Supporting textbook chapters for week 11: Chapters 10.3 & 10.4

Week 10, topics:

- Monte Carlo for Statistical Mechanics
  - Markov Chain
  - Simulated Annealing
  - Ising Model example

Monte Carlo simulations:

> Any simulation that uses random numbers to simulate random physical processes to estimate something about the outcome of that process.

`Newman, p. 476.`

We focus on statistical mechanics here.

Statistical mechanics: a review

- For a system in equilibrium at temperature T, the probability of finding the system in any particular state i is given by the Boltzmann distribution,
$$P(E_i) = \frac{\exp[-E_i/(k_B T)]}{Z}, \quad Z = \sum_{i=1}^{ALL} \exp[-E_i/(k_B T)]$$
where E_i is the energy of state i, k_B is Boltzmann's constant, Z is partition function
- System at temperature T undergoes transitions between states, with probability of being in a particular state $P(E_i)$

- To calculate expectation value of a macroscopic property X (e.g. total energy, magnetization, spin): average over the many microstates that the system visits
$$\langle X \rangle = \sum_{i=1}^{ALL} X_i P(E_i)$$
where X_i is the value of the quantity in the i^{th} microstate and P is the probability of finding the system in that microstate.
- Simple example: single mole of gas has $N_A \approx 6 \times 10^{23}$ molecules. Assume each molecule had only 2 possible spin states (gross underestimation), then the total number of spin microstates of the mole of gas is 2^{N_A}, which is huge.
- If we want to get any useful macroscopic information $\langle X \rangle$ about the system, we need to be more clever about how we count than just brute-force counting everything.

$$\langle X \rangle = \sum_{i=1}^{ALL} X_i P(E_i), \quad P(E_i) = \frac{\exp[-E_i/(k_B T)]}{Z}, \quad Z = \sum_{i=1}^{ALL} \exp[-E_i/(k_B T)]$$

- Huge number of terms in sum $\Rightarrow$ often impossible to perform analytically $\Rightarrow$ use Monte Carlo summation.
- Two difficulties to overcome:
  1. estimating $\langle X \rangle$: properly sampling which terms to sum over (*solution: importance sampling*),
  2. estimating Z (*solution: Markov Chain Monte Carlo*)

Importance sampling for Stat. Mech.

- Randomly sample the terms in the sum and only use those as an estimate. Replace $\langle X \rangle = \sum_{i=1}^{ALL} X_i P(E_i)$ with a sum over N randomly sampled microstates,
$$\langle X \rangle = \frac{\sum_{i=1}^{N} X_i P(E_i)}{\sum_{i=1}^{N} P(E_i)}.$$
  - Denominator ensures total probability over the sampled states is 1.
- To get a good estimate for the sum, it is only worth keeping the big terms
  - A lot of states have $E_i \gg k_B T$, therefore $P(E_i)$ really small since probability is proportional to $\exp[-E_i/(k_B T)]$
- Need to preferentially choose terms where the integrand is non-negligible, but assign them less weight individually (to not bias the final estimate) ... so use importance sampling!

- For a dicrete sum (see p. 478),
$$\langle X \rangle = \sum_{i=1}^{N} X_i P(E_i) \approx \frac{1}{N} \sum_{k=1}^{N} \frac{X_k P(E_k)}{w_k} \sum_{i=1}^{ALL} w_i.$$
- For weight w, use $P(E_i)$
$$\langle X \rangle \approx \frac{1}{N} \sum_{k=1}^{N} \underbrace{\frac{X_k P(E_k)}{P(E_k)}}_{=X_k} \underbrace{\sum_{i=1}^{ALL} P(E_i)}_{=1}.$$

In the end,

$$\langle X \rangle \approx \frac{1}{N} \sum_{k=1}^{N} X_k.$$

- Looks simple and no different from mean-value MC,
- but recall that the X_k's are drawn from non-uniform distribution: we randomly choose terms in the sum based on their Boltzmann probabilities, $P(E)$. But how? Recall
$$P(E_i) = \frac{\exp[-E_i/(k_B T)]}{Z}, \quad Z = \sum_{i=1}^{ALL} \exp[-E_i/(k_B T)]$$
- To do it this way, we need Z, which is a sum over all states. But if we could do this, we wouldn't need Monte Carlo in the first place!

Markov chain method

Mish-mashing [https://en.wikipedia.org/wiki/Markov_chain (https://en.wikipedia.org/wiki/Markov_chain)](https://en.wikipedia.org/wiki/Markov_chain) and [https://en.wikipedia.org/wiki/Markov_property (https://en.wikipedia.org/wiki/Markov_property)](https://en.wikipedia.org/wiki/Markov_property),

> A Markov chain is a stochastic model describing a sequence of possible events in which the probability of each event depends only on the state attained in the previous event. [...] (sometimes characterized as "memorylessness"). In simpler terms, it is a process for which predictions can be made regarding future outcomes based solely on its present state [...]. In other words, conditional on the present state of the system, its future and past states are independent.

- Random walks (Brownian motion) are Markov chains.
- Here: events are jumps in energy states, one after another.

Solution: Use the Markov chain method.

- Text goes into details on how to implement this method with a Metropolis algorithm.
- Crucial key: Metropolis does not directly compute probability to be in one state, but instead uses probability to transition between two states
  - Z cancels out in the process!
- In this lecture, we will summarize it algorithmically first, then briefly outline why it works mathematically.

Algorithm

1. Choose a random starting state i
2. Calculate the energy of that state E_i
3. Choose a transition to a new state j uniformly at random from allowed set
4. Calculate the energy of this new state, E_j
5. Calculate the acceptance probability for this transition:
   - $P_a = 1 \qquad \text{if } E_j \leq E_i$ (always accept a lower energy state)
   - $P_a = \exp\left(-\frac{E_j - E_i}{k_B T}\right) \quad \text{if } E_j > E_i$ (accept a higher energy state sometimes, more often for high T).
6. Accept/reject the move according to the acceptance probability
7. Measure the quantity X you want in its current state (new or old i) & store it
8. Repeat from step 2.

- How to implement the probability of the event in the previous slide?
  - $P_a = 1 \qquad \text{if } E_j \leq E_i$ (always accept a lower energy state)
  - $P_a = \exp\left(-\frac{E_j - E_i}{k_B T}\right) \quad \text{if } E_j > E_i$ (sometimes accept a higher energy state, more often for hight T).
- Draw a random number in $[0, 1)$. The statement

  ```
  if random() < exp(-(Ej-Ei)/kT):
  ```

  will introduce what to do if the move is accepted (`elif` will introduce what to do if rejected).
  - E.g., at very high T, $\exp(\ldots) \approx 1$ and almost all moves are accepted.
  - E.g., at low T, say, $\exp[-\Delta E/(k_B T)] = 1\%$, then `random()` has 1% chance of drawing a number that is $< 1\%$.
  - If $E_j \leq E_i$, then $\exp(\ldots) \geq 1$ and `if` statement automatically accepts.

Why does Metropolis create a system where each microstate has a probability $P(E_i)$, the Boltzmann distribution?

- Let τ_{ij} be transition probability from microstate i to microstate j, such that
$$\frac{\tau_{ij}}{\tau_{ji}} = \frac{P(E_j)}{P(E_i)},$$
which the Metropolis algorithm satisfies (see p. 482). For example, a small ratio above means
  - RHS: "*j is much less probable than i*" and equivalently,
  - LHS: "*probability of $j \to i$ is much higher than $i \to j$*",

  both statements being true in equal amounts.
- "In equal amounts" is crucial: it means that if you start from any initial state, your system will progressively evolve towards one where all microstates follow Boltzmann.

- Does it always converge? Yes. If you love linear algebra, see proof in Appendix D of Newman (it is actually quite elegant).

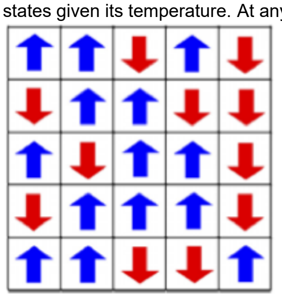
Example: Ising model

- Simple model of ferromagnetism, demonstrating many physical characteristics of fancier models.
- Assume an object is made up of a collection of dipoles (e.g., electron spins) and the net magnetization is the sum of the magnetization of all the spins.
- Ising model:
  - assume the spins can only point up or down.
  - the spins interact and favour parallel alignment of pairs of spins
  - the interactions are non-zero only between nearest neighbours (i.e., distance dependent).
- Macroscopic energy E and magnetization M (with no external field) are given by

$$E = -J \sum_{\langle ij \rangle} s_i s_j \quad \text{and} \quad M = \sum_i s_i$$

  where $s = +1$ if spin is up & $s = -1$ if spin is down.
  - Lowest energy occurs if the spins all line up.

- Spins can randomly flip as the system visits a set of allowable states given its temperature. At any particular moment the system may look like



Example in 1D

- Create array of dipoles, initial state: random spin at each location.
- Calculate energy & magnetization of state
- Implement Metropolis algorithm:
  - create new state: flip 1 spin randomly
  - calculate new total energy
  - calculate acceptance probability
  - decide whether to accept or reject new state
  - store 'new' energy & magnetization
  - repeat

In [ ]:

```
""" This program calculates the total energy and magnetization
for a 1D Ising model with N dipoles
Author: Nico Grisouard, University of Toronto """

import numpy as np
from random import random, randrange
import matplotlib.pyplot as plt

def energyfunction(J_, dipoles):
    energy = -J_*np.sum(dipoles[0:-1]*dipoles[1:])
    return energy

def acceptance(ARGUMENTS):
    """ Function for acceptance probability; to be completed """
    # Do stuff here
    return result  # result is True or False
```

In [ ]:

```
# define constants
kB = 1.0  # "Boltzmann" constant
T = 1.0  # "Temparature"
J = 1.0  # Interaction
num_dipoles = 100
N = 100  # number of flips

# generate array of dipoles and initialize diagnostic quantities
dipoles = np.ones(num_dipoles, int)  # hint: this will not work
energy = []
magnet = []
E = energyfunction(J, dipoles)
energy.append(E)
magnet.append(sum(dipoles))
```

In [ ]:
```python
print(dipoles)
```

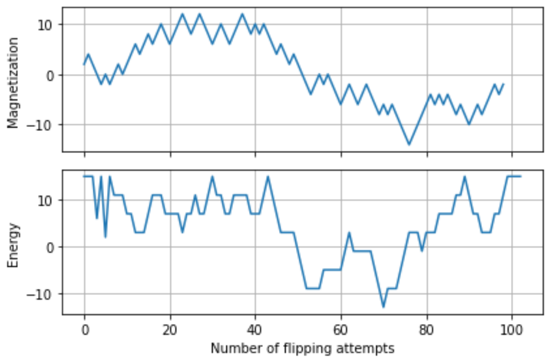
In [ ]:
```python
for i in range(N):
    picked = randrange(num_dipoles)  # choose a dipole
    dipoles[picked] *= -1  # propose to flip this dipole
    Enew = energyfunction(J, dipoles)  # compute Energy of proposed new state

    # calculate acceptance probability
    accepted = acceptance(Enew, E,)

    # store energy and magnetization
```

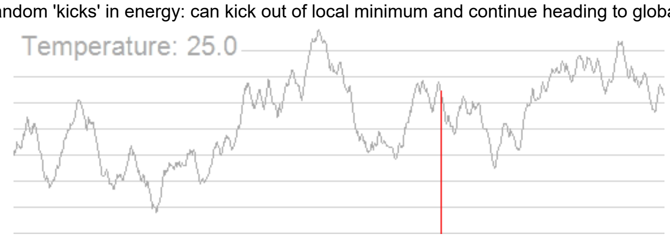
In [15]:
```python
# plot energy, magnetisation
fg, ax = plt.subplots(2, 1, sharex=True)
ax[0].plot(magnet)
ax[0].set_ylabel('Magnetization')
ax[0].grid()
ax[1].plot(energy)
ax[1].set_xlabel('Number of flipping attempts')
ax[1].set_ylabel('Energy')
ax[1].grid()

plt.tight_layout()
plt.show()
```



Simulated annealing

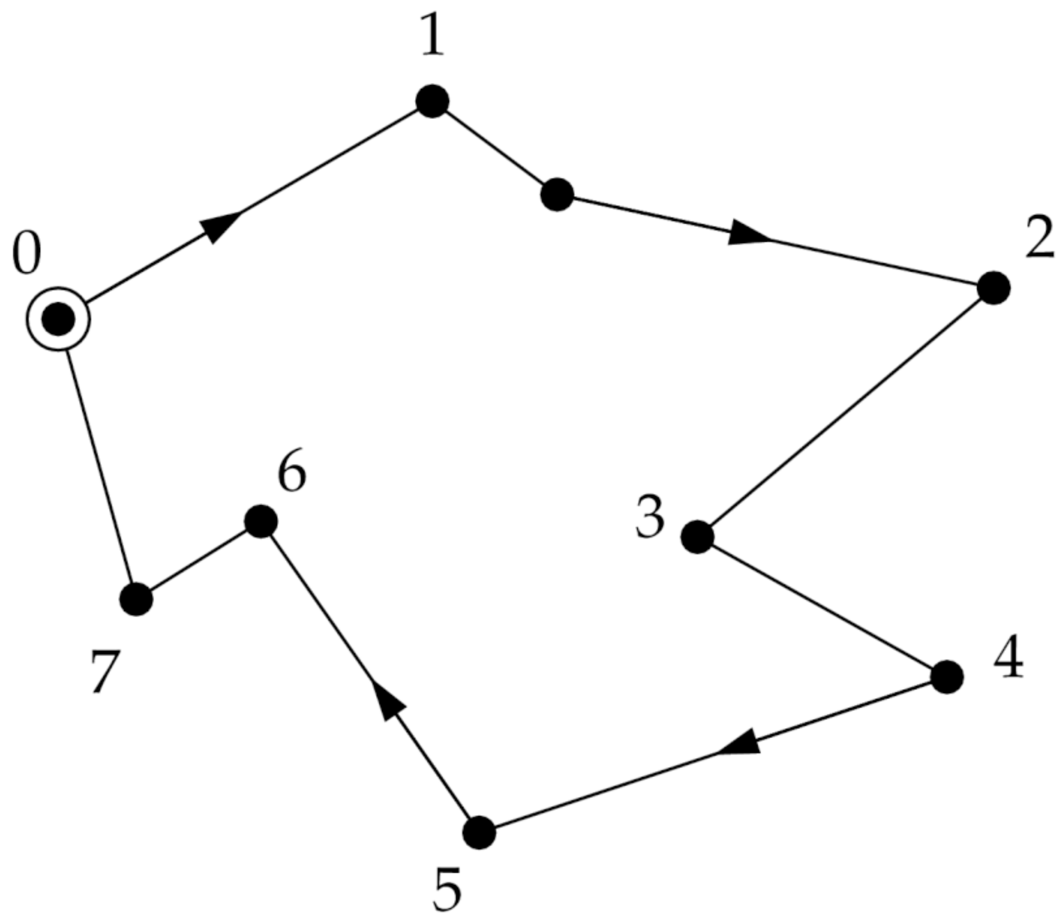
- Using Monte Carlo simulations to find **global** minima/maxima.
- In week 4 we talked about ways of finding local minima, which worked well if we had one, well-bracketed minimum. How about multiple local minima?
- How it works: rewrite max/min problem as looking for a "ground state energy" of a system.
  - Function f that you want the max/min of: make this the energy function.
  - how could you find ground state: reduce temperature until you reach the ground state.
- Issue: if you reduce temperature too quickly: might get caught in a local min instead of the global min.
- Solution: reduce temperature slowly. This way system has time to explore many microstates and find a good approximation to the global minimum.

- Visual Analogy: particle in a bumpy potential.
  - Too low energy: get stuck in nearest local minimum.
  - Keep low energy but allow some random 'kicks' in energy: can kick out of local minimum and continue heading to global minimum
  - 

    ([https://commons.wikimedia.org/wiki/File:Hill_Climbing_with_Simulated_Annealing.gif (https://commons.wikimedia.org/wiki/File:Hill_Climbing_with_Simulated_Annealing.gif)](https://commons.wikimedia.org/wiki/File:Hill_Climbing_with_Simulated_Annealing.gif))

Example: travelling salesman

- Famous NP-hard problem ([https://en.wikipedia.org/wiki/NP-hardness (https://en.wikipedia.org/wiki/NP-hardness)](https://en.wikipedia.org/wiki/NP-hardness)): what is the shortest route to visit a given set of locations on a map?
- Want global minimum of distance
- Start with random route, swap 2 cities, use Metropolis algorithm to determine whether to keep the swap
  - "energy" in this case is the total distance of the route
  - You can explore this problem using code from the book (`salesman.py`).



Summary

- Stat mech results often involve sums over impractical number of terms
  - Monte Carlo can sample a representative number of microstates: importance sampling
    - weight = probability of given microstate
  - How to compute partition function: Markov Chain using Metropolis algorithm.
    - Randomly explore states by transitioning from one microstate to the next
    - Works because the transition probability is closely related to the ratios of probabilities of being in either state.
    - Famous and fundamental example: the Ising model.
- Simulated annealing for finding global minimum of a function: let f be the "energy", and lower the "temperature" progressively
  - Famous example: travelling salesman problem