Chapter 15. Modeling of Data

15.0 Introduction

Given a set of observations, one often wants to condense and summarize the data by fitting it to a "model" that depends on adjustable parameters. Sometimes the model is simply a convenient class of functions, such as polynomials or Gaussians, and the fit supplies the appropriate coefficients. Other times, the model's parameters come from some underlying theory that the data are supposed to satisfy; examples are coefficients of rate equations in a complex network of chemical reactions, or orbital elements of a binary star. Modeling can also be used as a kind of constrained interpolation, where you want to extend a few data points into a continuous function, but with some underlying idea of what that function should look like.

The basic approach in all cases is usually the same: You choose or design a *figure-of-merit function* ("merit function," for short) that measures the agreement between the data and the model with a particular choice of parameters. The merit function is conventionally arranged so that small values represent close agreement. The parameters of the model are then adjusted to achieve a minimum in the merit function, yielding *best-fit parameters*. The adjustment process is thus a problem in minimization in many dimensions. This optimization was the subject of Chapter 10; however, there exist special, more efficient, methods that are specific to modeling, and we will discuss these in this chapter.

There are important issues that go beyond the mere finding of best-fit parameters. Data are generally not exact. They are subject to *measurement errors* (called *noise* in the context of signal-processing). Thus, typical data never exactly fit the model that is being used, even when that model is correct. We need the means to assess whether or not the model is appropriate, that is, we need to test the *goodness-of-fit* against some useful statistical standard.

We usually also need to know the accuracy with which parameters are determined by the data set. In other words, we need to know the likely errors of the best-fit parameters.

Finally, it is not uncommon in fitting data to discover that the merit function is not unimodal, with a single minimum. In some cases, we may be interested in global rather than local questions. Not, "how good is this fit?" but rather, "how sure am I that there is not a *very much better* fit in some corner of parameter space?" As we have seen in Chapter 10, especially §10.9, this kind of problem is generally quite difficult to solve.

The important message we want to deliver is that fitting of parameters is not the end-all of parameter estimation. To be genuinely useful, a fitting procedure

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should provide (i) parameters, (ii) error estimates on the parameters, and (iii) a statistical measure of goodness-of-fit. When the third item suggests that the model is an unlikely match to the data, then items (i) and (ii) are probably worthless. Unfortunately, many practitioners of parameter estimation never proceed beyond item (i). They deem a fit acceptable if a graph of data and model "looks good." This approach is known as *chi-by-eye*. Luckily, its practitioners get what they deserve.

CITED REFERENCES AND FURTHER READING:

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15.1 Least Squares as a Maximum Likelihood Estimator

Suppose that we are fitting N data points (x_i, y_i) $i = 1, \ldots, N$, to a model that has M adjustable parameters a_j, $j = 1, \ldots, M$. The model predicts a functional relationship between the measured independent and dependent variables,

$$y(x) = y(x; a_1 \ldots a_M) \tag{15.1.1}$$

where the dependence on the parameters is indicated explicitly on the right-hand side.

What, exactly, do we want to minimize to get fitted values for the a_j's? The first thing that comes to mind is the familiar least-squares fit,

$$\text{minimize over } a_1 \ldots a_M : \quad \sum_{i=1}^{N} [y_i - y(x_i; a_1 \ldots a_M)]^2 \tag{15.1.2}$$

But where does this come from? What general principles is it based on? The answer to these questions takes us into the subject of *maximum likelihood estimators*.

Given a particular data set of x_i's and y_i's, we have the intuitive feeling that some parameter sets $a_1 \ldots a_M$ are very unlikely — those for which the model function $y(x)$ looks *nothing like* the data — while others may be very likely — those that closely resemble the data. How can we quantify this intuitive feeling? How can we select fitted parameters that are "most likely" to be correct? It is not meaningful to ask the question, "What is the probability that a particular set of fitted parameters $a_1 \ldots a_M$ is correct?" The reason is that there is no statistical universe of models from which the parameters are drawn. There is just one model, the correct one, and a statistical universe of data sets that are drawn from it!

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