6.1 Introduction to Chi-Square Space

- the basic idea of searching chi-square space
- an example with two parameters and no error used to demonstrate salient features of chi-square space
- some comments about Mathcad contour graphs
- a look at two parameter chi-square space in the presence of random error
- changes in chi-square space as random errors increase
The Basic Idea

What happens if you have a non-linear equation that cannot be modified into, or approximated by, a linear form?

As long as $y$ has normally distributed error, a least-squares solution is still possible by empirically finding the equation coefficients which yield a minimum chi-square. The empirical procedures use repetitive guesses that "home-in" on the least-squares solution.

The guessing procedure is made logistically difficult as the number of parameters increases (dimensionality of the problem).

These are graphs of "chi-square space."
Two-Parameters, No Error (1)

This example will find the least-squares coefficients that minimize chi-square for the following non-linear function describing a peak. The true coefficient values were $a_0 = 50.69167$ and $a_1 = 2.13494$. With no noise $\sigma_y = 0$.

$$y(a_0, a_1, x) = \frac{1}{a_0 \sqrt{2\pi}} e^{-\frac{1}{2} \frac{(x-a_1)^2}{a_0^2}}$$

The following data were collected across the peak:

- (45, 0.005) (46, 0.017)
- (47, 0.042) (48, 0.084)
- (49, 0.137) (50, 0.177)
- (51, 0.185) (52, 0.155)
- (53, 0.104) (54, 0.056)
- (55, 0.024)
A chi-square map is a matrix of chi-square values plotted as a contour graph. The coefficients are varied over a range of values that is expected to include the minimum.

\[
\chi_{row,col} = \sum_{i=1}^{N} (y_i - y(a_{0\,row}, a_{1\,col}, x_i))^2
\]

In this case: $1.00 \leq a_0 \leq 3.00$, $\Delta a_0 = 0.02$

$50.00 \leq a_1 \leq 52.00$, $\Delta a_1 = 0.02$
• The data matrix and its contour graph have the rows and columns rotated by 90°.
• The default minimum is violet, which often makes the minimum difficult to locate. I plot the negative matrix to make red the minimum.
• A direct plot of the matrix has very little resolution near the minimum. I plot the natural log of the values to enhance small $\chi^2$ differences.
Random noise with $\sigma = 0.01$ was added to the data on slide 3. Trial #1 had the following values.

$$(45,0.001)(46,0.010)(47,0.037)(48,0.075)(49,0.120)(50,0.178)$$
$$(51,0.184)(52,0.160)(53,0.126)(54,0.064)(55,0.034)$$

Three sets of measurements were made. The graphs below show the three sets of data along with regression lines using the coefficients which gave a minimum in chi-square space.
Two Parameters with Error (2)

The contour graphs below show how the "details" of chi-square space change when error randomly moves the minimum.

- as with the linear least-squares, the minimum does not correspond to the true value (the true value is marked +)
- the contours are elliptically shaped, indicating that a change in $a_0$ affects chi-square more than an equal-sized change in $a_1$ ($a_0$ will be estimated more precisely)
- the non-concentric ellipses indicate that $\mu_0 - \Delta a_0$ affects the fit more than $\mu_0 + \Delta a_0$
- elliptical contours oriented at an angle to the parameter axes indicate that the two parameters have a non-zero covariance
Two Parameters with Error (3)

As the noise level increases, the graph flattens and the minimum can be found farther from the true value. In the contour plot at the right, the increased area of each contour is indicative of flattening. The graph below shows why chi-square space flattens near the minimum.

The black line in the graph at the left is the value of chi-square without error. To obtain the dashed red lines (chi-square with error) the horizontal blue lines were added to the black lines (before taking the log).