Homework 6

Due Friday, 9 March, at the beginning of class. Print out and turn in any Python/IDL/Matlab code you write.

Reading Assignment: Read Wall & Jenkins, Chapter 6, and Chapter 4 sections 4.1 & 4.2.

1 Introduction to χ^2 Minimization

The goal of this problem is to use χ^2 minimization to find a best fit line to a set of data, and to test the goodness-of-fit of the model to the data.

Download the data `hw6.dat` from the `Homework Assignments/data` folder. The data is in 3 column format x_i, y_i, σ_{y_i}, where the first column is data x value, second column is data y value, and the third column is the (known) uncertainty (square root of the variance) in the y value. (Assume the x values have no uncertainty.) For this data set, assume the data are independent, and that the y_i have Gaussian distributed noise (uncertainties). Our model for the data are that they lie along a line, $y_i = f(x_i; \theta_0, \theta_1) = \theta_0 + \theta_1 x_i$.

a) Write down the χ^2 statistic for the N-row 2-column datavector $\{x_i, y_i\}$, as a function of y_i, $\sigma^2_{y_i}$ and $f(x_i; \theta_0, \theta_1)$.

b) Use a minimization algorithm such as the `scipy.optimize.fmin` in Python, `amoeba` procedure in IDL, or the `fminunc` function in Matlab to find the minimum-χ^2 values of θ_0 and θ_1. Plot the data (w/error bars) along with your best-fit line. Using chi-by-eye, how well does the best-fit line fit the data (too well, well, not great, lousy)?

c) Report your minimum-χ^2 value, degrees of freedom (careful!), and probability to exceed (PTE) (one minus the cumulative probability) for your value of χ^2. How consistent is the (optimized) model with the data? Does this result agree with your chi-by-eye from part b)?

Here, you can see that mimimum-χ^2 estimation has the advantage of giving us a "goodness-of-fit" parameter which tells us how reasonable our model is (a line in this case).

2 Uncertainties for minimum-χ^2 Estimators

The goal of this problem is to understand how to estimate uncertainties and covariances matrices for minimum-χ^2 estimators.

In this problem, you are going to estimate the uncertainties on the line fit parameters that you obtained in Problem 1 above. You need to have successfully completed Problem 1 before proceeding here. Numerically, you should have obtained minimum-χ^2 parameter estimators of $\theta_0 = 37.5, \theta_1 = 3.14$ and $\chi^2 = 82.8$ at the minimum. Fix your code before proceeding if you did not obtain these values.

First, estimate the 2×2 covariance matrix for the fit parameters θ_0, θ_1 semi-analytically. To do this:

a) Write down the elements of the 2×2 curvature matrix $\mathcal{F}$ by taking the second derivatives of $\ln \mathcal{L}(\hat{\theta})$. (In this case, $\ln \mathcal{L}(\hat{\theta}) = -\chi^2/2$ from Prob. 1a above.)

b) Plug the data into your results from a) evaluated at the MLE values of θ_0, θ_1 to calculate a numerical estimate of the Fisher matrix $\hat{F}$

c) Invert $\hat{F}$ to find the covariance matrix $C_{\vec{\theta}}$ for the estimators $\hat{\vec{\theta}}$.

d) From the covariance matrix, what is your uncertainty on θ_0, marginalizing over θ_1, and for θ_1 marginalizing over θ_0, assuming the estimators are joint Gaussian distributed. (Hint: recall your results from Homework 3)

e) What is the correlation coefficient ρ in the uncertainties between the two parameters? Do you expect the parameter estimators to be correlated? Why or why not?

Now, you will numerically find $\Delta\chi^2$ contours and confidence regions for the two variables.

f) Evaluate the χ^2 statistic on a grid of points in the θ_0, θ_1 plane, centered on your mimimum-χ^2 values for these parameters, and with sufficient density to make the following contour plots look "smooth", i.e., the grid should be much smaller than the uncertainties in the parameter estimators. Using your grid map of χ^2, make a contour plot in the θ_0, θ_1 plane of $\Delta\chi^2$ with contours at $\Delta\chi^2 = 1^2, 2^2, 3^2 = 1, 4, 9$. Explain how the contours, projected onto the θ_0 and θ_1 axes are related to the marginal uncertainties for these two parameters. How do these marginal uncertainties compare to those you calculated from the curvature matrix in d)?

g) Using your grid map from f), plot the 68.3% and 95.4% confidence regions for the two parameters. What values of $\Delta\chi^2$ do these regions correspond to?

Note: the "true" parameter values used to generate the data are $\theta_0 = 42, \theta_1 = 3.2$. Where does this lie with respect to your confidence regions?