CHM 421/621
Statistical Mechanics

Lecture 17 Average, Variance and Uncertainty

Introduction and Review

Lecture Plan

Review of probability theory (ctd.)

- Probability Distributions - Discrete samples
- Probability Distributions - Continuous samples
- Averages and variances under a distribution
- Uncertainty

Averages and Variances

Average

Consider a property *g(x)* that depends on the variable (event) *x*.

We can compute an average value of *g* over a series of measurements of *x* as

$$\bar{g} = \frac{1}{N_{expt}} \sum_{i=1}^{N_{expt}} g(x_i)$$

Or, if we know the probability distribution *P*(*x*), as

$$\bar{g} = \sum_{x}^{N} g(x)P(x)$$

Or

$$\bar{g} = \int g(x)f(x)\ dx$$

Discrete

Continuous

Averages and Variances

Average

Consider the following distribution function for events

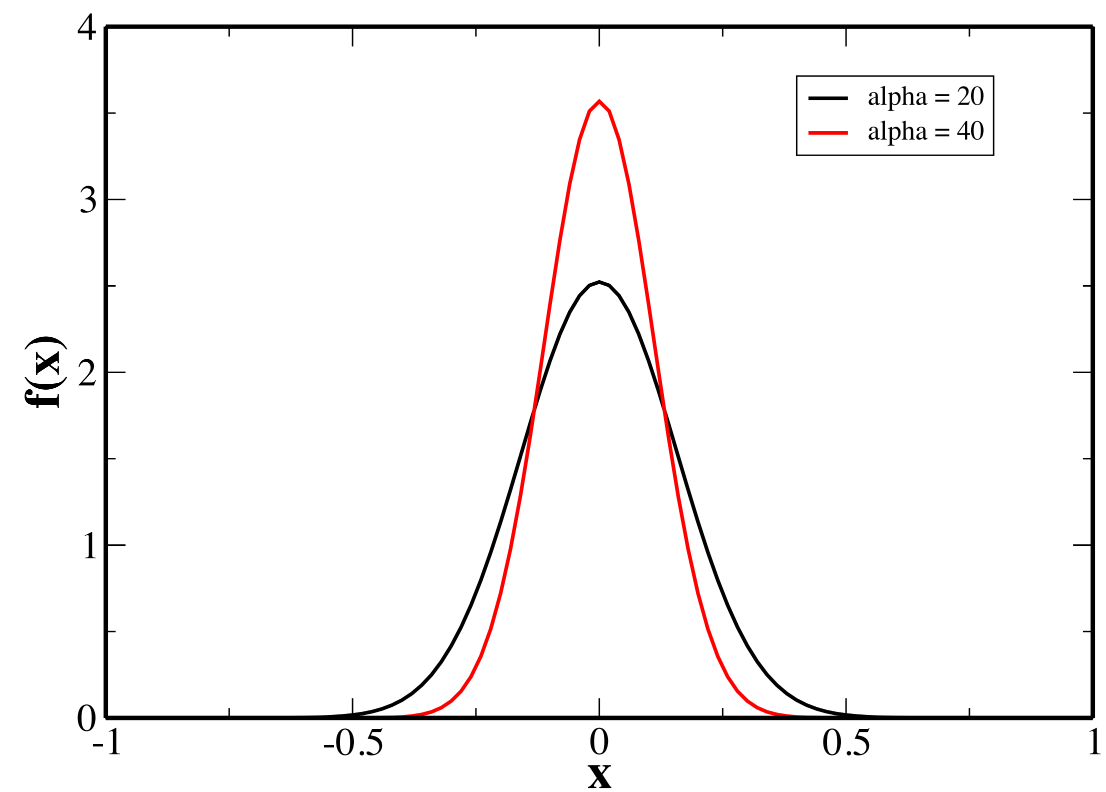
$$f(x) = \sqrt{\frac{\alpha}{\pi}} \exp\left(-\alpha x^2\right) \qquad -\infty \leq x \leq +\infty$$

Gaussian or normal distribution (Centred)

$$\bar{x} = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} x \exp\left(-\alpha x^2\right) \, dx = 0$$

$$\bar{x^2} = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} x^2 \exp\left(-\alpha x^2\right) \, dx = \frac{1}{2\alpha}$$

Thus, the smaller the value of α the fatter the curve



Averages and Variances

Average

Consider the following distribution function for events

$$f(x) = \sqrt{\frac{\alpha}{\pi}} \exp\left(-\alpha(x-x_0)^2\right) \quad -\infty \leq x \leq +\infty$$

Gaussian distribution (Off-centred / displaced)

$$\bar{x} = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} x \, \exp\left(-\alpha(x-x_0)^2\right) \, dx \quad = x_0$$

$$\overline{x^2} = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} x^2 \, \exp\left(-\alpha(x-x_0)^2\right) \, dx = \frac{1}{2\alpha} + x_0^2$$

However, note that

$$\overline{x^2} - \bar{x}^2 = \frac{1}{2\alpha}$$

Averages and Variances

Variance

Averages are not always the only important property to be extracted from a distribution.

We might also want to know how much the result of a particular experiment would differ from the expected average.

We can use the variance for this

$$\Delta\ x^2 = \frac{1}{N_{expt}} \sum_{i=1}^{N_{expt}} (x_i - \bar{x})^2$$

Why not $\overline{(x - \bar{x})}$?

Or, if we know the probability distribution *P*(*x*), as

$$\Delta\ x^2 = \sum_x^N (x - \bar{x})^2\ P(x)$$

Or

$$\Delta\ x^2 = \int (x - \bar{x})^2 f(x)\ dx$$

Discrete

Continuous

Averages and Variances

Variance

Note that

$$\mathrm{var(x)} = \Delta\ x^2 = \sum_x^N (x - \bar{x})^2\ P(x) = \overline{x^2} - \bar{x}^2$$

Square root of variance is called the standard deviation

$$\sigma(x) = \sqrt{\mathrm{var(x)}}$$

What is the standard deviation in the results in the case of rolling a single die?

Answer: $\sqrt{35/12}$

Averages and Variances

Normalised average value

The value of std. deviation helps in understanding the meaningfulness of an average and the spread of a distribution.

To quantify this we can define a normalised average value of *x*:

$$\mathrm{nav}(x) = \frac{\bar{x}}{\sigma(x)}$$

If $\mathrm{nav}(x) \ll 1$ then the average has no significance

If $\mathrm{nav}(x) \gg 1$ then the average is significant and the deviations from average are quite small

Most probable value

$$\left(\frac{\partial f(x)}{\partial x}\right)_{x_m} = 0$$

x_m is called the mode of the distribution

Uncertainty

Motivation

Rolling a true die *vs.* biased die

Case I. All numbers equally likely $P_i = 1/6$ (Most uncertain)

Case II. $P_i = 1/8$ ($i=1,5$) and $P_6=3/8$ (Lesser uncertainty than I)

Case III. $P_i = 0$ ($i=1,5$) and $P_6=1$ (Least uncertainty)

Case IV. $P_i = 1/8$ ($i=1,2,4,5,6$) and $P_3=3/8$ (Same as II)

Now consider rolling two dice, one true and one biased as in case III above.

The uncertainty in this case is the same as the case I. This can also be thought of as a sum of the individual uncertainties.

In the general case, the total uncertainty is at least that of either case. So the additivity of uncertainties of independent experiments is an appealing property to require.

Uncertainty

Desirable Properties

1. The uncertainty of an experiment consisting of two independent experiments should be a sum their individual uncertainties.
2. The uncertainty should depend on probabilities of all events.
3. The uncertainty should depend on the probabilities in a symmetric fashion.
4. The least uncertainty should occur when all but one event have probability 0. The maximum uncertainty should occur when all events have equal probability.

$$H(P_1, P_2, \cdots, P_N) = -\sum_{i=1}^{N} P_i \ln(P_i)$$ Discrete

$$H[f] = -\int f(x) \ln(f(x)) \, dx$$ Continuous

Uncertainty and information

A discrete example

Rolling a die assuming to be true:

$$H = 6 \times \frac{1}{6} \times \ln(6) = \ln(6) = 1.79$$

Suppose that before the die was rolled you received information that the die is biased towards 6 with P_6 = 3/8 (as in Case II).

The uncertainty is then

$$H = 5 \times \frac{1}{8} \times \ln(8) + \frac{3}{8} \times (\ln(8) - \ln(3)) = 1.67$$

The uncertainty reduces because of the new information obtained about the game.

We can say that you received 0.12 units of information.

Uncertainty and information

A continuous example

A particle is initially confined along a line $0 \leq x \leq 2$

If *f(x)* is the distribution function of the particle, then

$$\int_0^2 f(x)\; dx = 1$$

If we know nothing about the location then it is safe to assume all positions are equally likely. Which implies,

$$f(x) = \frac{1}{2}$$

So the uncertainty is

$$H[f] = \ln(2)$$

Uncertainty and information

A continuous example

If the confinement is relaxed a bit to $0 \le x \le 5$

Then, by the same calculation, the uncertainty becomes

$$H[f] = \ln(5)$$

We can say that by relaxing the confinement we lose some information about the particle's position. The amount of information lost is

$$\ln\left(\frac{5}{2}\right)$$

Uncertainty and information

The uncertainty is a reflection of the information we possess about the system. If we are told that an event *A* has occurred then it would affect our expectation of probabilities of the results. This can be captured through the conditional probability

$$H(A) = -\sum_i P(i|A)\ln P(i|A)$$

E.g., Someone tells us that a die only rolls numbers up to 4

$$H(i \leq 4) = -\sum_i P(i|i \leq 4)\ln\, P(i|i \leq 4)$$

$$P(i|i \leq 4) = \frac{1}{4}$$

$$H(i \leq 4) = \ln(4)$$