Error Propagation[1]

November 13, 2017

[1] HMS, 2017, v1.0

Chapter References

- Diez: None
- Navidi, Chapter 3

Motivation

$$\text{Measured Value} = \text{True Value} + \text{Bias} + \text{Random Error}$$

The bias refers to the systematic error due to bias in the instrument or bias in the human operator or even software.

Bias can be corrected.

Random errors however are not easily reduced and **propagate** into any additional calculations we may do with the data.

Motivation

- Let us measure the area of a circle: $A = \pi r^2$
- In measuring the area we note that there is uncertainty in our measurement of the radius, r. For example $r = 2.5 \pm 0.2$
- Given this uncertainty what is the uncertainty the computed area:

$$A \pm ?$$

Motivation

The reaction rate for an enzyme catalyzed reaction is given by:

$$v = \frac{V_m S}{K_m + S}$$

where V_m is the maximal velocity and K_m the substrate concentration, S at half the maximal rate.

The V_m and K_m are estimated to be 15.8 ± 0.9 mM/s and $0.5 \ \pm 0.05$ mM respectively.

At a substrate concentration of 5 mM, what is the reaction velocity and associated uncertainty?

Linear Combination of Measurements

If c is a constant, then:

$$\sigma_{cX} = |c|\sigma_X$$

$$\sigma_{c_1 X_1} + \sigma_{c_2 X_2} + \ldots = \sqrt{c_1^2 \sigma_{X_1}^2 + c_1^2 \sigma_{X_1}^2 + \ldots}$$

Important caveat: $X_1, X_2, \ldots$ are independent measurements.

Example

The radius of a circle, R, is measured to be 3.0 ± 0.1 cm. Estimate the circumference and find the uncertainty, σ_c, in the estimate.

$$R = 2\pi R$$

Using:

$$\sigma_{cX} = |c|\sigma_X$$

$$\sigma_c = |2\pi|\sigma_R = 0.63 \text{ cm}$$

The circumference is therefore: 18.85 ± 0.63 cm

Example

A surveyor is measuring the perimeter of a rectangular plot. Two adjacent sides are measured to be 50.11 ± 0.05m and 75.21 ± 0.08 cm. Estimate the perimeter of the lot and the uncertainty.

$$P = 2X + 2Y = 260.64 \text{ cm}$$

Using:

$$\sigma_{c_1 X_1} + \sigma_{c_2 X_2} + \ldots = \sqrt{c_1^2 \sigma_{X_1}^2 + c_1^2 \sigma_{X_1}^2 + \ldots}$$

$$\sigma_P = \sigma_{2X} + \sigma_{2Y} = \sqrt{4\sigma_X^2 + 4\sigma_2^2} = 0.19 \text{ m}$$

The perimeter is 250.64 ± 0.19 m

You cannot use $P = X + X + Y + Y$ and form $\sigma_P = \sigma_X + \sigma_X + \sigma_Y + \sigma_Y$ because $X + X$ is not the sum of independent quantities.

Dependent Measurements

For dependent measurements, one can compute an upper bound on the uncertainty in a linear combination:

$$\sigma_{c_1 X_1} + \sigma_{c_2 X_2} + \ldots \leq |c_1|\sigma_{X_1} + |c_2|\sigma_{X_2} + \ldots$$

Uncertainties for Functions of One Measurement

What happens if your function is nonlinear rather than a simple linear combination?

Given a random variable X, with known standard deviation σ_X and given $U = U(X)$ how do we compute σ_U?

Uncertainties for Functions of One Measurement

$$\sigma_U \approx \left| \frac{dU}{dX} \right| \sigma_X$$

Note the equation gives an approximate estimate.

Uncertainties for Functions of One Measurement

Going back to the first example of finding the area of a circle: $A = \pi R^2$. If $R = 5.00 \pm 0.01$ cm then find the area and the uncertainty in the Area.

$$\sigma_A \approx \left|\frac{dA}{dR}\right| \sigma_R$$

$$\begin{aligned} \frac{dA}{dR} &= 2\pi R \; \sigma_R \\ &= 10\pi \; 0.01 \\ &= 0.31 \text{ cm}^2 \end{aligned}$$

The area is therefore given by 78.5 ± 0.3 cm^2

Relative Uncertainties of One Measurement

If U is a measurement with true mean μ and uncertainty σ_U, then the relative uncertainty is:

$$\frac{\sigma_U}{U}$$

The relative uncertainty is also called the **coefficient of variation**

Relative Uncertainties of One Measurement

Recall the area of the circle in the previous example was 78.5 ± 0.3 cm^2. The absolute uncertainty was 0.3 cm^2.

The relative uncertainty is:

$$\begin{aligned} \frac{\sigma_A}{A} &= \frac{0.3}{78.5} \\ &= 0.004 \\ &= 0.4\% \end{aligned}$$

Uncertainties for Functions of Several Measurements

If $A, B, \ldots$, are independent measurements whose uncertainties are σ_A, σ_B, and if $U = U(A, B, \ldots)$ then

$$\sigma_U = \sqrt{\left(\frac{\partial U}{\partial A}\right)^2 \sigma_A^2 + \left(\frac{\partial U}{\partial B}\right)^2 \sigma_B^2 + \ldots}$$

Uncertainties for Functions of Several Measurements

Assume we have a function:

$$U = U(A, B)$$

The total deviation as a result of uncertainty in the measurements, A or B is given by:

$$dU = \frac{\partial U}{\partial A}\Delta A + \frac{\partial U}{\partial B}\Delta B$$

This assumes the deviations are small.

How to Propagate

$$\Delta U = \frac{\partial U}{\partial A}\Delta A + \frac{\partial U}{\partial B}\Delta B$$

The variance in U is given by:

$$\sigma_U^2 = \frac{1}{N}\sum_{i=1}^{N}(\Delta U_i)^2$$

The variances in the individual measurements, A and B are given by

$$\sigma_A^2 = \frac{1}{N}\sum_{i=1}^{N}(\Delta A_i)^2, \quad \sigma_B^2 = \frac{1}{N}\sum_{i=1}^{N}(\Delta B_i)^2,$$

How to Propagate

Inserting ΔU into σ_U^2

$$\sigma_U^2 = \frac{1}{N} \sum \left(\frac{\partial U}{\partial A} \Delta A_i + \frac{\partial U}{\partial B} \Delta B_i \right)^2$$

Expanding the squared term yields:

$$\sigma_U^2 = \frac{1}{N} \sum \left[\left(\frac{\partial U}{\partial A} \Delta A_i \right)^2 + \left(\frac{\partial U}{\partial B} \Delta B_i \right)^2 + 2 \frac{\partial U}{\partial A} \frac{\partial U}{\partial B} \Delta A_i \Delta B_i \right]$$

Let us assume that the errors are random and independent, this means that the cross-term will on average equal zero (positive and well as negative deviations are equally possible)

How to Propagate

We are therefore left with:

$$\sigma_U^2 = \frac{1}{N} \sum \left[\left(\frac{\partial U}{\partial A} \Delta A_i \right)^2 + \left(\frac{\partial U}{\partial B} \Delta B_i \right)^2 \right]$$

We can rearrange this equation by pulling out the derivatives:

$$\sigma_U^2 = \left(\frac{\partial U}{\partial A} \right)^2 \frac{1}{N} \sum (\Delta A_i)^2 + \left(\frac{\partial U}{\partial B} \right)^2 \frac{1}{N} \sum (\Delta B_i)^2$$

Do you recognized the terms: $\frac{1}{N} \sum (\Delta A_i)^2$ and $\frac{1}{N} \sum (\Delta B_i)^2$?

They are the variances for A and B, therefore...

How to Propagate

$$\sigma_U^2 = \left(\frac{\partial U}{\partial A}\right)^2 \sigma_A^2 + \left(\frac{\partial U}{\partial B}\right)^2 \sigma_B^2$$

A similar proof can also be made if the σ's are standard errors.

$$\sigma_U = \sqrt{\left(\frac{\partial U}{\partial A}\right)^2 \sigma_A^2 + \left(\frac{\partial U}{\partial B}\right)^2 \sigma_B^2 + \ldots}$$

General Expression for product/quotient

For the expression, $U = abc/(xyz)$ the uncertainty in U can be shown to be:

$$\frac{\sigma_U}{U} = \sqrt{\left(\frac{\sigma_a}{a}\right)^2 + \left(\frac{\sigma_b}{b}\right)^2 + \left(\frac{\sigma_c}{c}\right)^2 + \left(\frac{\sigma_x}{x}\right)^2 + \left(\frac{\sigma_y}{y}\right)^2 + \left(\frac{\sigma_z}{z}\right)^2}$$

General Rules

Addition/Subtraction	$x = a + b - c$	$\sigma_x = \sqrt{\sigma_a^2 + \sigma_b^2 + \sigma_c^2}$
Mutiplication/Division	$x = a \times b/c$	$\frac{\sigma_x}{x} = \sqrt{\left(\frac{\sigma_a}{a}\right)^2 + \left(\frac{\sigma_b}{b}\right)^2 + \left(\frac{\sigma_c}{c}\right)^2}$
Exponential	$x = a^k$	$\frac{\sigma_x}{x} = k\left(\frac{\sigma_a}{a}\right)$

Standard Error

Consider the mean $\bar{x}$:

$$\bar{x} = \frac{x_1 + x_2 + \ldots}{N}$$

In measuring an individual x_i there will be uncertainty in the x_i by an amount σ_{x_i}. Let us propagate the uncertainties in x_i into the mean standard deviation:

$$\sigma_{\bar{x}} = \sqrt{\left(\frac{\partial \bar{x}}{\partial x_1}\right)^2 \sigma_{x_1}^2 + \left(\frac{\partial \bar{x}}{\partial x_2}\right)^2 \sigma_{x_2}^2 + \ldots}$$

Standard Error

$$\sigma_{\bar{x}} = \sqrt{\left(\frac{\partial \bar{x}}{\partial x_1}\right)^2 \sigma_{x_1}^2 + \left(\frac{\partial \bar{x}}{\partial x_2}\right)^2 \sigma_{x_2}^2 + \ldots}$$

Let us assume that the uncertainties in each x_i are the same, that is

$$\sigma_{x_1} = \sigma_{x_2} = \ldots = \sigma_x$$

Since $\bar{x} = \sum x_i / N$ we can evaluate the partial derivatives:

$$\frac{\partial \bar{x}}{\partial x_1} = \frac{\partial \bar{x}}{\partial x_2} = \ldots = \frac{1}{N}$$

Inserting these into the propagation relationship yields:

Standard Error

$$\sigma_{\bar{x}} = \sqrt{\left(\frac{1}{N}\sigma_x\right)^2 + \left(\frac{1}{N}\sigma_x\right)^2 + \dots}$$

Rearranging yields:

$$\sigma_{\bar{x}} = \sqrt{N\frac{\sigma_x^2}{N^2}}$$

And finally:

$$\sigma_{\bar{x}} = \frac{\sigma_x}{\sqrt{N}}$$

The standard error simply expresses how uncertainty from the sampling propagates into the random variable that describes the means.

Example

Assume the mass of a rock is measured to be $m = 675.0 \pm 1$ gm and the volume is measured to be $V = 261.0 \pm 0.1$ mL. Estimate the density of the rock and the uncertainty of the estate.

$$\text{Density} = \frac{m}{V} = \frac{675.0}{261.0} = 2.582 \text{ g}$$

Apply

$$\sigma_D = \sqrt{\left(\frac{\partial D}{\partial m}\right)^2 \sigma_m^2 + \left(\frac{\partial D}{\partial V}\right)^2 \sigma_V^2 + \dots}$$

$$\frac{\partial D}{\partial m} = \frac{1}{m} = 0.0038 \text{ mL}^{-1}$$

$$\frac{\partial D}{\partial V} = -\frac{m}{V^2} = -0.0099 \; g/\text{mL}^2$$

Example

Assume the mass of a rock is measured to be $m = 675.0 \pm 1$ g and the volume is measured to be $V = 261.0 \pm 0.1$ mL.

$$\sigma_D = \sqrt{\left(\frac{\partial D}{\partial m}\right)^2 \sigma_m^2 + \left(\frac{\partial D}{\partial V}\right)^2 \sigma_V^2}$$

$$\sigma_D = 0.004 \text{ g/mL}$$

The density of the rock is: 2.582 ± 0.004 g/mL

Example

Suppose a concentration of a given solution is 13.7 ± 0.3 moles L^{-1}. A UV spec is used to measure the absorbance using a cuvette with a path length of 1.0 ± 0.1 cm. The absorbance is found to be 0.172807 ± 0.000008. Estimate the molar absorptivity, ε, using Beer's law $\varepsilon = A/(lc)$.

Since the expression is of the form product/quotient, we can use:

$$\frac{\sigma_\varepsilon}{\varepsilon} = \sqrt{\left(\frac{\sigma_A}{A}\right)^2 + \left(\frac{\sigma_l}{l}\right)^2 + \left(\frac{\sigma_c}{c}\right)^2}$$

Example

Inserting the values into the equation yields:

$$\frac{\sigma_\varepsilon}{\varepsilon} = \sqrt{\left(\frac{0.000008}{0.172807}\right)^2 + \left(\frac{0.1}{1}\right)^2 + \left(\frac{0.3}{13.7}\right)^2}$$

$$\frac{\sigma_\varepsilon}{\varepsilon} = 0.10237$$

Using Beer's law we can compute ε:

$$\varepsilon = 0.172807/(1 \times 13.7) = 0.012614 \text{ L mol}^{-1} \text{ cm}^{-1}$$

Therefore:

$$\varepsilon = 0.013 \pm 0.001 \text{ L mol}^{-1} \text{ cm}^{-1}$$

Effect on Error Bars

The following data was measured for an enzymatic reaction with standard error of 0.5 for each measurement

Substrate	Reaction Rate	Standard Error
1	0.363636364	0.5
2	0.533333333	0.5
3	0.631578947	0.5
4	0.695652174	0.5
5	0.740740741	0.5
6	0.774193548	0.5
7	0.8	0.5
8	0.820512821	0.5
9	0.837209302	0.5
10	0.85106383	0.5

Effect on Error Bars

The enzymatic reaction is governed by:

$$v = \frac{V_m\ s}{K_m + s}$$

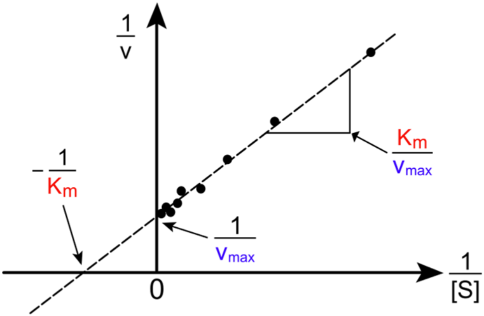
Transforming to:

$$\frac{1}{v} = \frac{K_m}{V_m}\frac{1}{s} + \frac{1}{V_m}$$

That is a plot of $1/v$ versus $1/s$ will yield a straight line.

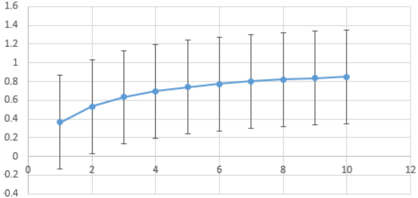
Effect on Error Bars

$$\frac{1}{v} = \frac{K_m}{V_m}\frac{1}{s} + \frac{1}{V_m}$$



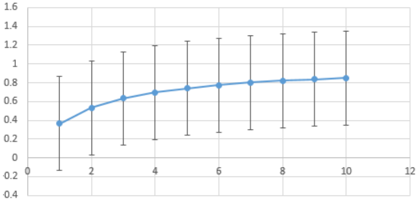
Effect on Error Bars

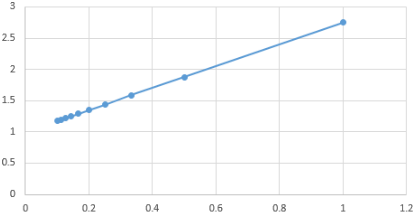
Plot of reaction velocity versus substrate concentration.



Effect on Error Bars

Left hand-side plot is reaction velocity versus substrate concentration.





Left plot is plot of $1/v$ versus $1/s$

Effect on Error Bars

How is the error propagated into $1/v$?

$$\frac{\sigma_x}{x} = \sqrt{\left(\frac{\sigma_a}{a}\right)^2 + \dots}$$

$$\frac{\sigma_{1/v}}{1/v} = \sqrt{\left(\frac{\sigma_v}{v}\right)^2} = \frac{\sigma_v}{v}$$

Therefore

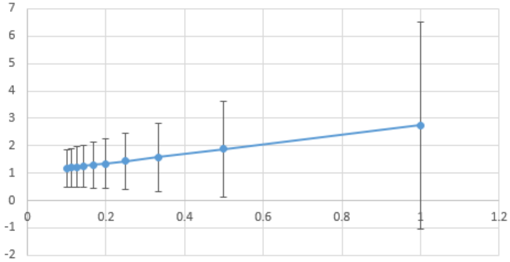
$$\sigma_{1/v} = \frac{\sigma_v}{v^2}$$

Effect on Error Bars

$$\sigma_{1/v} = \frac{\sigma_v}{v^2}$$

As at low v (high $1/v$), the uncertainty in $1/v$ significantly increases.

Effect on Error Bars



High v Low v

Error Propagation using Python

Use the uncertainties package:

```
te.installPackage('uncertainties')
```

Other Pythons use:

```
pip install --upgrade uncertainties
```

Error Propagation using Python

```
>>> from uncertainties import ufloat
>>> x = ufloat(1, 0.1)  # x = 1+/-0.1
>>> print 2*x
2.00+/-0.20
>>> v = ufloat (4.5, 0.25)
>>> print 1/v
0.222222222222222+/-0.012345679012345678
```

Error Propagation using Python

```
>>> from uncertainties import unumpy
>>>y = unumpy.uarray ([0.3636, 0.533, 0.631, 0.695, 0.7407,
                      0.774,0.8,0.821, 0.837, 0.851],
                      [0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5,0.5])
>>>print 1/y
[2.7502750275027505+/-3.7820063634526275
 1.876172607879924 8+/-1.7600118272794791
 1.5847860538827259+/-1.255773418290591
 1.4388489208633095+/-1.035143108534755
 1.3500742540839745+/-0.9113502457702002
 1.2919896640826873+/-0.8346186460482475
 1.25+/-0.7812499999999999
 1.218026796589525+/-0.7417946386050701
 1.1947431302270013+/-0.7137055736123066
 1.1750881316098707+/-0.6904160585251885]
>>>print 0.5/(0.3636*0.3636)
3.78200636345
```

Linear Regression

This leads eventually on to Linear Regression. But first we must introduce Analysis of Variance.