**A Gaussian Curve Fit to Experimental Data with Solver**

The function used to fit experimental data to a Gaussian curve is:



Where:

*yi* = the predicted value,

*h* = the peak height above the baseline,

*xi* = the value of the independent variable,

*µ* = the position of the maximum,

*σ* = the standard deviation, and

$b$ = the baseline offset.

We shall fit the 31 data points in Figure XX to a Gaussian curve by varying *h, µ* , *σ* and *b.* Clearly, 31 data points is too few for a good fit when four parameters are involved. However, it will demonstrate the procedure without overtaxing the reader with too much data entry.

1. Start a worksheet similar to that in Figure XX. Begin by entering the text in rows 1 to 9, and naming the cells B3:B6 with the text in column A. Temporarily ignore the values in B3:B7.
2. Enter the *x* and *y* values in rows 10 to 40 and construct a chart of the data. This will resemble the markers in the left-hand chart in Figure 10.25.

The starting values (B3:B6) are more critical than before. We are working with a more complex function and have more variable cells. If we start too far from the answer, Solver will reply, "You can't get there from here". Looking at the chart, a value of 1600 for *h* seems reasonable. The curve has its peak more or less midway between 2.5 and 2.66, so we will start with 0.255 in B4. Recalling that three standard deviations on each side of the mean encompasses most of a Gaussian curve, we compute a starting value for the standard deviation (B5) as =(0.27 - 0.24)/6 = 0.005. The tails of the curve are not far from zero, so a starting value of 0 for *b* would be appropriate.

1. With these values entered into B3:B6, enter this formula into C I 0 to compute the predicted value: =h\*EXP( - (((A10 - mu)/sig)^2)) + base. You may feel there is an extra set of parentheses but this is not so for we must allow for the fact that the negation operator has the highest priority. Copy the formula down to row 40.
2. Select C10:C40 and use the Copy tool. Click on the chart and use Paste Special to add a new data series. Your chart should now resemble the left-hand chart in Figure 10.25. Note how our analysis has generated a good starting fit to the experimental data.
3. Rather than adding another column to compute the squares of the residuals and adding these to get SSR, we will use the SUMXMY2 (Sum X Minus Y power of 2) function provided by Excel. This sums the squares of the differences of two ranges is just what we need. For our problem the two ranges are the *y* and *y'* ranges. In B7 enter the formula =SUMXMY2(B10:B40,C10:C40).
4. Use Solver to complete the task. The target cell is B7 which we wish to minimize by changing B3:B6. The resulting values are shown below.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *h* | *µ* | *σ* | *base* | resSqr |
| 1580.69 | 0.253959 | 0.003654 | 40.11852 | 114867.2 |

If you wish to experiment with larger, more realistic datasets and more complex problems (i.e. two overlapping Gaussian curves), the NIST web site provides some fine examples. Furthermore, it provides the values you should get for the parameters. To experiment with fitting a histogram to a normal curve; see Statics for Experiments.

Figure XX

|  |  |  |  |
| --- | --- | --- | --- |
| EXCEL | A | B | C |
| 1 | Gaussian Fit |  |  |
| 2 |  |  |  |
| 3 | h |  |  |
| 4 | mu |  |  |
| 5 | sig |  |  |
| 6 | base |  |  |
| 7 | resSq |  |  |
| 8 |  |  |  |
| 9 | x | y | y’ |
| 10 | 0.239 | 25 |  |
| 11 | 0.240 | 24 |  |
| 12 | 0.241 | 39 |  |
| 13 | 0.242 | 49 |  |
| 14 | 0.243 | 56 |  |
| 15 | 0.244 | 84 |  |
| 16 | 0.245 | 66 |  |
| 17 | 0.246 | 97 |  |
| 18 | 0.247 | 158 |  |
| 19 | 0.248 | 244 |  |
| 20 | 0.249 | 353 |  |
| 21 | 0.250 | 444 |  |
| 22 | 0.251 | 773 |  |
| 23 | 0.252 | 1196 |  |
| 24 | 0.253 | 1677 |  |
| 25 | 0.254 | 1654 |  |
| 26 | 0.255 | 1314 |  |
| 27 | 0.256 | 1173 |  |
| 28 | 0.257 | 933 |  |
| 29 | 0.258 | 550 |  |
| 30 | 0.259 | 220 |  |
| 31 | 0.260 | 101 |  |
| 32 | 0.261 | 97 |  |
| 33 | 0.262 | 39 |  |
| 34 | 0.263 | 26 |  |
| 35 | 0.264 | 11 |  |
| 36 | 0.265 | 16 |  |
| 37 | 0.266 | 10 |  |
| 38 | 0.267 | 13 |  |
| 39 | 0.268 | 8 |  |
| 40 | 0.269 | 5 |  |