Error Estimation

Source: *Richter "Estimating Errors in Least Square Fitting"*
http://ipnpr.jpl.nasa.gov/progress_report/42-122/122E.pdf

The problem:

Data of the form $(x_i, y_i), i \subset (1, \dots, N)$ is fitted by the function $y(x; a_1, \dots, a_M) \equiv y(x; \boldsymbol{a})$.

To determine the coefficients a_j, **it is sought to minimize**

$$\chi^2(\boldsymbol{a}) = \sum_{i=1}^{N} \frac{\big(y_i - y(x_i; \boldsymbol{a})\big)^2}{\sigma_i^2}$$

where σ_i is the standard deviation of the random errors of y_i (which are assumed to be normally distributed).

$\boldsymbol{a_0}$ is a coefficient vector that minimizes χ^2.

The variances of the elements a_j are given by $\sigma_{a_j}^2 = C_{jj}$: the diagonal elements of the covariance matrix $\boldsymbol{C}$ which is itself the inverse of the curvature or Hessian matrix $\boldsymbol{H}$.

The *weighted mean value of the variance of the fit is given by:* $\frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_y^2(x_i)}{\sigma_i^2} = \frac{M}{N}$ so that for constant data errors, **the mean standard error of the fit is**:

$$\overline{\sigma_y^2} = \frac{1}{N} \sum_{i=1}^{N} \sigma_y^2(x_i) = \frac{M}{N} \sigma^2$$

The **error in the value of the fitted function** is a function of x even when the σ_i are all the same and independent of x. Hence variance of the value of the fitted function (due to random data errors) is:

$$\sigma_y^2(x) = \sum_{j=1}^{M} \sum_{k=1}^{M} C_{jk} d_j(x) d_k(x) = \boldsymbol{d}(x)^T \boldsymbol{C} \boldsymbol{d}(x)$$

Where $d_j(x) = \left(\frac{\partial y(x{:}\boldsymbol{a})}{\partial a_j}\right)_{\boldsymbol{a_0}}$

For *linear* fitting where $y(x{:}\, \boldsymbol{a}) = \sum_{j=1}^{M} a_j X_j(x)$, $d_j(x) = X_j(x)$ and $\sigma_y^2(x) = \boldsymbol{x}(x)^T \boldsymbol{C} \boldsymbol{x}(x)$ where $\boldsymbol{x}$ is a column vector with elements $X_j(x)$.

Standard Error of Fit:

What is $\sigma_y(x)$, the standard error of the fit?

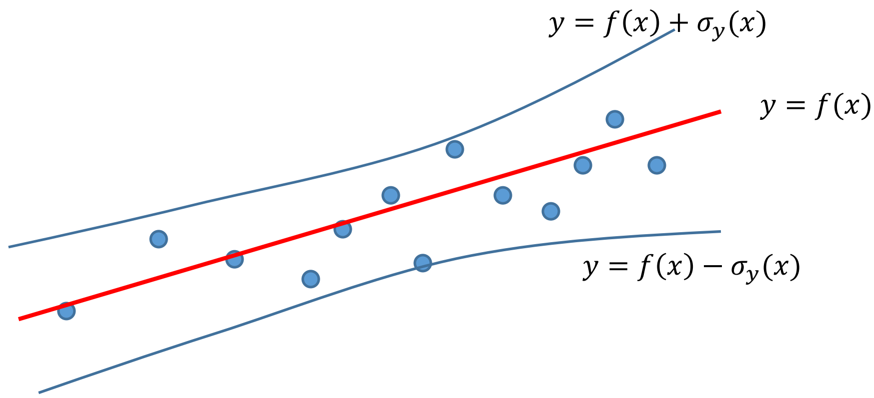

Figure 1: Illustration of standard error of fit $\sigma_y(x)$.

As is apparent from Figure 1, the standard error of fit is a very useful term! It is minimum at the centroid of the data points and maximum at the edges.

Least Squares Fitting:

$$\chi^2(\boldsymbol{a}) = \sum_{i=1}^{N} \frac{\left(y_i - y(x_i;\boldsymbol{a})\right)^2}{\sigma_i^2}$$

σ_i can be obtained from knowledge of experimental errors or from analysis of the data itself. It is assumed that the errors are normally distributed.

Linear Least Squares Fitting:

$$y(x;\boldsymbol{a}) = \sum_{j=1}^{M} a_j X_j(x)$$

$X_j(x)$ are arbitrary basis functions for the independent variable x.

In terms of linear algebra, the fitting function $y(x_i;\boldsymbol{a})$ is an N-element column vector, the coefficients a_j are elements of an M element column vector and the basis functions $X_j(x_i)$ are elements of an $N \times M$ matrix X_{ij}. Hence:

$$y(x_i;\boldsymbol{a}) = \sum_{j=1}^{M} a_j X_{ij}$$

i.e.

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{a}$$

Lets now define the column vector $b_i = \frac{y_i}{\sigma_i}$ and the matrix $A_{ij} = \frac{X_{ij}}{\sigma_i}$. Hence:

$$\chi^2(\boldsymbol{a}) = (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})$$

Extremum condition is: $\frac{\partial \chi^2}{\partial a_j} = 0$ i.e.[1]

$$\left(\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{A}\right)\boldsymbol{a} = \boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{b}$$

Hence:

$$\boldsymbol{a} = \left(\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{A}\right)^{-\mathbf{1}}\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{b} = \boldsymbol{C}\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{b}$$

Here $\boldsymbol{H} = \boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{A}$ and $\boldsymbol{C} = \boldsymbol{H}^{-\mathbf{1}}$ is the covariance matrix: a symmetric $M \times M$ matrix.

Hence:

$$a_j = a_j(y_1, y_2, \dots, y_N) = \sum_{k=1}^{N} C_{jk} \sum_{i=1}^{N} y_i \frac{X_k(x_i)}{\sigma_i^2}$$

Suitability of Basis Functions:

The value of χ^2 should be of the order $N - M \equiv \nu$: the number of **degrees of freedom** of this system. Hence

$$\chi_\nu^2 = \frac{\chi^2}{\nu} \approx 1$$

This is the condition for the fit to be meaningful. If $\nu \gg 1$, χ^2 is normally distributed with $\frac{\chi^2}{\nu}$ having mean 1 and standard deviation of $\sqrt{\frac{2}{\nu}}$.

[1] $\frac{\partial \chi^2}{\partial a_j} = (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T \frac{\partial(\boldsymbol{b}-\boldsymbol{A}\boldsymbol{a})}{\partial a_j} + \frac{\partial(\boldsymbol{b}-\boldsymbol{A}\boldsymbol{a})^T}{\partial a_j}(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a}) = -(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T\boldsymbol{A}\frac{\partial \boldsymbol{a}}{\partial a_j} - \frac{\partial \boldsymbol{a}^{\boldsymbol{T}}}{\partial a_j}\boldsymbol{A}^{\boldsymbol{T}}(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a}) = -(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T\boldsymbol{A}\frac{\partial \boldsymbol{a}}{\partial a_j} - (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T\left(\frac{\partial \boldsymbol{a}^{\boldsymbol{T}}}{\partial a_j}\boldsymbol{A}^{\boldsymbol{T}}\right)^{\boldsymbol{T}} = -(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T\boldsymbol{A}\frac{\partial \boldsymbol{a}}{\partial a_j} - (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T\boldsymbol{A}\frac{\partial \boldsymbol{a}}{\partial a_j} = \mathbf{-2}(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T\boldsymbol{A}\frac{\partial \boldsymbol{a}}{\partial a_j}$. Hence $\frac{\partial \chi^2}{\partial \boldsymbol{a}} = -2(\boldsymbol{b} - \boldsymbol{A}\boldsymbol{a})^T\boldsymbol{A} = -2\boldsymbol{b}^{\boldsymbol{T}}\boldsymbol{A} + 2(\boldsymbol{A}\boldsymbol{a})^T\boldsymbol{A} = -2\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{b} + 2\boldsymbol{A}^{\boldsymbol{T}}\boldsymbol{A}\boldsymbol{a}$

Standard Errors

$$\delta a_j = \sum_{i=1}^{N} \frac{\partial a_j}{\partial y_i} \delta y_i = \sum_{k=1}^{N} C_{jk} \sum_{i=1}^{N} \frac{X_k(x_i)}{\sigma_i^2} \delta y_i$$

In matrix form:

$$\delta \boldsymbol{a} = \boldsymbol{C} \boldsymbol{A}^{\boldsymbol{T}} \delta \boldsymbol{b}$$

The covariance of a_j and a_k is given by:

$$\boldsymbol{\sigma}_{\boldsymbol{a}}^{\boldsymbol{2}} = \langle \delta \boldsymbol{a} \delta \boldsymbol{a}^T \rangle = \boldsymbol{C} \boldsymbol{A}^{\boldsymbol{T}} \langle \delta \boldsymbol{b} \delta \boldsymbol{b}^T \rangle \boldsymbol{A} \boldsymbol{C}^{\boldsymbol{T}}$$

Since $\langle \delta y_i \delta y_k \rangle = \delta_{ik}$ (errors are uncorrelated), hence: $\langle \delta \boldsymbol{b} \delta \boldsymbol{b}^T \rangle = \boldsymbol{I}$**.** Hence[2],

$$\boldsymbol{\sigma}_{\boldsymbol{a}}^{\boldsymbol{2}} = \boldsymbol{C}\left(\boldsymbol{A}^{\boldsymbol{T}} \boldsymbol{A}\right) \boldsymbol{C}^{\boldsymbol{T}} = \boldsymbol{C}$$

Hence, the **errors in the coeffients are correlated**!

The variance of the coefficients are given by the **diagonal** elements:

$$\sigma_{a_j}^2 = C_{jj}$$

Hence:

$$\delta y(x; \boldsymbol{a}) = \sum_{j=1}^{M} \delta a_j X_j(x)$$

Hence the covariance:

$$\sigma_y^2(x, x') = \sum_{j=1}^{M} \sum_{k=1}^{M} \langle \delta a_j \delta a_k \rangle X_j(x) X_k(x') = \sum_{j=1}^{M} \sum_{k=1}^{M} C_{jk} X_j(x) X_k(x')$$

This is independent of parameter values a_j. For the special case where $x = x'$:

$$\sigma_y^2(x) = \sum_{j=1}^{M} \sum_{k=1}^{M} C_{jk} X_j(x) X_k(x) = \boldsymbol{X}^{\boldsymbol{T}} \boldsymbol{C} \boldsymbol{X}$$

Here $\boldsymbol{X}$ is a column vector whose elements are $X_j(x)$.

Hence, the **errors in** $y(x; \boldsymbol{a})$ **at two different values of** $\boldsymbol{x}$ **are correlated!**

The **weighted mean value of** $\boldsymbol{\sigma}_{\boldsymbol{y}}^{\boldsymbol{2}}(x)$ **over all** x is given by:

$$\overline{\sigma_y^2} = \frac{1}{N} \sum_{i=1}^{N} \frac{\sigma_y^2(x_i)}{\sigma_i^2} = \sum_{j=1}^{M} \sum_{k=1}^{M} C_{jk} \frac{1}{N} \sum_{i=1}^{N} \frac{X_j(x_i)}{\sigma_i} \frac{X_k(x_i)}{\sigma_i}$$

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[2] $\boldsymbol{C} = (\boldsymbol{A}^{\boldsymbol{T}} \boldsymbol{A})^{-\boldsymbol{1}}$ and $\boldsymbol{C}^{\boldsymbol{T}} = \boldsymbol{C}$

But $\frac{X_{ij}}{\sigma_i} = A_{ij}$. Hence:

$$\overline{\sigma_y^2} = \frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_y^2(x_i)}{\sigma_i^2} = \sum_{j=1}^{M}\sum_{k=1}^{M} C_{jk}\frac{1}{N}\sum_{i=1}^{N} A_{ij}A_{ik} = \sum_{j=1}^{M}\sum_{k=1}^{M} C_{jk}\frac{1}{N}\sum_{i=1}^{N} A_{ji}^{T}A_{ik}$$

Hence:

$$\overline{\sigma_y^2} = \sum_{j=1}^{M}\sum_{k=1}^{M} C_{jk}\frac{1}{N}\left(\boldsymbol{A^T A}\right)_{jk} = \frac{1}{N}\sum_{j=1}^{M}\sum_{k=1}^{M} C_{jk}\left(\boldsymbol{C^{-1}}\right)_{jk} = \frac{1}{N}\sum_{j=1}^{M} I_{jj} = \frac{M}{N}$$

Hence if $\sigma_i = \sigma$,

$$\overline{\sigma_y^2} = \frac{1}{N}\sum_{i=1}^{N}\sigma_y^2(x_i) = \frac{M}{N}\sigma^2$$

This is analogous to the variance of the mean for the case of one value of x where M=1. Hence, as a result of fitting to the function $y(x)$, **the variance of y is reduced by $\boldsymbol{\frac{M}{N}}$.** Hence the higher the value of M required to fit the data to reduce χ_v^2 to a value close to 1, the larger will be the errors in the values of the fitted function.

Very Important: For the fit to be meaningful:

1. $\chi_v^2 \approx 1$
2. Data errors (σ_i) have to be correctly chosen otherwise fit is not meaningful even with $\chi_v^2 \approx 1$.

Only if the fit is meaningful can one estimate the fitting errors meaningfully.

Non-Linear Least Squares Problem

No explicit solution for $\boldsymbol{a}$ exists and an iterative procedure must be followed.

$$y(x;\boldsymbol{a}) = y(x;\boldsymbol{a_0}) + \sum_{j=1}^{M}\left.\frac{\partial y(x;\boldsymbol{a})}{\partial a_j}\right|_{\boldsymbol{a_0}}\left(a_j - a_{0j}\right) = y(x;\boldsymbol{a_0}) + (\boldsymbol{a}-\boldsymbol{a_0})^{\boldsymbol{T}}\boldsymbol{d}(x;\boldsymbol{a_0})$$

Where $d_j(x;\boldsymbol{a_0}) = \left.\frac{\partial y(x;\boldsymbol{a})}{\partial a_j}\right|_{\boldsymbol{a_0}}$

And similarly:

$$\chi^2(\boldsymbol{a}) = \chi_{min}^2 + \frac{1}{2}\sum_{j=1}^{M}\sum_{k=1}^{M}\left.\frac{\partial^2\chi^2(\boldsymbol{a})}{\partial a_j\partial a_k}\right|_{\boldsymbol{a_0}}\left(a_j - a_{0j}\right)\left(a_k - a_{0k}\right) = \chi_{min}^2 + (\boldsymbol{a}-\boldsymbol{a_0})^T\boldsymbol{H}(\boldsymbol{a_0})(\boldsymbol{a}-\boldsymbol{a_0})$$

Here:

$$h_{jk}(\boldsymbol{a_0}) = \frac{1}{2}\left.\frac{\partial^2\chi^2(\boldsymbol{a})}{\partial a_j\partial a_k}\right|_{\boldsymbol{a_0}} = \sum_{i=1}^{N}\frac{1}{\sigma_i^2}\left.\frac{\partial y(x;\boldsymbol{a})}{\partial a_j}\right|_{\boldsymbol{a_0}}\left.\frac{\partial y(x;\boldsymbol{a})}{\partial a_k}\right|_{\boldsymbol{a_0}}$$

If we define:

$$A_{ij}(\boldsymbol{a}_0) = \frac{1}{\sigma_i}\frac{\partial y(x_i;\boldsymbol{a})}{\partial a_j}\bigg|_{\boldsymbol{a_0}} = \frac{d_{ij}(\boldsymbol{a_0})}{\sigma_i}$$

Then: $\boldsymbol{H} = \boldsymbol{A^T A},$ just like for linear least squares. The derivation then[3], on similar lines, leads to:

$$\boldsymbol{\sigma_a^2(a_0) = C(a_0) = H^{-1}(a_0)}$$

Hence also,

$$\sigma_y^2(x;\boldsymbol{a_0}) = \sum_{j=1}^{M}\sum_{k=1}^{M} C_{jk}(\boldsymbol{a_0})d_j(x;\boldsymbol{a_0})d_k(x;\boldsymbol{a_0}) = \boldsymbol{d^T C d}$$

i.e.

$$\overline{\sigma_y^2} = \frac{M}{N}\sigma^2$$

The standard error of regression is: $\sigma_R = \sqrt{\frac{\chi^2}{M-N}} = \sqrt{\chi_\nu^2}$

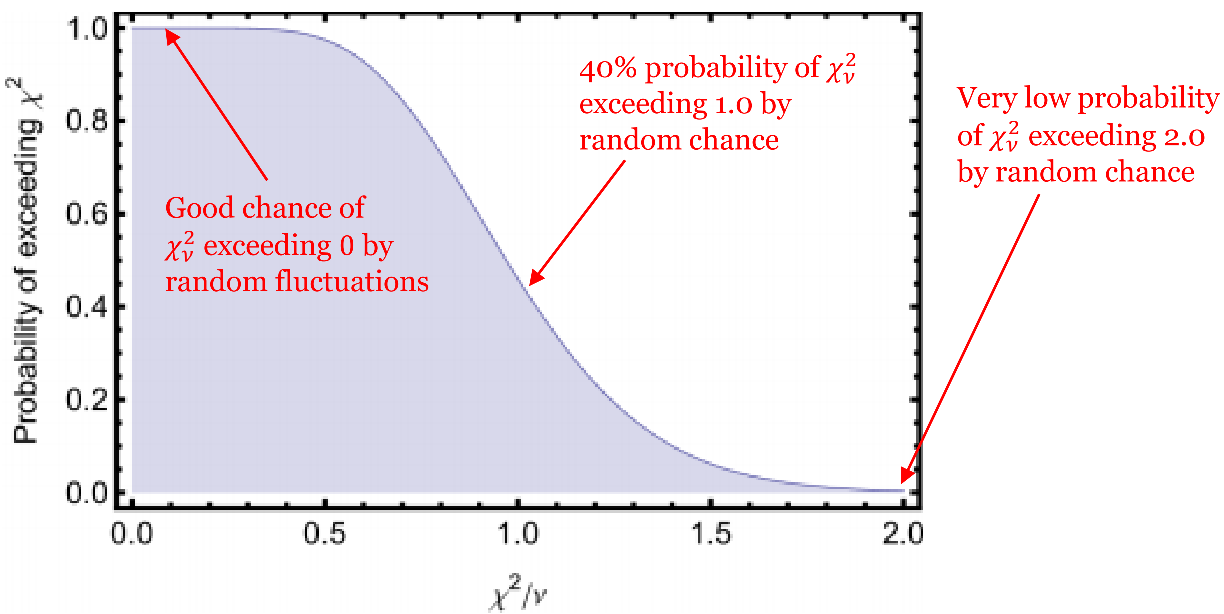
3 Here d_{ij} replaces X_{ij} of linear least squares.

$\pm\sigma_X$ is the 68.3% confidence limit

$\pm 2\sigma_X$ is the 95.4% confidence limit

$\pm 3\sigma_X$ is the 99.73% confidence limit

Note: Notice that $\boldsymbol{\sigma_a}$ and $\sigma_y(x)$ are not functions of $\chi^2(\boldsymbol{a_0})$. This is because the former are only meaningful if $\chi_v^2 \approx 1$ i.e. the χ^2 dependence is already baked in.



Null Hypothesis: The fit explains the data.

$\chi_v^2 \gg 1$ indicates a poor model fit: probability that the value of χ_v^2 occurred by random chance is very low.

$\chi_v^2 > 1$ indicates that fit has not fully captured the data but null hypothesis cannot be rejected.

$\chi_v^2 = 1$ indicates that the match between observation and estimate is in accord with the error variance. Null hypothesis cannot be rejected.

$\chi_v^2 < 1$ indicates *over-fitting* of data i.e. model is (improperly) fitting noise or the error variance has been over-estimated. Null hypothesis cannot be rejected.

Shapiro-Wilk test can be used to see if the residuals are normally distributed. If they are, then the student-t distribution can be used to verify that the mean is statistically zero.

Getting p-value for coefficient $\neq 0$.

The t –statistic to test if a given coefficient a_j is different from zero is:

$t_j = \frac{a_j}{\sigma_{a_j}}$. Get the value of $p = 1.0 - t.cdf(t_j, M - N)$ and if this is less the 0.05, then the value of a_j is significantly different from zero.

User's Guide to Error Analysis

http://www.colorado.edu/physics/EducationIssues/zwickl/Resources/Error%20Analysis%20Activity%202.pdf

What is least squares fitting:

$$\chi^2 = \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \left(y - y(x_i, \boldsymbol{a})\right)^2$$

Where there are N data points (x_i, y_i) and the fit function is given by $y(x, \boldsymbol{a})$ where $\boldsymbol{a}$ is a vector of the fit parameters.

Assumptions:

1. **Gaussian Distribution** of the random fluctuations in each y_i.
2. **Uncorrelated:** the random fluctuations in any one data point are uncorrelated with another data point.

If these two assumptions hold, minimizing χ^2 gives the *most likely* function that reproduces the observed data.

Uncertainty in the data σ_y^2 is calculated using the **residuals of the best fit**:

$$\sigma_y^2 = \frac{1}{N-n} \sum_{i=1}^{N} \left(y_i - y(x_i; \boldsymbol{a})\right)^2$$

This is analogous to finding the variance of a repeated measurement.

Note: This was not calculated in Richter's analysis.

The residuals must be randomly distributed about zero (no systematic variation).

Note: It is **not necessary** for a good fit line to pass through each set of error bars: though it should pass through most. If we have shown the error bars for standard error, then 68% of data points are expected to lie within their error bar.

Applying the chi-squared test:

The graph of the probability of $\chi_\nu^2 = \frac{\chi^2}{\nu}$ exceeding the observed value for ν degrees of freedom is available (cumulative density function CDF of the chi-squared distribution). This gives us the likelihood that the observed value of χ^2 occurred by chance.

The **null-hypothesis** for a chi-squared test is that the data are **independent** and **normally-distributed.** The **chi-squared** test for goodness-of-fit is used to *reject* the null hypothesis that the data are independent.

Note: It is possible to get a good looking χ_ν^2 by overestimating experimental errors (σ_i).

Interpreting Sum of Squares

http://facweb.cs.depaul.edu/sjost/csc423/documents/f-test-reg.htm

http://reliawiki.org/index.php/Simple_Linear_Regression_Analysis

For M observations and N regression parameters:

(1) Corrected Sum of Squares also called Sum of Squares of Regression :

$$SSM\ (or\ SSR) = \sum_{i=1}^{M} \frac{(y(x_i; \boldsymbol{a}) - \bar{y})^2}{\sigma_i^2}$$

$$\bar{y} = \frac{1}{M} \sum_{i=1}^{M} y_i$$

This is a measure of **explained variation**

(2) Sum of Squares for Error:

$$SSE = \sum_{i=1}^{M} \frac{\left(y_i - y(x_i; \boldsymbol{a})\right)^2}{\sigma_i^2}$$

This is a meaure of **unexplained variation**

(3) Corrected Sum of Squares (Total):

$$SST = \sum_{i=1}^{M} \frac{(y_i - \bar{y})^2}{\sigma_i^2}$$

(4) For multiple regression models:

$$SST = SSM + SSE$$

$$R^2 = \frac{SSM(or\ SSR)}{SST}$$

(5) Corrected Degrees of Freedom for Model:

$$DFM = N - 1$$

(6) Degrees of Freedom for Error:

$$DFE = M - N$$

(7) Corrected Degrees of Freedom Total:

$$DFT = DFM + DFE = M - 1$$

(8) Mean of Squares of Model:

$$MSM = \frac{SSM}{DFM}$$

(9) Mean of Squares for Error:

$$MSE = \frac{SSE}{DFE}$$

(10) Mean of Squares Total:

$$MST = \frac{SST}{DFT}$$

It is desirable to have MSM be large wrt MSE.

F-test

We want to test the following null hypothesis:

$$H_0: \beta_1 = \beta_2 = \cdots = \beta_{N-1} = 0$$

$$H_1: \beta_j \neq 0 \; for \; at \; least \; one \; value \; of \; j$$

Steps of the F-test.

1. State the null and alternative hypothesis.
2. Compute test statistics assuming null-hypothesis is true:
$$F = \frac{MSM}{MSE} = \frac{explained \; variance}{unexplained \; variance}$$
3. Find a (1-a)*100% confidence interval I for (DFM, DFE) degrees of freedom using an F-table or statistical software.
4. Accept the null-hypothesis if $\subset I$; else reject.
5. Use statistical software to determine the p value.

Implementation in Python

To implement this in Python, lets open a new file called *errorestimation.py*.

We need to import several things. See Figure 2

```
import scipy, numpy
import scipy.optimize, scipy.stats
import numpy.random
import matplotlib.pyplot as plt
import pandas as pd
import statsmodels
import statsmodels.stats
import statsmodels.stats.stattools as stools

plt.style.use("ggplot")
```

Figure 2: Various libraries that we need to import for analysis of a curve-fitting.

We define a function *fitdata* as shown in Figure 3. The inputs of the function are explained in the docstring (the green text in the triple quotes).

We will use the Levenberg-Marquadt algorithm to optimize the **p** (see discussion at the beginning of this chapter). This is a *non-linear* least square fitting.

The code corresponding to this is *within* the *fitdata* function's block. It appears in Figure 4. Sums of squares of various deviations appear in Figure 5 and analysis of goodness of fit appears in Figure 6.

The code for the plotting appears in Figure 7. The calculation of the standard error of the fit appears in Figure 8 and the code for formatting the axes in Figure 9.

See Figure 10, Figure 11 and Figure 12 for an illustration of importing, preparing and fitting data from an Excel sheet.

```python
def fitdata(f, Xdata, Ydata, Errdata, pguess, dict_data, ax = False, ax2 = False):
    '''
    fitdata(f, Xdata, Ydata, Errdata, pguess, dict_data)
        f = function f(X, p, dict_data)
        Xdata = array like object (k, M) shaped array for data with k predictors
        e.g. if X = (x1, x2, x3) then X =(X1, X2, X3) where X1 is a vector of x1 etc
        Ydata = array like object of length M
        Errdata = array like object of length M: error estimate of ydata.
        pguess = array like object of length N (vector of guess of parameters)
        dict_data = dictionary containing other data necessary for f
    Returns:
        popt = vector of length N of the optimized parameters
        pcov = Covariance matrix of the fit
        perr = vector of length N of the std-dev of the optimized parameters
        p95  = half width of the 95% confidence interval for each parameter i.e. popt-p95 and popt+p95
        p_p = vector of length N of the p-value for the parameters being zero
                (if p<0.05, null hypothesis rejected and parameter is non-zero)
        chisquared = (chisquared, chisquared_red, degfreedom, p)
        chisquared = chisquared value for the fit: sum of squares of weighted residuals
        chisquared_red = chisquared/degfreedom.  Value should be approx. 1 for a good fit.
        degfreedom = M - N the degrees of freedom of the fitting
        chisquare = (p, chisquared, chisquared_red, degfreedom)
                p = Probability of finding a chisquared value at least as extreme as the one shown
                    purely by random chance (should be high for good fit)
                chisquared =  chisquared value for the fit: sum of squares of weighted residuals
                chisquared_red = chisquared/degfreedom.  Value should be approx. 1 for a good fit.
                degfreedom = M - N the degrees of freedom of the fitting
                R2 = correlation coefficient or proportion of explained variance
                R2_adj = adjusted R2 taking into account number of predictors
        resanal = (p, w, mean, stddev) Analysis of residuals
                  p = Probability of finding a w at least as extreme as the one observed (should be high for good fit)
                  w = Shapiro-Wilk test criterion
                  mean = mean of residuals
                  p_res = probability that the mean value obtained is different from zero merely by chance
                  (should be low for good fit)
                  The mean must be within 1 stddev of zero for highly significant fitting.
                  F = F-statistic for the fit MSM/MSE.
                      Null hypothesis is that there is NO Difference between the two variances.
                  p_F = probability that this value of F can arise by chance alone.
                      p_F < 0.05 to reject null hypothesis and prove that the fit is good.
                  dw = Durbin_Watson statistic (value between 0 and 4).
                      2 = no-autocorrelation.  0 = +ve autocorrelation, 4 = -ve autocorrelation.
    '''
```

Figure 3: Function fitdata and its docstring explaining its inputs and outputs.

```python
'''
def error(p, Xdata, Ydata, Errdata, dict_data):
    Y = f(Xdata, p, dict_data)
    residuals = (Y - Ydata)/Errdata
    return residuals
res = scipy.optimize.leastsq(error, pguess, args=(Xdata, Ydata, Errdata, dict_data), full_output=1)
(popt, pcov, infodict, errmsg, ier) = res
perr = scipy.sqrt(scipy.diag(pcov))
```

*Figure 4: Code to optimize the parameters **p** using the scipy.optimize.leastsq module with full_output = 1. Also shown is **perr:** the vector of the standard-deviation for each of the **p** values.*

```
M = len(Ydata)
N = len(popt)
#Residuals
Y = f(Xdata, popt, dict_data)
residuals = (Y - Ydata)/Errdata
meanY = scipy.mean(Ydata)
squares = (Y - meanY)/Errdata
squaresT = (Ydata - meanY)/Errdata

SSM = sum(squares**2)   #Corrected Sum of Squares
SSE = sum(residuals**2) #Sum of Squares of Errors
SST = sum(squaresT**2)  #Total corrected sum of squares

DFM = N - 1  #Degrees of freedom for model
DFE = M - N  #Degrees of freedom for error
DFT = M - 1  #Degrees of freedom total

MSM = SSM/DFM  #Mean squares for model (explained variance)
MSE = SSE/DFE  #Mean squares for Error (should be small wrt MSM) Unexplained variance
MST = SST/DFT  #Mean squares for total

R2 = SSM/SST #proportion of explained variance
R2_adj = 1 - (1 - R2)*(M - 1)/(M - N - 1) #Adjusted R2
```

Figure 5: Code to analyse the sum of squares of various deviations of the fit. See the part about the F-test above.

```
#t-test to see if parameters are different from zero
t_stat = popt/perr  #t-statistic for popt different from zero
t_stat = t_stat.real
p_p = 1.0 - scipy.stats.t.cdf(t_stat, DFE) #should be low for good fit.
z = scipy.stats.t(M-N).ppf(0.95)
p95 = perr*z
#Chisquared Analysis on Residuals
chisquared = sum(residuals**2)
degfreedom = M - N
chisquared_red = chisquared/degfreedom
p_chi2 = 1.0 - scipy.stats.chi2.cdf(chisquared, degfreedom)
stderr_reg = scipy.sqrt(chisquared_red)
chisquare = (p_chi2, chisquared, chisquared_red, degfreedom, R2, R2_adj)

#Analysis of residuals
w, p_shapiro = scipy.stats.shapiro(residuals)
mean_res = scipy.mean(residuals)
stddev_res = scipy.sqrt(scipy.var(residuals))
t_res = mean_res/stddev_res #t-statistic to test that mean_res is zero.
p_res = 1.0 - scipy.stats.t.cdf(t_res, M-1)
    #if p_res < 0.05, null hypothesis rejected and mean is non-zero.
    #Should be high for good fit.
#F-test on residuals
F = MSM/MSE #explained variance/unexplained .  Should be Large
p_F = 1.0 - scipy.stats.f.cdf(F, DFM, DFE)
    #if p_F < 0.05, null-hypothesis is rejected
    #i.e. R^2 > 0 and at least one of the fitting parameters > 0.
dw = stools.durbin_watson(residuals)
resanal = (p_shapiro, w, mean_res, p_res, F, p_F, dw)
```

Figure 6: Test to see goodness of fit. p95 is the vector of the 95% confidence range of p i.e. p = p± p95 with 95% confidence. Shapiro test is to check if the residuals are normally distributed and the Durbin-Watson test is to check if they are correlated. p_shapiro should be > 0.05 and dw should be near 2 and away from 0 and 4.

```python
    if ax:
        formataxis(ax)
        ax.plot(Ydata, Y, 'ro')
        ax.errorbar(Ydata, Y, yerr = Errdata, fmt='.')
        Ymin, Ymax = min((min(Y),min(Ydata))), max((max(Y),max(Ydata)))
        ax.plot([Ymin, Ymax],[Ymin, Ymax],'b')

        ax.xaxis.label.set_text('Data')
        ax.yaxis.label.set_text('Fitted')

        sigmay, avg_stddev_data = get_stderr_fit(f, Xdata, popt, pcov, dict_data)
        Yplus = Y + sigmay
        Yminus = Y - sigmay
        ax.plot(Y, Yplus, 'c',alpha = 0.6, linestyle = '--', linewidth = 0.5)
        ax.plot(Y, Yminus, 'c', alpha = 0.6, linestyle = '--', linewidth = 0.5)
        ax.fill_between(Y, Yminus, Yplus, facecolor = 'cyan', alpha = 0.5)
        titletext = 'Parity plot for fit.\n'
        titletext += r'$r^2$ = %5.2f, $r^2_{adj}$ = %5.2f, '
        titletext += '$\sigma_{exp}$ = %5.2f, $\chi^2_{\nu}$ = %5.2f, $p_{\chi^2}$ = %5.2f,
        titletext += '$\sigma_{err}^{reg}$ = %5.2f'

        ax.title.set_text(titletext%(R2, R2_adj, avg_stddev_data, chisquared_red, p_chi2,stderr_reg))
        ax.figure.canvas.draw()

    if ax2:  #Test for homoscedasticity
        formataxis(ax2)
        ax2.plot(Y, residuals, 'ro')

        ax2.xaxis.label.set_text('Fitted Data')
        ax2.yaxis.label.set_text('Residuals')

        titletext = 'Analysis of Residuals\n'
        titletext += r'mean = %5.2f, $p_{res}$ = %5.2f, $p_{shapiro}$ = %5.2f, $Durbin-Watson$=%2.1f'
        titletext += '\n F = %5.2f,  $p_F$ = %3.2e'
        ax2.title.set_text(titletext%(mean_res, p_res, p_shapiro, dw, F, p_F))

        ax2.figure.canvas.draw()


    return popt, pcov, perr, p95, p_p, chisquare, resanal
```

Figure 7: Plotting and return

```python
def get_stderr_fit(f, Xdata, popt, pcov, dict_data):
    '''
    popt, pcov, perr, chisquare, shapiro = get_stderr_fit(f, Xdata, popt, pcov, dict_data)

    f = function f(X, p, dict_data)
    Xdata = array like object (k, M) shaped array for data with k predictors
    e.g. if X = (x1, x2, x3) then X =(X1, X2, X3) where X1 is a vector of x1 etc
    Ydata = array like object of length M
    popt = vector of length N of the optimized parameters
    pcov = Covariance matrix of the fit
    dict_data = dictionary containing other data necessary for f

    returns
    sigmay:  array like object of length M.  The standard deviations for error at a given value of X
    avg_stddev_data:  The constant standard deviation (experimental error) that would justify the given fit.
    '''
    Y = f(Xdata, popt, dict_data)
    listdY = []
    for i in xrange(len(popt)):
        p = popt[i]
        dp = abs(p)/1e6 + 1e-20
        popt[i] += dp
        Yi = f(Xdata, popt, dict_data)
        dY = (Yi - Y)/dp
        listdY.append(dY)
        popt[i] -= dp
    listdY = scipy.array(listdY)
    #listdY is an array with N rows and M columns N = len(popt), M = len(Xdata[0])
    #pcov is an array with N rows and N columns
    left = scipy.dot(listdY.T, pcov)
    #left is an array with M rows and N columns
    right = scipy.dot(left, listdY)
    #right is an M x M matrix.  The diagonals of this are what we need.
    sigma2y = right.diagonal()
    #sigmay is the standard error of the fit and is a function of X
    mean_sigma2y = scipy.mean(right.diagonal())
    M = Xdata.shape[1]
    N = len(popt)
    avg_stddev_data = scipy.sqrt(M*mean_sigma2y/N)
    #This is because if experimental error is constant at sig_dat, then mean_sigma2y = N/M*sig_dat**2
    sigmay = scipy.sqrt(sigma2y)
    return sigmay, avg_stddev_data
```

Figure 8: Code to calculate standard error of the fit.

```python
def formataxis(ax):
    ax.xaxis.label.set_fontname('Georgia')
    ax.xaxis.label.set_fontsize(12)
    ax.yaxis.label.set_fontname('Georgia')
    ax.yaxis.label.set_fontsize(12)
    ax.title.set_fontname('Georgia')
    ax.title.set_fontsize(12)



    for tick in ax.xaxis.get_major_ticks():
        tick.label.set_fontsize(8)
    for tick in ax.yaxis.get_major_ticks():
        tick.label.set_fontsize(8)
```

Figure 9: Code to format axis.

```python

def import_data(xlfile, sheetname):
    df = pd.read_excel(xlfile, sheetname = sheetname)
    return df

def prepare_data(df, Criterion, Predictors, Error = False):
    Y = scipy.array(df[Criterion])
    if Error:
        Errdata = scipy.array(df[Error])
    else:
        Errdata = scipy.ones(len(Y))
    Xdata = []
    for X in Predictors:
        X = list(df[X])
        Xdata.append(X)
    Xdata = scipy.array(Xdata)
    return Xdata, Y, Errdata
```

Figure 10: Code for importing data from an excel file and preparing it for fitting. See Figure 11 for illustration.

```python
if __name__ == "__main__":
    fig = plt.figure()
    ax = fig.add_subplot(111)
    fig.show()

    fig2 = plt.figure()
    ax2 = fig2.add_subplot(111)
    fig2.show()

#    #Make arbitrary function of three variables
    def f(X, p, dict_data):
        a = dict_data['a']
        b = dict_data['b']
        (x,y,z) = X
        Y = p[0]+ p[1]*x**2+p[2]*y + p[3]*z
        return Y


    #Get data from excel file using pandas
    df = import_data('SynthData.xlsx','Data')
    Xdata, Ydata, Errdata = prepare_data(df, 'Ydata',('x', 'y', 'z'),Error = 'err')

    #Intital Guess
    N = 4
    pguess = N*[0.0]

    popt, pcov, perr, p95, p_p, chisquare, resanal = fitdata(f, Xdata, Ydata, Errdata, pguess, dict_data, ax = ax, ax2 = ax2)
```

Figure 11: Illustration of use of importing, preparing and fitting data. The Excel file is named 'Synthdata.xlsx' and it contains a sheet called 'Data' formatted as shown in Figure 12

	A	B	C	D	E
1	x	y	z	Ydata	err
2	0	-1	-10	-26.312	10
3	0.052632	-0.78947	-9.42105	-33.0895	10
4	0.105263	-0.57895	-8.84211	-23.0898	10
5	0.157895	-0.36842	-8.26316	-26.3104	10
6	0.210526	-0.15789	-7.68421	-37.0378	10
7	0.263158	0.052632	-7.10526	-37.9639	10
8	0.315789	0.263158	-6.52632	-25.6197	10
9	0.368421	0.473684	-5.94737	-3.45358	10
10	0.421053	0.684211	-5.36842	-23.5125	10
11	0.473684	0.894737	-4.78947	-36.7872	10
12	0.526316	1.105263	-4.21053	-24.2072	10
13	0.578947	1.315789	-3.63158	-11.0806	10
14	0.631579	1.526316	-3.05263	12.43371	10
15	0.684211	1.736842	-2.47368	1.646041	10
16	0.736842	1.947368	-1.89474	22.93574	10
17	0.789474	2.157895	-1.31579	21.03534	10
18	0.842105	2.368421	-0.73684	19.66702	10
19	0.894737	2.578947	-0.15789	20.93693	10
20	0.947368	2.789474	0.421053	42.65305	10
21	1	3	1	71.88136	10
22					
23					
24					

Data

*Figure 12: The Excel sheet used for the above problem. Note that the **first** row is only the headings and the headings are referenced in the code of Figure 11.*