Assessing How Well a Model Fits the Data

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"Best" Fit

- Given a model depending on some parameters, and some data, we have said that certain parameter values "best" fit the data if they minimize the error quantified by the sum of the squares of the residuals:

$$E = \sum_{j=1}^{J} R_j^2$$

- Each residual R_j is the difference between the observed value y_j and the value the model predicts for this observation.
- While E quantifies the relative quality of different fits, the value of E is not so easy to interpret.

RMS Error

- The RMS error of a fit with residuals $R_1, \ldots, R_J$ is
$$\text{RMS error} = \sqrt{\frac{1}{J}\sum_{j=1}^{J} R_j^2}$$
- Minimizing the RMS error is equivalent to minimizing the sum-of-squares error E, but the RMS error has a more natural interpretation.
- The RMS error has the same units as the residuals and the data, unlike E.
- It is the root-mean-square average of the residuals, so it is not proportional to the number of data points like E is.

Does a parameter improve the model?

- Suppose we want to compare a model $f(t; \beta_1, \ldots, \beta_k, \beta_{k+1})$ to the model $f(t; \beta_1, \ldots, \beta_k, 0)$ with one fewer parameter.
- The best fit with the former model will always have an error no larger than the best fit with the latter model.
- How can we tell if the improvement is enough to make the additional parameter worth using?
- One approach is to develop a statistical model for the errors, in order to quantify the “significance” of the improvement.
- More simply (perhaps too simply), one can make a value judgment that (say) a 1% improvement is not worth the complication, but a 10% improvement is.

Does the parameter improve predictions?

- If the goal of the model is to predict data that hasn't yet or can't be measured, then we can assess whether the model with the additional parameter makes better predictions.
- Keep in mind that the more complicated model might make worse predictions than the simpler model.
- Thus, comparing the models' prediction residuals is more of a "fair fight" than comparing their residuals for the fitted data.
- How can we assess the quality of the predictions without waiting for new data to be available?

Training and Test Data

- A standard way to assess predictability of a model for data taken at a sequence of times starts by dividing the data into two time intervals.
- The data from the first time interval is called the training data set; the data from the second time interval is called the test data.
- The basic experiment is fit the model to the training data only, then see how well the parameters that best fit the training data are able to predict the test data.
- What proportion of the data to put in the training set depends on how much data you have and how far into the future you want the model to predict.

Interpreting the Results

- The RMS error for the test data, both by itself and in comparison with the RMS error for the training data, give some assessment of the model's predictiven power. However, comparing to the training RMS error is complicated if the two data sets have different amounts of variability.
- Comparing the test data RMS errors for two different models is a reasonable way to assess which makes better predictions (for the time interval of the test data, at least).
- Whatever conclusions you draw, they are more convincing if tested on multiple data sets.