Propagation of Systematic Uncertainties

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Methods for propagation of systematic uncertainties

You have probably become pretty comfortable by now with analyzing uncertainties in fitted parameters due to uncorrelated random errors in measured quantities. However, for many experiments systematic uncertainties are more important than random errors. Although there is no general theory of systematic uncertainties, one can usually make realistic estimates of their effects using relatively simple methods. One of the most important objectives of this course is to develop skill in analyzing systematic uncertainties and we expect you to estimate the systematic uncertainties in every derived quantity.

Let's start with a simple example. In the first experiment of this course, you will acquire data of the form $\{I_i, V_i\}$ where I is the current through and V is the voltage across a variable resistor connected in series to a battery. You will then fit the data using the model

$$V_i = \mathcal{E} - r\, I_i$$

where $\mathcal{E}$ is the open-circuit voltage of the battery and r is its internal resistance. The random uncertainties σ_I and σ_V in current and voltage measurements using a digital meter are about half of the least significant figure, primarily due to round-off. You can use standard fitting methods to deduce the parameters $\{\mathcal{E}, r\}$ and their uncertainties $\{\sigma_{\mathcal{E}}, \sigma_r\}$ due to the random errors in the current and voltage measurements. However, what happens if the calibration of meter is imperfect and all voltage readings are actually 1.5 % larger than the true voltage? What happens if there is an offset, such that all currents are about 0.1 A too small? These types of systematic errors would affect the values of the fitted parameters and those effects are often much larger than the random uncertainties estimated by least-squares analysis.

Assume that the response of the instrument is really linear, but that its calibration is imperfect. When you measure a voltage using a voltmeter, the output reading is supposed to be proportional to the input voltage and the manufacturer attempts to calibrate the instrument to read volts directly. However, the calibration cannot be expected to be perfect. Even if the performance of the instrument is truly linear, there can be a scale error and perhaps an offset. Therefore, we parametrize the instrumental response by

$$V_{\text{out}} = \lambda_V\, V_{\text{in}} + b_V$$

where V_{in} is the input voltage we seek to measure, V_{out} is the output voltage read from the meter, λ_V is a scale parameter, and b_V is an offset. Ideally, $\lambda_V \to 1$ and $b_V \to 0$ for a perfect instrument. Suppose that the specification sheet provided by the manufacturer claims that the accuracy for voltage measurements is $2\,\% \pm 0.01$, by which they mean: $\lambda_V = 1.00 \pm 0.02$ and $b_V = 0.00 \pm 0.01$ Volt. If $\lambda_V = 1.015$ for the meter that you actually use, then all of your voltage measurements would

be too high by the same factor. Your fitted value of $\mathcal{E}$ would also be too large by the same factor. We need a systematic procedure to analyze the effects of both scale and offset errors in both current and voltage upon derived quantities.

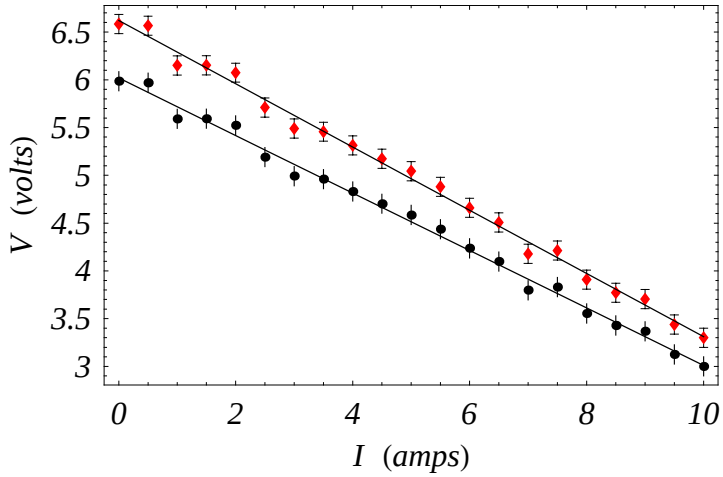
Consider the two data sets compared below with the corresponding linear fits. Both fits describe their data well, but the two sets of voltage data differ by a common scale factor λ_V. For the purposes of this illustration, we assumed that all other calibration parameters have their ideal values and we chose $\lambda_V = 1.1$, which would be a rather severe calibration error but it makes the effect easily visible. The scale error in the voltage calibration obviously affects both the vertical intercept $\mathcal{E}$ and the slope $-r$ fit to these data. The sensitivity of the physical parameters to the calibration parameters is gauged by the partial derivatives

$$\frac{\partial \mathcal{E}}{\partial \lambda_V} = \frac{\Delta \mathcal{E}}{\Delta \lambda_V}, \qquad \frac{\partial r}{\partial \lambda_V} = \frac{\Delta r}{\Delta \lambda_V}$$

where the right-hand sides are ratios between the change in the fitted quantity and the difference of the calibration parameter from its ideal value; in this $\Delta\lambda_V = 0.1$. For this data set we observe

$$\Delta\mathcal{E} \approx 0.6 \Longrightarrow \frac{\partial \mathcal{E}}{\partial \lambda_V} \approx 6.0$$

$$\Delta r \approx 0.23 \Longrightarrow \frac{\partial r}{\partial \lambda_V} \approx 2.3$$



This procedure can now be applied to each of the calibration parameters. We apply either a common scale factor or a common offset to the current or the voltage measurements, perform a least-squares fit, and determine how much the fitted parameters change from those obtained with nominal calibration parameters. This procedure is repeated for each known calibration parameter, one at a time. We assume that systematic errors in the calibration parameters are independent of each other and use standard propagation of uncorrelated errors to evaluate the net systematic uncertainties in fitted parameters according to

$$(\delta\mathcal{E}_{\text{sys}})^2 = \left(\frac{\partial \mathcal{E}}{\partial \lambda_V}\delta\lambda_V\right)^2 + \left(\frac{\partial \mathcal{E}}{\partial b_V}\delta b_V\right)^2 + \left(\frac{\partial \mathcal{E}}{\partial \lambda_I}\delta\lambda_I\right)^2 + \left(\frac{\partial \mathcal{E}}{\partial b_I}\delta b_I\right)^2$$

$$(\delta r_{\text{sys}})^2 = \left(\frac{\partial r}{\partial \lambda_V}\delta\lambda_V\right)^2 + \left(\frac{\partial r}{\partial b_V}\delta b_V\right)^2 + \left(\frac{\partial r}{\partial \lambda_I}\delta\lambda_I\right)^2 + \left(\frac{\partial r}{\partial b_I}\delta b_I\right)^2$$

where $\delta\lambda_{V,I}$ and $\delta b_{V,I}$ are estimated systematic uncertainties in the calibration constants for our instruments. We would then report our measurements in the form $\mathcal{E} \pm \sigma_{\mathcal{E}} \pm \delta\mathcal{E}_{\text{sys}}$ and $r \pm \sigma_r \pm \delta r_{\text{sys}}$ where the first uncertainty is random and the second systematic. Sometimes the two uncertainties are combined in quadrature, such that $(\delta\mathcal{E})^2 = \sigma_{\mathcal{E}}{}^2 + (\delta\mathcal{E}_{\text{sys}})^2$ and $(\delta r)^2 = \sigma_r{}^2 + (\delta r_{\text{sys}})^2$, but one should always remain aware of the relative sizes of the random and systematic contributions. Your lab reports should always compare random and systematic uncertainties.

In general we must evaluate the partial derivatives numerically — adjust each parameter one at a time, repeat the analysis, and determine the changes in the fitted parameters — but for the special case of a linear model and linear calibration parameters, we can evaluate and understand the partial derivatives algebraically instead. The substitutions

$$V \to \lambda_V\, V + b_V\,,\;\; I \to \lambda_I\, I + b_I \implies \lambda_V\, V_i + b_V \;=\; \mathcal{E} \;-\; r\,(\lambda_I\, I_i + b_I)$$

transform our model to

$$\lambda_V\, V_i + b_V \;=\; \mathcal{E} \;-\; r\,(\lambda_I\, I_i + b_I)$$

and after some rearrangement we find that

$$V_i \;=\; {\lambda_V}^{-1}(\mathcal{E} - b_V - r\, b_I) \;-\; r\,\lambda_I\,{\lambda_V}^{-1}\, I_i$$

takes the form

$$V_i \;=\; \mathcal{E}_{\text{eff}} \;-\; r_{\text{eff}}\, I_i$$

where

$$\mathcal{E}_{\text{eff}} \;=\; {\lambda_V}^{-1}(\mathcal{E} - b_V - r\, b_I)$$
$$r_{\text{eff}} \;=\; r\,\lambda_I\,{\lambda_V}^{-1}$$

are *effective* or modified parameters. If we assume that the changes in these parameters are small, the derivatives become

$$\frac{\partial \mathcal{E}_{\text{eff}}}{\partial \lambda_V} = -\frac{\mathcal{E}_{\text{eff}}}{\lambda_V} \implies \frac{\partial \mathcal{E}}{\partial \lambda_V} \approx -\mathcal{E}$$
$$\frac{\partial \mathcal{E}_{\text{eff}}}{\partial b_V} \;=\; -{\lambda_V}^{-1} \implies \frac{\partial \mathcal{E}}{\partial b_V} \approx -1$$
$$\frac{\partial \mathcal{E}_{\text{eff}}}{\partial \lambda_I} = 0 \implies \frac{\partial \mathcal{E}}{\partial \lambda_I} \approx 0$$
$$\frac{\partial \mathcal{E}_{\text{eff}}}{\partial b_I} \;=\; -r\,{\lambda_V}^{-1} \implies \frac{\partial \mathcal{E}}{\partial b_i} \approx -r$$
$$\frac{\partial r_{\text{eff}}}{\partial \lambda_V} = -\frac{r_{\text{eff}}}{\lambda_V} \implies \frac{\partial r}{\partial \lambda_V} \approx -r$$
$$\frac{\partial r_{\text{eff}}}{\partial b_V} \;=\; 0 \implies \frac{\partial r}{\partial b_V} \approx 0$$
$$\frac{\partial r_{\text{eff}}}{\partial \lambda_I} \;=\; \frac{r_{\text{eff}}}{\lambda_I} \implies \frac{\partial r}{\partial \lambda_I} \approx r$$
$$\frac{\partial r_{\text{eff}}}{\partial b_I} \;=\; 0 \implies \frac{\partial r}{\partial b_I} \approx 0$$

The intercept $\mathcal{E}$ scales with the voltage calibration factor or shifts with its offset, but the vertical intercept insensitve to scaling the horizontal variable. The effect of a current offset upon the voltage intercept is proportional to the slope r — there is little effect if the slope is flat or a large effect if it is steep. Similarly, the slope r is insensitive to offsets but is multiplied by a small change of scale, such that $\Delta r \approx \pm r\,\Delta\lambda$. These algebraic relationships conform perfectly with one's expectations based upon plotting rescaled or shifted data. Thus, we obtain

$$(\delta\mathcal{E}_{\text{sys}})^2 \;=\; (\mathcal{E}\,\delta\lambda_V)^2 \;+\; (\delta b_V)^2 \;+\; (r\,\delta b_I)^2$$
$$(\delta r_{\text{sys}})^2 \;=\; (r\,\delta\lambda_V)^2 \;+\; (r\,\delta\lambda_I)^2$$

where $\mathcal{E}$ and r are the fitted parameters using ideal calibration parameters ($\lambda_{V,I} \to 1$, $b_{V,I} \to 0$).

Suppose the fitted values are $\mathcal{E} = 5.91 \pm 0.03$ Volt and $r = 0.282 \pm 0.007\,\Omega$. Also suppose that the specification sheet provided by the multimeter manufacturer claims that $\delta\lambda = 0.02$ and $\delta b = 0.01$ for both voltage or current measurements, where b is in the appropriate units. The algebraic method then gives $\delta\mathcal{E}_{sys} = 0.12$ Volt and $\delta r_{sys} = 0.008\,\Omega$. Under these conditions the systematic uncertainty dominates for the voltage measurement while for the internal resistance systematic and random uncertainties are similar. Obviously, one cannot neglect the systematic errors and must consider both in drawing conclusions from an experiment.

Notice that systematic uncertainties are not reduced by taking more measurements. When systematic uncertainties are negligible, we can improve the accuracy of fitted quantities by taking more data to reduce the effect of random uncertainties. Once the random contributions to uncertainties in fitted parameters are reduced to the level of the systematic uncertainties, taking additional data provides little further improvement in the quality of the final results. Therefore, one must carefully consider systematic uncertainties when designing the experiment, for they ultimately determine its accuracy.

What if your data were collected using more than one scale setting of a particular meter? You would then assume that there are independent sets of calibration parameters for each scale and would have to apply scale factors or offsets to subsets of your data and evaluate their effects upon fitted parameters numerically — the algebraic method would no longer work. This is more work, but the computer won't complain. However, this shows that it is important to record in your lab notebook the scales that were used to acquire your data and to make note of all changes of scale. Try to minimize the number of scale changes, if that can be done without too large a fraction of your data near either end of the scale.

practice problem

Copy the data tabulated below into an *Excel* spreadsheet and use the *LinFit* macro to deduce $\mathcal{E}$ and r assuming ideal calibration parameters. Then evaluate the probability, $P[\chi^2_{red}]$, for your fit. Is it acceptable? Next, assume that $\delta\lambda = 0.03$ and $\delta b = 0.02$ for both current and voltage and estimate the systematic errors in $\mathcal{E}$ and r algebraically. Then evaluate the contributions of each calibration to the systematic uncertainties numerically by using *LinFit* on suitably modified data. These two methods should give similar results, but conducting this exercise manually is instructive. The numerical method is often easier than the algebraic method, especially for nonlinear models.

I	V	σ_V
0.00	6.0	0.1
0.50	5.9	0.1
1.00	5.7	0.1
1.50	5.5	0.1
2.00	5.4	0.1
2.50	5.4	0.1
3.00	5.0	0.1
3.50	4.9	0.1
4.00	4.9	0.1
4.50	4.6	0.1
5.00	4.5	0.1
5.50	4.4	0.1
6.00	4.1	0.1
6.50	4.2	0.1
7.00	3.8	0.1
7.50	3.8	0.1
8.00	3.7	0.1
8.50	3.6	0.1
9.00	3.2	0.1
9.50	3.0	0.1
10.00	3.0	0.1