This is a testfile for vscode

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摘要

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Contents

1 This is a section

Hello world! Hello Ali! As shown in figure 1

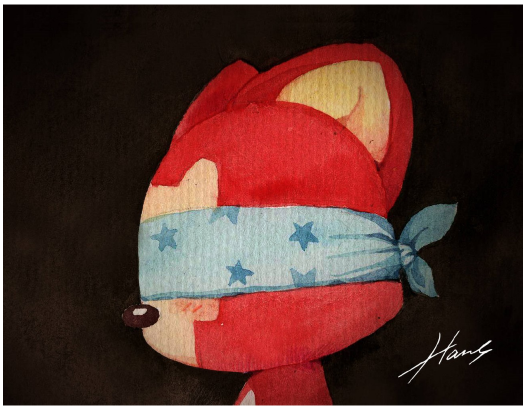

图 1: this is Sihan Cao

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

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)

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

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

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

3.1.3 Statistical Property

Variance: ”cumulant”

$$Var(X) = \langle X^2 \rangle - \langle X \rangle^2 \tag{3}$$

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

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

3.2 Lattice Model

Space is discretizied, and each discrete cell can hold 0 or 1 particle. Microstate <—> Combinations

For the probablistic mechanics, the multi-cimponents 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 artifical intelligence for engineers

4.1 Lecture

4.1.1 Lecture 3

Gradient decsent

All samples.

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

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

4.1.1.3 Batch Gradient Descent

4.1.1.4 mini Batch Gradient Descent

One mini batch is one epoch. «deeplearning.ai» deeplearning.ai

4.1.1.5 Cost function:

the landsacpe is settle (The cost function is the same)

4.1.1.6 Evaluation matrices:

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

4.1.1.7 Training and Test Set:

5 Computer Version

5.1 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:

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

5.2 Lecture

5.2.1 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.

6 Homework Part

Stirling's approximation

$$N! = (\frac{N}{e})^N \ln N! \approx N \ln N - N \tag{5}$$

6.1 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).

6.1.1 (a)

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

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

To calculate A and B:

$$A = 2 * (\frac{\sigma^{12}}{d^{12}}) + 2 * (\frac{\sigma^{12}}{(2d)^{12}}) + 2 * (\frac{\sigma^{12}}{(3d)^{12}}) + ... = 2.0005(\frac{\sigma^{12}}{d^{12}}) \tag{7}$$

$$B = 2 * (\frac{\sigma^6}{d^6}) + 2 * (\frac{\sigma^6}{(2d)^6}) + 2 * (\frac{\sigma^6}{(3d)^6}) + 2 * (\frac{\sigma^6}{(4d)^6}) + ... = 1.0173(\frac{\sigma^6}{d^6}) \tag{8}$$

Then,

$$U = \frac{1}{2}N4\epsilon[2.0005\frac{\sigma^1 2}{d^1 2} - 1.0173\frac{\sigma^6}{d^6}] \tag{9}$$

To calculate the equilibirium space d,

$$\frac{\mathrm{d}U}{\mathrm{d}r} = 0 \tag{10}$$

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

6.1.2 b

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

6.1.3 c

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

6.2 Problem 6

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

6.2.1 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 $1g/cm^3 = 1g/(10^6 nm)^3$. So the number of molecules can be calculated through the following formulation:

$$Mole = \frac{4}{3}\pi \cdot (1nm)^3 \cdot 1g/(10^6 nm)^3 \div 18g/mol = 2.327 \times 10^{-19} mole \tag{11}$$

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

$$Number = 2.327 \times 10^{-19} mole \times 6.022 \times 10^{23} = 140132 \approx 1.4 \times 10^5 \tag{12}$$

6.2.2 diameter of 1μ m

Same method just changed the volume of the drop:

$$\frac{4}{3}\pi \cdot (10^3 nm)^3 \cdot 1g/(10^6 nm)^3 \div 18g/mol \times 6.022 \times 10^{23} \approx 1.4 \times 10^{14} \tag{13}$$

6.2.3 diameter of 1 mm

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

6.3 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:

$$3(A-1) \cdot 3(A-2) \cdot \cdots \cdot 3(2) \cdot 3(1) = 3^{A-1} \times (A-1)! \tag{15}$$

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

6.4 c

6.5 Problem 8

6.5.1 a

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

6.5.2 b

The total number of combinations is C_{2N}^{2n}

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.