III. STATISTICAL ANALYSIS

Suppose you have a dataset in the form:

Frequency [Hz]	Stopping potential [V]
$f_1 \pm \delta f_1$	$V_{s1} \pm \delta V_{s1}$
$f_2 \pm \delta f_2$	$V_{s2} \pm \delta V_{s2}$
$f_3 \pm \delta f_3$	$V_{s3} \pm \delta V_{s3}$
$f_4 \pm \delta f_4$	$V_{s4} \pm \delta V_{s4}$
$f_5 \pm \delta f_5$	$V_{s5} \pm \delta V_{s5}$

The model, also known as the fit model, also known as the fit function, is linear:

$$\hat{V}_s = b_0 + b_1 f, \tag{9}$$

where $\hat{V}_s$ is the predicted value for the stopping potential, and b_0 and b_1 are the fit parameters. The former is called the y-intercept and the latter is referred to as the slope. The goal is to obtain the best-fit values for the fit parameters, $b_0 = \beta_0 \pm \delta\beta_0$ and $b_1 = \beta_1 \pm \delta\beta_1$, as well as the correlation between the fit parameters.

We note that if we perform a naive linear regression for example using MS Excel's `LINEST()` function, we incorrectly estimate the uncertainties for the fit parameters. Below, we discuss all possible cases for the given data set and present a minimal working example (MWE) to illustrate the differences.

A. Case of $\delta f_i = 0$ and $\delta V_{si} = 0$ for all i

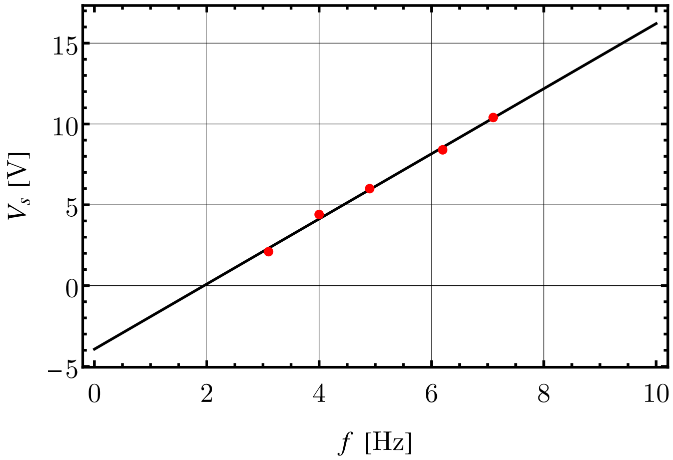
Use the simple linear regression by all means and trust in $\delta\beta_0$ and $\delta\beta_1$.

Consider the example dataset:

```
f = {3.1, 4.0, 4.9, 6.2, 7.1};
Vs = {2.1, 4.4, 6.0, 8.4, 10.4};
```

We obtain

$$b_0 = -3.93165 \pm 1.62777, \tag{10}$$
$$b_1 = 2.01416 \pm 0.309315, \tag{11}$$
$$\rho = -0.961519. \tag{12}$$



B. Case of $\delta f_i = 0$ and $\delta V_{si} \neq 0$ for all i

When the dependent variable has uncertainties, we perform a *weight fit*. We define a χ^2 function as

$$\chi^2 = \sum_{i=1}^{5} \frac{[V_{si} - \hat{V}_s(f_i)]^2}{\delta V_{si}^2} = \sum_{i=1}^{5} \frac{[V_{si} - (b_0 + b_1 f_i)]^2}{\delta V_{si}^2}. \tag{13}$$

This is just a quadratic function of b_0 and b_1. We compute the first partial derivatives with respect to b_0 and b_1, set them equal to zero, and solve them for $b_0 = \beta_0$ and $b_1 = \beta_1$:

$$\left[\frac{\partial \chi^2}{\partial b_0}\right]_{b_0=\beta_0} = 0, \quad \left[\frac{\partial \chi^2}{\partial b_1}\right]_{b_1=\beta_1} = 0. \tag{14}$$

Then we compute the hessian of the χ^2 function and evaluate it at $b_0 = \beta_0$ and $b_1 = \beta_1$:

$$\mathcal{F} = \frac{1}{2} \begin{pmatrix} \frac{\partial^2 \chi^2}{\partial b_0^2} & \frac{\partial^2 \chi^2}{\partial b_0 \partial b_1} \\ \frac{\partial^2 \chi^2}{\partial b_0 \partial b_1} & \frac{\partial^2 \chi^2}{\partial b_2^2} \end{pmatrix}_{b_0=\beta_0, b_1=\beta_1} . \tag{15}$$

This is called the Fisher information matrix. The inverse of the Fisher matrix gives the covariance matrix, $\mathcal{V}$, which looks like

$$\mathcal{V} = \mathcal{F}^{-1} = \begin{pmatrix} \sigma_0^2 & \rho\sigma_0\sigma_1 \\ \rho\sigma_0\sigma_1 & \sigma_1^2 \end{pmatrix}, \tag{16}$$

where σ_0 and σ_1 are the uncertainties in β_0 and β_1, respectively, and ρ is their correlation.

Consider the example dataset:

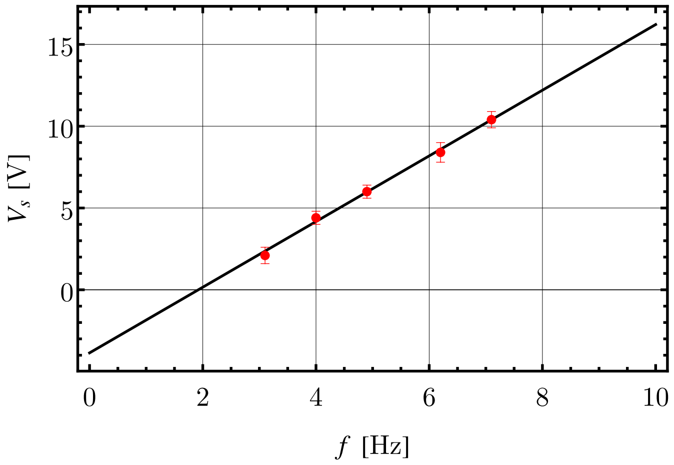
```
f = {3.1, 4.0, 4.9, 6.2, 7.1};
Vs = {2.1, 4.4, 6.0, 8.4, 10.4};
dVs = {0.5, 0.4, 0.4, 0.6, 0.5};
```

We obtain

$$b_0 = -3.85697 \pm 0.780734, \tag{17}$$

$$b_1 = 2.00722 \pm 0.154176, \tag{18}$$

$$\rho = -0.964117. \tag{19}$$



C. Case of $\delta f_i \neq 0$ and $\delta V_{si} = 0$ for all i

The weighted fit of the previous section will not work here because of vanishing uncertainties in the dependent variable. The trick is to define a new model by treating V_s as the independent variable and f as the dependent one:

$$\hat{f} = c_0 + c_1 V_s. \tag{20}$$

We repeat the analysis of the previous section by simply swapping fs by V_ss and by replacing bs by cs. We obtain the best-fit values for the fit parameters as $c_0 = \gamma_0 \pm \delta\gamma_0$ and $c_1 = \gamma_1 \pm \delta\gamma_1$. Then noting that

$$V_s = \frac{f - c_0}{c_1} = -\frac{c_0}{c_1} + \frac{1}{c_1} f, \tag{21}$$

which gives us

$$b_0 = -\frac{c_0}{c_1}, \quad b_1 = \frac{1}{c_1}, \tag{22}$$

we obtain the best-fit values for b_0 and b_1 by letting the errors propagate through

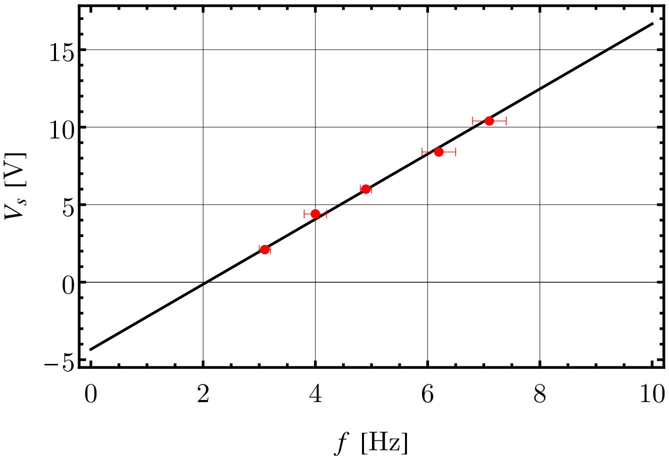
$$\beta_0 \pm \delta\beta_0 = -\frac{\gamma_0 \pm \delta\gamma_0}{\gamma_1 \pm \delta\gamma_1}, \quad \beta_1 = \frac{1}{\gamma_1 \pm \delta\gamma_1}. \tag{23}$$

Consider the example dataset:

```
f = {3.1, 4.0, 4.9, 6.2, 7.1};
df = {0.1, 0.2, 0.1, 0.3, 0.3};
Vs = {2.1, 4.4, 6.0, 8.4, 10.4};
```

We obtain

$$b_0 = -4.33441 \pm 0.524907, \tag{24}$$
$$b_1 = 2.10011 \pm 0.119775, \tag{25}$$
$$\rho = -0.967084. \tag{26}$$



D. Case of $\delta f_i \neq 0$ and $\delta V_{si} \neq 0$ for all i

In this most general case, we apply the method of *orthogonal distance regression*, where our χ^2 function is of the form

$$\chi^2 = \sum_{i=1}^{5} \left(\frac{\Delta f_i^2}{\delta f_i^2} + \frac{\Delta V_{si}^2}{\delta V_{si}^2} \right), \tag{27}$$

where each Δf_i is now an auxiliary fit parameter, and $\Delta V_{si} = b_0 + b_1(f_i + \Delta f_i) - V_i$. This is now a quadratic function of seven variables (two original fit parameters b_0 and b_1, and five Δf_i); nevertheless, the idea is the same: set the first partial derivatives equal to zero, obtain the best-fit values to obtain the Fisher information matrix. Once we have the Fisher matrix, the rest is the same as in earlier sections, namely the parts where we invert the Fisher matrix to obtain the uncertainties and the correlation.

Consider the example dataset:

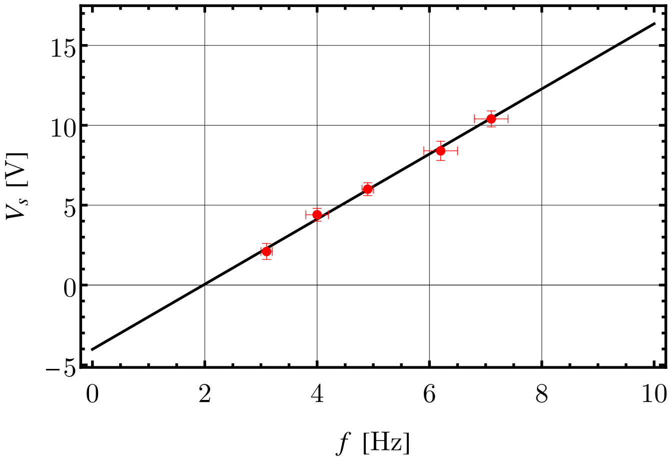
```
f = {3.1, 4.0, 4.9, 6.2, 7.1};
df = {0.1, 0.2, 0.1, 0.3, 0.3};
Vs = {2.1, 4.4, 6.0, 8.4, 10.4};
dVs = {0.5, 0.4, 0.4, 0.6, 0.5};
```

We obtain

$$b_0 = -4.02244 \pm 1.03016, \tag{28}$$

$$b_1 = 2.03759 \pm 0.213709, \tag{29}$$

$$\rho = -0.966788. \tag{30}$$



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This document can be obtained from

https://kagsimsek.github.io/files/teaching/lab7_notes.pdf

The Mathematica notebook with the code for all these cases can be obtained from

https://kagsimsek.github.io/files/teaching/mwe_stat_analysis.nb