# 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

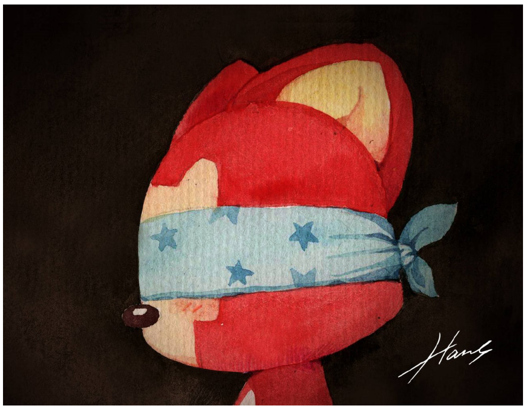

图 1: this is Sihan Cao

# 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,

$$U = \frac{1}{2}N4\epsilon[2.0005\frac{\sigma^12}{d^12} - 1.0173\frac{\sigma^6}{d^6}] \tag{9}$$

To calculate the equilibirium space d,

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

So the $d$ is $\sqrt[6]{\frac{2\times2.0005}{1.0173}}\sigma = 1.2564\sigma$
The d just depend on length scale $\sigma$, but has no relationship with energy scale $\epsilon$

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

## 6.2 Problem 8

### 6.2.1 a

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

### 6.2.2 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.