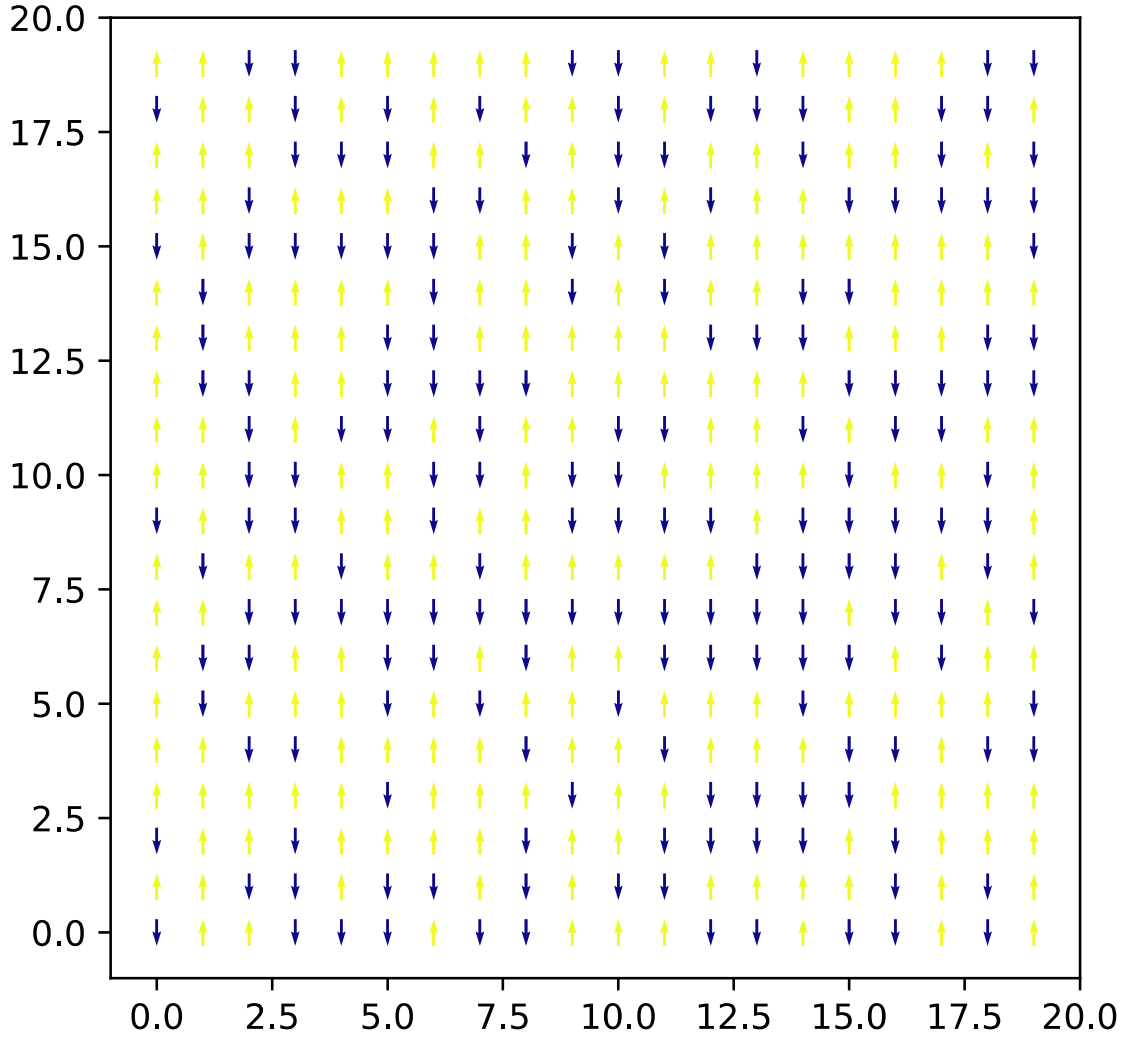
$$E = -J \sum_{\langle i,j \rangle} s_i s_j$$

  - Where $\langle i, j \rangle$ indicate neighboring spins
  - *J* is the interaction strength
    - If J > 0 aligned spins are preferred
    - If J < 0 antialigned spins are preferred

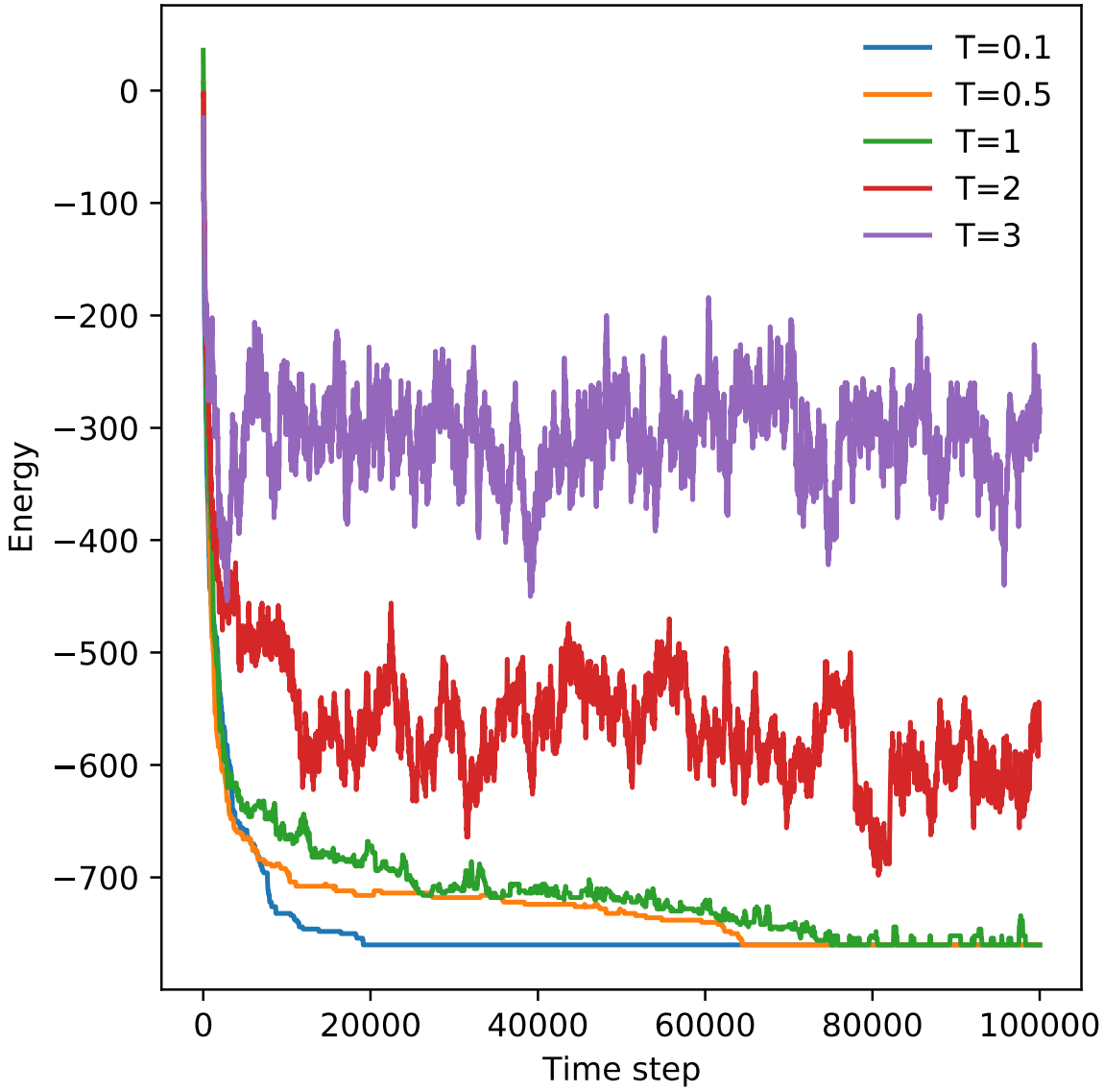
Monte Carlo simulation: Ising model on square lattice

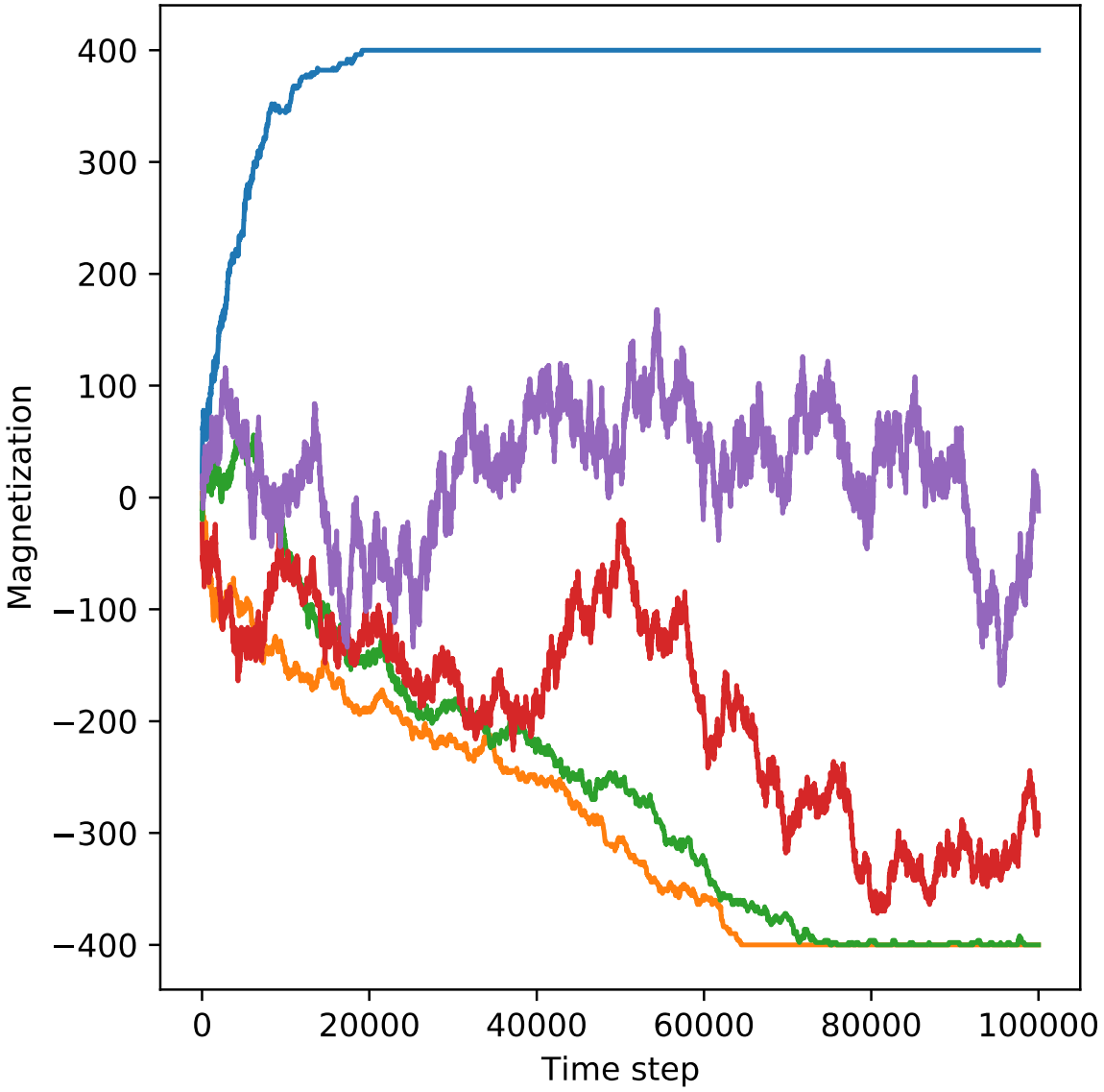
- 20 x 20 square lattice of spins
- Initialized randomly
- Move set: Flip a random spin
  - If it lowers the energy, accept
  - If it raises the energy, accept with Boltzmann probability
- Can also monitor magnetization

$$M = \sum_i s_i$$

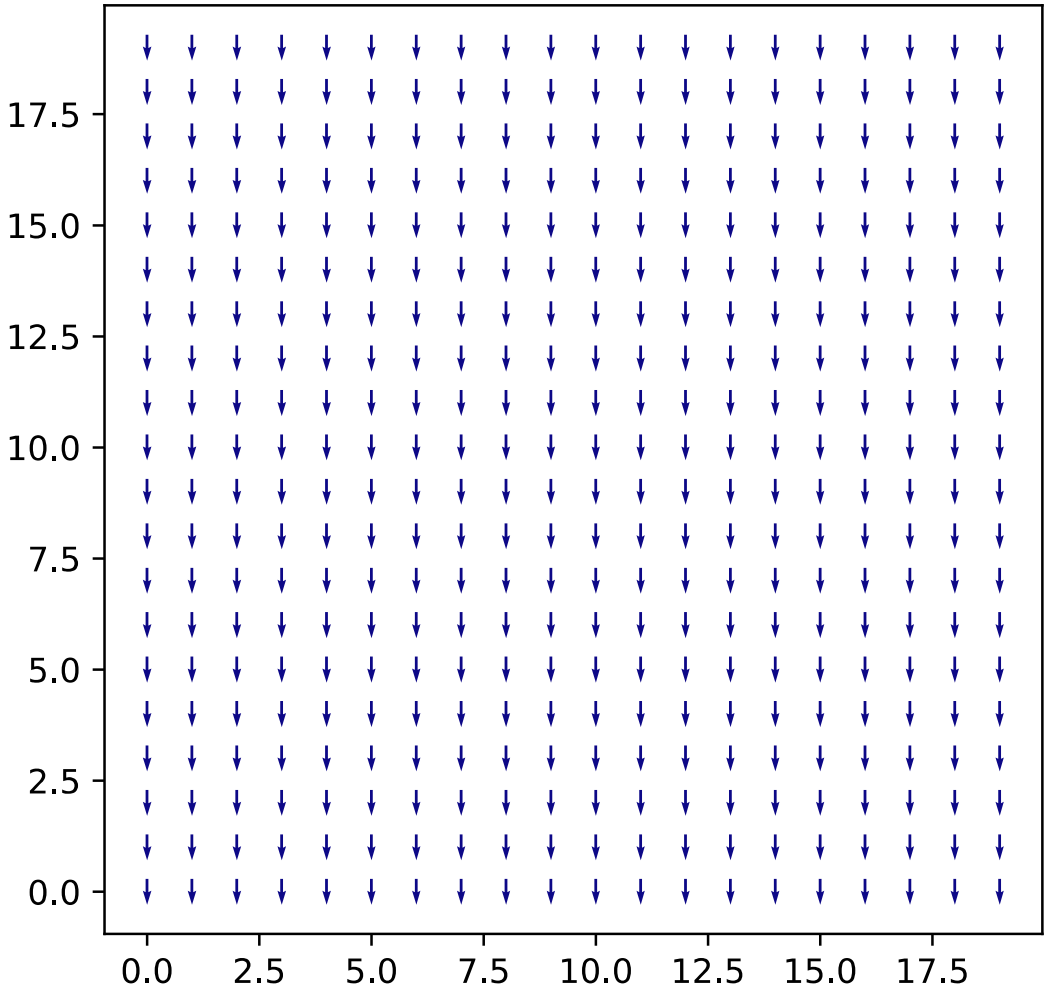


Ising model on square lattice versus T

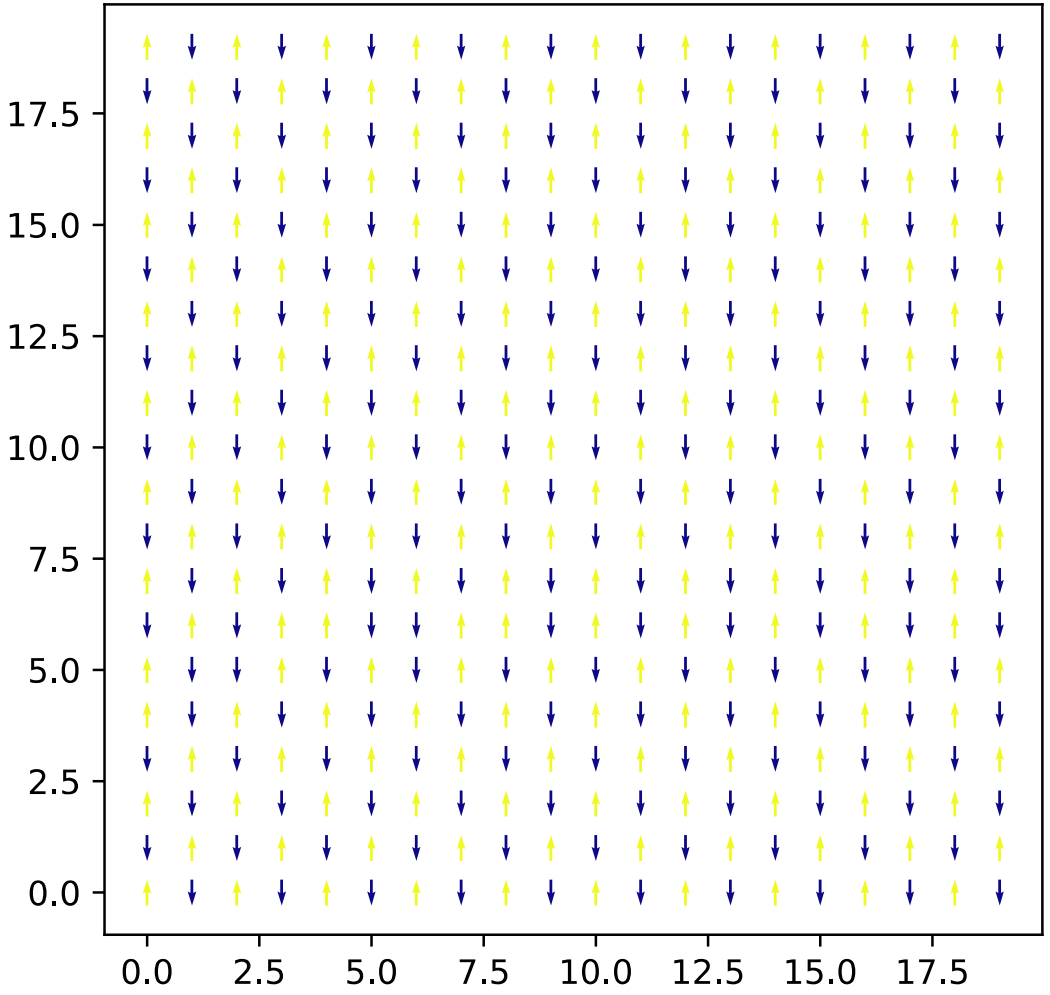




Ferromagnetic for J > 0,



Antiferromagnetic for J < 0



Today's lecture:
Stochastic methods

- Monte Carlo simulation in Stat Mech: The Ising model
- Simulated Annealing: Travelling salesman problem
- Genetic algorithms
- Quantum Monte Carlo

Simulated annealing (Newman Sec. 10.4)

- Monte Carlo methods can also be used for numerical optimization
- Optimization methods discussed so far only give local minima
- Global optimization problems are very challenging
- Simulated annealing borrows ideas from statistical physics/materials science to tackle this problem
  - Annealing: Heat treatment of materials to remove defects by allowing atoms to move to their equilibrium structure

Statistical mechanics for optimization

- Recall the Boltzmann probability:

$$P(E_i) = \frac{e^{-\beta E_i}}{Z}, \qquad Z = \sum_i e^{-\beta E_i}$$

- Assume we have single, unique ground state
- Choose energy scale so that the ground state configuration is 0 energy
- If we cool the system to $T = 0$, then the probability distribution is:

$$P(E_i) = \begin{cases} 1 & \text{if } E_i = 0 \\ 0 & \text{if } E_i > 0 \end{cases}$$

- By cooling the system, we can find the ground state

Statistical mechanics for optimization

- We can use the same strategy (cooling the system) for finding the minimum of a function
  - Take the value of the function to be the “energy”
  - Take the values of independent variables to define a state of the system

- But how can we avoid getting trapped in a local minima?
  - Energy of all nearby states are higher in energy, will not accept moves for low *T*

- Solution: “Anneal” by cooling slowly so system can find its way to the global minimum
  - Guaranteed to converge to global minimum if we cool slowly enough (often not possible)

Simulated annealing approach

- Choose $k_B T$ to be significantly greater than the typical energy change from a singe Monte Carlo move
  - Then:

$$\beta(E_j - E_i) \ll 1 \quad \Longrightarrow \quad P_a \simeq 1$$

  - Most moves accepted, state of the system rapidly randomized

- Make a cooling "schedule," e.g.:

$$T = T_0 e^{-t/\tau}$$

- Choice of τ require some trial and error, slower cooling is more likely to find ground state, but simulation takes longer

Example: Travelling salesman problem

- Find the shortest route that visits a given set of locations on a map
- One of the most famous optimization problems (NP hard)
- We will assume the salesman can travel between the *N* points on the map in straight lines (i.e., the world is flat)
  - *N* cities are chosen at random in a 2D square of unit length
- Want to minimize total distance travelled over the tour:

$$D = \sum_{i=0}^{N-1} |\mathbf{r}_{i+1} - \mathbf{r}_i|$$

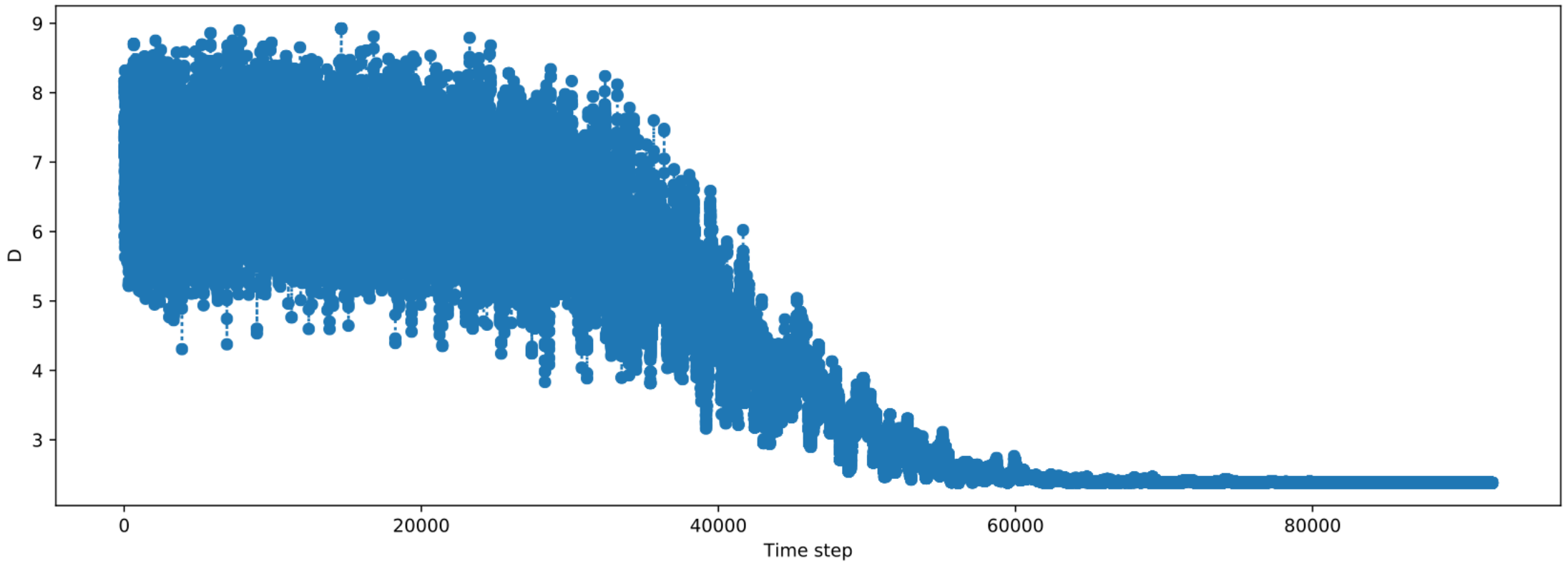
Markov chain Monte Carlo for traveling salesman

$$D = \sum_{i=0}^{N-1} |\mathbf{r}_{i+1} - \mathbf{r}_i|$$

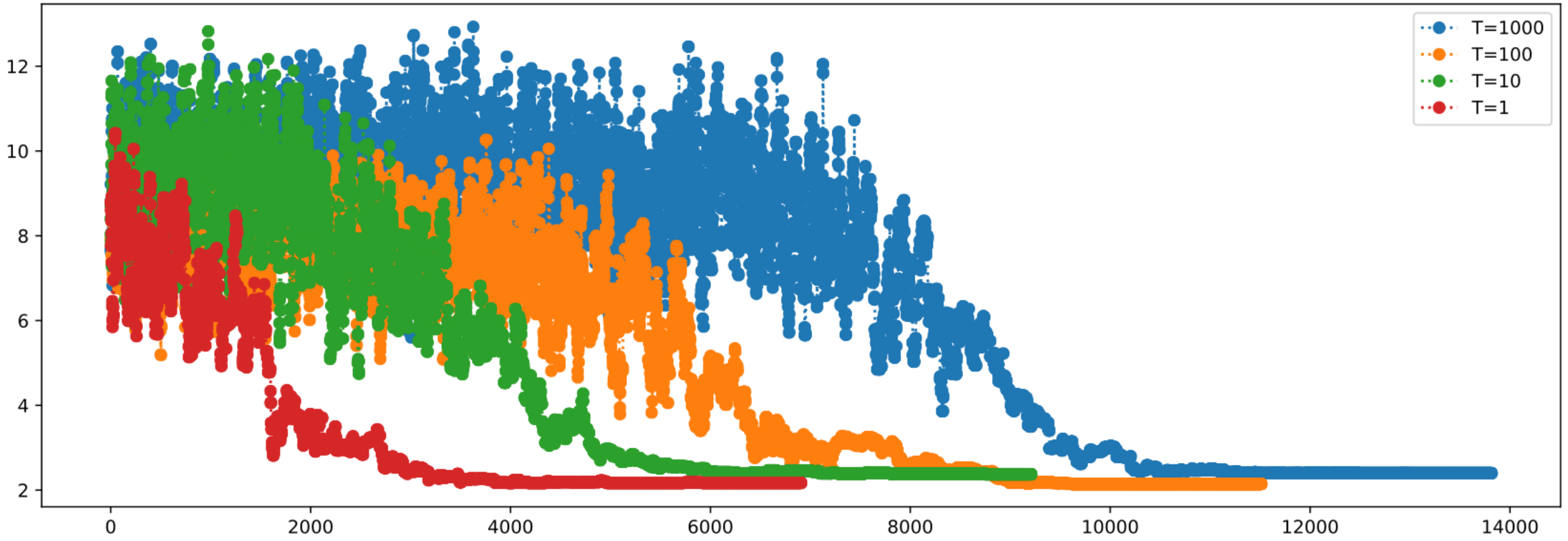
- Minimize *D* over set of all possible tours

- First set up an initial tour
- Then choose from set of moves: Swap pairs of cities
  - Accept if swap shortens the tour
  - If it lengthens the tour, accept with Boltzmann probability, energy replaced by distance D

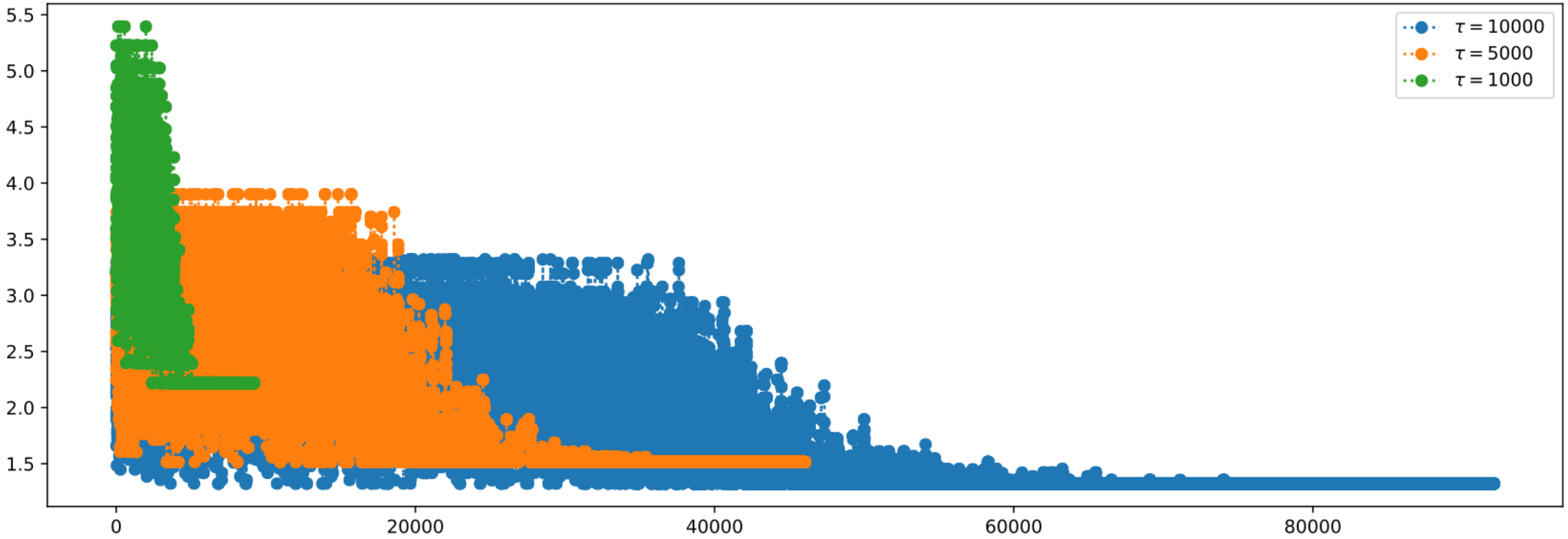
Simulated annealing for traveling salesman



Simulated annealing for traveling salesman: Different starting temperatures



Simulated annealing for traveling salesman: Different cooling rates temperatures



Today's lecture:
Stochastic methods

- Monte Carlo simulation in Stat Mech: The Ising model
- Simulated Annealing: Travelling salesman problem
- Genetic algorithms
- Quantum Monte Carlo

Genetic Algorithms (Pang Ch. 11)

- We saw in the case of simulated annealing:
  - Finding global minima is difficult
  - We can use inspiration from physics in solving unrelated problems in optimization

- Genetic algorithms are techniques for optimization inspired by biology
  - Create “organisms” that store a set of chromosomes
  - Create new organisms by mixing the genes of parents, and allowing for mutations

Steps for the genetic algorithm

- The problem: find the global minimum of multi-variable function $g(r_1,r_2,\ldots,r_n)$

- 1. Create a gene pool, i.e., an initial population of configurations
  - Configurations are values of variables
  - Can be binary or continuous
- 2. Selection: Choose members to be parents
- 3. Crossover: Produce offspring by mixing their genes
  - Parent chromosomes are cut into segments, exchanged, and joined together
- 4. Mutation: Create random changes to the chromosomes
- 5. In all of the steps above, make sure the configurations with lowest cost (evaluation of g) survive

Example: the Thomson problem

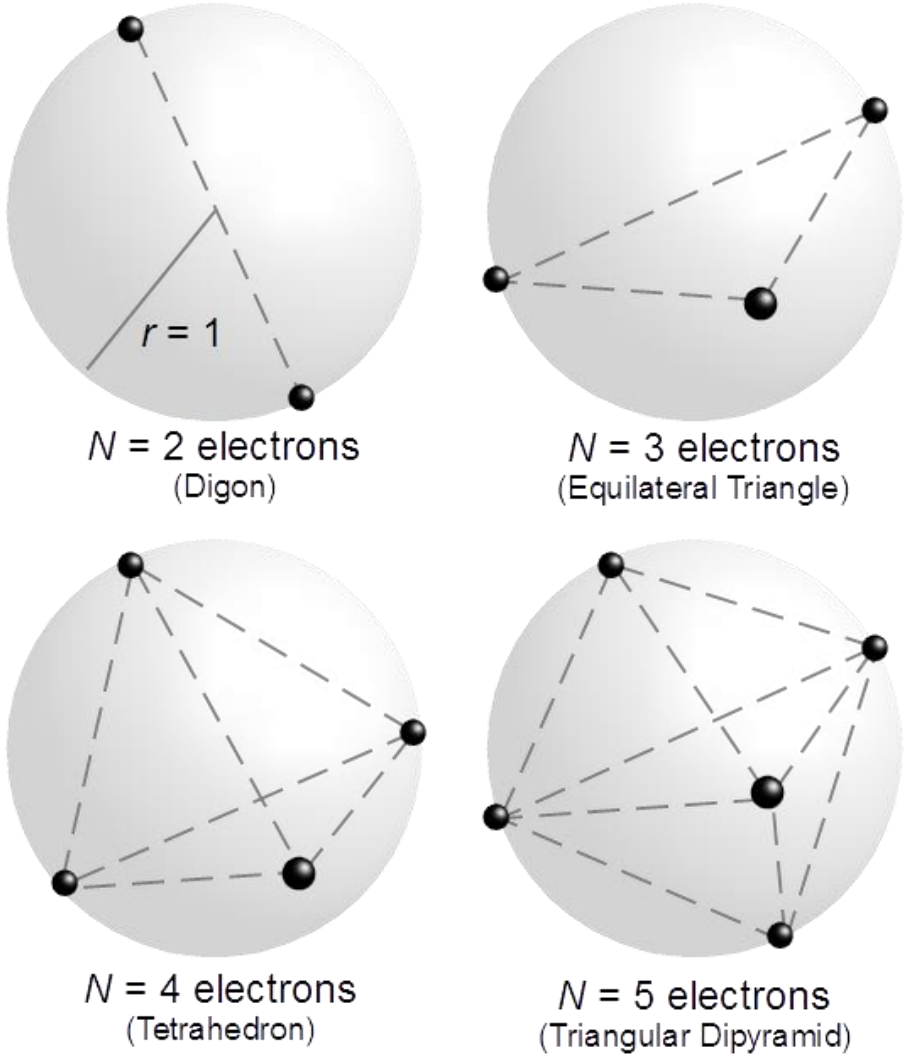
- Consider placing like charges on a unit sphere
- What is the optimal arrangement to reduce the electrostatic energy:

$$U = \frac{q^2}{4\pi\epsilon_0} \sum_{i>j=1}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

- Inspired by J.J. Thomson's "plum pudding model" for atoms

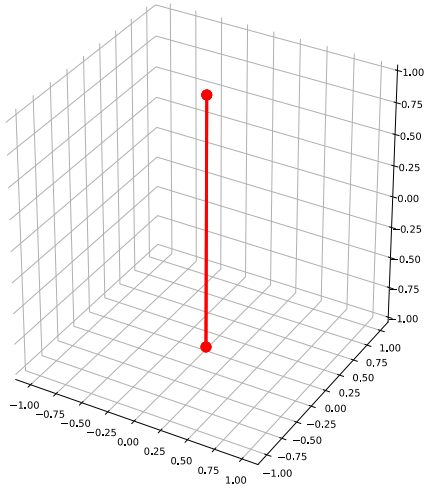
Solutions to the Thomson problem

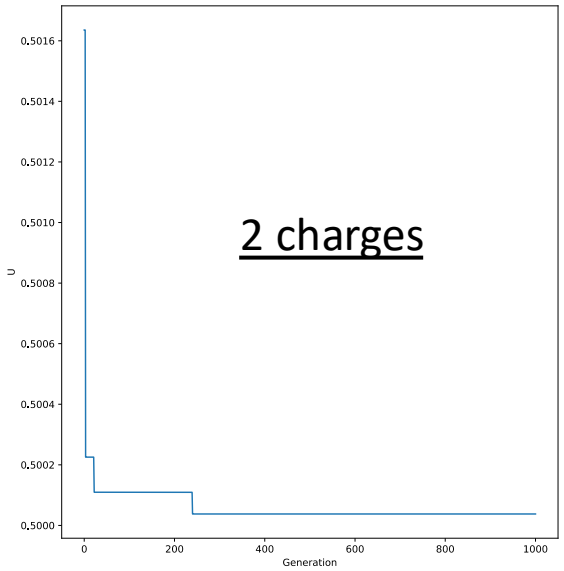
N	E_1	Symmetry	$\left\|\sum \mathbf{r}_i\right\|$	v_3	v_4	v_5	v_6	v_7	v_8	e	f_3	f_4	θ_1	Equivalent polyhedron
2	0.500000000	$D_{\infty h}$	0	–	–	–	–	–	–	2	–	–	180.000°	digon
3	1.732050808	D_{3h}	0	–	–	–	–	–	–	3	2	–	120.000°	triangle
4	3.674234614	T_d	0	4	0	0	0	0	0	6	4	0	109.471°	tetrahedron
5	6.474691495	D_{3h}	0	2	3	0	0	0	0	9	6	0	90.000°	triangular dipyramid
6	9.985281374	O_h	0	0	6	0	0	0	0	12	8	0	90.000°	octahedron
7	14.452977414	D_{5h}	0	0	5	2	0	0	0	15	10	0	72.000°	pentagonal dipyramid
8	19.675287861	D_{4d}	0	0	8	0	0	0	0	16	8	2	71.694°	square antiprism
9	25.759986531	D_{3h}	0	0	3	6	0	0	0	21	14	0	69.190°	triaugmented triangular prism
10	32.716949460	D_{4d}	0	0	2	8	0	0	0	24	16	0	64.996°	gyroelongated square dipyramid
11	40.596450510	C_{2v}	0.013219635	0	2	8	1	0	0	27	18	0	58.540°	edge-contracted icosahedron
12	49.165253058	I_h	0	0	0	12	0	0	0	30	20	0	63.435°	icosahedron (geodesic sphere $\{3,5+\}_{1,0}$)
13	58.853230612	C_{2v}	0.008820367	0	1	10	2	0	0	33	22	0	52.317°	
14	69.306363297	D_{6d}	0	0	0	12	2	0	0	36	24	0	52.866°	gyroelongated hexagonal dipyramid
15	80.670244114	D_3	0	0	0	12	3	0	0	39	26	0	49.225°	
16	92.911655302	T	0	0	0	12	4	0	0	42	28	0	48.936°	
17	106.050404829	D_{5h}	0	0	0	12	5	0	0	45	30	0	50.108°	double-gyroelongated pentagonal dipyramid
18	120.084467447	D_{4d}	0	0	2	8	8	0	0	48	32	0	47.534°	
19	135.089467557	C_{2v}	0.000135163	0	0	14	5	0	0	50	32	1	44.910°	
20	150.881568334	D_{3h}	0	0	0	12	8	0	0	54	36	0	46.093°	
21	167.641622399	C_{2v}	0.001406124	0	1	10	10	0	0	57	38	0	44.321°	
22	185.287536149	T_d	0	0	0	12	10	0	0	60	40	0	43.302°	



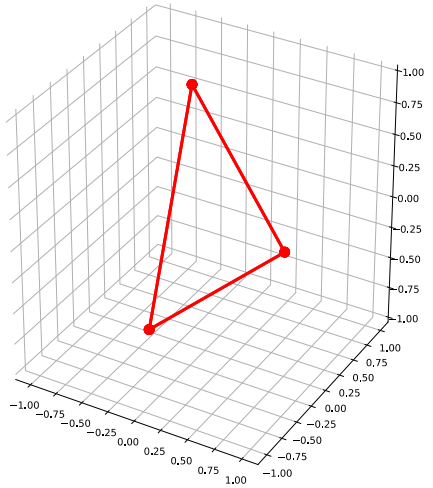
https://en.wikipedia.org/wiki/Thomson_problem

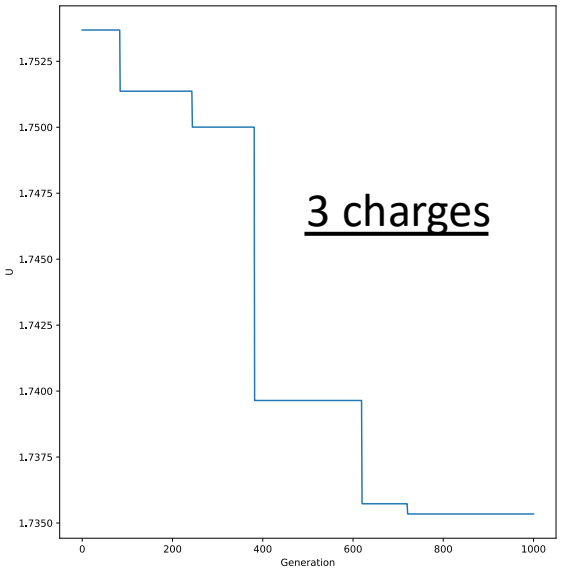
Solutions to the Thomson problem



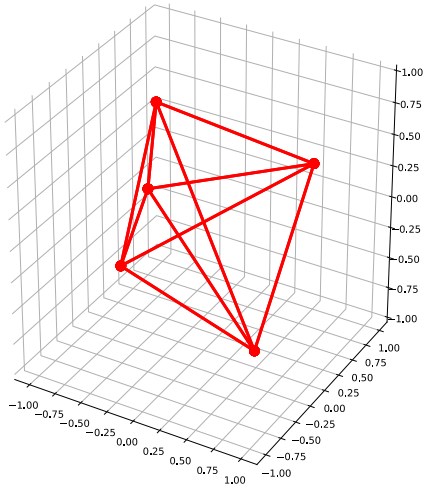


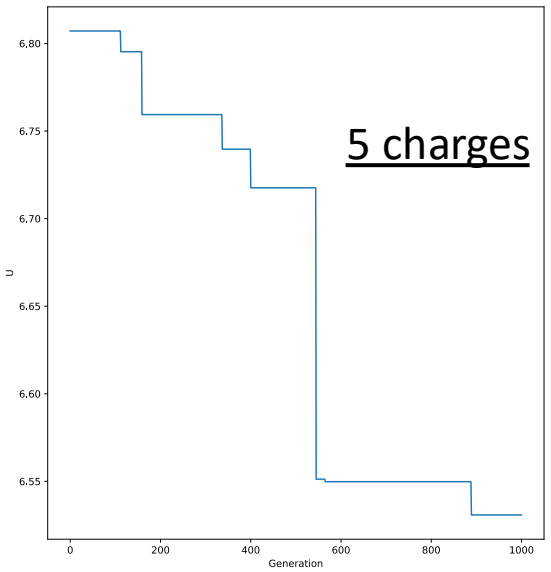
2 charges



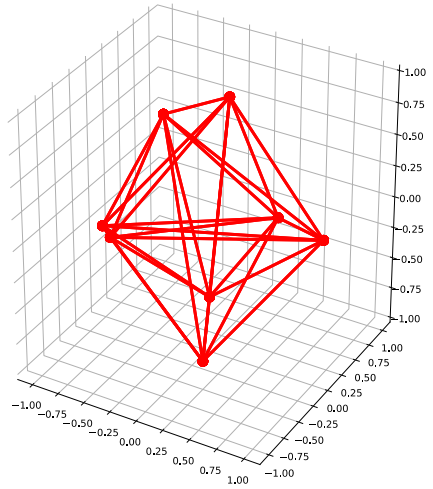


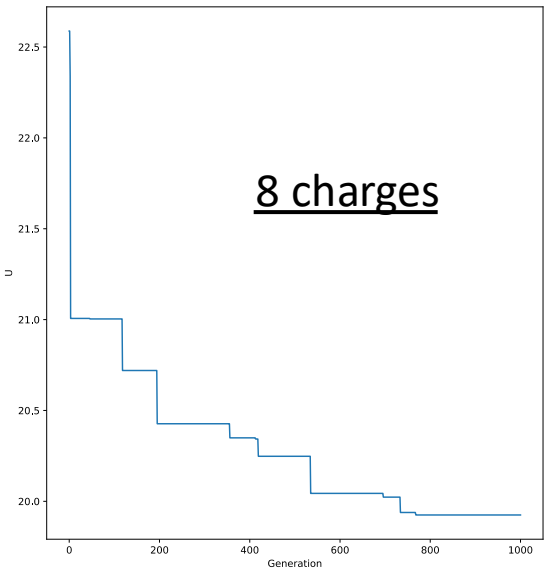
3 charges





5 charges





8 charges

Today's lecture:
Stochastic methods

- Monte Carlo simulation in Stat Mech: The Ising model
- Simulated Annealing: Travelling salesman problem
- Genetic algorithms
- Quantum Monte Carlo

Quantum Monte Carlo (Pang Sec. 10.5)

- So far, we have studied classical systems
- Monte Carlo algorithm can be generalized to study quantum systems
- Most direct generalization of the Metropolis algorithm: Variational quantum Monte Carlo
- We will just introduce some basic concepts in QMC and show how what we learned on classical systems transfers

General many-body quantum problem:

- We are seeking approximate solutions of the Hamiltonian:

$$H = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m_i} \nabla_i^2 + U_{\text{ext}}(\mathbf{r}_i) \right] + \sum_{i>j} V(\mathbf{r}_i, \mathbf{r}_j)$$

Kinetic energy

External potential

Electron-electron interaction

General many-body quantum problem:

- We are seeking approximate solutions of the Hamiltonian:

$$H = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m_i} \nabla_i^2 + U_{\text{ext}}(\mathbf{r}_i) \right] + \sum_{i>j} V(\mathbf{r}_i, \mathbf{r}_j)$$

- Time-independent many-body Schrödinger equation

$$H\Psi_n(\mathbf{R}) = E_n \Psi_n(\mathbf{R})$$

- $\mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ is the positions of all particles

- In general, cannot obtain analytic solution for more than two particles
- Numerically exact solutions are also limited to few particles

The many-body ground state

- Often, we would like to study the ground state of the system
- In that case, we can make use of the variational principle
  - Any other state has higher energy than the ground state
  - Introduce a trial state Φ to approximate the ground state, and minimize with respect to some set of parameters α_i

$$E[\alpha_i] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} \geq E_0$$

- Minimize by taking parameters in the Euler-Lagrange equation

$$\frac{\delta E[\alpha_i]}{\delta \alpha_i} = 0$$

Variational minimization of many-body ground state

- We can write:

$$E[\alpha_i] = \frac{\int \Phi^\dagger(\mathbf{R}) H \Phi(\mathbf{R}) d\mathbf{R}}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'} \equiv \int \mathcal{W}(\mathbf{R}) \mathcal{E}(\mathbf{R}) d\mathbf{R}$$

- Where:

$$\mathcal{W}(\mathbf{R}) = \frac{|\Phi(\mathbf{R})|^2}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'}, \qquad \mathcal{E}(\mathbf{R}) = \frac{1}{\Phi(\mathbf{R})} H \Phi(\mathbf{R})$$

Distribution function

Local energy of specific **R**

Variational minimization of many-body ground state

- We can write:

$$E[\alpha_i] = \frac{\int \Phi^\dagger(\mathbf{R}) H \Phi(\mathbf{R}) d\mathbf{R}}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'} \equiv \int \mathcal{W}(\mathbf{R}) \mathcal{E}(\mathbf{R}) d\mathbf{R}$$

- Where:

$$\mathcal{W}(\mathbf{R}) = \frac{|\Phi(\mathbf{R})|^2}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'}, \qquad \mathcal{E}(\mathbf{R}) = \frac{1}{\Phi(\mathbf{R})} H \Phi(\mathbf{R})$$

- If we know these, we can evaluate the expression via Monte Carlo
- Then vary α_i to minimize $E[\alpha_i]$

The trial wavefunction

- Common choice for trial wavefunctions:

$$\Phi(\mathbf{R}) = D(\mathbf{R})e^{-U(\mathbf{R})}$$

- $D(\mathbf{R})$ is a constant for bosons and a Slater determinant of single-particle orbitals for fermion systems
- $U(\mathbf{R})$ is ”Jastrow factor”:

$$U(\mathbf{R}) = \sum_{i=1}^{N} u_i(\mathbf{r}_i) + \sum_{i>j}^{N} u_2(\mathbf{r}_i, \mathbf{r}_j) + \dots$$

Comes from the interaction of particles with external potential

Comes from the interparticle interactions

The trial wavefunction

- Common choice for trial wavefunctions:

$$\Phi(\mathbf{R}) = D(\mathbf{R})e^{-U(\mathbf{R})}$$

- $D(\mathbf{R})$ is a constant for bosons and a Slater determinant of single-particle orbitals for fermion systems
- $U(\mathbf{R})$ is ”Jastrow factor”:

$$U(\mathbf{R}) = \sum_{i=1}^{N} u_i(\mathbf{r}_i) + \sum_{i>j}^{N} u_2(\mathbf{r}_i, \mathbf{r}_j) + \dots$$

- The key to the method is to choose a trial wavefunction that contains the necessary physics

Procedure for variational QMC

- 1. Choose a basis of single-particle orbitals
- 2. For fermions, construct Slater determinant (by a linear combination of atomic orbitals, or a by single-particle method like Hartree-Fock or DFT)
- 3. Determine the interparticle interactions
- 4. Perform Metropolis steps, e.g., by altering particle positions $\mathbf{r}_i$
- 5. Use as the probability in the Markov chain: $\mathcal{W}(\mathbf{R}) = \frac{|\Phi(\mathbf{R})|^2}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'}$
- 6. Accumulate average energy via local energy: $E = \frac{1}{M} \sum_{m=1}^{M} \mathcal{E}(\mathbf{R}_m)$

After class tasks

- Homework 5 due November 19

- Readings:
  - Simulated annealing: Newman Sec. 10.4
  - Genetic algorithms:
    - https://en.wikipedia.org/wiki/Thomson_problem
    - Pang Ch. 11
  - QMC:
    - Pang Secs. 10.5, 10.6
    - https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.73.33
    - https://journals.aps.org/prb/abstract/10.1103/PhysRevB.16.3081