Lecture 5
Maximum Likelihood Method

- Suppose we are trying to measure the true value of some quantity (x_T).
  - We make repeated measurements of this quantity $\{x_1, x_2, \ldots x_n\}$.
  - The standard way to estimate x_T from our measurements is to calculate the mean value:

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

    - set $x_T = \mu_x$.
    - DOES THIS PROCEDURE MAKE SENSE???
    - MLM: a general method for estimating parameters of interest from data.
- Statement of the Maximum Likelihood Method
  - Assume we have made N measurements of x $\{x_1, x_2, \ldots x_n\}$.
  - Assume we know the probability distribution function that describes x: $f(x, \alpha)$.
  - Assume we want to determine the parameter α.
    - *MLM: pick α to maximize the probability of getting the measurements (the x_i's) that we did!*
- How do we use the MLM?
  - The probability of measuring x_1 is $f(x_1, \alpha)dx$
  - The probability of measuring x_2 is $f(x_2, \alpha)dx$
  - The probability of measuring x_n is $f(x_n, \alpha)dx$
  - If the measurements are independent, the probability of getting the measurements we did is:

$$L = f(x_1,\alpha)dx \cdot f(x_2,\alpha)dx \cdots f(x_n,\alpha)dx = f(x_1,\alpha)\cdot f(x_2,\alpha)\cdots f(x_n,\alpha)dx^n$$

  - We can drop the dx^n term as it is only a proportionality constant

$$L = \prod_{i=1}^{N} f(x_i,\alpha)$$

Likelihood Function

- We want to pick the α that maximizes L:

$$\left.\frac{\partial L}{\partial \alpha}\right|_{\alpha=\alpha^*} = 0$$

- Both L and $\ln L$ have maximum at the same location.
  - maximize $\ln L$ rather than L itself because $\ln L$ converts the product into a summation.

$$\ln L = \sum_{i=1}^{N} \ln f(x_i, \alpha)$$

  - new maximization condition:

$$\left.\frac{\partial \ln L}{\partial \alpha}\right|_{\alpha=\alpha^*} = \sum_{i=1}^{N} \frac{\partial}{\partial \alpha} \ln f(x_i, \alpha)\Big|_{\alpha=\alpha^*} = 0$$

    - α could be an array of parameters (e.g. slope and intercept) or just a single variable.
    - equations to determine α range from simple linear equations to coupled non-linear equations.

- Example:
  - Let $f(x, \alpha)$ be given by a Gaussian distribution.
  - Let $\alpha = \mu$ be the mean of the Gaussian.
  - We want the best estimate of α from our set of n measurements $\{x_1, x_2, \ldots x_n\}$.
  - Let's assume that σ is the same for each measurement.

$$f(x_i, \alpha) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\alpha)^2}{2\sigma^2}}$$

  - The likelihood function for this problem is:

$$L = \prod_{i=1}^{n} f(x_i, \alpha) = \prod_{i=1}^{n} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x_i-\alpha)^2}{2\sigma^2}} = \left[\frac{1}{\sigma\sqrt{2\pi}}\right]^n e^{-\frac{(x_1-\alpha)^2}{2\sigma^2}} e^{-\frac{(x_2-\alpha)^2}{2\sigma^2}} \cdots e^{-\frac{(x_n-\alpha)^2}{2\sigma^2}} = \left[\frac{1}{\sigma\sqrt{2\pi}}\right]^n e^{-\sum_{i=1}^{n}\frac{(x_i-\alpha)^2}{2\sigma^2}}$$

- Find α that maximizes the log likelihood function:

$$\frac{\partial \ln L}{\partial \alpha} = \frac{\partial}{\partial \alpha}\left[n \ln\left(\frac{1}{\sigma\sqrt{2\pi}}\right) - \sum_{i=1}^{n} \frac{(x_i - \alpha)^2}{2\sigma^2} \right] = 0$$

$$\frac{\partial}{\partial \alpha} \sum_{i=1}^{n} (x_i - \alpha)^2 = 0$$

$$\sum_{i=1}^{n} 2(x_i - \alpha)(-1) = 0$$

$$\sum_{i=1}^{n} x_i = n\alpha$$

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

Average

- If σ are different for each data point
  - α is just the weighted average:

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

Weighted average

- Example
  - Let $f(x, \alpha)$ be given by a Poisson distribution.
  - Let $\alpha = \mu$ be the mean of the Poisson.
  - We want the best estimate of α from our set of n measurements $\{x_1, x_2, \ldots x_n\}$.
  - The likelihood function for this problem is:

$$L = \prod_{i=1}^{n} f(x_i, \alpha) = \prod_{i=1}^{n} \frac{e^{-\alpha}\alpha^{x_i}}{x_i!} = \frac{e^{-\alpha}\alpha^{x_1}}{x_1!}\frac{e^{-\alpha}\alpha^{x_2}}{x_2!}\cdots\frac{e^{-\alpha}\alpha^{x_n}}{x_n!} = \frac{e^{-n\alpha}\alpha^{\sum_{i=1}^{n} x_i}}{x_1!x_2!..x_n!}$$

  - Find α that maximizes the log likelihood function:

$$\frac{d\ln L}{d\alpha} = \frac{d}{d\alpha}\left(-n\alpha + \ln\alpha \cdot \sum_{i=1}^{n} x_i - \ln(x_1!x_2!..x_n!)\right) = -n + \frac{1}{\alpha}\sum_{i=1}^{n} x_i = 0$$

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

Average

Some general properties of the Maximum Likelihood Method

- ☺ For large data samples (large n) the likelihood function, L, approaches a Gaussian distribution.
- ☺ Maximum likelihood estimates are usually *consistent*.
  - For large n the estimates converge to the true value of the parameters we wish to determine.
- ☺ Maximum likelihood estimates are usually *unbiased*.
  - For all sample sizes the parameter of interest is calculated correctly.
- ☺ Maximum likelihood estimate is *efficient*: the estimate has the smallest variance.
- ☺ Maximum likelihood estimate is *sufficient*: it uses all the information in the observations (the x_i's).
- ☺ The solution from MLM is unique.
- ☹ Bad news: we must know the correct probability distribution for the problem at hand!

Maximum Likelihood Fit of Data to a Function

- Suppose we have a set of n measurements:

  $$x_1,\ y_1 \pm \sigma_1$$
  $$x_2,\ y_2 \pm \sigma_2$$
  $$\ldots$$
  $$x_n,\ y_n \pm \sigma_n$$

  - Assume each measurement error (σ) is a standard deviation from a Gaussian pdf.
  - Assume that for each measured value y, there's an x which is known exactly.
  - Suppose we know the functional relationship between the y's and the x's:

    $$y = q(x, \alpha, \beta, \ldots)$$

    - α, β...are parameters.
  - MLM gives us a method to determine α, β... from our data.
- Example: Fitting data points to a straight line:

  $$q(x, \alpha, \beta, \ldots) = \alpha + \beta x$$

  $$L = \prod_{i=1}^{n} f(x_i, \alpha, \beta) = \prod_{i=1}^{n} \frac{1}{\sigma_i \sqrt{2\pi}} e^{-\frac{(y_i - q(x_i, \alpha, \beta))^2}{2\sigma_i^2}} = \prod_{i=1}^{n} \frac{1}{\sigma_i \sqrt{2\pi}} e^{-\frac{(y_i - \alpha - \beta x_i)^2}{2\sigma_i^2}}$$

  - Find α and β by maximizing the likelihood function L likelihood function:

$$\frac{\partial \ln L}{\partial \alpha} = \frac{\partial}{\partial \alpha} \sum_{i=1}^{n} \left[\ln\left(\frac{1}{\sigma_i \sqrt{2\pi}} \right) - \frac{(y_i - \alpha - \beta x_i)^2}{2\sigma_i^2} \right] = \sum_{i=1}^{n} \left[-\frac{2(y_i - \alpha - \beta x_i)(-1)}{2\sigma_i^2} \right] = 0$$

$$\frac{\partial \ln L}{\partial \beta} = \frac{\partial}{\partial \beta} \sum_{i=1}^{n} \left[\ln\left(\frac{1}{\sigma_i \sqrt{2\pi}} \right) - \frac{(y_i - \alpha - \beta x_i)^2}{2\sigma_i^2} \right] = \sum_{i=1}^{n} \left[-\frac{2(y_i - \alpha - \beta x_i)(-x_i)}{2\sigma_i^2} \right] = 0$$

two linear equations with two unknowns

- Assume all σ's are the same for simplicity:

$$\sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \alpha - \sum_{i=1}^{n} \beta x_i = 0$$

$$\sum_{i=1}^{n} y_i x_i - \sum_{i=1}^{n} \alpha x_i - \sum_{i=1}^{n} \beta x_i^2 = 0$$

- We now have two equations that are linear in the two unknowns, α and β.

$$\sum_{i=1}^{n} y_i = n\alpha + \beta \sum_{i=1}^{n} x_i$$

$$\sum_{i=1}^{n} y_i x_i = \alpha \sum_{i=1}^{n} x_i + \beta \sum_{i=1}^{n} x_i^2$$

Matrix form →

$$\begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} y_i x_i \end{bmatrix} = \begin{bmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

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

Taylor Eqs. 8.10-12

  - We will see this problem again when we talk about "least squares" ("chi-square") fitting.

- EXAMPLE:
  - A trolley moves along a track at constant speed. Suppose the following measurements of the time vs. distance were made. From the data find the best value for the velocity (v) of the trolley.

Time t (seconds)	1.0	2.0	3.0	4.0	5.0	6.0
Distance d (mm)	11	19	33	40	49	61

  - Our model of the motion of the trolley tells us that:

$$d = d_0 + vt$$

- We want to find v, the slope (β) of the straight line describing the motion of the trolley.
- We need to evaluate the sums listed in the above formula:

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{6} t_i = 21\ s$$

$$\sum_{i=1}^{n} y_i = \sum_{i=1}^{6} d_i = 213\ mm$$

$$\sum_{i=1}^{n} x_i y_i = \sum_{i=1}^{6} t_i d_i = 919\ s \cdot mm$$

$$\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{6} t_i^2 = 91\ s^2$$

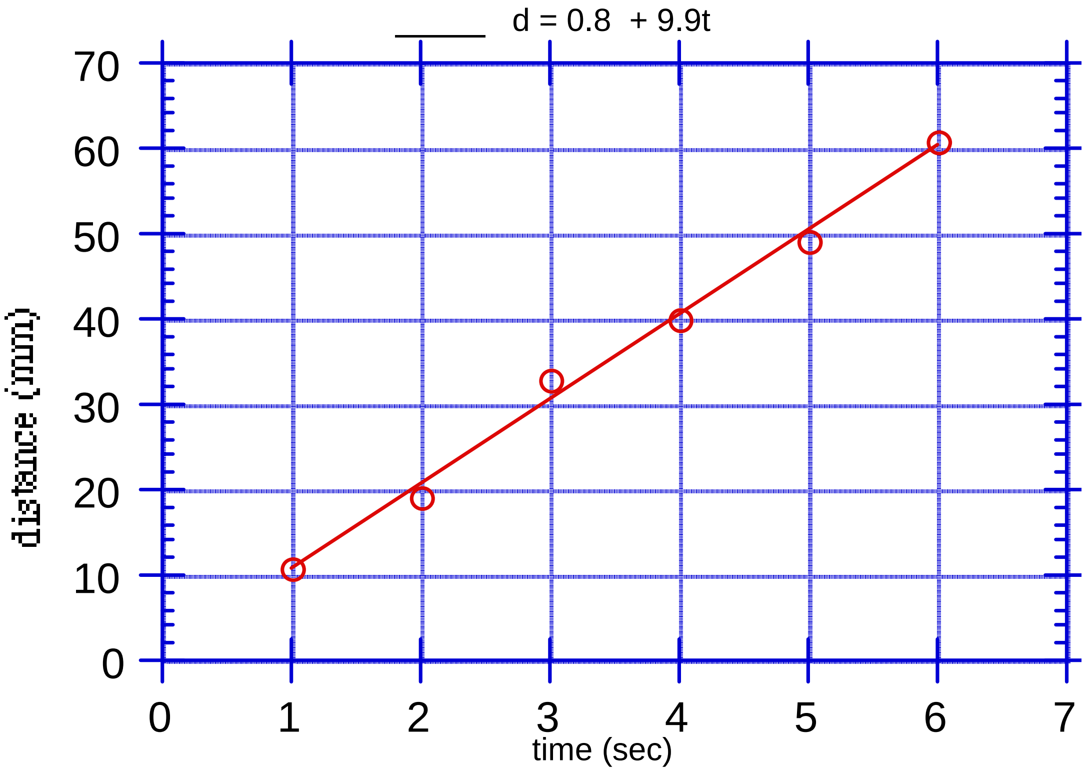
$$v = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i}{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2} = \frac{6\times 919 - 21\times 213}{6\times 91 - 21^2} = 9.9\, mm/s$$

best estimate of the speed

$$d_0 = 0.8\ mm$$

best estimate of the starting point

MLM fit to the data for $d = d_0 + vt$



- The line best represents our data.
- Not all the data points are "on" the line.
- The line minimizes the sum of squares of the deviations between the line and our data (d_i):

$$\delta = \sum_{i=1}^{n} [\text{data}_i - \text{prediction}_i]^2 = \sum_{i=1}^{n} [d_i - (d_0 + vt_i)]^2$$

Least square fit