

This is a testfile for vscode

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摘要

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1 This is a section

Hello world! Hello Ali! As shown in figure 1

2 Molecular Dynamics

Classical mechanics can not be the whole story. Statistical Mechanics, (some system that not seem to go to the lowest energy) Today I watch 46:43



图 1: this is Sihan Cao

3 Probability Theory:

3.1 Probability Distribution

All Probability Distribution must be normalized: sum over all possible outcomes must be "1"! flip coin is a discrete variable (The outcome only has finite value), but in molecular dynamics we mainly think of continous variable.

3.1.1 Normalization for continous variable

$$: \int_{-\infty}^{+\infty} p(x)dx = 1$$

3.1.2 Expected Value (aka Mean value, first moment of the distribution)

$$\langle X \rangle = \int_{-\infty}^{+\infty} xp(x)dx \quad (1)$$

The n_{th} order moment can be calculated through:

$$\langle X^n \rangle = \int_{-\infty}^{+\infty} x^n p(x)dx \quad (2)$$

3.1.3 Statistical Property

Variance: "cumulant"

$$Var(X) = \langle X^2 \rangle - \langle X \rangle^2 \quad (3)$$

Standard Deviation: Not cumulant, but has same unit as X

$$std(x) = \sqrt{Var(X)} \quad (4)$$

3.2 Lattice Model

Space is discretized, and each discrete cell can hold 0 or 1 particle. Microstate \longleftrightarrow Combinations

For the probabilistic mechanics, the multi-components system go to the (macro) state with the highest multiplicity (combos) 这句话是测试能否进行引用及支持中文^[1]。

4 Machine Learning and artificial intelligence for engineers

4.1 Lecture

4.1.1 Lecture 2

4.1.1.1 Linear Regression To measure the error, just calculate the difference between the prediction result derived from the hypothesis, and calculate the difference between result and the ground truth. $d_1 = \theta x^{(1)} - y^{(1)}, d_2 = \theta x^{(2)} - y^{(2)}, \dots, d_m = \theta x^{(m)} - y^{(m)}$. We should square it otherwise it will offset each other.

We calculate the distance, square it, and sum it to get our "OBJECTIVE FUNCTION", So the objective function (I think one type of objective function):

$$\sum_{i=1}^m (y^i - h(x^i))^2 \quad (5)$$

The m is the number of training data point in our dataset.

所以，目标函数的意义就是，衡量一个拟合函数表现得好坏的工具。并且我们的参数是根据优化这个函数来计算得到的。

4.1.2 Lecture 3

Gradient descent

All samples.

4.1.2.1 Stochastic Gradient Descent SGD (Stochastic Gradient Descent), don't sum all the samples, just do it one by one. Stochastic (S) comes from

4.1.2.2 Epoch one epoch is go through all the data points from 1 to m. When to stop training: the cost function.

4.1.2.3 Batch Gradient Descent

4.1.2.4 mini Batch Gradient Descent One mini batch is one epoch. «deeplearning.ai»
deeplearning.ai

4.1.2.5 Cost function: the landscape is settle (The cost function is the same)

4.1.2.6 Evaluation matrices: SSE, sum square error (sum of square error for each sample) MSE (Mean Square Error), divide SSE by m, which is the data points you have.

4.1.2.7 Training and Test Set:

4.1.3 Lecture 4

5 Probability and Estimation Method for Engineering System

5.1 Lecture

5.1.1 Lecture 3

5.1.1.1 probability function

5.1.1.2 Total Probability and Bayes' formula Conditional Distributions are distributions conditional expectation and variance

5.1.1.2.1 Hw Independent event diagram

6 Computer Version

6.1 Rotation Matrix

$$\begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

For the linear transformation we only need to care about

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

which is the x-axis unit vector of the original coordinate and

$$\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

which is the y-axis unit vector of the original coordinate. Just draw a circle, and calculate the coordinate of the unit vector after rotation. The coordinate for the x-axis unit vector is the first column of the rotation matrix, and the y-axis is the second column. To use the rotation Matrix it's

just like:

$$\begin{bmatrix} x^1 \\ y^1 \end{bmatrix} = A \begin{bmatrix} x \\ y \end{bmatrix}$$

6.2 Lecture

6.2.1 Lecture1

Think image as a function, a color image is just like:

$$f(x, y) = \begin{bmatrix} r(x, y) \\ g(x, y) \\ b(x, y) \end{bmatrix}$$

For the image Processing, there are point operation and neighborhood operation.

7 Molecular Dynamics

7.1 Lecture

7.1.1 Lecture 3

8 Homework Part

Stirling's approximation

$$N! = \left(\frac{N}{e}\right)^N \ln N! \approx N \ln N - N \quad (6)$$

8.1 Problem 5

Lennard Jones law: $4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6]$ For a FCC material $U(d) = \frac{1}{2}4\epsilon$

The r^{12} term is the short term repulsive term (describe Pauli Repulsion), and the r^6 is the long term attractive term (describe van der Waals force or dispersion force).

8.1.1 (a)

The sum of the energy of the material could be written as:

$$U = 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6] = \frac{1}{2}N4\epsilon(\frac{(\sigma)^{12}}{(d)^{12}}A - \frac{(\sigma)^6}{(d)^6}B) \quad (7)$$

To calculate A and B:

$$A = 2 * (\frac{\sigma^{12}}{d^{12}}) + 2 * (\frac{\sigma^{12}}{(2d)^{12}}) + 2 * (\frac{\sigma^{12}}{(3d)^{12}}) + \dots = 2.0005(\frac{\sigma^{12}}{d^{12}}) \quad (8)$$

$$B = 2 * (\frac{\sigma^6}{d^6}) + 2 * (\frac{\sigma^6}{(2d)^6}) + 2 * (\frac{\sigma^6}{(3d)^6}) + 2 * (\frac{\sigma^6}{(4d)^6}) + \dots = 1.0173(\frac{\sigma^6}{d^6}) \quad (9)$$

Then,

$$U = \frac{1}{2}N4\epsilon[2.0005\frac{\sigma^{12}}{d^{12}} - 1.0173\frac{\sigma^6}{d^6}] \quad (10)$$

To calculate the equilibrium space d ,

$$\frac{dU}{dr} = 0 \quad (11)$$

So the d is $\sqrt[6]{\frac{2 \times 2.0005}{1.0173}} \sigma = 1.2564 \sigma$

The d just depend on length scale σ , but has no relationship with energy scale ϵ

8.1.2 b

If there is no energy dissipation, the total system will vibrate like a wave.

8.1.3 c

The total energy of the system is $U = 2N\epsilon[A\frac{\sigma^{12}}{r^{12}} - B\frac{\sigma^6}{r^6}]$, so $\frac{d^2u}{dr^2} = 2N\epsilon[A\sigma^{12}(12 \times 13r^{-14}) - B\sigma^6(42r^{-8})] = 2N\epsilon[2.0005\sigma^{12} \times 156 \times (1.2564\sigma)^{-14} - 1.0173\sigma^6 \times 42 \times (1.2564\sigma)^{-8}]$ So the effective spring constant equals: $11.7938N\epsilon\sigma^{-2}$

8.2 Problem 6

The weight of one mole water is 18 g/mol, and the density of water is 1g/mL.

8.2.1 diameter of 1 nm:

The volume of the water drop is $\frac{4}{3}\pi r^3$, so the volume of the drop is $\frac{4}{3}\pi \cdot (1nm)^3$. The density is 1g/mL, which could be written as $1g/cm^3 = 1g/(10^6nm)^3$. So the number of molecules can be calculated through the following formulation:

$$Mole = \frac{4}{3}\pi \cdot (1nm)^3 \cdot 1g/(10^6nm)^3 \div 18g/mol = 2.327 \times 10^{-19}mole \quad (12)$$

To get the number of molecules just multiply the mole with Avogadro's number:

$$Number = 2.327 \times 10^{-19}mole \times 6.022 \times 10^{23} = 140132 \approx 1.4 \times 10^5 \quad (13)$$

8.2.2 diameter of 1μ m

Same method just changed the volume of the drop:

$$\frac{4}{3}\pi \cdot (10^3nm)^3 \cdot 1g/(10^6nm)^3 \div 18g/mol \times 6.022 \times 10^{23} \approx 1.4 \times 10^{14} \quad (14)$$

8.2.3 diameter of 1 mm

$$\frac{4}{3}\pi \cdot (10^6nm)^3 \cdot 1g/(10^6nm)^3 \div 18g/mol \times 6.022 \times 10^{23} \approx 1.4 \times 10^{23} \quad (15)$$

8.3 b

Note that there are "A" water molecules. There are 3A atoms in the system. For the first water molecule, its atoms could have (3A-3) interactions. For the second water molecule, its atoms

have (3A-6). Based on this pattern, the total pairs is:

$$3(A-1) \cdot 3(A-2) \cdot \dots \cdot 3(2) \cdot 3(1) = 3^{A-1} \times (A-1)! \quad (16)$$

So, for the waterdrop with 1 nm, the number of pairs is; For the mm pair, the number of pair is $3^{1.4 \times 10^{23}} \times (1.4 \times 10^{23} - 1)!$

8.4 c

When I try to print the number, there is a overflow error in python.

8.5 Problem 7

8.6 Problem 8

8.6.1 a

For one lattice, the combination is C_N^n . Because the system has two lattices, so the total number of combinations is $C_N^n \cdot C_N^n = (C_N^n)^2$

8.6.2 b

The total number of combinations is C_{2N}^{2n} . The W_A could be written as $\frac{N!}{n!(N-n)!} \cdot \frac{N!}{n!(N-n)!}$, and the W_B could be written as $\frac{(2N)!}{(2n)!(2N-2n)!}$. Based on the form of sterling approximation, when N is really large is $N! = N^N e^{-N}$, So the ratio between W_A and W_B could be calculated through:

$$\frac{W_B}{W_A} = \frac{(2N)!}{(2n)!(2N-2n)!} \cdot \frac{n!n!}{(N-n)!(N-n)!} \cdot \frac{(N-n)!(N-n)!}{(2N-2n)!} \quad (17)$$

We could use $\frac{N!N!}{(2N)!}$ as an example:

$$\frac{\left(\frac{2N}{e}\right)^{2N}}{\left(\frac{N}{e}\right)^{2N}} = 2^{2N} \quad (18)$$

So the second term is just using n to replace the N in the previous equation, so it is $\frac{1}{2^{2n}}$ and the third term is $\frac{1}{2^{2N-2n}}$.

So the result is the total Product of the three term:

$$2^{2N} \cdot \frac{1}{2^{2n}} \cdot \frac{1}{2^{2N-2n}} = 1 \quad (19)$$

8.6.3 c

Based on the previous question, the entropy difference could be calculated as following:

$$\Delta S = k \ln\left(\frac{W_B}{W_A}\right) = k \ln(1) = 0 \quad (20)$$

参考文献

- [1] G. J. Pottie and W. J. Kaiser. Embedding the internet: Wireless integrated network sensors. *Communications of the Acm*, 43, 2000.