

# Probability

①

Discrete events:

Consider a random process which has a limited number of outcomes

tossing a coin:  $n=2$

rolling a die:  $n=6$

answering a SAT question:  $n=4$

The outcomes have associated values  $E_1, E_2, \dots, E_n$

In each experiment (trial) only one outcome is observed.

Probability is defined as:

$$P(E_j) = \lim_{N \rightarrow \infty} \frac{N_j}{N}$$

← number of trials with outcome  $E_j$   
← number of trials performed

$$P_j = \lim_{N \rightarrow \infty} \frac{N_j}{N}$$

Examples: Coin:  $E_1 = \text{heads}$   
 $E_2 = \text{tails}$

$$P(E_1) = P_1 = \frac{1}{2}$$

$$P(E_2) = P_2 = \frac{1}{2}$$

Die:  $E_1 = 1$   $E_2 = 2$   $\dots$   $E_6 = 6$

$$P(E_1) = P(E_2) = \dots = P(E_6) = \frac{1}{6}$$

Because  $N_1 + N_2 + \dots + N_n = N = \sum_{j=1}^n N_j$

(each trial had to result in one of the outcomes  
so total trials is sum of trials in each outcome)

That means we have limits on the value of each probability

$$0 \leq P(E_j) \leq 1$$

We also need to note that the combined probability of each event is 100%: (That is, there must be an outcome of each trial) This is called normalization:

$$\begin{aligned} \sum_{j=1}^n P(E_j) &= \sum_{j=1}^n \lim_{N \rightarrow \infty} \frac{N_j}{N} \\ &= \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^n N_j \\ &= \lim_{N \rightarrow \infty} \frac{N}{N} = 1 \end{aligned}$$

Now, consider an experiment in which two events A & B can or cannot occur. We define the outcomes as:

<u>Possible Results</u>	<u>Number of occurrences</u>
A and B	$N_1$
A, but not B	$N_2$
B, but not A	$N_3$
neither A nor B	$N_4$

We know right away that  $N = N_1 + N_2 + N_3 + N_4$  and from the table we can deduce the probability of A or B separately)

$$P(A) = \frac{N_1 + N_2}{N} \quad P(B) = \frac{N_3 + N_4}{N}$$

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The Joint probability is the probability of A & B happening together

$$P(A, B) = \frac{N_1}{N}$$

Conditional probability, given that B occurs, what's the probability of A?

$$P(A|B) = \frac{N_1}{N_1 + N_3}$$

Similarly, probability of B given observation of A:

$$P(B|A) = \frac{N_1}{N_1 + N_2}$$

Playing around with these terms gives us a general result:

$$P(B|A) P(A) = \frac{N_1}{N_1 + N_2} \cdot \frac{N_1 + N_2}{N} = \frac{N_1}{N} = P(A, B)$$

$$P(A|B) P(B) = \frac{N_1}{N_1 + N_3} \cdot \frac{N_1 + N_3}{N} = \frac{N_1}{N} = P(A, B)$$

$$\begin{array}{c} \swarrow \quad \uparrow \\ P(A \text{ given } B) \cdot P(B) = P(A \text{ and } B) \end{array}$$

One interesting variant is what this implies for mutually exclusive A & B. That is if A precludes B,  $P(A, B) = 0$

$$P(A|B) = P(B|A) = 0$$

For independent A & B A has no effect on appearance of B (or vice versa) so

$$P(B|A) = P(B)$$

$$P(A|B) = P(A)$$

$$\therefore P(B|A)P(A) = P(B)P(A) = P(A, B)$$

product of independent probabilities      joint probability

Averages

Average roll of a die gives what?

$$\bar{X} = \langle x \rangle = \sum_j x_j P(x_j)$$

← probability of outcome j

↑ value of outcome j

$$= 1 \cdot \frac{1}{6} + 2 \cdot \frac{1}{6} + 3 \cdot \frac{1}{6} + 4 \cdot \frac{1}{6} + 5 \cdot \frac{1}{6} + 6 \cdot \frac{1}{6}$$

$$= \frac{1+2+3+4+5+6}{6} = \frac{21}{6} = 3.5$$

↑ note that this is not one of the outcomes!

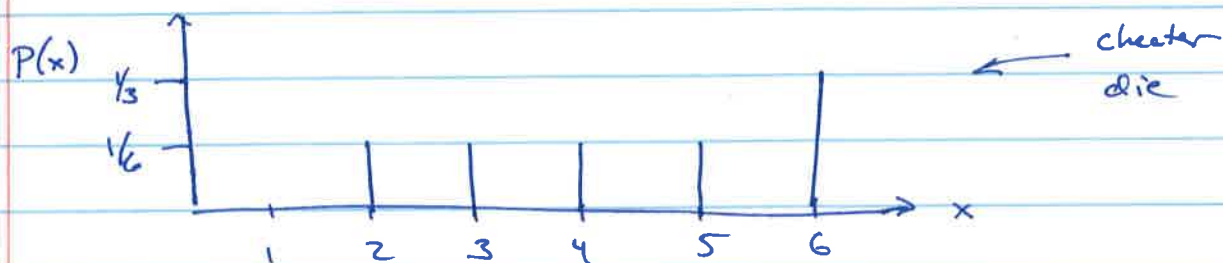
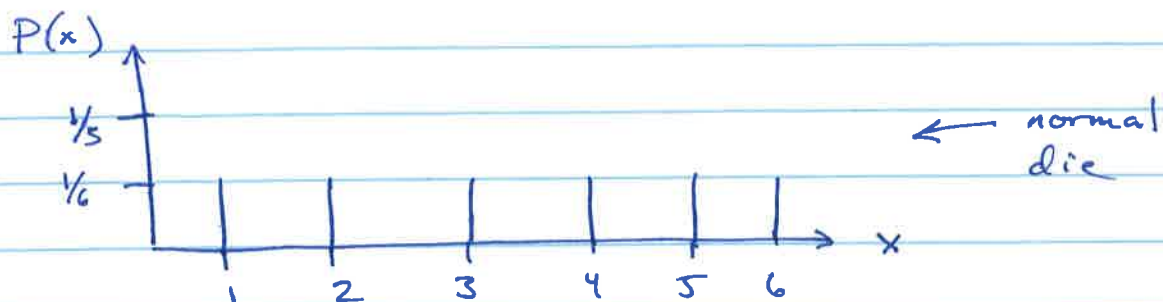
Loaded dice give very different means (we'll construct a die that gives 6 more often):

$$\langle x \rangle_{\text{cheater}} = 1 \cdot (0) + 2 \cdot \frac{1}{6} + 3 \cdot \frac{1}{6} + 4 \cdot \frac{1}{6} + 5 \cdot \frac{1}{6} + 6 \cdot \frac{1}{3}$$

$$= \frac{2+3+4+5+12}{6} = \frac{26}{6} = 4 \frac{1}{3}$$

We can plot  $p(x_j)$  ← the probability of outcome  $x_j$

vs. the value  $x_j$



The second moment

$$\langle x^2 \rangle = \sum_j x_j^2 P(x_j)$$

↗ average value of  
the square of the  
outcome

Examples: Normal die:  $\langle x^2 \rangle = \frac{1+4+9+16+25+36}{6} = 15.1\bar{6}$

Cheater die:  $\langle x^2 \rangle = \frac{4+9+16+25}{6} + \frac{36}{3} = \frac{27+36}{3}$

$$= 21$$

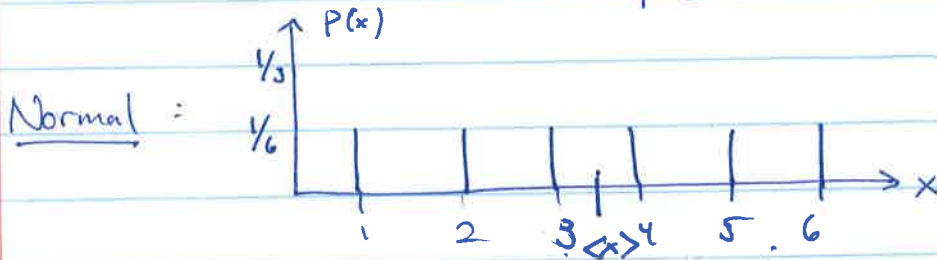
The standard deviation:

$\sigma_x$  easiest to define as its square

$$\sigma_x^2 = \langle (x - \bar{x})^2 \rangle$$

Back to our dice example:

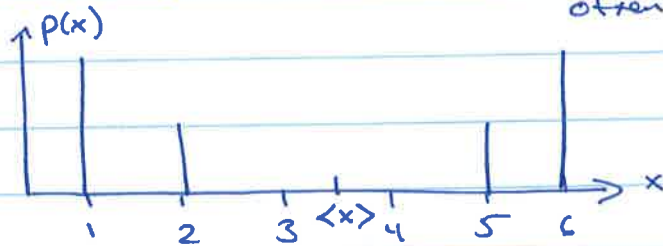
6



Average

$$\langle x \rangle = \bar{x} = \sum_{j=1}^n x_j \cdot P(x_j) = \frac{1+2+3+4+5+6}{6} = 3.5$$

Cheater (super secret): This die rolls 6 & 1 twice as often but never rolls 3 or 4.



$$\begin{aligned} \text{Average: } \langle x \rangle &= 1\left(\frac{1}{3}\right) + 2\left(\frac{1}{6}\right) + 5\left(\frac{1}{6}\right) + 6\left(\frac{1}{3}\right) \\ &= 3.5 \end{aligned}$$

Last time we defined 2 quantities

$$\langle x^2 \rangle = \text{second moment} = \sum_{j=1}^n x_j^2 P(x_j)$$

= the average value of the square of the dice roll.

$$\text{For normal die: } \langle x^2 \rangle = \frac{1+4+9+16+25+36}{6} = 15.1\bar{6}$$

$$\text{For this cheater } \langle x^2 \rangle = \frac{1+36}{3} + \frac{4+25}{6} = 17.1\bar{6}$$

Also the Standard deviation  $\sigma_x$

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle$$

Let's parse that

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle$$

The average square of the deviation from the average.

"On average how far are we (in absolute terms) from average behavior"

One of the things you'll prove in the HW is:

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

Here's a hint:

$$\sigma_x^2 = \sum_{j=1}^n (x_j - \langle x \rangle)^2 P(x_j)$$

So how does this work for the dice:

Normal

$$\langle x \rangle = 3.5$$

$$\langle x^2 \rangle = 15.16\bar{6}$$

$$\sigma_x = \sqrt{15.16\bar{6} - (3.5)^2}$$

$$= 1.708$$

Super-secret cheater

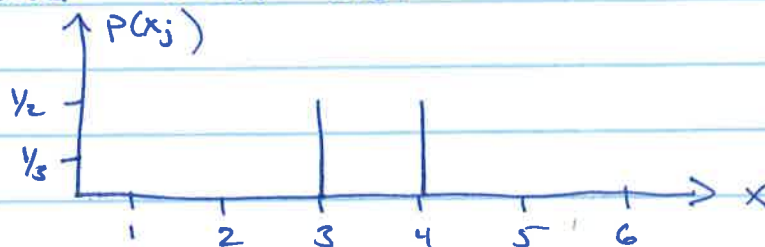
$$\langle x \rangle = 3.5$$

$$\langle x^2 \rangle = 17.16\bar{6}$$

$$\sigma_x = \sqrt{17.16\bar{6} - (3.5)^2}$$

$$= 2.217$$

Here's another cheater die:



OK, you work this one:

$$\langle x \rangle = \frac{1}{2} \cdot 3 + \frac{1}{2} \cdot 4 = \frac{7}{2} = 3.5$$

$$\langle x^2 \rangle = \frac{1}{2} \cdot 9 + \frac{1}{2} \cdot 16 = \frac{25}{2} = 12.5$$

$$\sigma_x^2 \text{ in 2 ways: } \sigma_x^2 = \frac{1}{2} (3-3.5)^2 + \frac{1}{2} (4-3.5)^2$$

$$= \frac{1}{2} \left(-\frac{1}{2}\right)^2 + \frac{1}{2} \left(\frac{1}{2}\right)^2$$

$$= \frac{1}{2} \left(\frac{1}{4}\right) + \frac{1}{2} \left(\frac{1}{4}\right)$$

$$\sigma_x^2 = \frac{1}{4}$$

$$\sigma_x = \frac{1}{2}$$

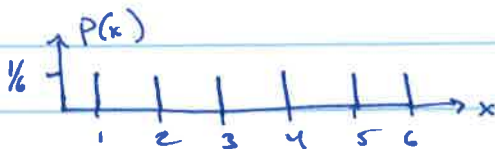
$$\text{Also: } \sigma_x = \sqrt{12.5 - (3.5)^2} = \sqrt{\frac{1}{4}} = \frac{1}{2}$$

So for this cheater, on average, we deviate from the mean (3.5) by a value of  $\frac{1}{2}$ .

The more sharply peaked a distribution is around  $\langle x \rangle$ , the smaller  $\sigma_x$  will be!

### Different kinds of distributions

A regular die has a uniform distribution





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That is, for every possible outcome the probability is identical:

$$P(x_j) = \frac{1}{n} \leftarrow \text{total \# of outcomes possible.}$$

Another very common discrete probability distribution is called the Poisson distribution

$$P(j) = \frac{a^j}{j!} e^{-a}$$

where  $j = 0, 1, 2, 3, \dots$   
and  $a$  is a constant.

This distribution governs discrete events that occur during a fixed time period (i.e. # of text messages you receive per day, # of mutations on a DNA strand / month, cars arriving at a traffic light, # of pieces of mail / day)

It is a shockingly common law at all lengths & time scales.

First, let's show it is normalized:

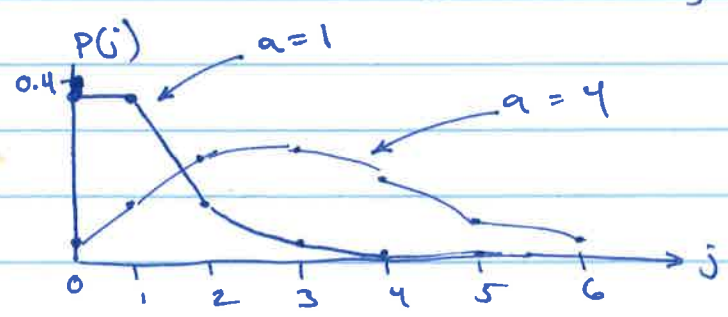
$$\begin{aligned} \sum_{j=0}^{\infty} P(j) &= \sum_{j=0}^{\infty} \frac{a^j}{j!} e^{-a} \\ &= e^{-a} \sum_{j=0}^{\infty} \frac{a^j}{j!} = e^{-a} \left( 1 + a + \frac{a^2}{2!} + \frac{a^3}{3!} + \dots \right) \\ &= e^{-a} (e^a) = 1 \end{aligned}$$

What about the average?

$$\begin{aligned}
\langle j \rangle &= \sum_{j=0}^{\infty} j P(j) \\
&= \sum_{j=0}^{\infty} j \frac{a^j}{j!} e^{-a} \\
&= e^{-a} \sum_{j=0}^{\infty} \frac{j a^j}{j!} \\
&= e^{-a} \sum_{j=0}^{\infty} \frac{a^j}{(j-1)!} \\
&= e^{-a} \sum_{j=0}^{\infty} a \frac{a^{j-1}}{(j-1)!} \\
&= a e^{-a} e^a \\
&= a
\end{aligned}$$

(-1)! = ∞  
so the first term goes away!)

This distribution is fascinating



We can generalize a few of the quantities we've defined:

n<sup>th</sup> moment :  $\langle x^n \rangle$

n<sup>th</sup> central moment :  $\langle (x - \langle x \rangle)^n \rangle$

1<sup>st</sup> central moment:  $\langle (x - \langle x \rangle) \rangle$

$$= \langle x \rangle - \langle \langle x \rangle \rangle$$

$$= \langle x \rangle - \langle x \rangle$$

$$= 0$$

2<sup>nd</sup> central moment  $\equiv$  variance:  $\langle (x - \langle x \rangle)^2 \rangle$

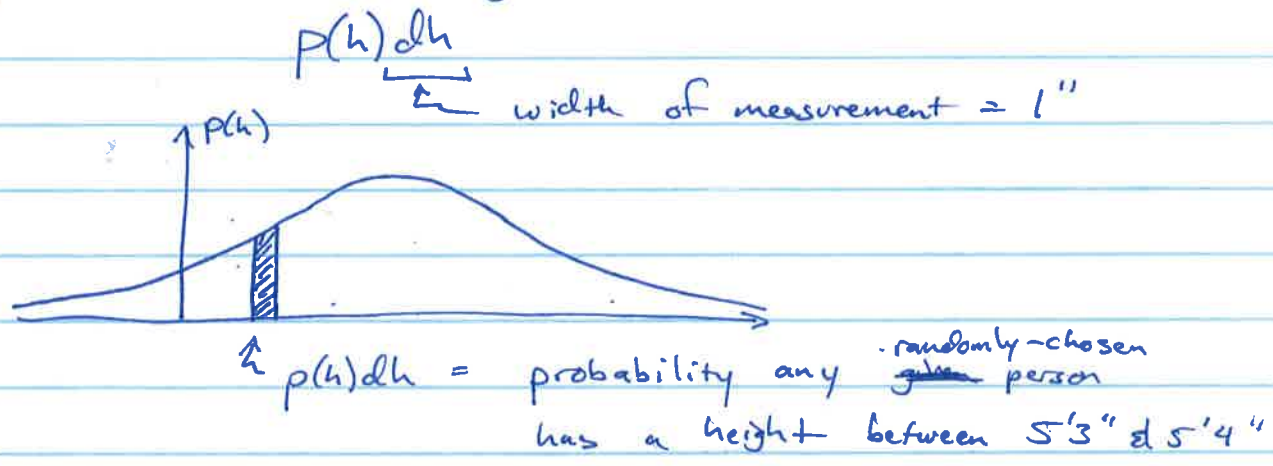
$$\equiv \sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2$$

Since  $\sigma_x^2 \geq 0$ , it must be true that

$$\langle x^2 \rangle \geq \langle x \rangle^2$$

Continuous Distributions

Consider probabilities of finding a chemistry professor with a height between 5'3" & 5'4"



Some analogies between dice (discrete outcomes) and height (continuous outcomes)

	<u>Discrete</u>	<u>Continuous</u>
Boundedness:	$0 \leq p_j \leq 1$	<u>Not true</u> : $0 \leq p(h) \leq 1$
Conservation:	$\sum_{j=1}^n p_j = 1$	$\int_{-\infty}^{\infty} p(h)dh = 1$
Mean	$\langle x \rangle = \sum_{j=1}^n x_j p(x_j)$	$\langle h \rangle = \int_{-\infty}^{\infty} h p(h)dh$

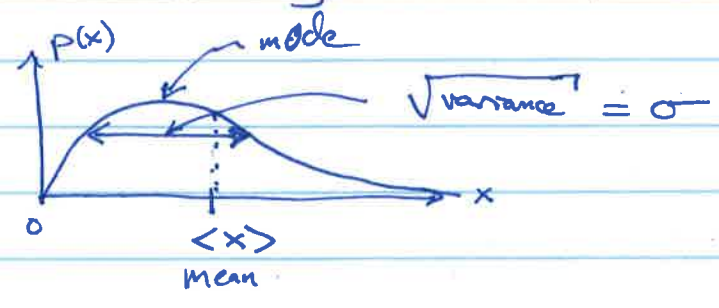
2<sup>nd</sup> moment  $\langle x^2 \rangle = \sum_{j=1}^n x_j^2 p_j$  Discrete

$\langle h^2 \rangle = \int_{-\infty}^{\infty} h^2 p(h) dh$  Continuous

Std. Dev.  $\sigma_x^2 = \sum_{j=1}^n (x_j - \langle x \rangle)^2 p_j$

$\sigma_h^2 = \int_{-\infty}^{\infty} (h - \langle h \rangle)^2 p(h) dh$

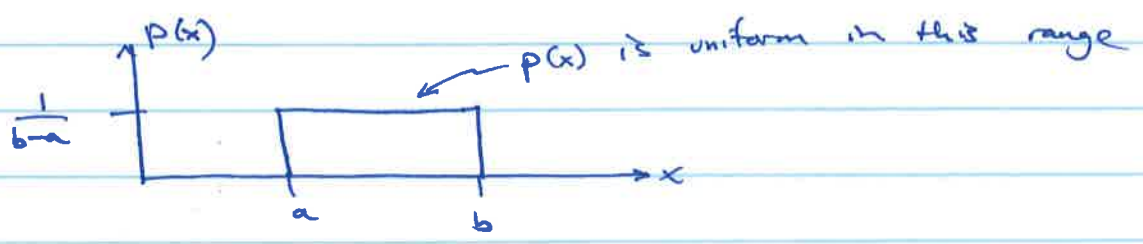
Consider an arbitrary distribution



Examples

Uniform probability density

$$p(x) = \begin{cases} \frac{1}{b-a} & a \leq x \leq b \\ 0 & \text{otherwise} \end{cases}$$



Normalization check:

$$\begin{aligned} \int_{-\infty}^{\infty} p(x) dx &= \int_a^b \frac{1}{b-a} dx \\ &= \frac{1}{b-a} [x]_a^b \\ &= \frac{b-a}{b-a} = 1 \end{aligned}$$

Mean:

$$\begin{aligned} \langle x \rangle &= \int_a^b x p(x) dx = \int_a^b \frac{x}{b-a} dx \\ &= \frac{1}{b-a} \left[ \frac{x^2}{2} \right]_a^b = \frac{b^2 - a^2}{2(b-a)} \\ &= \frac{(b+a)(b-a)}{2(b-a)} = \frac{b+a}{2} \end{aligned}$$

2<sup>nd</sup> moment:

$$\begin{aligned} \langle x^2 \rangle &= \int_a^b x^2 p(x) dx = \int_a^b \frac{x^2}{b-a} dx \\ &= \frac{1}{b-a} \left[ \frac{x^3}{3} \right]_a^b = \frac{b^3 - a^3}{3(b-a)} \\ &= \frac{b^2 + ab + a^2}{3} \end{aligned}$$

Variance: 
$$\begin{aligned} \sigma^2 &= \langle x^2 \rangle - \langle x \rangle^2 = \frac{b^2 + ab + a^2}{3} - \frac{(b+a)^2}{4} \\ &= \frac{(b-a)^2}{12} \end{aligned}$$

Next time: error

## Treatment of Experimental Data

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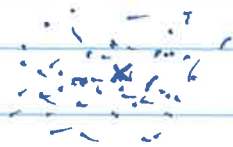
Types of error - All experiments contain sources of error, so it is important to determine the accuracy of measurements

Exact values:  $x$

Measured values:  $\cdot$



good accuracy  
& precision



poor accuracy  
poor precision



poor accuracy  
good precision

- Systematic errors: same direction & magnitude for each repetition of the experiment: affect accuracy without affecting precision
- Random errors: do not have the same direction & magnitude each time: affects both accuracy & precision.

## Statistical treatment of random errors

- Sample: A limited number of actual measurements
- Population: An imaginary set of an infinite number of repetitions of a perfect experiment.

We use samples to infer properties of populations.

Properties of a population  
probability distribution of

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a property  $x$ :  $f(x)$  N.B:  $\int_{-\infty}^{\infty} f(x) dx = 1$

Population mean:  $\mu = \int_{-\infty}^{\infty} x f(x) dx$

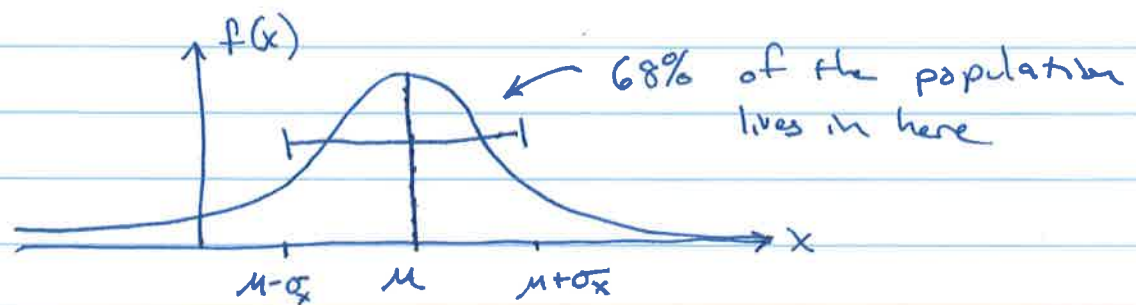
Population variance:  $\sigma_x^2 = \int_{-\infty}^{\infty} (x-\mu)^2 f(x) dx$

Population Std. Deviation:  $\sigma_x = [\sigma_x^2]^{1/2}$

We can often make the assumption that any population of experimental results is governed by the Gaussian or Normal distribution:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma_x^2}} e^{-\frac{(x-\mu)^2}{2\sigma_x^2}}$$

where  $\mu = \text{mean}$ ,  $\sigma_x^2 = \text{variance}$



For 68.3% of the population  $\mu - \sigma_x \leq x \leq \mu + \sigma_x$

For 95% of the population

$$\mu - 1.96\sigma_x \leq x \leq \mu + 1.96\sigma_x$$

The Central Limit Theorem: If a random experimental error arises from the sum of many contributions, then the errors will be governed by a Gaussian distribution.

Properties of a sample:

sample mean:  $\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i$

$i$  = individual experiments

$N$  = total experiments

$x_i$  = measurement of  $x$  in experiment  $i$

sample variance:  $S_x^2 = \frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2$

sample std. dev:  $S_x = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2}$

We use  $N-1$  in the denominator to create an unbiased estimate of  $S_x$ .

$N = N$  pieces of information =  $N-1$  pieces of information in addition to the mean.

Scientists often report data such that the reported value will be correct 95% of the time. This requires the 95% confidence interval.

That is the correct value is

$$\mu = \bar{x} \pm \epsilon$$

where 95% of the time  $\mu$  lies between

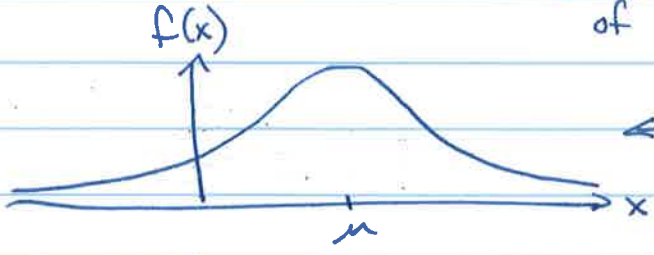
$$\bar{x} - \epsilon \leq \mu \leq \bar{x} + \epsilon$$



If we knew  $\sigma$ , the population std. dev., we could say with 95% confidence that

$$\mu = x \pm 1.96 \sigma$$

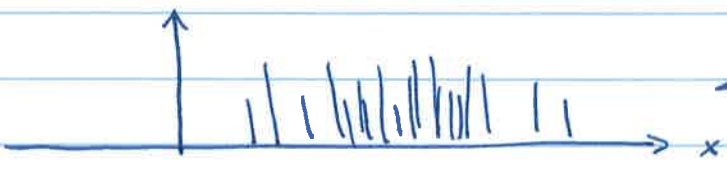
↗ outcome of a single measurement of the population mean



← original population with  $\sigma$  &  $\mu$



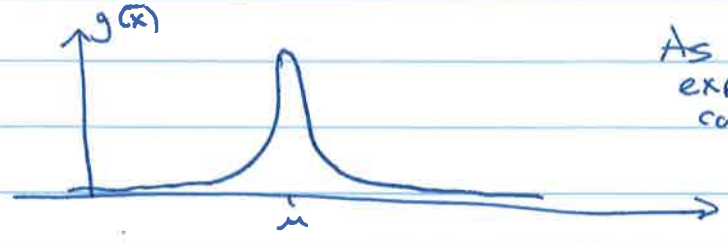
← multiple experiments, each to measure mean value



← values of  $\bar{x}$  for N measurements

Standard Deviation of the measurements of the mean

$$\sigma_m = \frac{\sigma}{\sqrt{N}}$$



As we do more experiments we become confident that our mean-of-means is closer to the correct value.

$$g(\bar{x}) = \frac{1}{\sqrt{2\pi} \sigma_m} e^{-\frac{(\bar{x}-\mu)^2}{2\sigma_m^2}}$$

Taking more measurements of a mean gives you less error in  $\bar{x}$ . Reducing error by 4 times requires 4 times as much data.

$$E = 1.96 \sigma_m = \frac{1.96 \sigma}{\sqrt{N}}$$

We still don't know  $\sigma$ , but

$$E = \frac{1.96 S_x}{\sqrt{N}}$$

is a reasonable guess. The correct estimate of  $E$  is

$$E = \frac{t(\nu, 0.05) S}{\sqrt{N}}$$

where  $t$  is called "Student's  $t$ -factor" and  $\nu = N - 1$ .

### Propagation of Errors

Consider a quantity that is calculated from 2 measured quantities

$$a = \bar{a} \pm E_a$$

$\nwarrow$  error confidence limits for  $a$   
 $\nearrow$  mean value of  $a$

$$b = \bar{b} \pm E_b$$

$$c = \bar{a} + \bar{b}$$

How do we calculate the error in  $\bar{c}$  from  $E_a$  &  $E_b$ ?

More generally:

$$y = y(x_1, x_2, \dots, x_n)$$

$$x_i = \bar{x}_i \pm E_i \quad (i=1, \dots, n)$$

First, create differential:

$$dy = \left(\frac{\partial y}{\partial x_1}\right) dx_1 + \left(\frac{\partial y}{\partial x_2}\right) dx_2 + \dots + \left(\frac{\partial y}{\partial x_n}\right) dx_n$$

White size errors

$$\Delta y = \left(\frac{\partial y}{\partial x_1}\right) \Delta x_1 + \left(\frac{\partial y}{\partial x_2}\right) \Delta x_2 + \dots + \left(\frac{\partial y}{\partial x_n}\right) \Delta x_n$$

Square this:

$$(\Delta y)^2 = \left(\left(\frac{\partial y}{\partial x_1}\right) \Delta x_1 + \dots + \left(\frac{\partial y}{\partial x_n}\right) \Delta x_n\right)^2$$

The leading direct terms: There are others that couple the measurements too, but let's ignore for now.

$$(\Delta y)^2 \approx \left(\frac{\partial y}{\partial x_1}\right)^2 \Delta x_1^2 + \dots + \left(\frac{\partial y}{\partial x_n}\right)^2 \Delta x_n^2$$

$$\epsilon_y \approx \sqrt{\left(\frac{\partial y}{\partial x_1}\right)^2 \epsilon_1^2 + \left(\frac{\partial y}{\partial x_2}\right)^2 \epsilon_2^2 + \dots}$$

As the errors  $\epsilon_1, \dots, \epsilon_n \rightarrow 0$  this becomes exact.

For  $C = a + b$

$$\frac{\partial c}{\partial a} = 1 \quad \frac{\partial c}{\partial b} = 1$$

$$\therefore \epsilon_c = \sqrt{\epsilon_a^2 + \epsilon_b^2}$$

Example:

Suppose we measure the frequency  $\omega$  from an IR spectrum

$$\omega \pm \epsilon_\omega \leftarrow 95\% \text{ confidence limits}$$

And we know a mass from mass spectrometry

$$m \pm \epsilon_m$$

Now, if we want the spring constant

$$k = m\omega^2$$

$$\frac{\partial k}{\partial m} = \omega^2 \quad \frac{\partial k}{\partial \omega} = 2m\omega$$

$$\epsilon_k = \sqrt{\omega^2 \epsilon_m^2 + 2m\omega \epsilon_\omega^2}$$

{

95% confidence interval in spring constant.

## Linear Regression

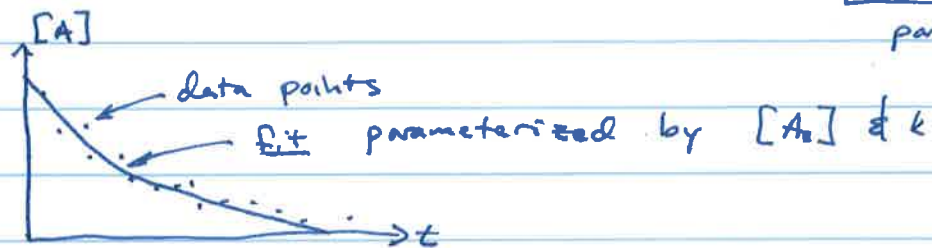
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Consider a function  $y$  of an independent variable  $x$ :

$$y = y(x) = f(x; \underbrace{a_1, a_2, \dots, a_p}_{\text{parameters or constants}})$$

We'd like the best set of parameters to fit a collection of data  $\{x_i, y_i\}$  to a model

Example:  $[A] = [A_0] e^{-kt} = f(t; \underbrace{[A_0], k}_{\text{parameters}})$



A residual for the  $i^{\text{th}}$  data point is the discrepancy between the measured values and the value of the function at that point:



$$r_i = y_i - f(x_i; a_1, \dots, a_p)$$

$\left\{ \begin{array}{l} \uparrow \\ \text{residual} \end{array} \right.$   $\left\{ \begin{array}{l} \uparrow \\ \text{actual value} \end{array} \right.$   $\left\{ \begin{array}{l} \uparrow \\ \text{independent variable} \end{array} \right.$

A perfect fit would have  $r_i = 0$  for all points  $i$ . The best fit to the data (given a particular model) minimizes the sum of squares of the residuals

This is called the method of least squares or a regression.

That is:

$$R = \sum_{i=1}^N \left[ y_i - f(x_i; a_1, \dots, a_p) \right]^2$$

← number of data points

We minimize  $R$  with respect to  $\{a_1, \dots, a_p\}$

$$\frac{\partial R}{\partial a_1} = 0, \quad \frac{\partial R}{\partial a_2} = 0, \quad \dots$$

This usually generates a set of nonlinear equations that must be solved iteratively, and the tools to do this (like Q+Grace) can require some expertise.

For linear functions like  $y = mx + b$ , the parameters  $m$  &  $b$  can be determined exactly.

$$R = \sum_{i=1}^N (y_i - mx_i - b)^2$$

$$\frac{\partial R}{\partial m} = 2 \sum_{i=1}^N (y_i - mx_i - b)(-x_i) = 0$$

$$\frac{\partial R}{\partial b} = 2 \sum_{i=1}^N (y_i - mx_i - b)(-1) = 0$$

Rewriting these:

$$m \sum_{i=1}^N x_i^2 + b \sum_{i=1}^N x_i = \sum_{i=1}^N x_i y_i$$

$$m \sum_{i=1}^N x_i + b \sum_{i=1}^N 1 = \sum_{i=1}^N y_i$$

To solve these, let's define

$$\begin{cases}
 S_x = \sum_{i=1}^N x_i & S_y = \sum_{i=1}^N y_i \\
 S_{xy} = \sum_{i=1}^N x_i y_i & S_{x^2} = \sum_{i=1}^N x_i^2
 \end{cases}$$

→ All of these come from our measured experimental data

$$\begin{aligned}
 m S_{x^2} + b S_x &= S_{xy} \\
 m S_x + b N &= S_y
 \end{aligned}$$

we want this vector

$$\begin{pmatrix} S_{x^2} & S_x \\ S_x & N \end{pmatrix} \begin{pmatrix} m \\ b \end{pmatrix} = \begin{pmatrix} S_{xy} \\ S_y \end{pmatrix}$$

Using Cramer's rule:

$$m = \frac{1}{D} (N S_{xy} - S_x S_y)$$

$$b = \frac{1}{D} (S_{x^2} S_y - S_x S_{xy})$$

$$D = N S_{x^2} - (S_x)^2 \quad \leftarrow \text{determinant}$$

The hardest part is finding a suitable linear model. For example, here's some data on the vapor pressure of water

<u>T (°C)</u>	<u>P (torr)</u>
0	4.579
5	6.543
10	9.209
15	12.788
20	17.535
25	23.756

The model :  $p = c e^{-\Delta H_m / RT}$  ← not linear!   
 *heat of vaporization*

$$\ln p = \ln c - \frac{\Delta H_m}{RT}$$

So, if we let  $y = \ln p$  and  $x = \frac{1}{T}$  we'll have a linear model with

$$m = \frac{-\Delta H_m}{R} \quad b = \ln c$$

$y = \ln p$	$x = 1/T \text{ (K}^{-1}\text{)}$
1.521	0.00366
1.878	0.00360
2.220	0.00353
2.549	0.00347
2.864	0.00341
3.168	0.00335

$$S_x = 0.0210$$

$$S_y = 14.200$$

$$S_{xy} = 0.0494$$

$$S_{x^2} = 7.3731 \times 10^{-5}$$

$$\left[ \begin{array}{l} m = -5.3645 \times 10^3 \\ b = 21.16355 \end{array} \right]$$

The correlation coefficient

$$r = \frac{N S_{xy} - S_x S_y}{\sqrt{(N S_{x^2} - (S_x)^2)(N S_{y^2} - (S_y)^2)}}$$



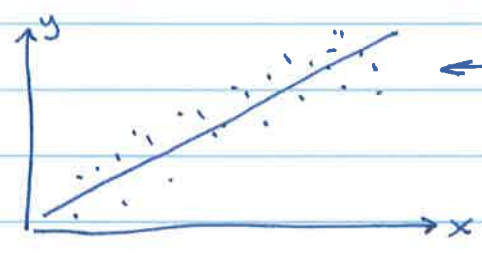
If this is close to 1, we have a good fit



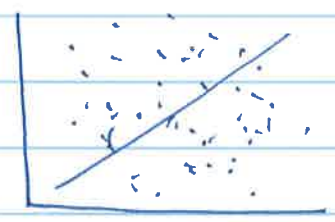
Note:

$$r = \frac{\text{Covariance}(X, Y)}{\sigma_x \sigma_y}$$

$$\text{Covariance}(x, y) = \sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y})$$

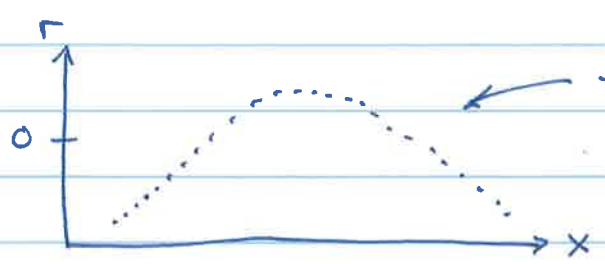
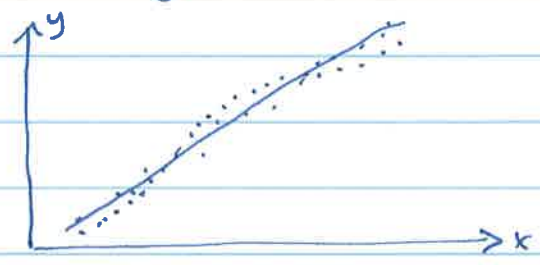


← r tells you something about the width of the scatter around the best linear model  
 r = 1 → all points are on the line



r = 0 → no particular correlation

Plotting residuals can sometimes reveal flaws in your model



← this structure means we're missing something parabolic in our model for the data