Lecture 7

Some Advanced Topics using Propagation of Errors and Least Squares Fitting

Error on the mean (review from Lecture 4)

- Question: If we have a set of measurements of the same quantity:
  $x_1 \pm \sigma_1 \; x_2 \pm \sigma_2 \ldots \; x_n \pm \sigma_n$
  - What's the best way to combine these measurements?
  - How to calculate the variance once we combine the measurements?
  - Assuming Gaussian statistics, the Maximum Likelihood Methods combine the measurements as:

$$x = \frac{\sum_{i=1}^{n} x_i/\sigma_i^2}{\sum_{i=1}^{n} 1/\sigma_i^2}$$

weighted average: bigger σ →less weight

  - If all the variances ($\sigma_1^2 = \sigma_2^2 = \ldots \sigma_n^2$) are the same:

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

unweighted average

  - The variance of the weighted average can be calculated using propagation of errors:

$$\sigma_x^2 = \sum_{i=1}^{n}\left[\frac{\partial}{\partial x_i}x\right]^2 \sigma_i^2 = \sum_{i=1}^{n}\frac{1/\sigma_i^4}{\left[\sum_{i=1}^{n} 1/\sigma_i^2\right]^2}\sigma_i^2 = \frac{\sum_{i=1}^{n} 1/\sigma_i^2}{\left[\sum_{i=1}^{n} 1/\sigma_i^2\right]^2}$$

$$\sigma_x^2 = \frac{1}{\sum_{i=1}^{n} 1/\sigma_i^2}$$

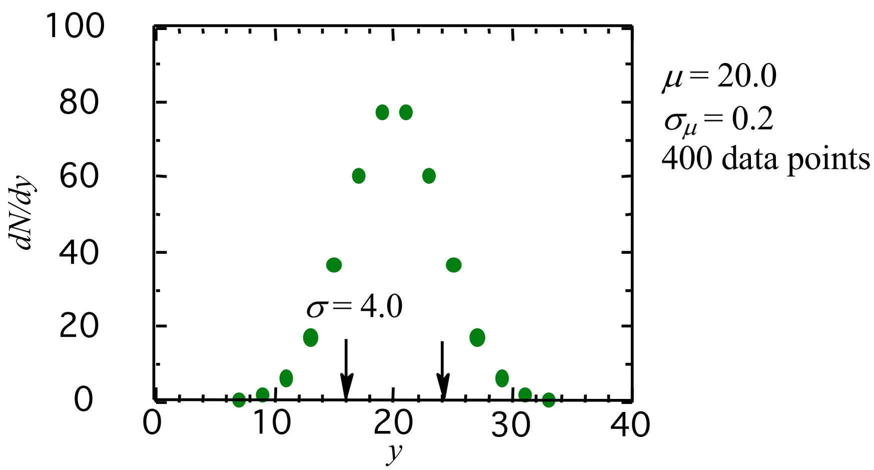
σ_x is the error in the weighted mean

◆ If all the variances are the same:

$$\sigma_x^2 = \frac{1}{\sum_{i=1}^{n} 1/\sigma_i^2} = \frac{1}{n/\sigma^2} = \frac{\sigma^2}{n}$$

Lecture 4

- The error in the mean (σ_x) gets smaller as the number of measurements (n) increases.
- Don't confuse the error in the mean (σ_x) with the standard deviation of the distribution (σ)!
- If we make more measurements
  - the standard deviation (σ) of the distribution remains the same
  - the error in the mean (σ_x) decreases



More on Least Squares Fit (LSQF)

- In Lec 5, we discussed how we can fit our data points to a linear function (straight line) and get the "best" estimate of the slope and intercept. However, we did not discuss two important issues:
  - How to estimate the uncertainties on our slope and intercept obtained from a LSQF?
  - How to apply the LSQF when we have a non-linear function?

- Estimation of Errors from a LSQF
  - Assume we have data points that lie on a straight line:

    $y = \alpha + \beta x$
    - Assume we have n measurements of x's and y's.
    - For simplicity, assume that each y measurement has the same error σ.
    - Assume that x is known much more accurately than y.
      - ☞ ignore any uncertainty associated with x.
    - Previously we showed that the solution for the intercept α and slope β is:

$$\alpha = \frac{\sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} y_i x_i \sum_{i=1}^{n} x_i}{n \sum_{i=1}^{n} x_i^2 - \left[\sum_{i=1}^{n} x_i\right]^2}$$

$$\beta = \frac{n \sum_{i=1}^{n} y_i x_i - \sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i}{n \sum_{i=1}^{n} x_i^2 - \left[\sum_{i=1}^{n} x_i\right]^2}$$

    - Since α and β are functions of the measurements (y_i's)
      - ☞ use the Propagation of Errors technique to estimate σ_α and σ_β.

$$\sigma_Q^2 = \sigma_x^2 \left(\frac{\partial Q}{\partial x}\right)^2 + \sigma_y^2 \left(\frac{\partial Q}{\partial y}\right)^2 + 2\sigma_{xy} \left(\frac{\partial Q}{\partial x}\right)\left(\frac{\partial Q}{\partial y}\right)$$

      - ★ Assumed that each measurement is independent of each other:

$$\sigma_Q^2 = \sigma_x^2 \left(\frac{\partial Q}{\partial x}\right)^2 + \sigma_y^2 \left(\frac{\partial Q}{\partial y}\right)^2$$

$$\sigma_\alpha^2 = \sum_{i=1}^{n} \sigma_{y_i}^2 \left(\frac{\partial \alpha}{\partial y_i}\right)^2 = \sigma^2 \sum_{i=1}^{n} \left(\frac{\partial \alpha}{\partial y_i}\right)^2$$

$$\frac{\partial \alpha}{\partial y_i} = \frac{\partial}{\partial y_i} \frac{\sum_{i=1}^n y_i \sum_{j=1}^n x_j^2 - \sum_{i=1}^n y_i x_i \sum_{j=1}^n x_j}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2} = \frac{\sum_{j=1}^n x_j^2 - x_i \sum_{j=1}^n x_j}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2}$$

$$\sigma_\alpha^2 = \sigma^2 \sum_{i=1}^n \left(\frac{\sum_{j=1}^n x_j^2 - x_i \sum_{j=1}^n x_j}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2} \right)^2 = \sigma^2 \sum_{i=1}^n \frac{\left(\sum_{j=1}^n x_j^2\right)^2 + x_i^2 \left(\sum_{j=1}^n x_j\right)^2 - 2x_i \sum_{j=1}^n x_j \sum_{j=1}^n x_j^2}{\left(n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2\right)^2}$$

$$\sigma_\alpha^2 = \sigma^2 \frac{n\left(\sum_{j=1}^n x_j^2\right)^2 + \sum_{i=1}^n x_i^2 \left(\sum_{j=1}^n x_j\right)^2 - 2\left(\sum_{j=1}^n x_j\right)^2 \sum_{j=1}^n x_j^2}{\left(n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2\right)^2}$$

$$\sigma_\alpha^2 = \sigma^2 \frac{n\left(\sum_{j=1}^n x_j^2\right)^2 - \left(\sum_{j=1}^n x_j\right)^2 \sum_{j=1}^n x_j^2}{\left(n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2\right)^2}$$

$$\sigma_\alpha^2 = \sigma^2 \sum_{j=1}^n x_j^2 \frac{n \sum_{j=1}^n x_j^2 - \left(\sum_{j=1}^n x_j\right)^2}{\left(n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2\right)^2}$$

$$\sigma_\alpha^2 = \sigma^2 \frac{\sum_{j=1}^n x_j^2}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2}$$

variance in the intercept

★ We can find the variance in the slope (β) using the same procedure:

$$\sigma_\beta^2 = \sum_{i=1}^{n} \sigma_{y_i}^2 \left(\frac{\partial \beta}{\partial y_i}\right)^2 = \sigma^2 \sum_{i=1}^{n} \left(\frac{\partial \beta}{\partial y_i}\right)^2 = \sigma^2 \sum_{i=1}^{n} \left(\frac{\partial}{\partial y_i} \frac{n \sum_{i=1}^{n} y_i x_i - \sum_{i=1}^{n} y_i \sum_{j=1}^{n} x_j}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}\right)^2$$

$$\sigma_\beta^2 = \sigma^2 \sum_{i=1}^{n} \left(\frac{n x_i - \sum_{j=1}^{n} x_j}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}\right)^2 = \sigma^2 \frac{n^2 \sum_{j=1}^{n} x_j^2 + n\left(\sum_{j=1}^{n} x_j\right)^2 - 2n \sum_{i=1}^{n} x_i \sum_{j=1}^{n} x_j}{\left(n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2\right)^2}$$

$$\sigma_\beta^2 = \sigma^2 \frac{n^2 \sum_{j=1}^{n} x_j^2 - n\left(\sum_{j=1}^{n} x_j\right)^2}{\left(n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2\right)^2}$$

$$\sigma_\beta^2 = \frac{n\sigma^2}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

variance in the slope

■ If we don't know the true value of σ,

☞ estimate variance using the spread between the measurements (y_i's) and the fitted values of y:

$$\sigma^2 \approx \frac{1}{n-2} \sum_{i=1}^{n} \left(y_i - y_i^{fit}\right)^2 = \frac{1}{n-2} \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2$$

★ $n - 2$ = number of degree of freedom

= number of data points – number of parameters (α, β) extracted from the data

- If each y_i measurement has a different error σ_i:

$$\sigma_\alpha^2 = \frac{1}{D}\sum_{i=1}^{n}\frac{x_i^2}{\sigma_i^2}$$

$$\sigma_\beta^2 = \frac{1}{D}\sum_{i=1}^{n}\frac{1}{\sigma_i^2}$$

$$D = \sum_{i=1}^{n}\frac{1}{\sigma_i^2}\sum_{i=1}^{n}\frac{x_i^2}{\sigma_i^2} - \left(\sum_{i=1}^{n}\frac{x_i}{\sigma_i^2}\right)^2$$

Weighted slope and intercept

  - ★ The above expressions simplify to the "equal variance" case.
    - Don't forget to keep track of the "n's" when factoring out σ. For example

$$\sum_{i=1}^{n}\frac{1}{\sigma_i^2} = \frac{n}{\sigma^2} \quad \text{not} \quad \frac{1}{\sigma^2}$$

- LSQF with non-linear functions:
  - For our purposes, a non-linear function is a function where one or more of the parameters that we are trying to determine (e.g. α, β from the straight line fit) is raised to a power other than 1.
    - Example: functions that are non-linear in the parameter τ:

$$y = A + x/\tau$$
$$y = A + x\tau^2$$
$$y = Ae^{-x/\tau}$$

      - ★ These functions are linear in the parameters A.

- The problem with most non-linear functions is that we cannot write down a solution for the parameters in a closed form using, for example, the techniques of linear algebra (i.e. matrices).
  - Usually non-linear problems are solved numerically using a computer.
  - Sometimes by a change of variable(s) we can turn a non-linear problem into a linear one.
    - ★ Example: take the natural log of both sides of the above exponential equation:

$$\ln y = \ln A - \frac{x}{\tau} = C - Dx$$

      - A linear problem in the parameters C and D!
      - In fact its just a straight line!
      - ☞ To measure the lifetime τ (Lab 7) we first fit for D and then transform D into τ.
- Example: Decay of a radioactive substance. Fit the following data to find N_0 and τ:

$$N = N_0 e^{-x/\tau}$$

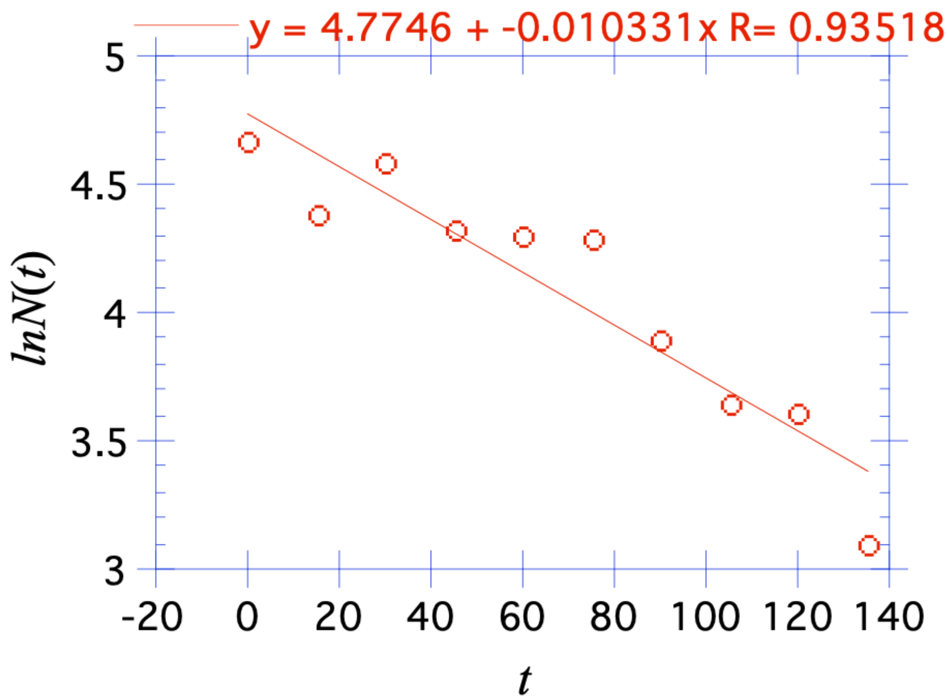
  - N represents the amount of the substance present at time t.
  - N_0 is the amount of the substance at the beginning of the experiment ($t = 0$).
  - τ is the lifetime of the substance.

i	1	2	3	4	5	6	7	8	9	10
t_i	0	15	30	45	60	75	90	105	120	135
N_i	106	80	98	75	74	73	49	38	37	22
$y_i = \ln N_i$	4.663	4.382	4.585	4.317	4.304	4.290	3.892	3.638	3.611	3.091

$$D = -\beta = -\frac{n\sum_{i=1}^{n} y_i x_i - \sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i}{n\sum_{i=1}^{n} x_i^2 - \left[\sum_{i=1}^{n} x_i\right]^2} = \frac{10\times 2560.41 - 40.733\times 675}{10\times 64125 - 675^2} = 0.01033$$

$$\tau = \frac{1}{D} = 96.80\ sec$$

- The intercept is given by: $C = 4.77 = \ln A$ or $A = 117.9$



- Example: Find the values A and τ taking into account the uncertainties in the data points.
  - The uncertainty in the number of radioactive decays is governed by Poisson statistics.
  - The number of counts N_i in a bin is assumed to be the average (μ) of a Poisson distribution:

    $\mu = N_i =$ Variance
  - The variance of y_i ($= \ln N_i$) can be calculated using propagation of errors:

$$\sigma_y^2 = \sigma_N^2(\partial y/\partial N)^2 = \sigma_N^2(\partial \ln N/\partial N)^2 = N(1/N)^2 = 1/N$$

- The slope and intercept from a straight line fit that includes uncertainties in the data points:

$$\alpha = \frac{\sum_{i=1}^{n}\frac{y_i}{\sigma_i^2}\sum_{i=1}^{n}\frac{x_i^2}{\sigma_i^2} - \sum_{i=1}^{n}\frac{x_i y_i}{\sigma_i^2}\sum_{i=1}^{n}\frac{x_i}{\sigma_i^2}}{\sum_{i=1}^{n}\frac{1}{\sigma_i^2}\sum_{i=1}^{n}\frac{x_i^2}{\sigma_i^2} - \left(\sum_{i=1}^{n}\frac{x_i}{\sigma_i^2}\right)^2} \text{ and } \beta = \frac{\sum_{i=1}^{n}\frac{1}{\sigma_i^2}\sum_{i=1}^{n}\frac{x_i y_i}{\sigma_i^2} - \sum_{i=1}^{n}\frac{x_i}{\sigma_i^2}\sum_{i=1}^{n}\frac{y_i}{\sigma_i^2}}{\sum_{i=1}^{n}\frac{1}{\sigma_i^2}\sum_{i=1}^{n}\frac{x_i^2}{\sigma_i^2} - \left(\sum_{i=1}^{n}\frac{x_i}{\sigma_i^2}\right)^2}$$

  - ★ If all the σ's are the same then the above expressions are identical to the unweighted case.

  Taylor P. 201 and Problem 8.9

  α = 4.725 and β = -0.00903

  τ = -1/β = 1/0.00903 = 110.7 sec

- To calculate the error on the lifetime, we first must calculate the error on β:

$$\sigma_\beta^2 = \frac{\sum_{i=1}^{n}\frac{1}{\sigma_i^2}}{\sum_{i=1}^{n}\frac{1}{\sigma_i^2}\sum_{i=1}^{n}\frac{x_i^2}{\sigma_i^2} - \left(\sum_{i=1}^{n}\frac{x_i}{\sigma_i^2}\right)^2} = \frac{652}{652\times 2684700 - 33240^2} = 1.01\times 10^{-6}$$

$$\sigma_\tau^2 = \sigma_\beta^2 (\partial\tau/\partial\beta)^2$$

$$\sigma_\tau = \sigma_\beta\left(\frac{1}{\beta^2}\right) = \frac{1.005\times 10^{-3}}{(9.03\times 10^{-3})^2} = 12.3$$

☞ The experimentally determined lifetime is

τ = 110.7 ± 12.3 sec.