PHYS 232 March 22, 2024

- Assignment #6 will be posted this weekend
- Formal Report due Apr. 10 @ 11 am

Last Time:

Fit data to:

$$y(x) = a_1 f_1(x) + a_2 f_2(x) + \ldots + a_m f_m(x)$$

Meas. $(x_i, y_i \pm \sigma_i)$ for $i = 1..N$

Want to determine:

$$a_1 \pm \sigma_{a_1}, \; a_2 \pm \sigma_{a_2}, \ldots, \; a_m \pm \sigma_{a_m}$$

We found the a_k values from

$$\boxed{\underline{a} = \underline{\underline{\varepsilon}}\, \underline{\beta}}$$

Diagonal elements of $\underline{\underline{\Sigma}}$ give the square of the uncertainty in the best-fit parameters

$$a_1 \pm \sqrt{\Sigma_{11}}$$
$$a_2 \pm \sqrt{\Sigma_{22}}$$
$$\vdots$$
$$a_m \pm \sqrt{\Sigma_{mm}}$$

<u>Today</u>: Nonlinear Fits

Examine the case of a non-linear fit,

i.e. $y(x)$ is <u>not</u> of the form $\sum_{k=1}^{m} a_k f_k(x)$

Eg. $y(x) = a_1 \sin(a_2 x)$

Compare & contrast linear & non-linear fits.

linear case

$$y = a_1 + a_2 x$$

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - y(x_i)}{\sigma_i} \right)^2$$

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - a_1 - a_2 x_i}{\sigma_i} \right)^2$$

$$\frac{\partial \chi^2}{\partial a_1} = 2 \sum \frac{y_i - a_1 - a_2 x_i}{\sigma_i} \left(-\frac{1}{\sigma_i} \right) = 0$$

$$\therefore \sum \frac{y_i}{\sigma_i^2} = \sum \frac{a_1 + a_2 x_i}{\sigma_i^2} \quad (1)$$

no a_1 or a_2

$$\frac{\partial \chi^2}{\partial a^2} = 2 \sum \left(\frac{y_i - a_1 - a_2 x_i}{\sigma_i} \right) \left(-\frac{x_i}{\sigma_i} \right) = 0$$

$$\sum \frac{x_i y_i}{\sigma_i^2} = \sum \frac{x_i}{\sigma_i^2} (a_1 + a_2 x_i) \quad (2)$$

no a_1 or a_2

non-linear case

$$y = a_1 \sin(a_2 x)$$

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - y(x_i)}{\sigma_i} \right)^2$$

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - a_1 \sin(a_2 x_i)}{\sigma_i} \right)^2$$

$$\frac{\partial \chi^2}{\partial a_1} = 2 \sum \frac{y_i - a_1 \sin(a_2 x_i)}{\sigma_i} \cdot \left(-\frac{\sin(a_2 x_i)}{\sigma_i} \right) = 0$$

$$\underbrace{\sum \frac{y_i \sin(a_2 x_i)}{\sigma_i^2}}_{\text{involves } a_2} = \sum \frac{a_1 \sin^2(a_2 x_i)}{\sigma_i^2} \quad (1')$$

$$\frac{\partial \chi^2}{\partial a_2} = 2 \sum \frac{y_i - a_1 \sin(a_2 x_i)}{\sigma_i} \cdot \left(-\frac{x_i a_1}{\sigma_i} \cos(a_2 x_i) \right) = 0$$

have a_1 & a_2

$$\sum \frac{x_i y_i}{\sigma_i^2} a_1 \cos(a_2 x_i) \quad (2')$$

$$= \sum \frac{x_i}{\sigma_i^2} a_1^2 \cos(a_2 x_i) \sin(a_2 x_i)$$

For linear fit, can express ① & ② as a matrix eq'n w/ a_k parameters in a single column matrix

$$\underbrace{\begin{pmatrix} \sum \frac{y_i}{\sigma_i^2} \\ \sum \frac{x_i y_i}{\sigma_i^2} \end{pmatrix}}_{\underline{\beta}} = \underbrace{\begin{pmatrix} \sum \frac{1}{\sigma_i^2} & \sum \frac{x_i}{\sigma_i^2} \\ \sum \frac{x_i}{\sigma_i^2} & \sum \frac{x_i^2}{\sigma_i^2} \end{pmatrix}}_{\underline{\underline{\alpha}}} \underbrace{\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}}_{\underline{a}}$$

$$\Rightarrow \quad \underline{a} = \underline{\underline{\alpha}}^{-1} \underline{\beta}$$

For non-linear fit, the a_k's in (1') & (2') are on both sides of eq'ns & a_2 is inside trig. fcns, cannot write down an equiv. matrix eq'n for this case.

$\Rightarrow$ need a new fitting method.

One method for non-linear fits:

Objective is still to minimize

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - y(x_i)}{\sigma_i} \right)^2$$

For example, want to minimize:

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - a_1 \sin(a_2 x_i)}{\sigma_i} \right)^2$$

Strategy 1.

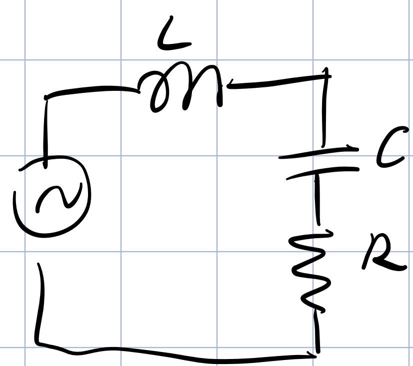
Pick a range of possible values for a_1 & a_2.

$$\left.\begin{aligned} a_{1,min} &\le a_1 \le a_{1,max} \\ a_{2,min} &\le a_2 \le a_{2,max} \end{aligned}\right\}$$

have to know something about physical system to select reasonable ranges for parameters

Eg. LRC circuit.

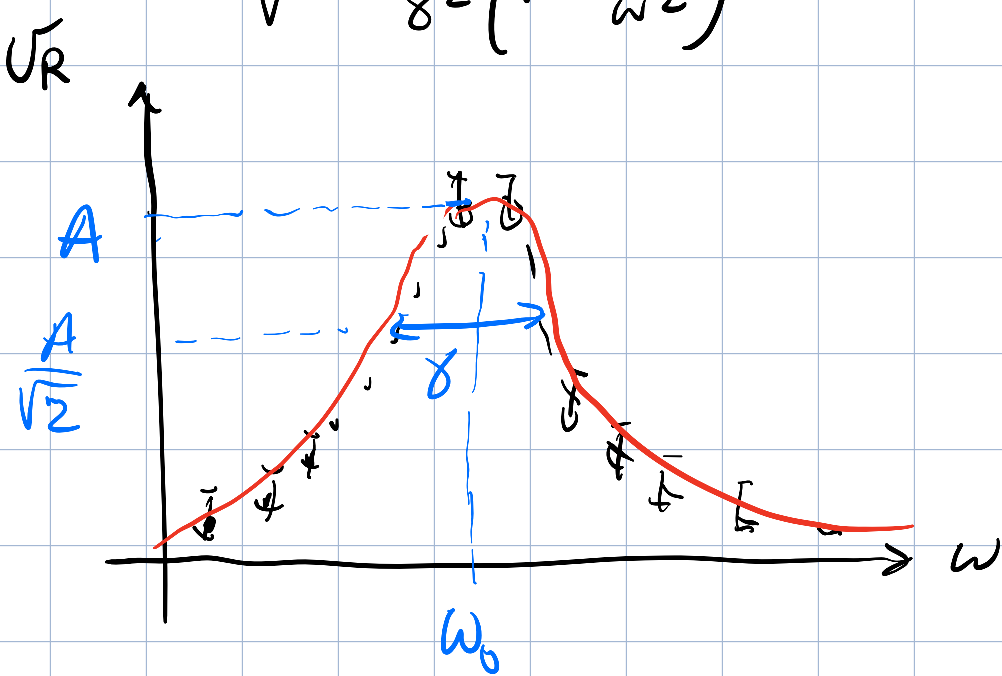
Voltage across R in:



$$V_R = \frac{A}{\sqrt{1 + \frac{\omega^2}{\gamma^2}\left(1 - \frac{\omega_0^2}{\omega^2}\right)^2}}$$

meas. V_R vs ω

→ fit parameters are A, γ, ω_0

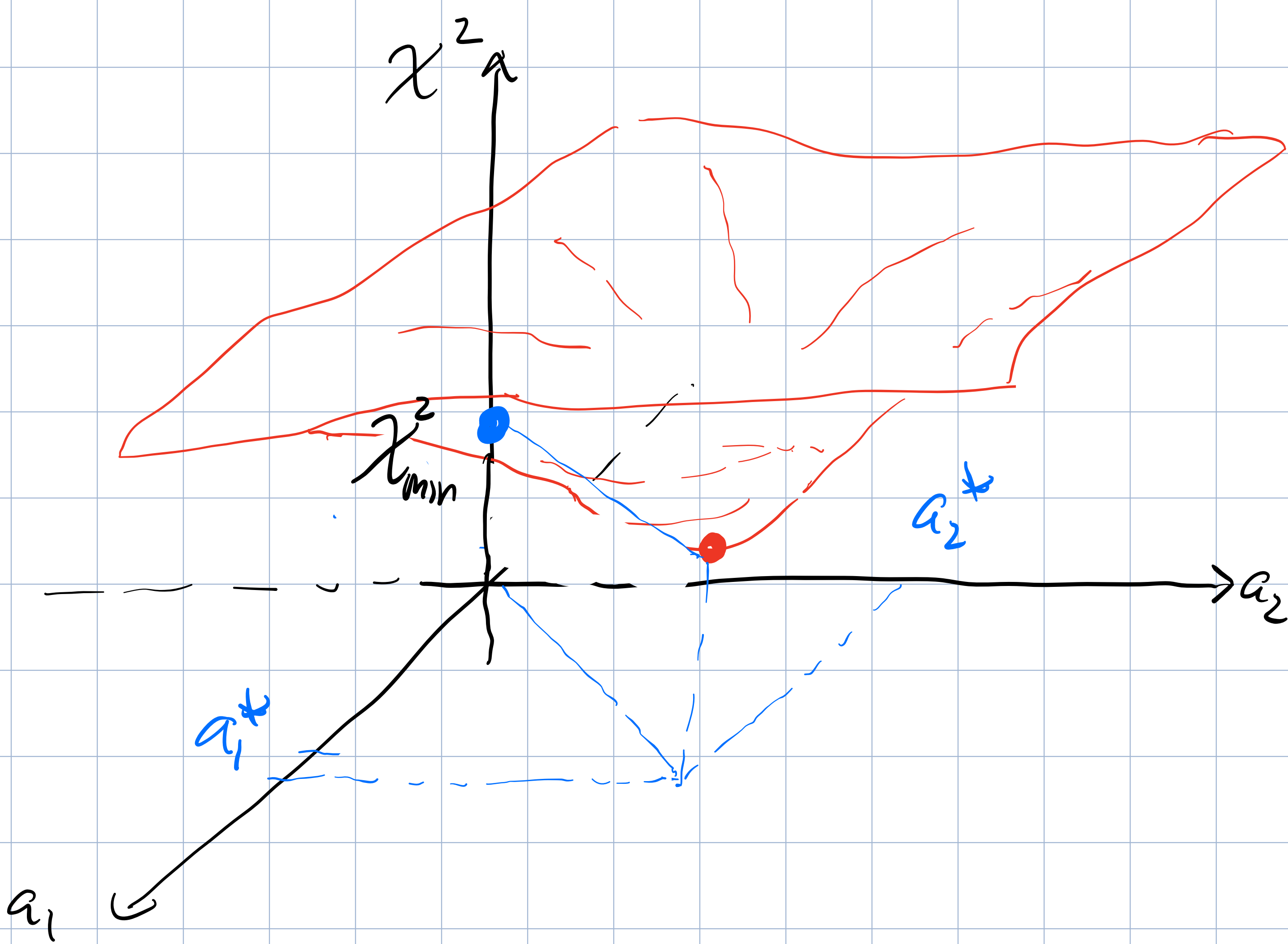


Use measured data to est. what the fit parameters are likely to be.

2. Pick a step size Δa_1 & Δa_2 for each parameter

- small Δa_1, Δa_2 good for high resolution, but takes longer to calc. all χ^2 values.

3. Evaluate χ^2 at all possible combos of (a_1, a_2). Best-fit parameters are the values that minimize χ^2.



If (a_1^*, a_2^*) give the minimum value of χ^2, then they are our estimates of the best-fit parameters.

If the non-linear fcn is very complicated, the χ^2 surface can have local & global minima. Can get trapped in a local minimum & miss the global minimum.