CAP Program Tutorial: Model Fitting in Python

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Please retrieve the zip file from http://github.com/capprogram/FittingTutorial and unzip the file in your working space. In the folder there are python codes (paramfit1.py and paramfit2.py) that contain partial answers for you to fill out. Two additional activities are codes to write on your own. Solutions are also available for all of the activities (with the extension .sln).

Why do we fit models to our data?

- To understand the underlying distribution of our data
- To test hypotheses or competing theoretical models
- To predict values for future observations

These are just a few examples of why we might want to fit a model to our data. In this tutorial we will go through the basics of fitting model parameters to data using two different techniques: Maximum Likelihood Estimation and Bayesian Analysis.

Part I: Linear Least Squares Fitting & Maximum Likelihood Estimation:

Least Squares Fitting is based on the assumption that the uncertainty in your measurements follows a Gaussian distribution. In the linear case, the best solution is given by the slope & y-intercept parameters that minimize the root mean square (rms) of the residuals in the y-direction.

The rms squared is given by: $rms^2 = \sum \frac{(y_i - (\alpha x_i + \beta))^2}{\sigma_i^2}$ where x_i is the independent variable, y_i is the dependent variable with uncertainty σ_i, and α and β are the slope and y-intercept parameter values.

Least Squares Fitting falls within the category of parameter fitting known as *Maximum Likelihood Estimation (*MLE). In this method, we measure the likelihood for a given model using the χ^2 statistic:

The likelihood is given by: $L = \exp\left(\frac{-\chi^2}{2}\right)$ where $\chi^2 = \sum \frac{(y_{value,i} - y_{model,i})^2}{\sigma_i^2}$

To find the MLE solution to our model, we maximize the likelihood function by taking the derivative with respect to each parameter (the slope and y-intercept in the case of a linear fit) and by solving for where each derivative is equal to 0. To simplify the math, we first take the natural log of the likelihood function. For least squares fitting, it is possible to obtain an analytical solution for the slope and y-intercept. The derivation is shown below:

take the natural log of the likelihood function $\ln(L) = -\left(\frac{1}{2}\right)\chi^2 = -\left(\frac{1}{2}\right)\sum \frac{(y_i - (\alpha x_i + \beta))^2}{\sigma_i^2}$

take the derivatives of ln(L) with respect to α and β and set those equations to 0

$$\frac{d\ln(L)}{d\alpha} = -1 \frac{\sum (y_i - (\alpha x_i + \beta))(-x_i)}{\sigma_i^2} = 0 \qquad \frac{d\ln(L)}{d\beta} = -1 \frac{\sum (y_i - (\alpha x_i + \beta))(-1)}{\sigma_i^2} = 0$$

if we assume σ_i are all the same, we have two equations for two unknowns to solve

eqn 1: $\sum y_i x_i - \alpha \sum x_i^2 - \beta \sum x_i = 0$ **eqn 2:** $\sum y_i - \alpha \sum x_i - N\beta = 0$

multiply eqn 1 by N and multiply eqn 2 by $\sum x_i$

eqn1: $N \sum y_i x_i - N\alpha \sum x_i^2 - N\beta \sum x_i = 0$ **eqn2:** $\sum x_i \sum y_i - \alpha \sum x_i \sum x_i - N\beta \sum x_i = 0$

now we can set these two equations equal to each other and solve for α

$$N \sum y_i x_i - N\alpha \sum x_i^2 = \sum x_i \sum y_i - \alpha \left(\sum x_i\right)^2$$

$$\alpha = \frac{\sum x_i \sum y_i - N \sum (x_i y_i)}{\left(\sum x_i\right)^2 - N \sum x_i^2}$$ *divide top and bottom by N^2* $$\alpha = \frac{\frac{1}{N^2} \sum x_i \sum y_i - \frac{1}{N} \sum (x_i y_i)}{\frac{1}{N^2}\left(\sum x_i\right)^2 - \frac{1}{N} \sum x_i^2}$$

$$\alpha = \frac{\bar{x}\,\bar{y} - \overline{xy}}{\bar{x}\,\bar{x} - \left(\overline{x^2}\right)}$$ *where the bar over the variable signifies the mean value of that quantity*

now we can go back and solve for β:

from **eqn 2** $N\beta = \sum y_i - \alpha \sum x_i$ ====> $\beta = \frac{1}{N} \sum y_i - \frac{\alpha}{N} \sum x_i$ ====> $\beta = \bar{y} - \alpha \bar{x}$

For more complicated functions or if the uncertainties are not uniform, the derivatives of the likelihood may not be possible to solve analytically, and we can use programs such as **np.polyfit** to determine the parameters numerically.

Activity 1: paramfit1.py

In paramfit1.py we create fake data with known slope and y-intercept. We then compute the maximum likelihood estimated slope and y-intercept for the fake data. Fill in lines ending with "?" Solutions are provided in paramfit1.py.sln

a) Run the program paramfit1.py and plot the data. What does **npr.normal** do?

b) Read over the MLE derivation for the linear least squares analytical solution (above) and compute the slope and y-intercept for the fake data set. Plot the best fit solution on top of the data. What is the assumption that we made for the uncertainties on our fake data?

c) For linear least squares fitting, we can obtain analytical solutions to the uncertainties on the slope and y-intercept estimates, which I have provided below.

$$\sigma_\alpha = \sqrt{\frac{\sum (y_i - (\alpha x_i + \beta))^2}{(N-2) \sum (x_i - \bar{x})^2}}$$ $$\sigma_\beta = \sqrt{\left(\frac{\sum (y_i - (\alpha x_i + \beta))^2}{N-2}\right) * \left(\frac{1}{N} + \frac{(\bar{x})^2}{\sum (x_i - \bar{x})^2}\right)}$$

See http://mathworld.wolfram.com/LeastSquaresFitting.html for the full derivation. Compute the uncertainties for the slope and y-intercept analytically. Which parameter has larger fractional uncertainty?

Read up on **np.polyfit**: http://docs.scipy.org/doc/numpy/reference/generated/numpy.polyfit.html

d) Use **np.polyfit** to compute the MLE slope and y-offset for the data set. Do you get the same result as in the analytical case from part b? Note that **np.polyfit** does not automatically take an array of uncertainties on the y value. If our uncertainties on each data point are different, we can input an optional weight vector: **fit=np.polyfit(xval, yval, 1, w=1/sig)** where sig is an array containing the uncertainty on each data point. Note that the input is 1/sig rather than 1/sig**2 as you might expect from the equations above. The np.polyfit function squares the weight value within the source code.

In this example we have assumed that the uncertainty on all of our data points is the same. This simplified assumption is often not the case. If the uncertainties are different, then must include each data point's uncertainty within the MLE calculation.

e) Another method to determine the uncertainties is to use the covariance matrix:

$$C=\begin{pmatrix}\sigma_{\alpha}^{2} & cov(\alpha,\beta)\\ cov(\alpha,\beta) & \sigma_{\beta}^{2}\end{pmatrix}$$ which is the inverse of the Hessian Matrix (in pre-tutorial reading)

np.polyfit will compute the covariance matrix numerically if you add cov= “True” to the **np.polyfit** function call. Print out the uncertainties computed using the covariance matrix. Are they the same as the analytical solution? What happens to the uncertainties if you increase/decrease the number of data points? What happens to the percentage difference between the analytical and numerical methods if you increase/decrease the number of data points?

Optional Activity 2: zombies 1

If you are running low on time, skip this activity on move on to Part II. For this activity you will write your own code, but remember that you can take portions of previous code to make the process faster. Pull up the python quick reference card (http://user.physics.unc.edu/~sheila/PythonQuickReference.pdf) and codes from previous tutorials to help you write the code for this activity. Please feel free to work together on this part. My solutions are provided in zombies1.py.sln

A virus has gotten out that is turning humans into zombies. You have been recording the % of zombies ever since the outbreak (~14 days ago). However the power has gone out for the past four days and your generator just kicked in allowing you to analyze the data and determine when there will be no humans left (% humans = [1-% zombies] = 0). Your data are in percentzombie.txt where time=0 is the present day (time = -14 is 14 days ago when you started taking data).

a) Read in your data and plot it as time vs. % human as blue stars. Our best estimate of the uncertainty on the time at which you take each data point about the zombie percentage that is about half a day. ***Note that we are putting time on the y-axis because it is the variable with the measurement errors.***

b) Evaluate the MLE slope & y-intercept and overplot the best fit line in green. What does the y-intercept value mean in the context of this situation? Are you a zombie?

c) In the above step you have fit the data minimizing residuals in the y-direction (time). How could you use **np.polyfit** to fit the data minimizing residuals in the x-direction (% humans)? Keep in mind that you can rewrite a line y=a*x + b as x =(1/a)*y – (b/a). Over plot this fit in red – how does the y-intercept value change? In which variable should you minimize residuals to get the most accurate prediction of the time when there will be no humans left?

d) In a new plotting window, plot the residuals of the linear fit from step 2 as green stars. Evaluate the reduced χ^2 for your data (refer to the Correlations and Tests Tutorial from June 9). Is your model a good fit to the data? Often times we think the R value from the Pearson correlation test tells us how good the fit is, but a reduced χ^2 actually gives a better estimate of how good your model is, not just whether the correlation is strong.

e) What happens when you increase the order of the fit? Overplot the higher order fits on figure 1. What happens to the residuals if you increase the order of the fit (see **np.polyfit**, and **np.polyval**)? Overplot the new residuals in time compared to the residuals from the linear fit on figure 2.

f) Calculate the reduced χ^2 for these higher order fits – do they yield as good a fit to the data as the linear fit?

Part II: Bayesian Estimation:

Bayesian analysis presents an entirely different philosophy in determining model parameters compared to the traditional MLE. In part I we determined the likelihood of the data given the model, which involved one model and many data sets. In the Bayesian framework, we determine the likelihood of the model given the data, which involves many models and one data set.

Bayes's Theorem $$P(M|D)=\frac{P(D|M)*P(M)}{P(D)}$$

$P(D|M)$ --- the likelihood (as in part I), note this is read as "probability of data given model"

$P(M)$ --- the prior probability (known information about the model, an example is a flat prior, which weights all parameter possibilities equally)

$P(D)$ --- probability of the data, essentially a normalization factor

$P(M|D)$ --- the posterior probability of the model given the data

In Bayesian analysis we turn from maximizing the likelihood function and finding the single "best" set of parameters to constructing the distribution of likelihoods for a grid of parameter space where we think our parameters are likely to be. We first must set up the model grid with known *priors* on the possible range and distribution of our model parameters. We then compute the combined likelihood of the data and the prior for all possible values over the defined grid of parameters to obtain our posterior probability distribution. In many problems scientists will assume a flat prior (all grid points weighted equally), and then the posterior probability distribution is proportional to the likelihood.

Activity 3: paramfit2.py

In paramfit2.py we use the same fake data set created in paramfit1.py. This time, however, we will determine the slope and y-intercept through Bayesian analysis by constructing a grid of possible values of the slope and y-intercept and evaluate the likelihood of each grid point. Fill in any lines ending in "?"

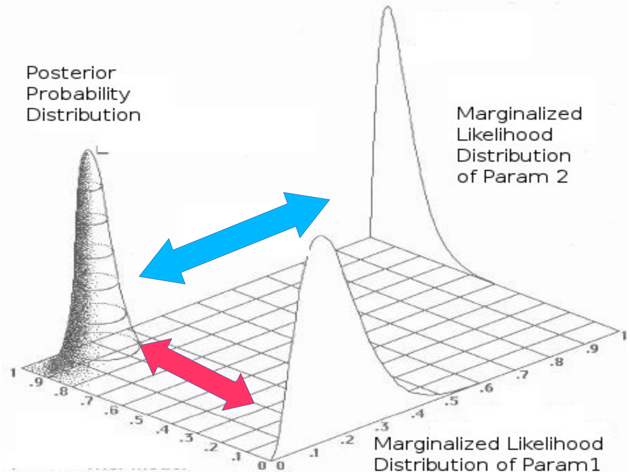
a) Run paramfit2.py and plot the fake data. Set up grids for the y-intercept and slope values that we are considering. What values are we considering for the slope and the y-intercept? What is the implicit prior on the slope and y-intercept that we are considering?

b) Check that the model space from the choice of grid values for both the y-intercept and slope is also uniformly distributed. To do this plot a series of lines using all possible y-intercepts (y=x+beta_i) and then all possible slopes (y=x*alpha_i). Is the model space from the y-intercept parameter evenly spaced? Is the model space from the slope parameter evenly spaced? Note that the evenly spaced grid for the slope values does not result in an evenly spaced grid set of angles (or tan[y/x])

c) Read through: http://jakevdp.github.io/blog/2014/06/14/frequentism-and-bayesianism-4-bayesian-in-python/ How can we write a prior that compensates for the non-uniform weighting of the angles.
Note that in this article alpha and beta are reversed: y= α + β*x

d) Compute the posterior probability distributions for the entire grid assuming 1) a flat prior on the values of the slopes and y-intercepts (non-uniform in the angle) and 2) the prior that compensates and creates a uniform angular distribution. Pay attention to where the prior appears in the equation for computing the likelihood.

e) Now that we have our entire likelihood distribution over the entire parameter space, we can see the distributions of our individual parameters by summing the probability distribution of the other parameters (i.e., if we want to look at the posterior likelihood distribution of the slope, we sum over the likelihood distribution of the y-intercept). We call this procedure "marginalizing." (see diagram at right)


Posterior Probability Distribution
Marginalized Likelihood Distribution of Param 2
Marginalized Likelihood Distribution of Param1
1
.9
.8
.7
.6
.5
.4
.3
.2
.1
0
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1

Plot the likelihood distributions of the slope using the two different priors (green for flat and red for compensating). Are there any differences (you may need to zoom in)?
How do the likelihood distributions of the slope compare with the MLE values from paramfit1.py? Estimate the uncertainty on the slope value by eye. How does the uncertainty on the slope compare with the MLE value? Do the same for the y-intercept. What happens to the marginalized likelihood distributions for the slope and y-intercept if you change the number of data points (try N=100, N=10)? What happens if you change the grid spacing (try slope ranges from 1-10 in steps of 0.1, y-int ranges from 1-10 in steps of 1)?

In Bayesian analysis, it is important to think about the questions you are trying to answer when setting up the problem. Starting with a well understood model and prior is key. In this case do you want a flat prior on the slope and y-intercept, or do you want a prior that compensates for the unequal distribution in in angles. What range do you want to compute your data over? How finely should you bin the grids?

<u>*Optional - Activity 4: zombies 2*</u>
For this activity you will write your own code (but remember that you can take portions of previous code to make the process faster).

A virus has gotten out that is turning humans into zombies. You as a scientist have been recording the % of zombies ever since the outbreak (~14 days ago). However the power has gone out for the past four days and your generator just kicked in allowing you to analyze the data and determine when there will be no humans left (% humans = [1-% zombies] = 0). where time=0 is the present day (time = -14 is 14 days ago when you started taking data).Use your Bayesian skills now to perform this analysis.

a) Read in the data and plot it as time vs. % human in blue stars.

b) Create grids to test your parameter space assuming a linear model for the data. Based on your output from zombies1.py, what ranges should you try? Compute the full likelihood distribution. Which prior do you want to use?

c) Determine the marginalized likelihood distribution for the time at which there are 0% humans. Which parameter must you marginalize over?

d) Using the prior that you yourself are not a zombie yet and that you have provisions for another month, recompute the posterior likelihood distribution and determine the marginalized likelihood distribution for the time at which there are 0% humans.

e) How does the Bayesian analysis for determining the time when there are 0% humans compare with the MLE fit from the second activity? Can you think of a better model for the data?

For more information on the Bayesian approach, tutorials are available on the website below, which are all provided in python notebooks) http://jakevdp.github.io/blog/2014/06/14/frequentism-and-bayesianism-4-bayesian-in-python/ .

Optional - Activity 5:Optimization

In the above tutorials we have looked at different methods for determining model parameters for our data sel. These methods fall within the larger category of mathematical optimization, which seeks to determine the best value for a given problem, while minimal computational effort.

Read through optimizationTutorial.pdf, written by Zane Beckwith, (a former CAP REU graduate assistant). It provides an overview of the topic of optimization along with several different examples of different types of optimization algorithms.

At the end of the write up, Zane has a short tutorial for which he has provided two codes: scatter.py & neldermead.py. Both of these python programs actually contain function definitions and can be read into your own code using the **import** command. To complete the activity, you would use the function **minimize** from neldermead.py to find minima of the Himmelblau function, which is provided by the function **simulate** in scatter.py. I have provided my own example of how to do this in zanesprob.py.