ME170b Lecture 5

2/22/23

Experimental Techniques

Last time:

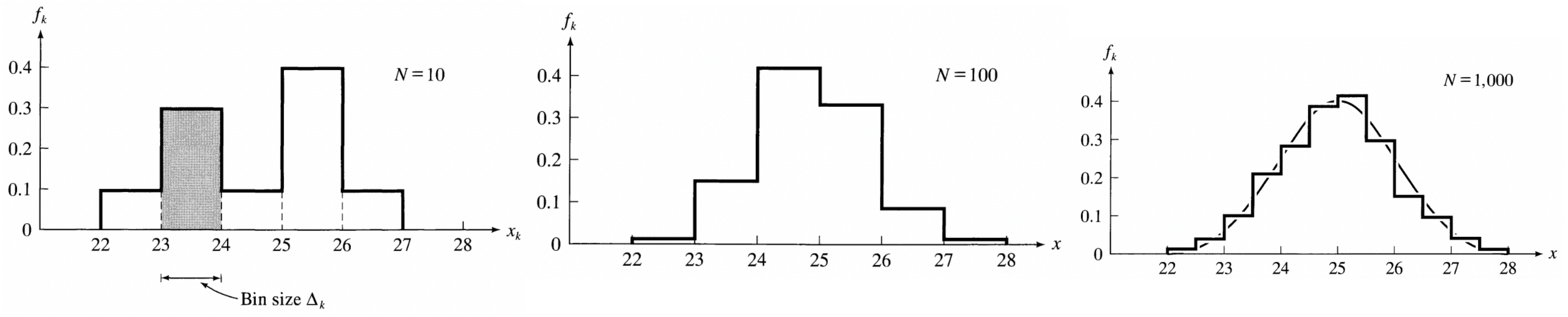
> Normal Distribution

Today:

> Ch.6/7/8

- > Rejection of data
- > Weighted Averages
- > Least Squares

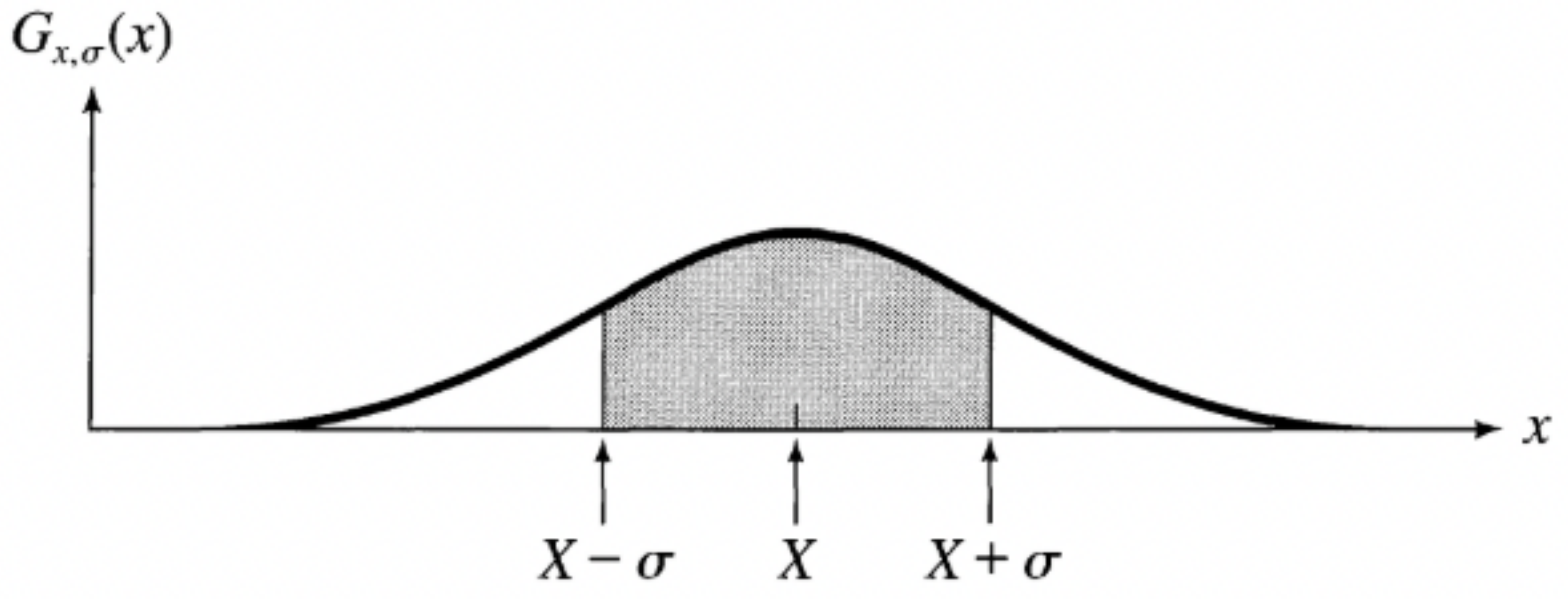
Last time: Limiting Distributions



Key Idea: As N-> infinity, the distribution approaches a definite, continuous curve — this curve is called the “limiting distribution”

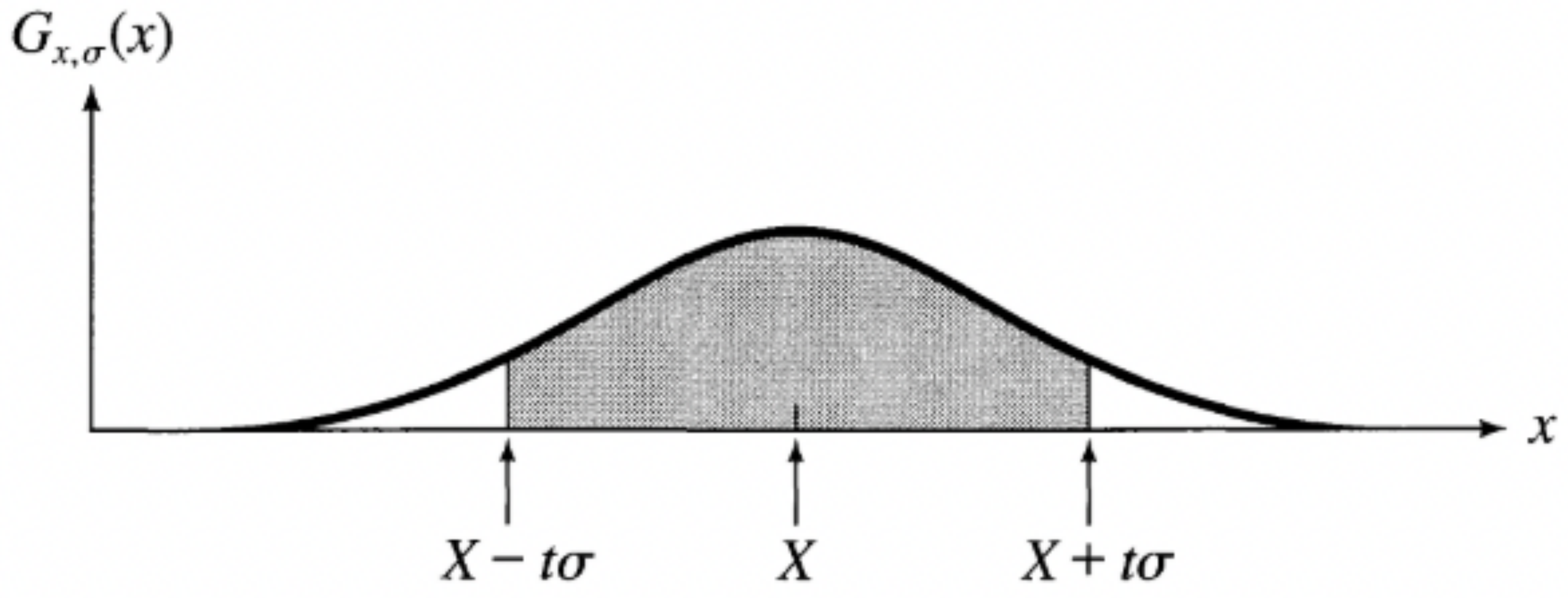
The standard deviation as 68% confidence limit

$$Prob(\text{within } \sigma) = \frac{1}{\sqrt{2\pi}} \int_{-1}^{1} e^{-z^2/2}\, dz.$$



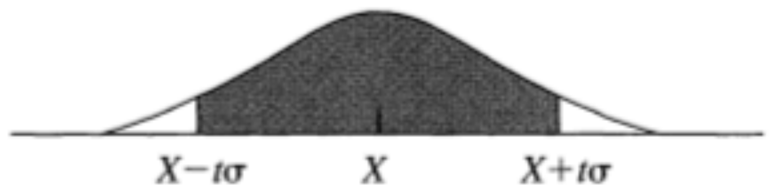
More generally, what is the probability a measurement falls within t*sigma?

$$Prob(\text{within } t\sigma) = \frac{1}{\sqrt{2\pi}} \int_{-t}^{t} e^{-z^2/2}\, dz$$



Gaussian probability table

Table A. The percentage probability, $Prob(\text{within } t\sigma) = \int_{X-t\sigma}^{X+t\sigma} G_{X,\sigma}(x)\,dx$, as a function of t.



t	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09
0.0	0.00	0.80	1.60	2.39	3.19	3.99	4.78	5.58	6.38	7.17
0.1	7.97	8.76	9.55	10.34	11.13	11.92	12.71	13.50	14.28	15.07
0.2	15.85	16.63	17.41	18.19	18.97	19.74	20.51	21.28	22.05	22.82
0.3	23.58	24.34	25.10	25.86	26.61	27.37	28.12	28.86	29.61	30.35
0.4	31.08	31.82	32.55	33.28	34.01	34.73	35.45	36.16	36.88	37.59
0.5	38.29	38.99	39.69	40.39	41.08	41.77	42.45	43.13	43.81	44.48
0.6	45.15	45.81	46.47	47.13	47.78	48.43	49.07	49.71	50.35	50.98
0.7	51.61	52.23	52.85	53.46	54.07	54.67	55.27	55.87	56.46	57.05
0.8	57.63	58.21	58.78	59.35	59.91	60.47	61.02	61.57	62.11	62.65
0.9	63.19	63.72	64.24	64.76	65.28	65.79	66.29	66.80	67.29	67.78
1.0	68.27	68.75	69.23	69.70	70.17	70.63	71.09	71.54	71.99	72.43
1.1	72.87	73.30	73.73	74.15	74.57	74.99	75.40	75.80	76.20	76.60
1.2	76.99	77.37	77.75	78.13	78.50	78.87	79.23	79.59	79.95	80.29
1.3	80.64	80.98	81.32	81.65	81.98	82.30	82.62	82.93	83.24	83.55
1.4	83.85	84.15	84.44	84.73	85.01	85.29	85.57	85.84	86.11	86.38
1.5	86.64	86.90	87.15	87.40	87.64	87.89	88.12	88.36	88.59	88.82
1.6	89.04	89.26	89.48	89.69	89.90	90.11	90.31	90.51	90.70	90.90
1.7	91.09	91.27	91.46	91.64	91.81	91.99	92.16	92.33	92.49	92.65
1.8	92.81	92.97	93.12	93.28	93.42	93.57	93.71	93.85	93.99	94.12
1.9	94.26	94.39	94.51	94.64	94.76	94.88	95.00	95.12	95.23	95.34
2.0	95.45	95.56	95.66	95.76	95.86	95.96	96.06	96.15	96.25	96.34
2.1	96.43	96.51	96.60	96.68	96.76	96.84	96.92	97.00	97.07	97.15
2.2	97.22	97.29	97.36	97.43	97.49	97.56	97.62	97.68	97.74	97.80
2.3	97.86	97.91	97.97	98.02	98.07	98.12	98.17	98.22	98.27	98.32
2.4	98.36	98.40	98.45	98.49	98.53	98.57	98.61	98.65	98.69	98.72
2.5	98.76	98.79	98.83	98.86	98.89	98.92	98.95	98.98	99.01	99.04
2.6	99.07	99.09	99.12	99.15	99.17	99.20	99.22	99.24	99.26	99.29
2.7	99.31	99.33	99.35	99.37	99.39	99.40	99.42	99.44	99.46	99.47
2.8	99.49	99.50	99.52	99.53	99.55	99.56	99.58	99.59	99.60	99.61
2.9	99.63	99.64	99.65	99.66	99.67	99.68	99.69	99.70	99.71	99.72
3.0	99.73									
3.5	99.95									
4.0	99.994									
4.5	99.9993									
5.0	99.99994									

Maximum likelihood estimator

$$x_1, x_2, \ldots, x_N,$$ data points

Suppose we know the 'center' and 'width' parameters of a Gaussian that describes our finite set of data points

We can estimate the probability of observing x_1 given our Gaussian parameters :

$$Prob(x \text{ between } x_1 \text{ and } x_1 + dx_1) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x_1 - X)^2/2\sigma^2}\, dx_1.$$

$$Prob(x_1) \propto \frac{1}{\sigma} e^{-(x_1 - X)^2/2\sigma^2}$$

We can do the same for x_2 … x_n:

$$Prob(x_2) \propto \frac{1}{\sigma} e^{-(x_2 - X)^2/2\sigma^2} \qquad Prob(x_N) \propto \frac{1}{\sigma} e^{-(x_N - X)^2/2\sigma^2}$$

Maximum likelihood estimator

We can estimate the probability of obtaining each of the readings, x_1, x_2 … x_n:

$$Prob_{X,\sigma}(x_1, \ldots, x_N) = Prob(x_1) \times Prob(x_2) \times \ldots$$

or

$$Prob_{X,\sigma}(x_1, \ldots, x_N) \propto \frac{1}{\sigma^N} e^{-\Sigma(x_i - X)^2/2\sigma^2}$$

In reality, the Gaussian parameters X and sigma can not be known!

By iteratively adjusting X and sigma to maximize the probability of observing the data we can get a good estimate of X and sigma from our data points!

Maximum likelihood estimator: summary

Given: N observations, x_1, x_2 … x_n
Find: X and Sigma, expected value (mean) and standard deviation of the limiting distributions

The best estimate, maximizes the following probability:

$$Prob_{X,\sigma}(x_1, \ldots, x_N) \propto \frac{1}{\sigma^N} e^{-\Sigma(x_i - X)^2/2\sigma^2}.$$

mle

Maximum likelihood estimates

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MATLAB MLE function

Syntax

```
phat = mle(data)
phat = mle(data,Name,Value)
[phat,pci] = mle( __ )
```

Rejection of Data - Ch.6

3.8, 3.5, 3.9. 3.9, 3.4, 1.8

What's wrong with this data set? Why does it matter? What can we do about it?

Rejection of Data

3.8, 3.5, 3.9. 3.9, 3.4, 1.8

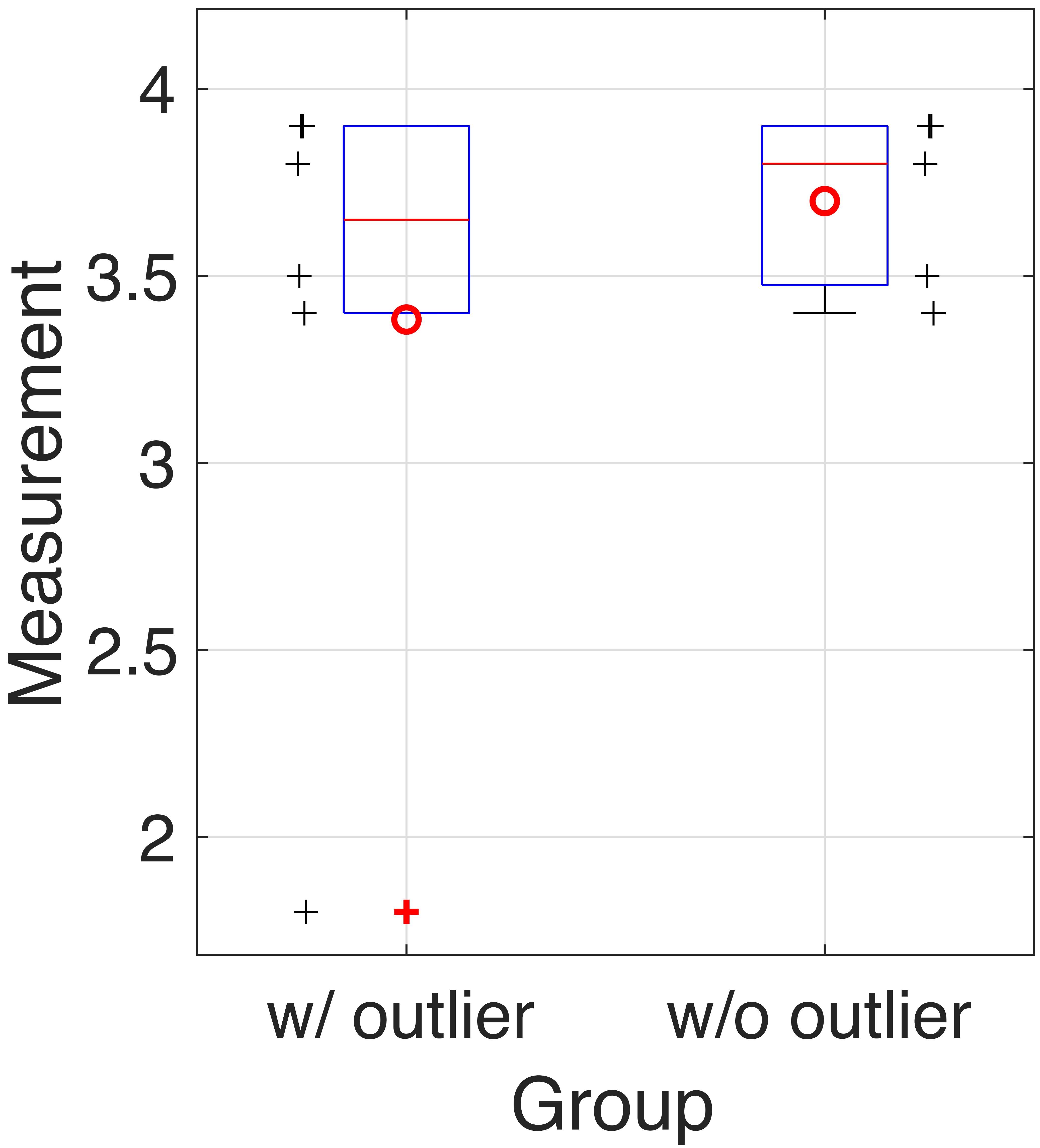
Let’s calculate our an estimate of x with and without the “outlier”

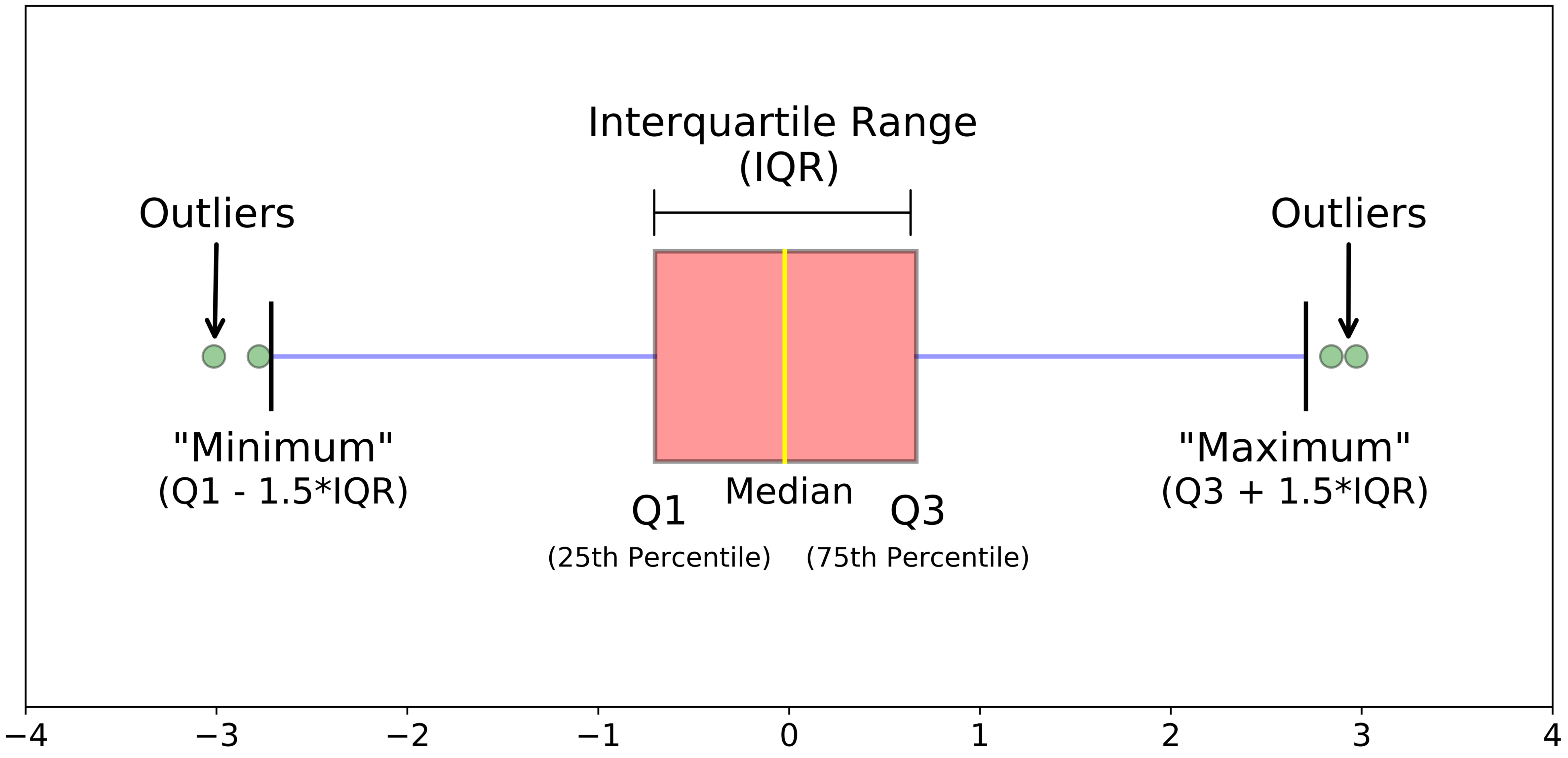
3.4 +/- 0.1 vs 3.70 +/- 0.05

These are significantly different!

Rejection of Data

3.8, 3.5, 3.9. 3.9, 3.4, 1.8





Rejection of Data

3.8, 3.5, 3.9. 3.9, 3.4, 1.8

What should we do about it?

When should an experimenter “reject data”?

Controversial topic!

- Some experiments think you should never “remove” data
- ultimately rejection of data is subjective!

Chauvenet's criterion: a means of assessing whether one piece of experimental data — an outlier — from a set of observations, is likely to be spurious

Chauvenet's criterion

3.8, 3.5, 3.9, 3.9, 3.4, 1.8

Let's calculate the mean and std

$$\bar{x} = 3.4 \text{ s}$$

$$\sigma_x = 0.8 \text{ s.}$$

What's the probability of obtaining the outlier measurement?

$$Prob(\text{within } t\sigma) = \frac{1}{\sqrt{2\pi}} \int_{-t}^{t} e^{-z^2/2}\, dz$$

3.4 - 1.8 = 1.6 = 2\sigma

$$\begin{aligned} Prob(\text{outside } 2\sigma) &= 1 - Prob(\text{within } 2\sigma) \\ &= 1 - 0.95 \\ &= 0.05. \end{aligned}$$

Chauvenet's criterion

3.8, 3.5, 3.9, 3.9, 3.4, 1.8

What's the probability of obtaining the outlier measurement?

$$Prob(\text{within } t\sigma) = \frac{1}{\sqrt{2\pi}} \int_{-t}^{t} e^{-z^2/2} \, dz$$

3.4 - 1.8 = 1.6 = 2\sigma

$$\begin{aligned} Prob(\text{outside } 2\sigma) &= 1 - Prob(\text{within } 2\sigma) \\ &= 1 - 0.95 \\ &= 0.05. \end{aligned}$$

What does this mean?

5% of measurements should be as deviant as the outlier

1/20 measurements!

$$\begin{aligned} &(\text{expected number as deviant as 1.8 s}) \\ &\quad = (\text{number of measurements}) \times Prob(\text{outside } 2\sigma) \\ &\quad = 6 \times 0.05 = 0.3. \end{aligned}$$

We expect 0.3 samples as deviant as 1.8

Chauvenet's criterion: main idea

Set a probability boundary do decide if data is an outlier:
if the expected number of measurements at least as deviant as the suspect measurement is less than one-half, then the suspect measurement should be rejected.

$$x_1, \ldots, x_N$$

From all N measurements, you calculate $\bar{x}$ and σ_x

$$t_{sus} = \frac{|x_{sus} - \bar{x}|}{\sigma_x} \qquad Prob(\text{outside } t_{sus}\sigma)$$

$$\begin{aligned} n &= (\text{expected number as deviant as } x_{sus}) \\ &= N \times Prob(\text{outside } t_{sus}\sigma). \end{aligned}$$

If this expected number n is less than one-half, then, according to Chauvenet's criterion, you can reject X_sus

Chauvenet's criterion: what to do if you have an outlier?

If you do decide to reject x_{sus}, you would naturally recalculate $\bar{x}$ and σ_x using just the remaining data; in particular, your final answer for x would be this new mean, with an uncertainty equal to the new SDOM.

Chauvenet's criterion: example

$$46, 48, 44, 38, 45, 47, 58, 44, 45, 43$$

$$\bar{x} = 45.8 \quad \text{and} \quad \sigma_x = 5.1$$

$$t_{\text{sus}} = \frac{x_{\text{sus}} - \bar{x}}{\sigma_x} = \frac{58 - 45.8}{5.1} = 2.4.$$

$$\begin{aligned} Prob(\text{outside } 2.4\sigma) &= 1 - Prob(\text{within } 2.4\sigma) \\ &= 1 - 0.984 \\ &= 0.016. \end{aligned}$$

In 10 measurements, he would therefore expect to find only 0.16 of one measurement as deviant as his suspect result. Because 0.16 is less than the number 0.5 set by Chauvenet's criterion, he should at least consider rejecting the result.

$$\bar{x} = 44.4 \quad \text{and} \quad \sigma_x = 2.9$$

Discussion: this topic is still contentious

Let’s think about the issues, what’s wrong with ‘rejecting data’

- some scientists believe that data should never be rejected without external evidence that the measurement in question is incorrect
- reasonable compromise is to use Chauvenet’s criterion to identify data that could be considered for rejection; having made this identification, you could do all subsequent calculations twice, once including the suspect data and once excluding them, to see how much the questionable values affect your final conclusion.
- the choice of one-half as the boundary of rejection (in the condition that $n < 5$) is arbitrary.
- Perhaps even more important, unless you have made a very large number of measurements ($N \sim 50$, say), the value of sigma, is extremely uncertain as an estimate for the true standard deviation of the measurements — number t_{sus} in (6.4) is very uncertain.

Chauvenet’s criterion should be used only as a last resort, when you cannot check your measurements by repeating them!

Weigted Averages — CH. 7

How can we combine two or more separate and independent measurements of a single physical quantity?

$$\text{Student } A: \quad x = x_A \pm \sigma_A$$

$$\text{Student } B: \quad x = x_B \pm \sigma_B$$

Before combining measurements must check consistency

$$\text{Student } A: \quad x = x_A \pm \sigma_A$$

$$\text{Student } B: \quad x = x_B \pm \sigma_B$$

How?

The discrepancy | x_a - x_b| should not be significantly larger than both simga_a and sigma_b

Naive approach — let's just average?

$$(x_A + x_B)/2$$

Why is this not appropriate?

- the average is unsuitable if the two uncertainties sigma_1, and sigma_b, are unequal
- gives equal importance to both measurements

What if sigma_a << sigma_b — we should 'trust' x_a more then!

We can use principles of maximum likelihood to solve this

assuming that both measurements are governed by the Gauss distribution

- errors are only random
- measurements are distributed normally

$$Prob_X(x_A) \propto \frac{1}{\sigma_A} e^{-(x_A - X)^2/2\sigma_A^2}$$

$$Prob_X(x_B) \propto \frac{1}{\sigma_B} e^{-(x_B - X)^2/2\sigma_B^2}$$

We don’t know true value X

$$Prob_X(x_A, x_B) = Prob_X(x_A)\, Prob_X(x_B) \propto \frac{1}{\sigma_A \sigma_B} e^{-\chi^2/2},$$

$$\chi^2 = \left(\frac{x_A - X}{\sigma_A}\right)^2 + \left(\frac{x_B - X}{\sigma_B}\right)^2$$

sum of the squares of the deviations from X of the two measurements, each divided by its corresponding uncertainty.

We can use principles of maximum likelihood to solve this

ML principle: our best estimate for the unknown true value X is that value for which the actual observations x_a and x_b are most likely

$$
\begin{aligned}
Prob_X(x_A, x_B) &= Prob_X(x_A)\, Prob_X(x_B) \\
&\propto \frac{1}{\sigma_A \sigma_B} e^{-\chi^2/2},
\end{aligned}
$$

Need to find X that maximize this probability

$$\chi^2 = \left(\frac{x_A - X}{\sigma_A}\right)^2 + \left(\frac{x_B - X}{\sigma_B}\right)^2$$

corresponding to minimizing CHI^2

$$2\frac{x_A - X}{{\sigma_A}^2} + 2\frac{x_B - X}{{\sigma_B}^2} = 0.$$

$$(\text{best estimate for } X) = \left(\frac{x_A}{{\sigma_A}^2} + \frac{x_B}{{\sigma_B}^2}\right) \Big/ \left(\frac{1}{{\sigma_A}^2} + \frac{1}{{\sigma_B}^2}\right).$$

We can use principles of maximum likelihood to solve this

$$(\text{best estimate for } X) = \left(\frac{x_A}{\sigma_A^2} + \frac{x_B}{\sigma_B^2}\right) \bigg/ \left(\frac{1}{\sigma_A^2} + \frac{1}{\sigma_B^2}\right).$$

$$(\text{best estimate for } X) = x_{\text{wav}} = \frac{w_A x_A + w_B x_B}{w_A + w_B}$$

$$w_A = \frac{1}{\sigma_A^2} \quad \text{and} \quad w_B = \frac{1}{\sigma_B^2}.$$

analogy: it is similar to the formula for the center of gravity of two bodies, where w_a, and w_b, are the actual weights of the two bodies, and x_a, and x_b, their positions.

Quick Check 7.1. Workers from two laboratories report the lifetime of a certain particle as 10.0 ± 0.5 and 12 ± 1, both in nanoseconds. If they decide to combine the two results, what will be their respective weights as given by (7.8) and their weighted average as given by (7.9)?

QC7.1. Weights $=$ 4 and 1; weighted average $=$ 10.4 ns.

Easily generalizes for N measurements

$$x_1 \pm \sigma_1, \quad x_2 \pm \sigma_2, \ldots, \quad x_N \pm \sigma_N$$

$$x_{\text{wav}} = \frac{\sum w_i x_i}{\sum w_i},$$

$$w_i = \frac{1}{\sigma_i^2}$$

Uncertainty of the weighted average?

Because the weighted average is a function of the original measured values the uncertainty in x, can be calculated using error propagation.

$$\sigma_{\text{wav}} = \frac{1}{\sqrt{\sum w_i}}.$$

Uncertainty of the weighted average?

Because the weighted average is a function of the original measured values the uncertainty in x, can be calculated using error propagation.

$$\sigma_{\text{wav}} = \frac{1}{\sqrt{\sum w_i}}.$$

Least-Squares — Ch.8

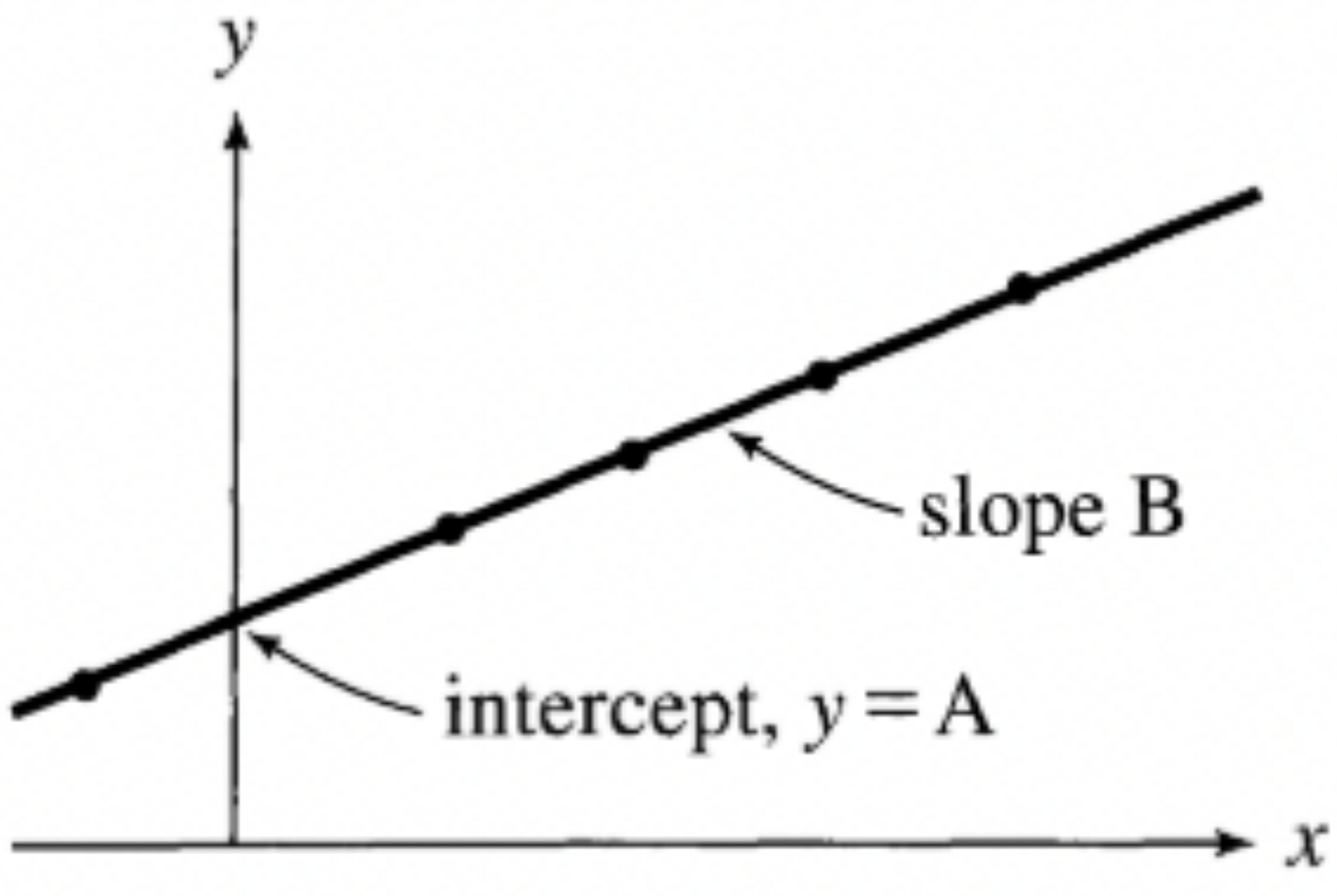
One of the most common and interesting types of experiment involves the measurement of several values of two different physical variables to investigate the mathematical relationship between the two variables.

y, and x, are measured

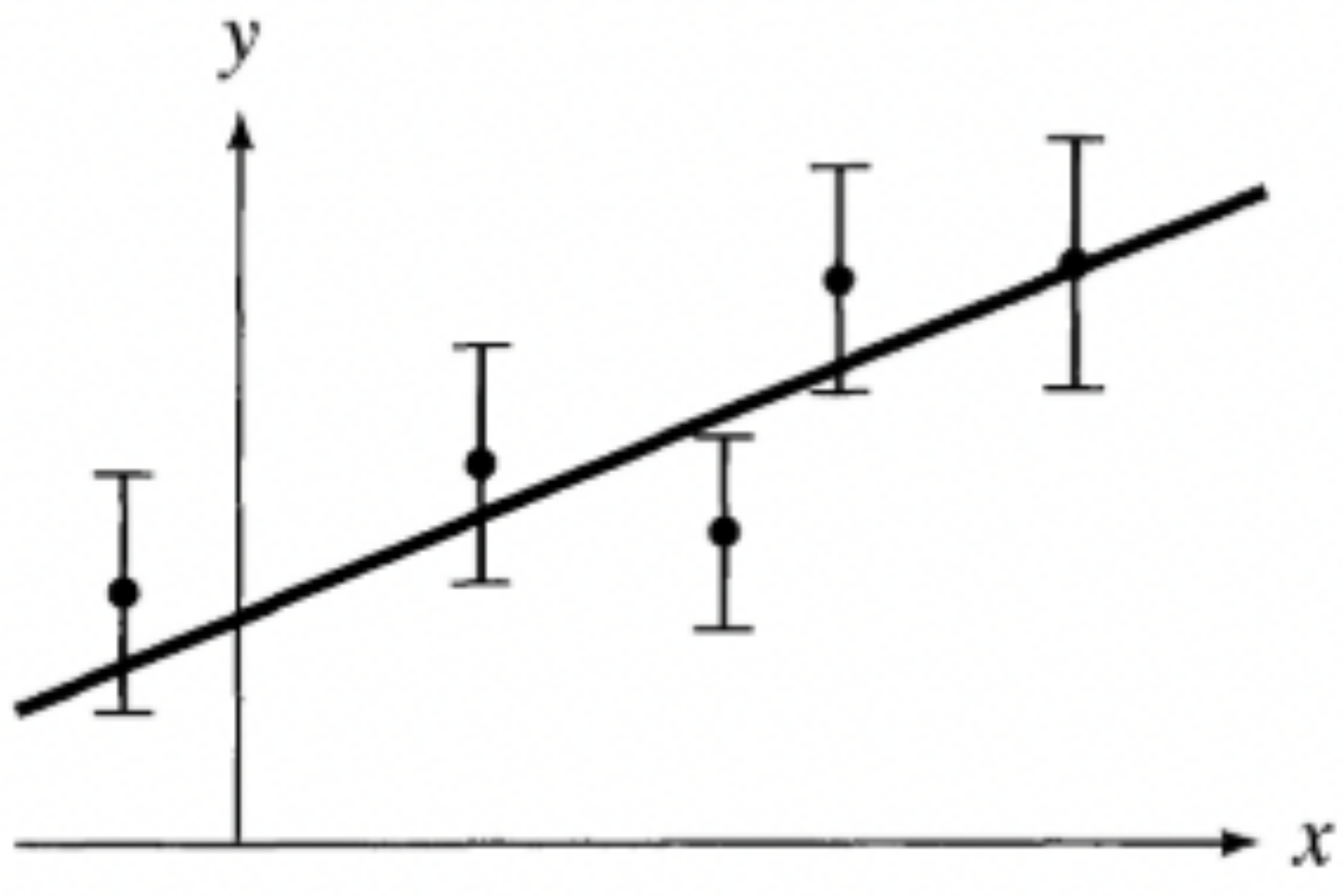
$$y = A + Bx$$

linear relationships is perhaps the most important

The least squares problem: how to find best fit?



No uncertainty —
relationship is clear



Uncertainty, we need a
technique to find the ‘best’ line

Using principle of maximum likelihood we can find the best straight line to fit a series of experimental points. This is called linear regression, or the least-squares fit for a line

What is the purpose?

$$y = A + Bx$$

1. We want to estimate the coefficients A and B

2. Another important determination is whether the data (x_i, y_i) rally are linear — "how <u>well</u> does the data fit our model?" (Ch.9)

How to estimate A and B?

$$(x_1, y_1), \ldots, (x_N, y_N)$$

assume y suffer appreciable uncertainty, the uncertainty in our measurements of x is negligible.

let's use ML. first proceed as if we know A and B:

$$(\text{true value for } y_i) = A + Bx_i$$

$$Prob_{A,B}(y_i) \propto \frac{1}{\sigma_y} e^{-(y_i - A - Bx_i)^2/2\sigma_y{}^2}$$

$$Prob_{A,B}(y_1, \ldots, y_N) = Prob_{A,B}(y_1) \cdots Prob_{A,B}(y_N)$$

$$\propto \frac{1}{\sigma_y{}^N} e^{-\chi^2/2},$$

$$\chi^2 = \sum_{i=1}^{N} \frac{(y_i - A - Bx_i)^2}{\sigma_y{}^2}$$

Best estimates of A and B maximize the probability, which corresponds to minimizing the CHI^2 term (hence least squares)

How to estimate A and B?

$$\chi^2 = \sum_{i=1}^{N} \frac{(y_i - A - Bx_i)^2}{\sigma_y^2}$$

How to find and expression for the minimum?

$$\frac{\partial \chi^2}{\partial A} = \frac{-2}{\sigma_y^2} \sum_{i=1}^{N} (y_i - A - Bx_i) = 0$$

$$AN + B\sum x_i = \sum y_i$$

$$\frac{\partial \chi^2}{\partial B} = \frac{-2}{\sigma_y^2} \sum_{i=1}^{N} x_i(y_i - A - Bx_i) = 0.$$

$$A\sum x_i + B\sum x_i^2 = \sum x_i y_i$$

Two unknowns, two equations!

How to estimate A and B?

$$A = \frac{\sum x^2 \sum y - \sum x \sum xy}{\Delta}$$

$$B = \frac{N \sum xy - \sum x \sum y}{\Delta}$$

$$\Delta = N \sum x^2 - \left(\sum x\right)^2$$

How to estimate uncertainty in y?

Remember that the numbers y_1, y_2, … y_N are not N measurements of the same quantity. (They might, for instance, be the times for a stone to fall from N different heights.)

The measurement of each y, is (we are assuming) normally distributed about its true value A + Bx,, with width parameter sigma.

$$\sigma_y = \sqrt{\frac{1}{N}\Sigma(y_i - A - Bx_i)^2}.$$

$$\sigma_y = \sqrt{\frac{1}{N-2}\sum_{i=1}^{N}(y_i - A - Bx_i)^2},$$

How to estimate uncertainty in A and B?

The uncertainties in A and B are given by simple error propagation in terms of those in y_1 … y_N

$$\sigma_A = \sigma_y \sqrt{\frac{\sum x^2}{\Delta}}$$

$$\sigma_B = \sigma_y \sqrt{\frac{N}{\Delta}}$$

Some caveats

1. What if the uncertainty of y is <u>not</u> equal for all measurements?

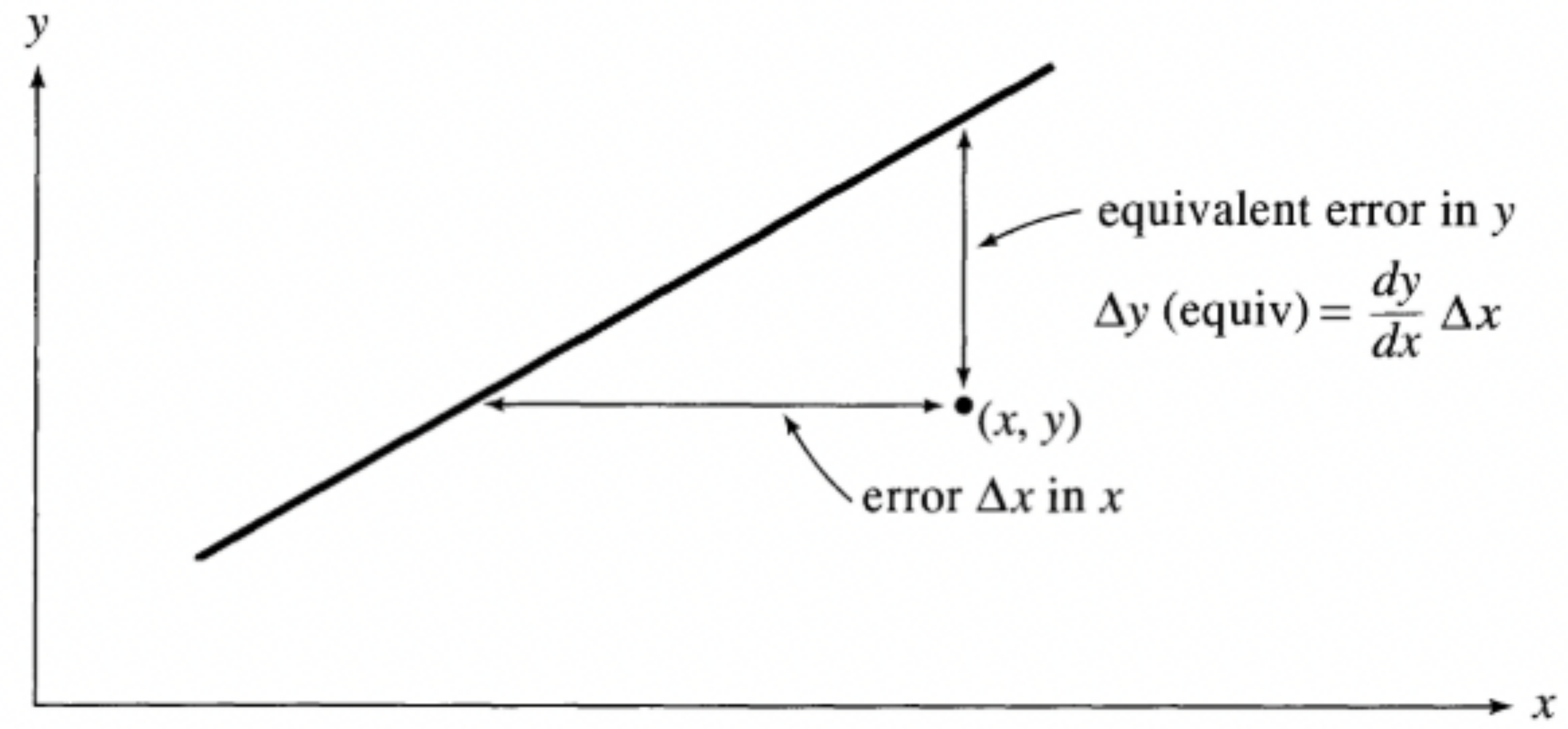
we can use the method of weighted least squares,
(ex. in Prob. 8.9)

2. What if both x and y have uncertainties

actually doesn't make a bog difference

What if both x and y have uncertainties

Assume error in x only



$$\sigma_y(\text{equiv}) = \frac{dy}{dx}\sigma_x. \qquad \sigma_y(\text{equiv}) = B\sigma_x$$

if all the uncertainties sigma_x, are equal, the same is true of the equivalent uncertainties simga_y(equiv).

What if both x and y have uncertainties

Now for the case that both x and y have uncertainties.

$$\sigma_y(\text{equiv}) = \sqrt{\sigma_y^2 + (B\sigma_x)^2}$$

If both x and y have uncertainties, we can combine in quadrature and replace with a single uncertainty

The most complicated case is when each measurement x_i and y_i have their own uncertainties, then we need to use the equivalence and a weighted least squares

We can use least squares to fit nonlinear curves!

$$y = A + Bx + Cx^2$$

polynomial

$$Prob(y_1, \ldots, y_N) \propto e^{-\chi^2/2},$$

$$\chi^2 = \sum_{i=1}^{N} \frac{(y_i - A - Bx_i - Cx_i^2)^2}{\sigma_y^2}.$$

system of equations N+1 degree of poly

$$\begin{aligned} AN + B\sum x + C\sum x^2 &= \sum y, \\ A\sum x + B\sum x^2 + C\sum x^3 &= \sum xy, \\ A\sum x^2 + B\sum x^3 + C\sum x^4 &= \sum x^2 y. \end{aligned}$$

General case when least squares can fit

problems in which the function y = f(x) depends linearly on the parameters A, B, C, …

$$y = A \sin x + B \cos x.$$

$$y = Ae^{Bx} \qquad \ln y = \ln A + Bx$$