

# BPhO

Computational  
Challenge

## Seminar 01: Incorporating experimental error in calculations

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## Standard form

Very small and very large quantities are tedious (and *error prone*) to write out using full decimal notation.

**Standard form:** e.g.  $6.67 \times 10^{-11}$

is an *integer* between 1 and 9 followed by  $N - 1$  digits, where  $N$  is the number of **significant figures** of the quantity.

The power of 10 (the ‘exponent’) gives you an *immediate sense of scale*.

1 light-year  $1\text{ly} = 9.461 \times 10^{15} \text{ m}$

proton radius  $r \approx 8.42 \times 10^{-16} \text{ m}$

**Precision.** A precise measurement is performed to a **high number of significant figures**. This typically means the *random error* in the measurement (i.e. the **standard deviation**) is *very small* compared to the **mean value**. In calculations, one should quote an answer to the *worst precision* (i.e. lowest number of significant figures) of the *input values*.

$$x = 123.4, \quad y = 56.7, \quad z = 8.9$$

$$\therefore x = 1.234 \times 10^2, \quad y = 5.67 \times 10^1, \quad z = 8.9$$

lowest precision  
i.e. 2 s.f.

$$a = \frac{xy}{z} = \frac{123.4 \times 56.7}{8.9} = 786.1550\dots \quad (\text{unrounded})$$

$$a = 7.9 \times 10^2 \quad \text{to 2.s.f}$$

**Accuracy** relates to the degree of *systematic error*. A time of **12.345s** may be *very precise*, but could easily be **2.000s** out from a **true value of 10.345s** if there is some form of accidental offset in the timing system.

## PRECISION VS ACCURACY



✓ Precision  
✗ Accuracy



✗ Precision  
✓ Accuracy



✗ Precision  
✗ Accuracy



✓ Precision  
✓ Accuracy

# Mean and standard deviation

If you have a *sample* of data, which you believe represents a quantity  $x$  subject to *random error*:

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

is an *unbiased estimator* of the **mean value** of the quantity  $x$ .  
 $N$  is the number of measurements, and  $x_i$  is the  $i^{\text{th}}$  measurement.

$$\sigma_x = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2}$$

is an *unbiased estimator* of the **error** in this measurement. This is *not quite* the *standard deviation*, which involves an  $N$  factor rather than  $N - 1$  in the fraction preceding the sum.

The measurement  $x$  can therefore be quoted:

$$x = \bar{x} \pm \sigma_x$$

## ERROR CALCULATION

Excel spreadsheet  
example

ACTUAL X VALUE 123

### X VALUES WITH RANDOM ERROR

121	121	125	122	120	128	120	121	124	119	N
										10

MEAN X  $\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i$

122

$$(x_i - \bar{x})^2$$

1.21	1.21	8.41	0.01	4.41	34.8	4.41	1.21	3.61	9.61
------	------	------	------	------	------	------	------	------	------

ERROR IN X  $\sigma_x = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2}$

3

SO:  $X = ( 122 \quad +/- \quad 3 \quad )$

The presentation of numeric information can be as important as the numbers themselves. CLARITY is key. Not only do you want to efficiently compute a number from variable inputs, *you need a sanity check that the calculation is correct.*

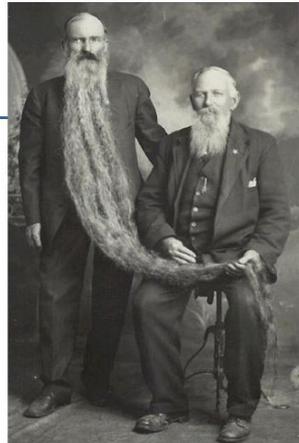
Use a spreadsheet to construct a **visual calculator**.

SPEED CONVERTER	
SPEED IN METRES PER SECOND	
<input type="text" value="20"/>	
SPEED / KM PER HOUR	72.00 
SPEED / MILES PER HOUR	44.74 
SPEED / NAUTICAL MILES PER HOUR	38.88 
SPEED / NANOPARSEC PER BEARD-INCH	2.94 

$speed = \frac{distance}{time}$   
 mile = 1609m  
 nmile = 1852m  
 $ms^{-1} = 2.237mph$   
 $ms^{-1} = 3.600kmh^{-1}$   
 parsec =  $3.086 \times 10^{16} m$   
 beard-inch = 7.5 weeks



$$\frac{\text{nanoparsec}}{\text{beard-inch}} = \frac{10^{-9} \times 3.086 \times 10^{16} m}{7.5 \times 7 \times 24 \times 3600s} = 6.80ms^{-1}$$



Zachariah Taylor Wilcox  
 Born April 1847 14 feet  
 Original caption: "Here is the longest beard in the world, for it has been growing for 41 years"

**Errors.** All measurable quantities will be subject to *uncertainty*. If quantities  $x, y, \dots$  are within a known range, we can use **upper and lower bounds** to determine the range of combined quantities.

e.g.  $x_- \leq x \leq x_+$        $y_- \leq y \leq y_+$

Therefore:  $x_-^2 y_- \leq x^2 y \leq x_+^2 y_+$        $x_-^2 / y_+ < x^2 / y < x_+^2 / y_-$

Note the mixing of *upper and lower bounds* in the last example.

Another example:  $1.23 \leq x \leq 4.56, \quad 7.89 \leq y \leq 11.2$

$$z = \frac{\sqrt{y}}{x}$$

$$\frac{\sqrt{7.89}}{4.56} < z < \frac{\sqrt{11.2}}{1.23}$$

$$0.616 < z < 2.721$$

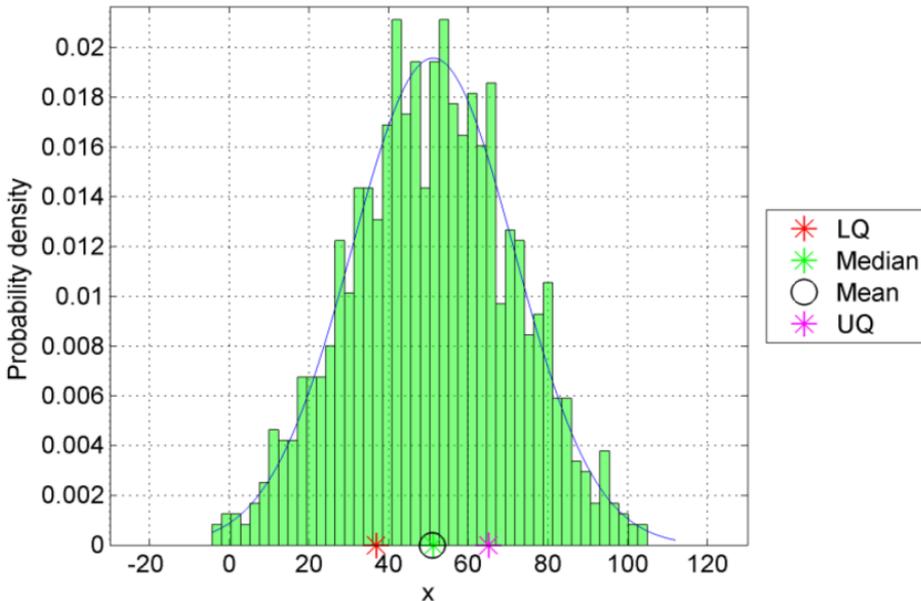
# Laws of Errors – but only if you think errors are *normally distributed*

If errors are *normally distributed*, the ‘**Law of Errors**’ can be useful (although may result in an artificially tighter uncertainty than upper and lower bounds). Let  $f(x, y, z, \dots)$  be a function of measurable quantities e.g.  $x = \bar{x} \pm \sigma_x$ .

$$f = \bar{f} \pm \sigma_f \text{ where } \bar{f} = f(\bar{x}, \bar{y}, \bar{z}, \dots) : \quad \sigma_f^2 = \left( \frac{\partial f}{\partial x} \sigma_x \right)^2 + \left( \frac{\partial f}{\partial y} \sigma_y \right)^2 + \left( \frac{\partial f}{\partial z} \sigma_z \right)^2 + \dots$$

If  $f(x, y, \dots) = kx^a y^b \dots \Rightarrow \left( \frac{\sigma_f}{f} \right)^2 = \left( \frac{a\sigma_x}{x} \right)^2 + \left( \frac{b\sigma_y}{y} \right)^2 + \dots$  You *add* the (power weighted) squares of fractional errors.

Normalized histogram with fitted PDF  
 Mean=50.8773, Median=51.1451  
 STD=20.3984, SKEW=-0.018384  
 LQ=36.8502, UQ=65.0277, IQR=28.1775  
 Number of samples = 1000



Example:

$$f = 3x^2 y^{-\frac{1}{2}}, \quad x = 20 \pm 3, \quad y = 40 \pm 5$$

$$\therefore \left( \frac{\sigma_f}{\bar{f}} \right)^2 = \left( \frac{2\sigma_x}{\bar{x}} \right)^2 + \left( \frac{\frac{1}{2}\sigma_y}{\bar{y}} \right)^2$$

$$\bar{f} = 3 \times 20^2 \times 40^{-\frac{1}{2}} = 189.7366\dots$$

$$\therefore \sigma_f = \bar{f} \sqrt{\left( \frac{2 \times 3}{20} \right)^2 + \left( \frac{\frac{1}{2} \times 5}{40} \right)^2} = 58.14\dots$$

$$\therefore f = (1.9 \pm 0.6) \times 10^2$$

## UPPER AND LOWER BOUND CALCULATION VS LAWS OF ERRORS

k =

w =  +/-   
 x =  +/-   
 y =  +/-   
 z =  +/-

a =   
 b =   
 c =   
 d =

$$f(w, x, y, z) = \frac{kw^a x^b}{y^c z^d}$$

$$f = 3x^2 y^{-\frac{1}{2}}$$

$$x = 20 \pm 3$$

$$y = 40 \pm 5$$

Paste as values to here. THEN SAVE BEFORE RUNNING MATLAB CODE.

mean f

fmean =

upper bound for f

fmax =

lower bound for f

fmin =

fmean +

fzmean -

Gaussian error in f

$$f(w, x, y, z) = \frac{kw^a x^b}{y^c z^d}$$

$$\sigma_f^2 = \left( \frac{\partial f}{\partial x} \sigma_x \right)^2 + \left( \frac{\partial f}{\partial y} \sigma_y \right)^2 + \left( \frac{\partial f}{\partial z} \sigma_z \right)^2 + \dots$$

$$f(x, y, \dots) = kx^a y^b \dots \Rightarrow \left( \frac{\sigma_f}{f} \right)^2 = \left( \frac{a\sigma_x}{x} \right)^2 + \left( \frac{b\sigma_y}{y} \right)^2 + \dots$$

# UPPER AND LOWER BOUND CALCULATION VS LAWS OF ERRORS

k = 3.00

w =	1.00	+/-	0.00	a =	0.00
x =	20.00	+/-	3.00	b =	2.00
y =	40.00	+/-	5.00	c =	0.50
z =	1.00	+/-	0.00	d =	0.00

$$f(w, x, y, z) = \frac{k w^a x^b}{y^c z^d}$$

Paste as values to here. THEN SAVE BEFORE RUNNING MATLAB CODE.

mean f	fmean =	189.74	fmean +	78.52
upper bound for f	fmax =	268.25	fzmean -	60.49
lower bound for f	fmin =	129.24		

Gaussian error in f 58.14

$$f(w, x, y, z) = \frac{k w^a x^b}{y^c z^d}$$

$$\sigma_f^2 = \left(\frac{\partial f}{\partial x} \sigma_x\right)^2 + \left(\frac{\partial f}{\partial y} \sigma_y\right)^2 + \left(\frac{\partial f}{\partial z} \sigma_z\right)^2 + \dots$$

$$f(x, y, \dots) = k x^a y^b \dots \Rightarrow \left(\frac{\sigma_f}{f}\right)^2 = \left(\frac{a \sigma_x}{x}\right)^2 + \left(\frac{b \sigma_y}{y}\right)^2 + \dots$$

Excel display

MATLAB command window display

$$z = 3x^2 y^{-\frac{1}{2}}$$

$$x = 20 \pm 3$$

$$y = 40 \pm 5$$

```

UPPER AND LOWER BOUND CALCULATOR
f = k * w^a * x^b / ( y^c * z*d )

k = 3
w = 1 +/- 0, a = 0
x = 20 +/- 3, b = 2
y = 40 +/- 5, c = 0.5
z = 1 +/- 0, d = 0

Mean f = 189.7367
Upper f - Mean f = 78.5153
Mean f - Lower f = 60.4919
Gaussian f error = 58.1431

fx EDU>>
    
```

To avoid tedium,  
we ingest these  
from the Excel  
sheet

```
1 %Upper and lower bound error calculator
2 % f = k * w^a * x^b / ( y^c * z^d )
3 function upper_and_lower_bounds
4 clc; disp(' '); disp(' UPPER AND LOWER BOUND CALCULATOR ');
5 disp(' f = k * w^a * x^b / ( y^c * z^d ) '); disp(' ');
6
7 %Get parameters from Excel
8 [k,w,x,y,z,sigma_w,sigma_x,sigma_y,sigma_z,a,b,c,d] = get_data_from_excel;
9
10 %Calculate outputs
11 mean_f = k * (w^a) * (x^b) / ( (y^c) * (z^d) );
12 f_upper = k *...
13     ( ( (w+sigma_w)^a ) * ( (x+sigma_x)^b ) ) /...
14     ( ( ( y - sigma_y)^c ) * (( z-sigma_z)^d ) );
15 f_lower = k *...
16     ( ( (w-sigma_w)^a ) * ( (x-sigma_x)^b ) ) /...
17     ( ( ( y + sigma_y)^c ) * (( z+sigma_z)^d ) );
18
19 gaussian_f_error = mean_f *...
20     sqrt( ( a*sigma_w/w)^2 + ( b*sigma_x/x)^2 +...
21     ( c*sigma_y/y)^2 + ( d*sigma_z/z)^2 );
22
23 %Display message to command window
24 disp([' k = ',num2str(k) ]);
25 disp([' w = ',num2str(w), ' +/- ',num2str(sigma_w), ', a = ',num2str(a) ]);
26 disp([' x = ',num2str(x), ' +/- ',num2str(sigma_x), ', b = ',num2str(b) ]);
27 disp([' y = ',num2str(y), ' +/- ',num2str(sigma_y), ', c = ',num2str(c) ]);
28 disp([' z = ',num2str(z), ' +/- ',num2str(sigma_z), ', d = ',num2str(d) ]);
29 disp(' ');
30 disp([' Mean f = ',num2str(mean_f) ] );
31 disp([' Upper f - Mean f = ',num2str(f_upper - mean_f) ] );
32 disp([' Mean f - Lower f = ',num2str(mean_f - f_lower) ] );
33 disp([' Gaussian f error = ',num2str(gaussian_f_error) ] ); disp(' ');
34
35 %%
36
```

MATLAB  
code to evaluate  
upper and  
lower bound  
calculations.

Although you  
have to 'think  
in arrays',  
dealing with  
word-variables  
is easier than cell  
references!

## UPPER AND LOWER BOUND CALCULATION VS LAWS OF ERRORS

$k = 3.95$

$w = 23.08$	$\pm$	$0.55$	$a = 2.47$
$x = 60.43$	$\pm$	$0.12$	$b = 2.85$
$y = 65.94$	$\pm$	$0.18$	$c = 3.36$
$z = 22.71$	$\pm$	$0.69$	$d = 1.82$

Paste as values to here. THEN SAVE BEFORE RUNNING MATLAB CODE.

```

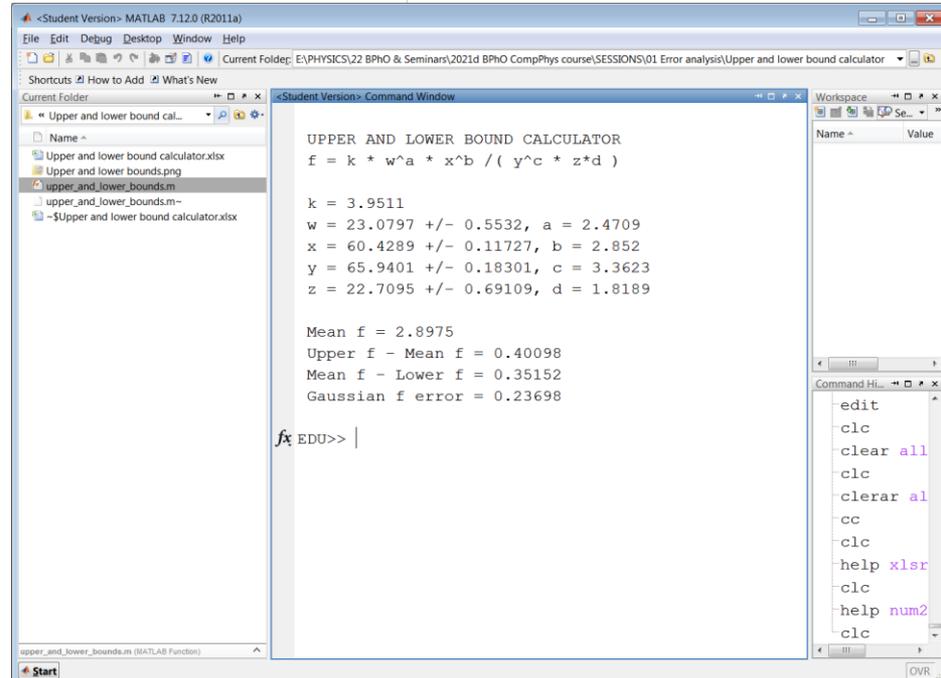
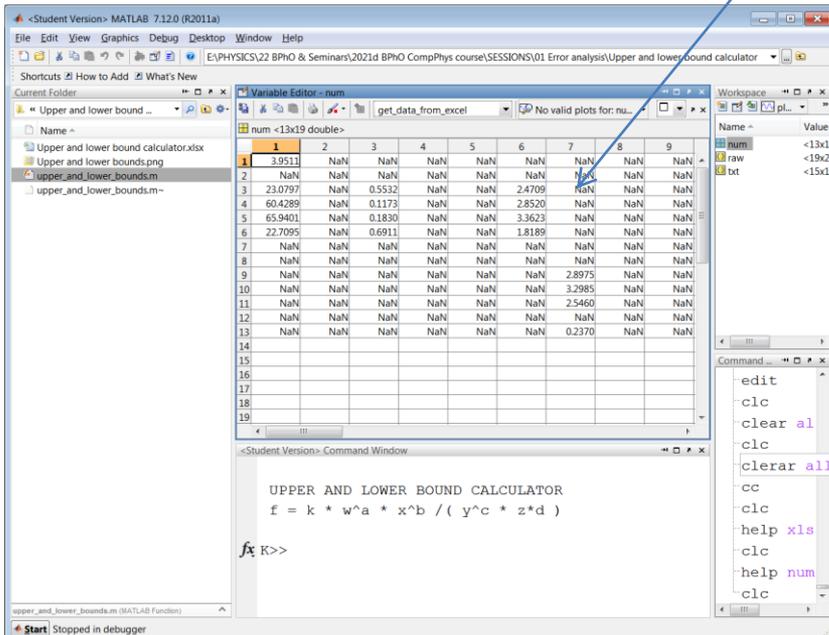
36
37 %Get parameters from Excel
38 function [k,w,x,y,z,sigma_w,sigma_x,sigma_y,sigma_z,a,b,c,d] = get_data_from_excel
39 [num,txt,row] = xlsread('upper and lower bound calculator.xlsx');
40 k = num(1,1);
41 w = num(3,1); sigma_w = num(3,3); a = num(3,6);
42 x = num(4,1); sigma_x = num(4,3); b = num(4,6);
43 y = num(5,1); sigma_y = num(5,3); c = num(5,6);
44 z = num(6,1); sigma_z = num(6,3); d = num(6,6);

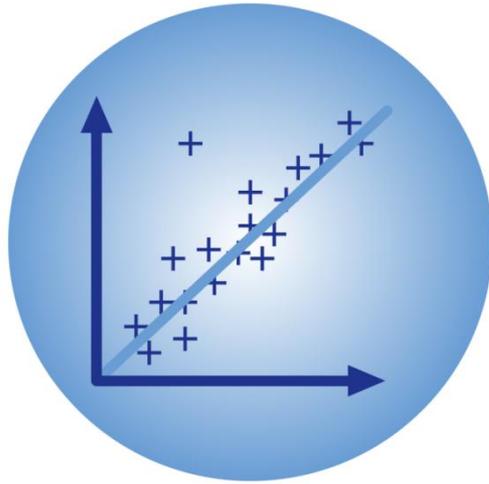
```

In this example, to avoid tedious hard coding, we ingest the data directly from Excel into MATLAB.

Note we ingest the full precision of the stored numbers. They have been chosen to be displayed to 2.d.p. in Excel.

This function performs the ingest into MATLAB





# BPhO

## Computational Challenge

- Suggested homework
- Q&A