# 16. 1stOpt 多峰拟合及分峰

多峰拟合是比较常见的非线性拟合问题，1stOpt 不仅可以轻松求解多峰模型拟合问题，还可以非常方便进行分峰处理。

## 16.1 案例

模型拟合公式如下，由 4 个高斯函数组成；拟合数据及数据图见下表 16-1 和图 16-1。

$$y = y_0 + \sum_{i=1}^{4}\left(\left(\frac{a_i}{w_i\sqrt{\frac{\pi}{2}}}\right)\exp\left(-2\left(\frac{x - xc_i}{w_i}\right)^2\right)\right) \tag{16-1}$$

表 16.1 数据：

| | |
|---|---|
| x | 0.0000, 0.2857, 0.5714, 0.8571, 1.1429, 1.4286, 1.7143, 2.0000, 2.2857, 2.5714, 2.8571, 3.1429, 3.4286, 3.7143, 4.0000, 4.2857, 4.5714, 4.8571, 5.1429, 5.4286, 5.7143, 6.0000, 6.2857, 6.5714, 6.8571, 7.1429, 7.4286, 7.7143, 8.0000, 8.2857, 8.5714, 8.8571, 9.1429, 9.4286, 9.7143, 10.0000, 10.2857, 10.5714, 10.8571, 11.1429, 11.4286, 11.7143, 12.0000, 12.2857, 12.5714, 12.8571, 13.1429, 13.4286, 13.7143, 14.0000, 14.2857, 14.5714, 14.8571, 15.1429, 15.4286, 15.7143, 16.0000, 16.2857, 16.5714, 16.8571, 17.1429, 17.4286, 17.7143, 18.0000, 18.2857, 18.5714, 18.8571, 19.1429, 19.4286, 19.7143, 20.0000, 20.2857, 20.5714, 20.8571, 21.1429, 21.4286, 21.7143, 22.0000, 22.2857, 22.5714, 22.8571, 23.1429, 23.4286, 23.7143, 24.0000, 24.2857, 24.5714, 24.8571, 25.1429, 25.4286, 25.7143, 26.0000, 26.2857, 26.5714, 26.8571, 27.1429, 27.4286, 27.7143, 28.0000, 28.2857, 28.5714, 28.8571, 29.1429, 29.4286, 29.7143, 30.0000, 30.2857, 30.5714, 30.8571, 31.1429, 31.4286, 31.7143, 32.0000, 32.2857, 32.5714, 32.8571, 33.1429, 33.4286, 33.7143, 34.0000, 34.2857, 34.5714, 34.8571, 35.1429, 35.4286, 35.7143, 36.0000, 36.2857, 36.5714, 36.8571, 37.1429, 37.4286, 37.7143, 38.0000, 38.2857, 38.5714, 38.8571, 39.1429, 39.4286, 39.7143, 40.0000 |
| y | 0.0169, 0.0294, 0.0540, 0.0832, 0.1769, 0.3010, 0.4822, 0.8909, 1.4673, 2.6091, 3.9487, 6.1861, 10.2854, 14.1971, 20.8154, 27.9622, 34.1893, 50.9944, 52.8896, 74.7148, 78.2739, 94.8341, 97.1913, 106.9074, 110.5764, 99.7094, 95.2368, 100.9800, 95.3051, 84.7236, 72.5028, 63.7613, 53.8688, 45.3433, 47.6868, 39.2611, 41.2603, 38.4826, 41.0614, 42.8718, 52.4247, 54.6309, 58.5655, 57.6910, 62.2335, 63.6598, 74.5593, 76.3657, 76.8343, 76.4166, 73.9337, 83.6326, 79.5735, 77.3333, 82.7579, 74.8436, 70.2986, 69.1072, 62.9654, 63.9911, 63.3608, 54.3341, 54.7983, 54.1602, 50.5028, 46.6765, 37.3148, 35.4733, 31.4011, 31.6141, 29.3181, 29.2092, 25.6456, 23.5434, 21.6426, 20.5469, 21.0379, 23.0230, 23.3786, 22.6132, 28.5862, 29.2285, 34.6253, 40.5241, 43.5328, 44.4078, 55.3422, 63.8790, 70.3837, 64.7925, 84.1060, 85.2346, 96.3957, 101.5065, 101.5635, 125.4770, 123.0295, 116.8548, 132.5786, 146.0718, 152.3447, 149.5277, 149.2917, 167.8167, 140.3957, 146.2560, 140.2877, 150.3306, 151.0844, 135.0494, 124.1520, 128.2794, 121.8187, 127.7168, 109.3237, 98.8645, 101.0413, 95.4619, 82.9761, 108.2798, 173.0225, 125.9043, 55.3894, 48.4749, 40.5538, 32.5134, 30.7203, 26.0722, 21.6562, 19.8353, 16.4291, 14.3602, 11.6957, 8.8610, 7.2047, 6.0873, 5.1435, 4.1757, 3.0479, 2.7644, 2.1079 |

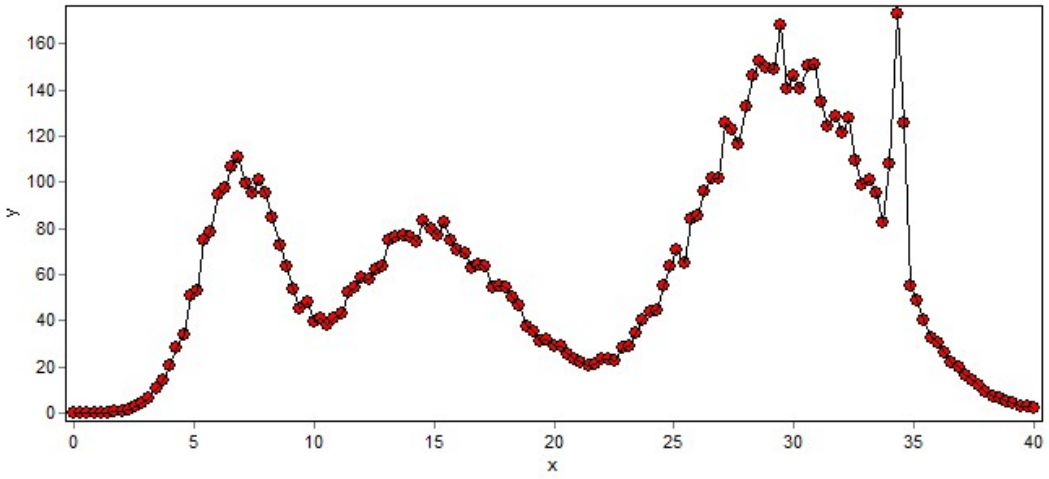



图 16.1 多峰函数数据图

## 16.2 多峰函数拟合求解

该多峰拟合函数是 4 个高斯函数的组合，广义而言就是一个普通的非线性拟合问题，但高斯峰函数尤其特殊性，一些参数是有明确的数学几何意义的，比如参数 xc 代表峰值对应的 x 坐标值，参考图 16.1 可以明确知道 4 个峰对应的 xc 值范围应该在自变量 x 值范围之内，即[0,40]之间，因此求解代码加了一句“Parameter xc(4)=[0,40];”，对参数 xc 进行访问限制。虽然 1stOpt 可以不需要猜测参数初值，但如果给出合理的求解范围无疑会加快得到全局最优解的速度，同时也增加得到全局最优解的概率，尤其对本案例，第 4 个峰只有仅仅 3 个数据点，求解难度较大。下面代码几乎可以 100%得到全局最优解。

代码 16-1

```
Parameter xc(4)=[0,40];
Function y=y0+Sum(i=1:4,A,w,xc)((A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2));
Data;
//x    y
0.0000      0.0169
0.2857      0.0294
0.5714      0.0540
0.8571      0.0832
1.1429      0.1769
….
```

结果：

```
Root of Mean Square Error (RMSE): 3.99446092891712
Sum of Squared Residual: 2249.756253883
```

Correlation Coef. (R): 0.995956951587509
R-Square: 0.991930249415483
Adjusted R-Square: 0.991813296508461
Determination Coef. (DC): 0.991930249415483
Chi-Square: 23.838094271931
F-Statistic: 1311.14205027548

| Parameter | Best Estimate |
|---|---|
| xc1 | 29.7237852683356 |
| xc2 | 14.8189007168224 |
| xc3 | 6.85943495716345 |
| xc4 | 34.340829577245 |
| y0 | -0.340779521137444 |
| a1 | 1351.67408949051 |
| w1 | 7.09493440428869 |
| a2 | -670.622634994602 |
| w2 | -6.76753411792903 |
| a3 | 408.386651256984 |
| w3 | 3.16442539003381 |
| a4 | 61.8474317626829 |
| w4 | 0.443632255572946 |

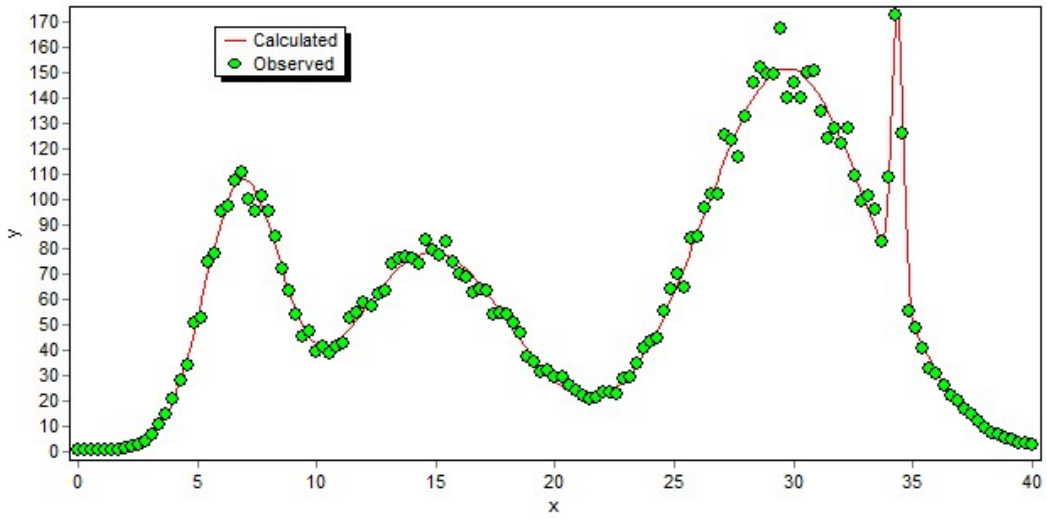



图 16.2 多峰函数拟合计算对比图

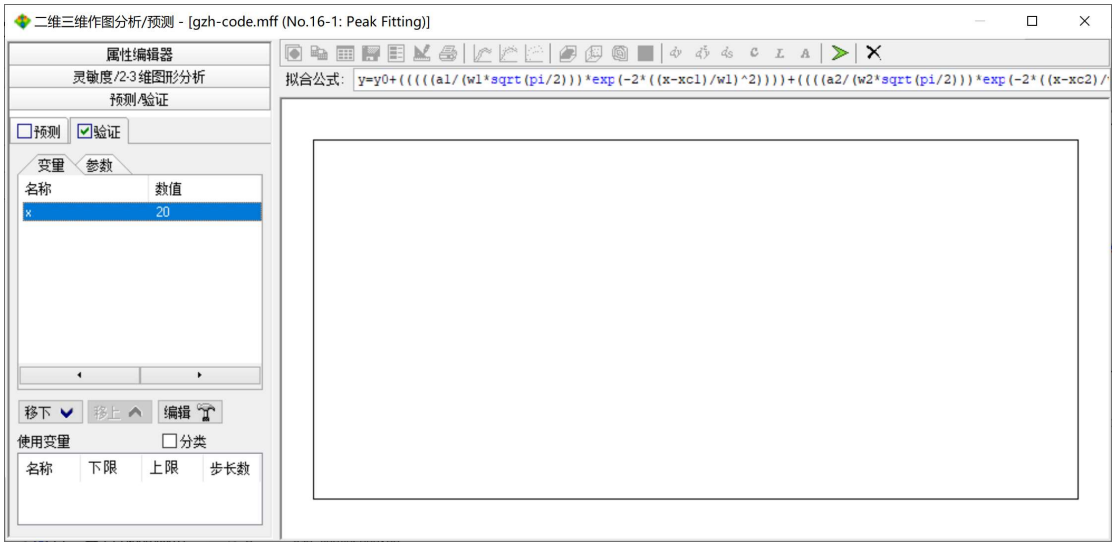
## 16.3 多峰函数分峰

前面拟合计算结束、各参数值求出之后即可进行分峰。有两种方式可供选择。

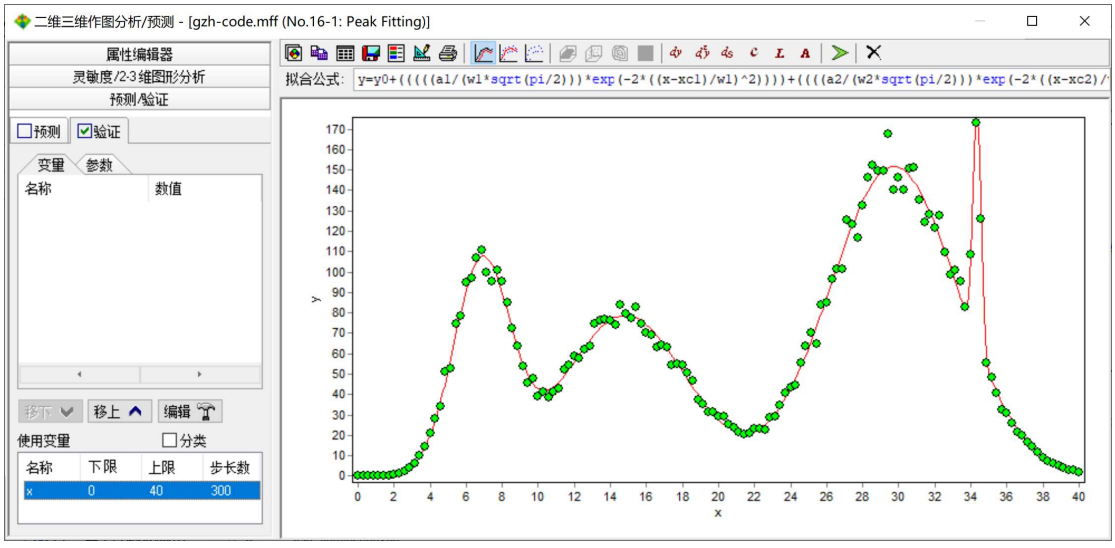
1) 分析-预测窗口实现分峰

拟合计算完毕，点击“二维-三维分析/预测”按钮。

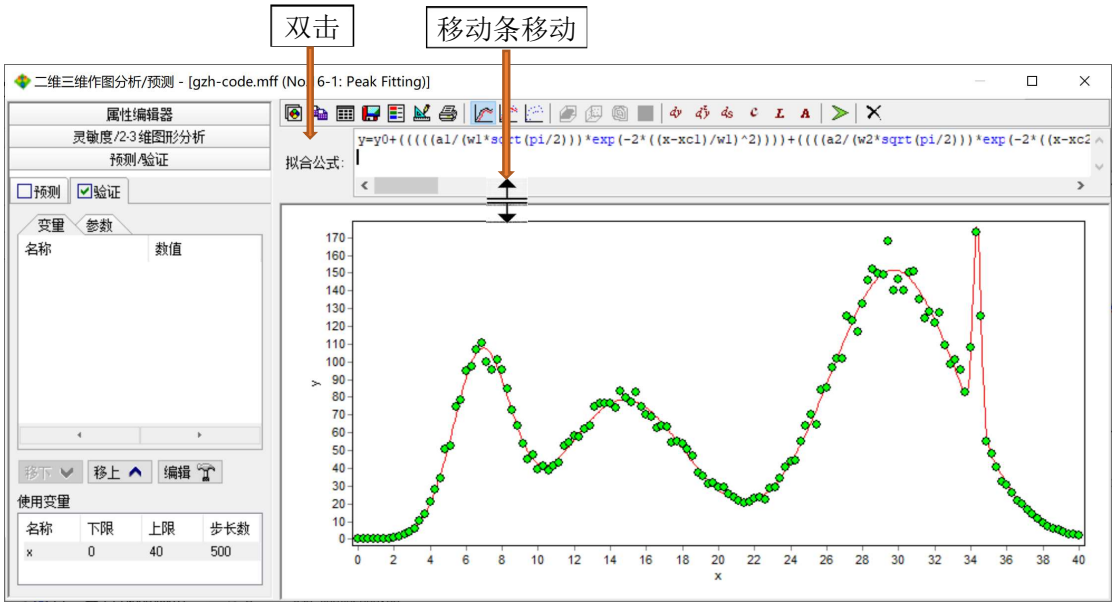
选“验证”页面：



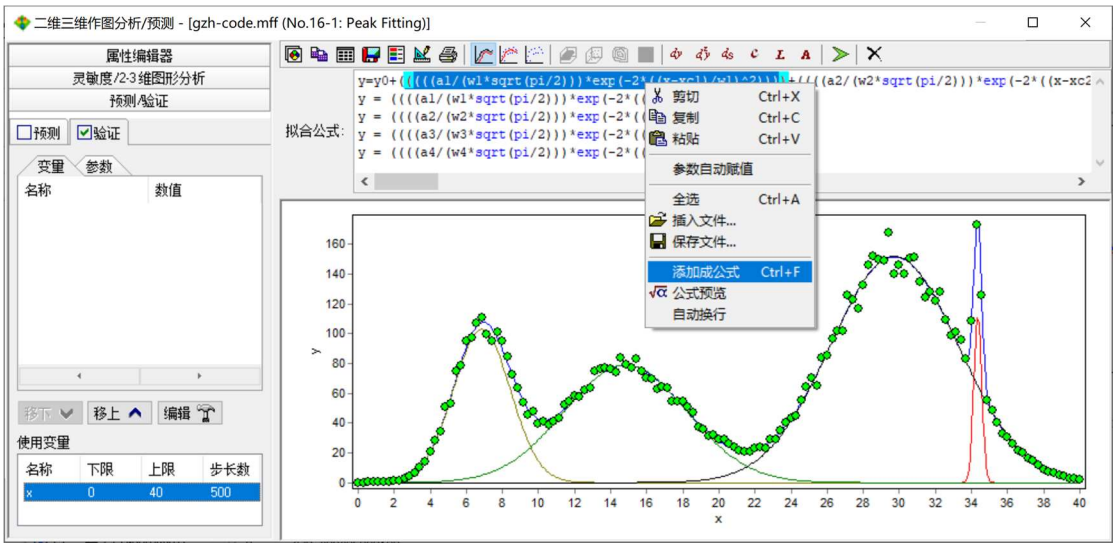

选择 x 自变量项，按“移下”按钮，或双击所选 x 自变量项：



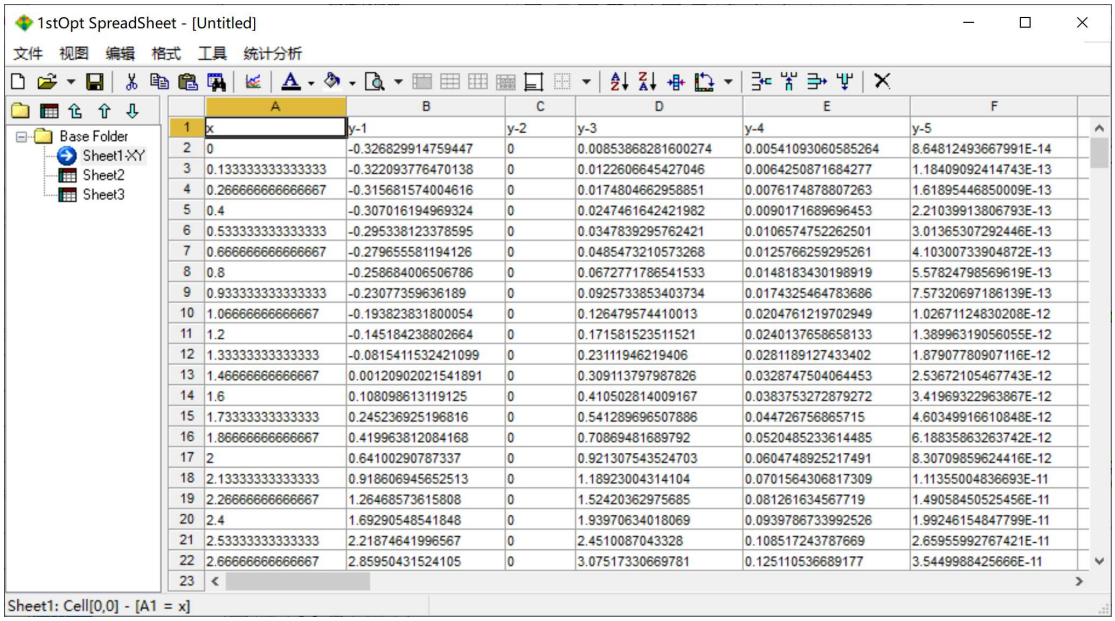
双击或通过移动条扩大函数窗口：




选择各峰函数表达式，右键弹出菜单“添加成公式”：




点击上图工具栏左起第三个按钮可查看详细计算数据值：




| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| 1 | x | y-1 | y-2 | y-3 | y-4 | y-5 |
| 2 | 0 | -0.326829914759447 | 0 | 0.00853868281600274 | 0.00541093060585264 | 8.64812493667991E-14 |
| 3 | 0.133333333333333 | -0.322093776470138 | 0 | 0.0122606645427046 | 0.0064250871684277 | 1.18409092414743E-13 |
| 4 | 0.266666666666667 | -0.315681574004616 | 0 | 0.0174804662958851 | 0.0076174878807263 | 1.61895446850009E-13 |
| 5 | 0.4 | -0.307016194969324 | 0 | 0.0247461642421982 | 0.0090171689696453 | 2.21039913806793E-13 |
| 6 | 0.533333333333333 | -0.295338123378595 | 0 | 0.0347839295762421 | 0.0106574752262501 | 3.01365307292446E-13 |
| 7 | 0.666666666666667 | -0.279655581194126 | 0 | 0.0485473210573268 | 0.0125766259295261 | 4.10300733904872E-13 |
| 8 | 0.8 | -0.258684006506786 | 0 | 0.0672771786541533 | 0.0148183430198919 | 5.57824798569619E-13 |
| 9 | 0.933333333333333 | -0.23077359636189 | 0 | 0.0925733853403734 | 0.0174325464783686 | 7.57320697186139E-13 |
| 10 | 1.06666666666667 | -0.193823831800054 | 0 | 0.126479574410013 | 0.0204761219702949 | 1.02671124830208E-12 |
| 11 | 1.2 | -0.145184238802664 | 0 | 0.171581523511521 | 0.0240137658658133 | 1.38996319056055E-12 |
| 12 | 1.33333333333333 | -0.0815411532421099 | 0 | 0.23111946219406 | 0.0281189127433402 | 1.87907780907116E-12 |
| 13 | 1.46666666666667 | 0.00120902021541891 | 0 | 0.309113797987826 | 0.0328747504064453 | 2.53672105467743E-12 |
| 14 | 1.6 | 0.108098613119125 | 0 | 0.410502814009167 | 0.0383753272879272 | 3.41969322963867E-12 |
| 15 | 1.73333333333333 | 0.245236925196816 | 0 | 0.541289696507886 | 0.044726756865715 | 4.60349916610848E-12 |
| 16 | 1.86666666666667 | 0.419963812084168 | 0 | 0.70869481689792 | 0.0520485233614485 | 6.18835863263742E-12 |
| 17 | 2 | 0.64100290787337 | 0 | 0.921307543524703 | 0.0604748925217491 | 8.30709859624416E-12 |
| 18 | 2.13333333333333 | 0.918606945652513 | 0 | 1.18923004314104 | 0.0701564306817309 | 1.11355004836693E-11 |
| 19 | 2.26666666666667 | 1.26468573615808 | 0 | 1.52420362975685 | 0.081261634567719 | 1.49058450525456E-11 |
| 20 | 2.4 | 1.69290548541848 | 0 | 1.93970634018069 | 0.0939786733992526 | 1.99246154847799E-11 |
| 21 | 2.53333333333333 | 2.21874641996567 | 0 | 2.4510087043328 | 0.108517243787669 | 2.65955992767421E-11 |
| 22 | 2.66666666666667 | 2.85950431524105 | 0 | 3.07517330669781 | 0.125110536689177 | 3.54499884256666E-11 |
| 23 | | | | | | |

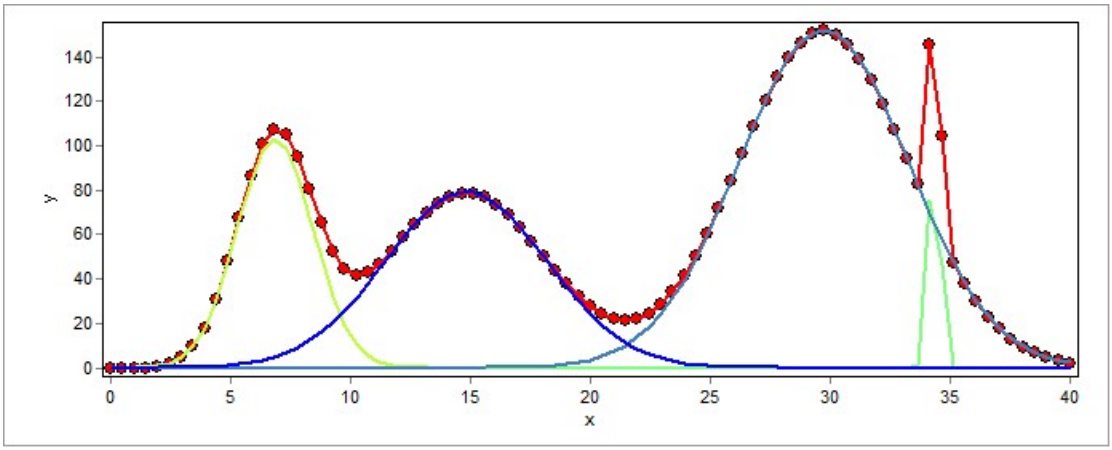
2) 代码实现分峰

除了上面介绍的在预测窗口界面化实现分峰外，还可以通过作图代码实现分峰，即将拟合计算所得的参数值作为常数，由下面代码实现。

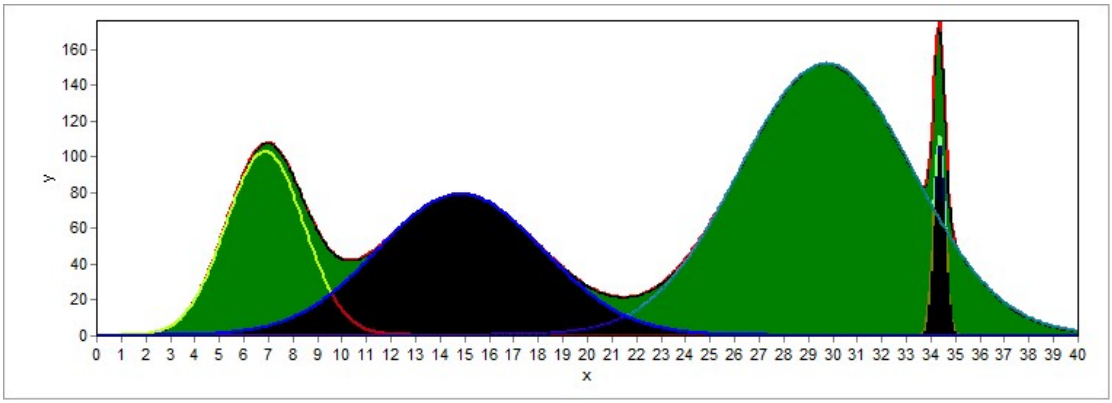
代码 16-2

```
Constant xc1=6.85943495851161,xc2=34.3408295929302,xc3=29.723785268395,xc4=14.8189007181235,
y0=-0.340779543600283,a1=408.386651225468,w1=3.16442538987146,a2=-61.8474317431603,w2=-
0.443632252924537,
a3=-1351.67408940441,w3=-7.0949344015555,a4=-670.622634909386,w4=-6.7675341163538;
//Integration = 1; //1: Simpson, 2: Trapezium, 3: Left EndPoint, 4: Right EndPoint;
Variable x=[0:0.5:40],y;
PlotFunction
y = y0+(a1/(w1*sqrt(pi/2)))*exp(-2*((x-xc1)/w1)^2)+(a2/(w2*sqrt(pi/2)))*exp(-2*((x-
xc2)/w2)^2)+(a3/(w3*sqrt(pi/2)))*exp(-2*((x-xc3)/w3)^2)+(a4/(w4*sqrt(pi/2)))*exp(-2*((x-xc4)/w4)^2);
y = (a1/(w1*sqrt(pi/2)))*exp(-2*((x-xc1)/w1)^2);
y = (a2/(w2*sqrt(pi/2)))*exp(-2*((x-xc2)/w2)^2);
y = (a3/(w3*sqrt(pi/2)))*exp(-2*((x-xc3)/w3)^2);
y = (a4/(w4*sqrt(pi/2)))*exp(-2*((x-xc4)/w4)^2);
```

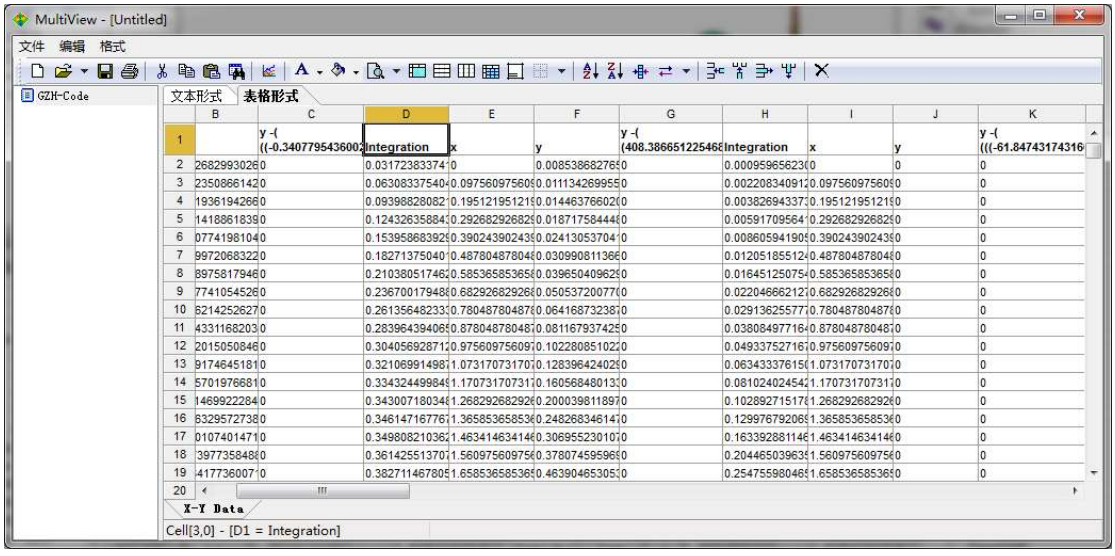
执行上述代码，可得如下结果分峰结果图：



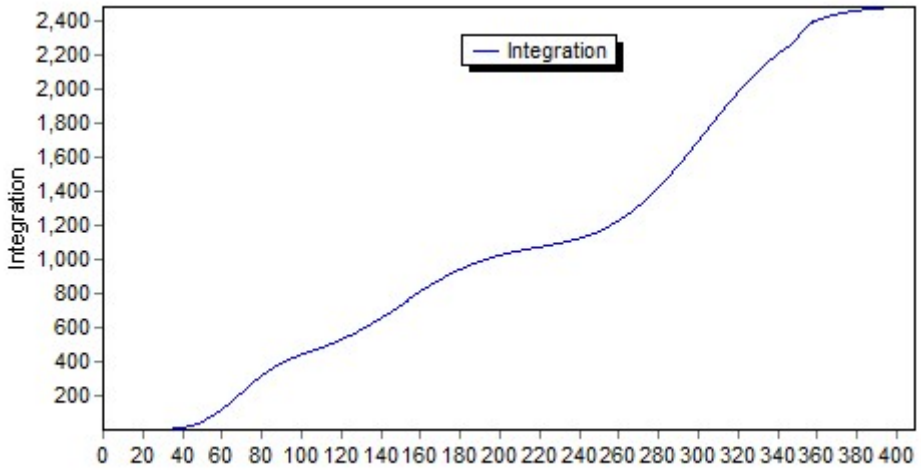

上述代码中，如果加一句“Integration = 1;”，还可以计算出每个峰曲线与 x 坐标轴间的面积：



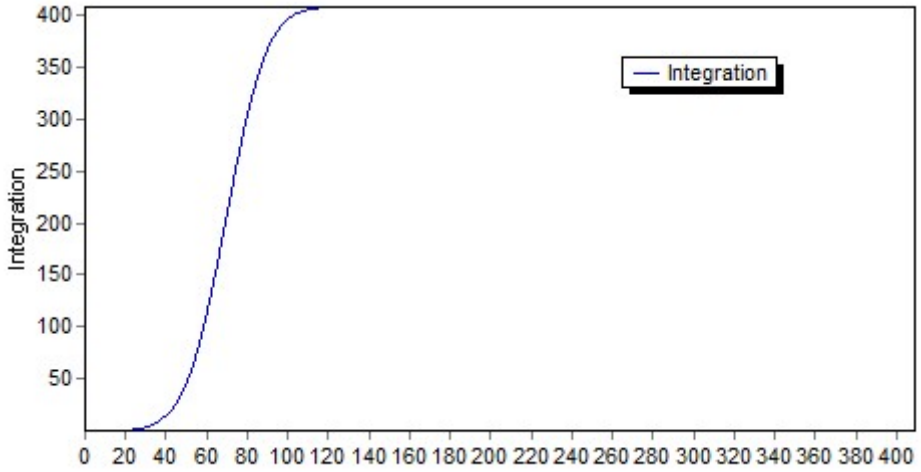

在结果报表中可以看到详细的面积数值数据：



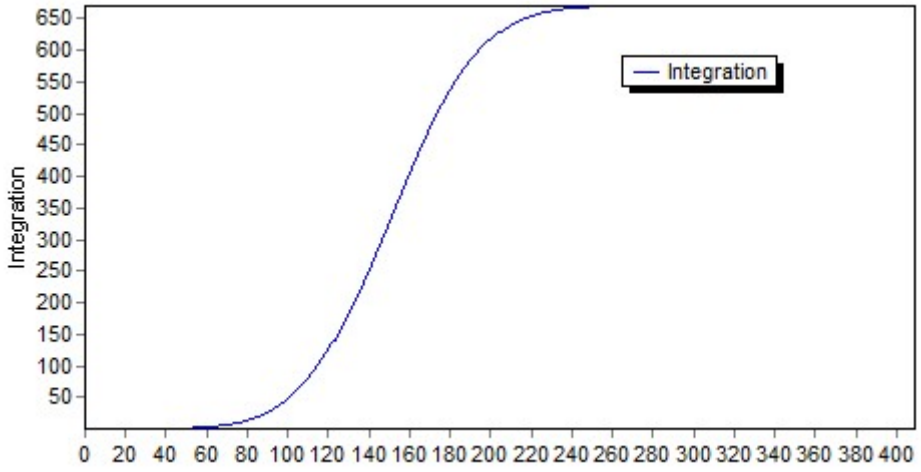

由上述计算所得面积变化数据值，可得到整体及每个单峰面积变化图。
整体复合峰面积变化图：



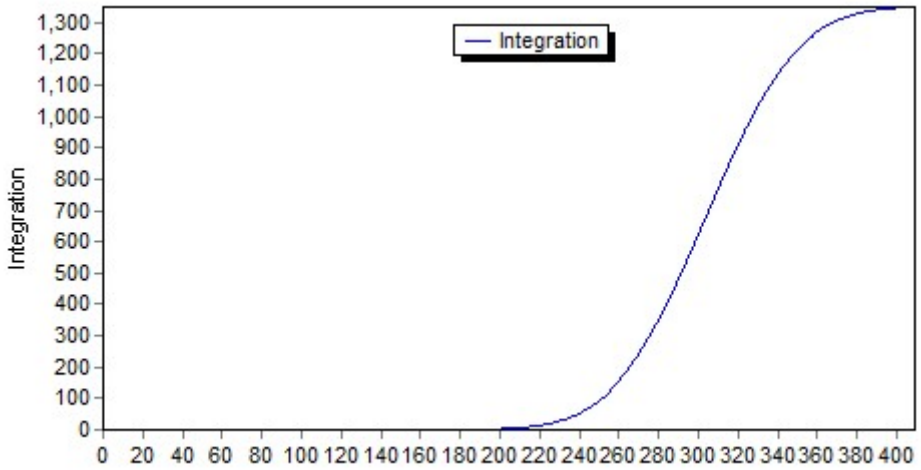

单峰一面积变化图：



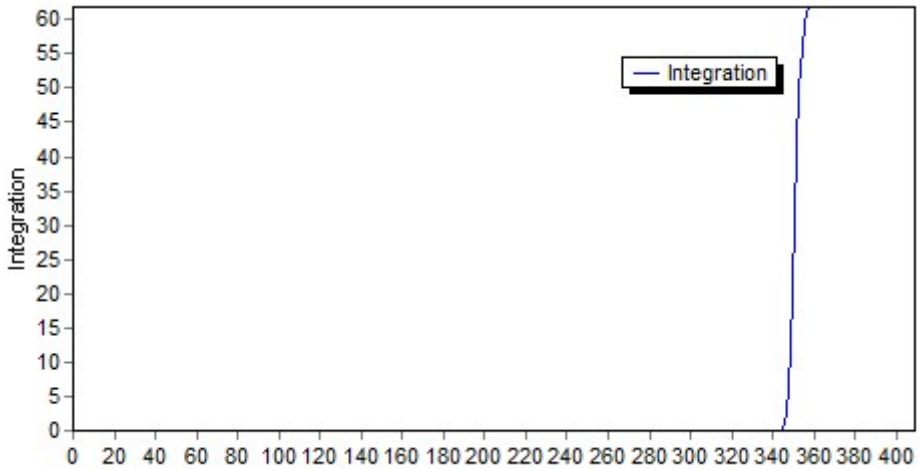

单峰二面积变化图：




单峰三面积变化图：




单峰四面积变化图：




## 16.4 小结

1stOpt 可以非常方便处理应对多峰函数拟合及后期的分峰问题，此外还可求得各峰面积。