

# 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 |

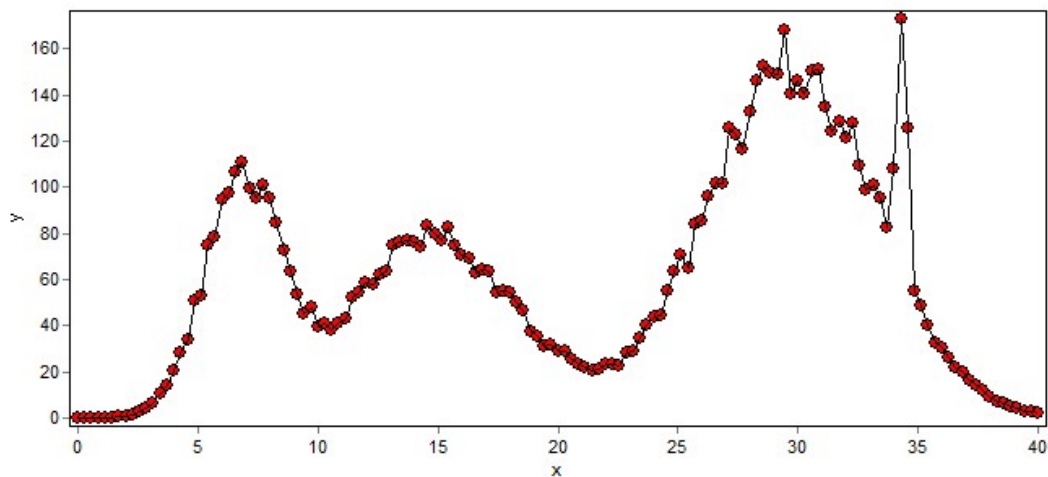


图 16.1 多峰函数数据图

## 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

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```

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:

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```

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

```

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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  |

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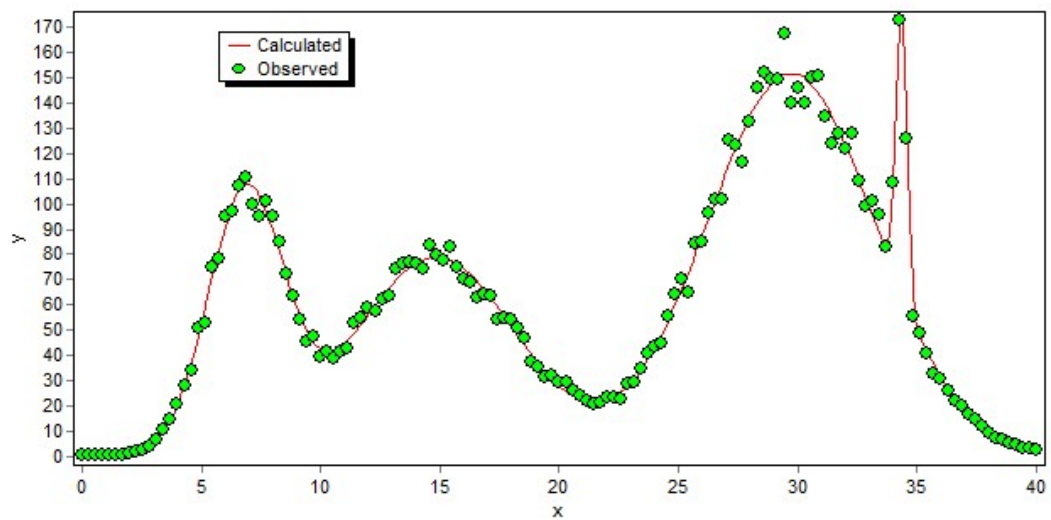


图 16.2 多峰函数拟合计算对比图

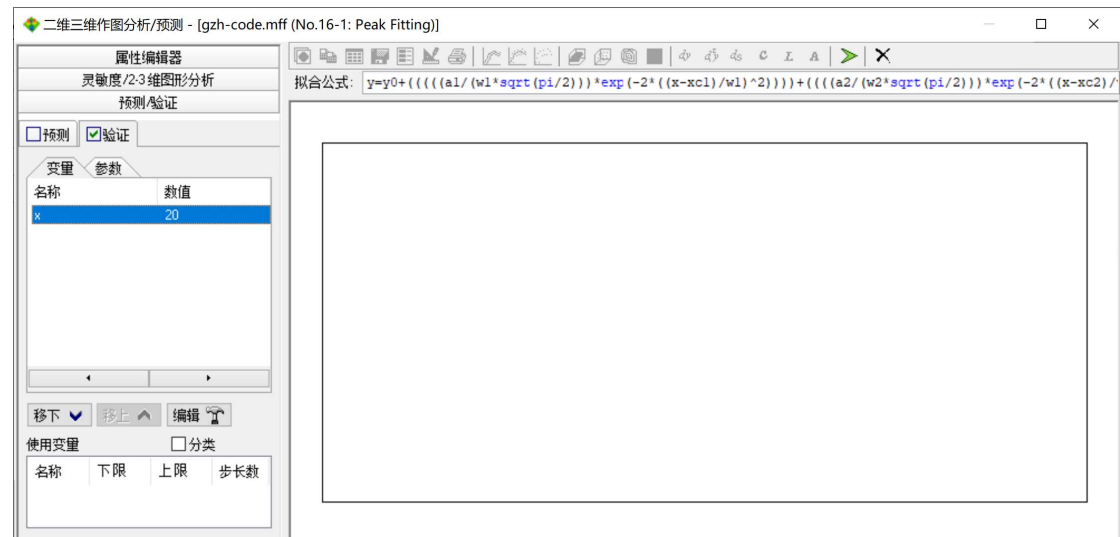
## 16.3 多峰函数分峰

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。

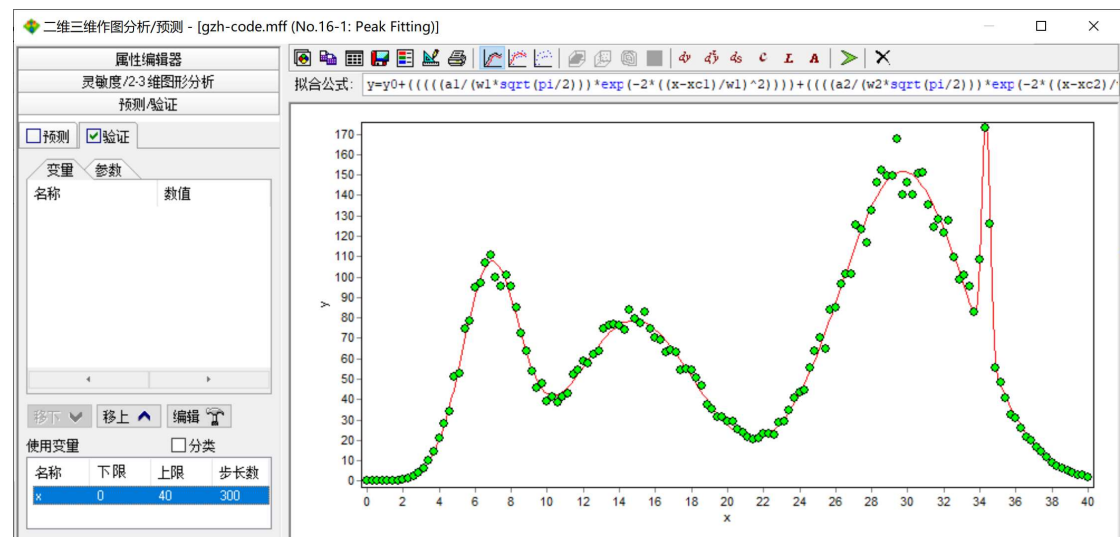
### 1) 分析-预测窗口实现分峰

拟合计算完毕，点击“二维-三维分析/预测”按钮。

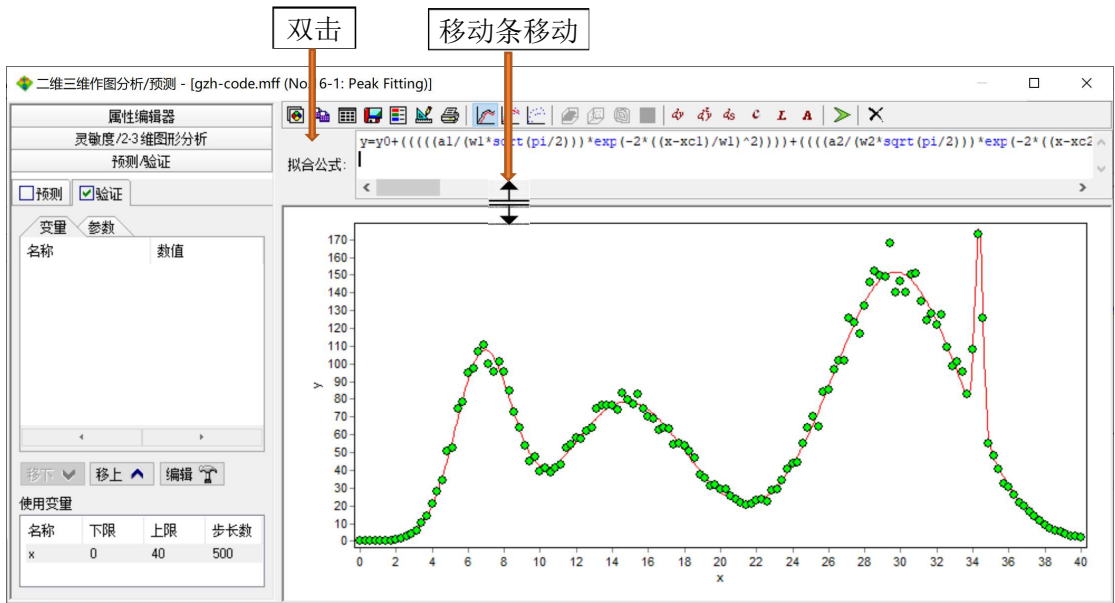
选“验证”页面：



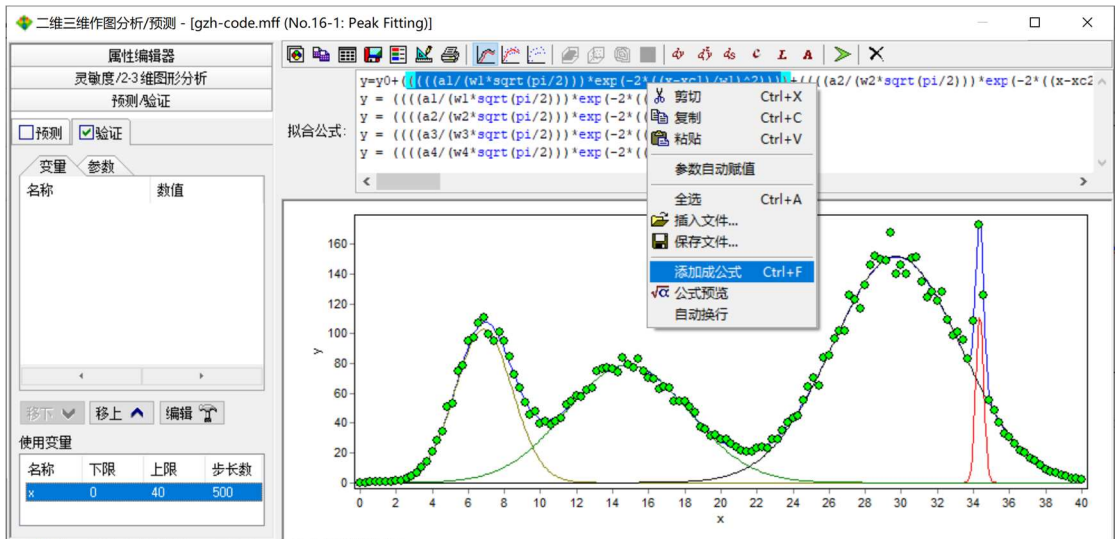
选择 x 自变量项，按“移下”按钮，或双击所选 x 自变量项：



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   | 3.5449988425666E-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

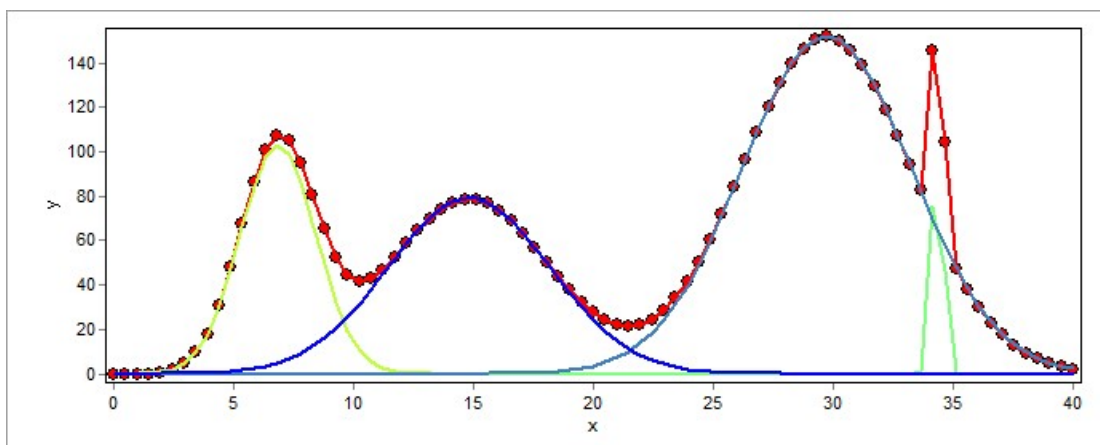
```

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);

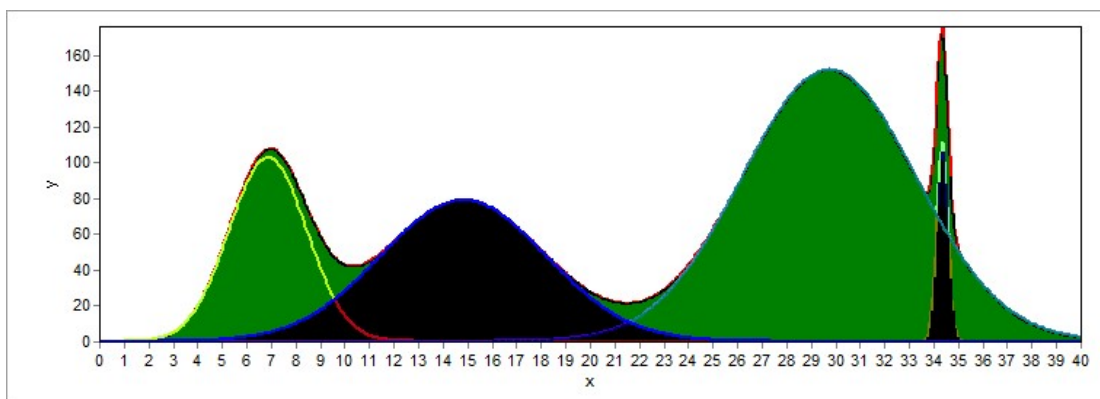
```

执行上述代码，可得如下结果分峰结果图：





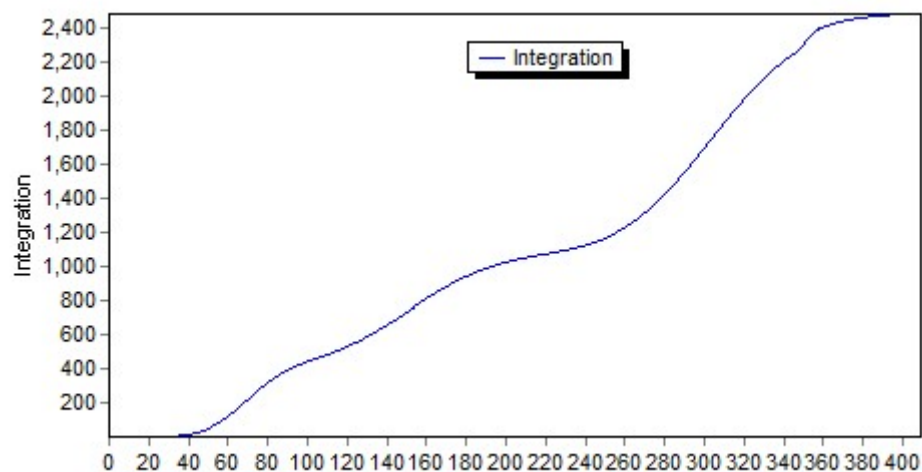
上述代码中，如果加一句“Integration = 1;”，还可以计算出每个峰曲线与 x 坐标轴间的面积：



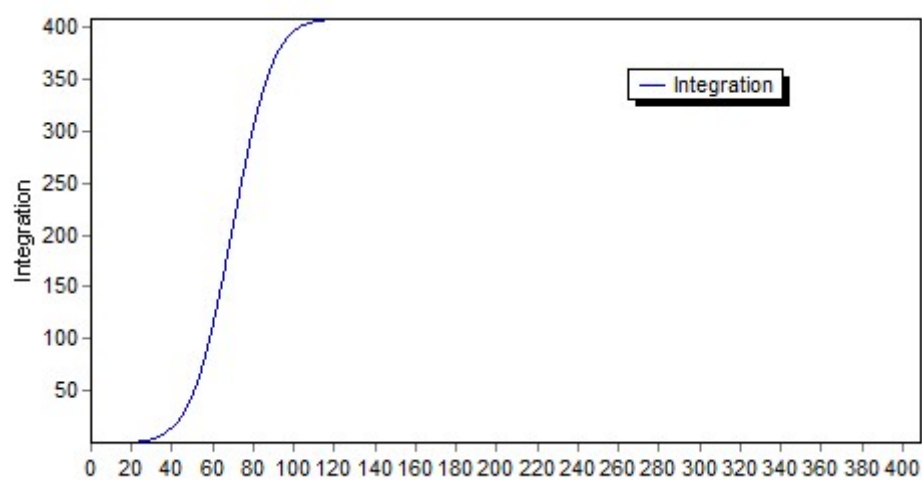
在结果报表中可以看到详细的面积数值数据：

| MultiView - [Untitled]         |            |                    |               |               |   |               |                   |             |   |   |
|--------------------------------|------------|--------------------|---------------|---------------|---|---------------|-------------------|-------------|---|---|
| 文件 编辑 格式                       |            |                    |               |               |   |               |                   |             |   |   |
| GZH-Code                       |            |                    |               |               |   |               |                   |             |   |   |
| 文本形式 表格形式                      |            |                    |               |               |   |               |                   |             |   |   |
| 1                              | B          | C                  | D             | E             | F | G             | H                 | I           | J | K |
|                                | y-1        | ((-0.3407795436002 | Integration   | x             | y | y-1           | (408.386651225468 | Integration | x | y |
| 2                              | 2682993028 | 0.03172383374      | 0             | 0.00853868276 | 0 | 0.00095965623 | 0                 | 0           | 0 | 0 |
| 3                              | 2350866142 | 0.06308337540      | 0.09756097560 | 0.01134269955 | 0 | 0.00220834091 | 0.09756097560     | 0           | 0 | 0 |
| 4                              | 1936194268 | 0.09398828082      | 0.19512195121 | 0.01446376602 | 0 | 0.00382694337 | 0.19512195121     | 0           | 0 | 0 |
| 5                              | 1418861838 | 0.12432635884      | 0.29268292682 | 0.01871758444 | 0 | 0.00591709564 | 0.29268292682     | 0           | 0 | 0 |
| 6                              | 0774198104 | 0.15395868392      | 0.39024390243 | 0.02413053704 | 0 | 0.00860594190 | 0.39024390243     | 0           | 0 | 0 |
| 7                              | 9872068322 | 0.18271375040      | 0.48780487804 | 0.03099081136 | 0 | 0.01205185512 | 0.48780487804     | 0           | 0 | 0 |
| 8                              | 8975817948 | 0.21038051746      | 0.58536585365 | 0.03965040962 | 0 | 0.01645125075 | 0.58536585365     | 0           | 0 | 0 |
| 9                              | 7741054528 | 0.23670017948      | 0.68292682926 | 0.05053720077 | 0 | 0.02204666212 | 0.68292682926     | 0           | 0 | 0 |
| 10                             | 8214252627 | 0.26135648233      | 0.78048780487 | 0.06416873238 | 0 | 0.02913625577 | 0.78048780487     | 0           | 0 | 0 |
| 11                             | 4331168203 | 0.28396439408      | 0.87804878048 | 0.08116793742 | 0 | 0.03808497716 | 0.87804878048     | 0           | 0 | 0 |
| 12                             | 2015050848 | 0.30405692871      | 0.97560975609 | 0.10228085102 | 0 | 0.04933752716 | 0.97560975609     | 0           | 0 | 0 |
| 13                             | 9174845181 | 0.32106991498      | 1.07317073170 | 0.12839642402 | 0 | 0.06343337615 | 1.07317073170     | 0           | 0 | 0 |
| 14                             | 5701976681 | 0.33432449984      | 1.17073170731 | 0.16056848013 | 0 | 0.08102402454 | 1.17073170731     | 0           | 0 | 0 |
| 15                             | 1469922284 | 0.34300718034      | 1.26829268292 | 0.20003981189 | 0 | 0.10289271517 | 1.26829268292     | 0           | 0 | 0 |
| 16                             | 8329572738 | 0.34614716776      | 1.36585365853 | 0.24826834614 | 0 | 0.12997679206 | 1.36585365853     | 0           | 0 | 0 |
| 17                             | 0107401471 | 0.34980821036      | 1.46341463414 | 0.30695523010 | 0 | 0.16339288114 | 1.46341463414     | 0           | 0 | 0 |
| 18                             | 3977358480 | 0.36142551370      | 1.56097560975 | 0.37807459596 | 0 | 0.20446503963 | 1.56097560975     | 0           | 0 | 0 |
| 19                             | 4177360070 | 0.38271146780      | 1.65853658536 | 0.46390465305 | 0 | 0.25475598046 | 1.65853658536     | 0           | 0 | 0 |
| 20                             |            |                    |               |               |   |               |                   |             |   |   |
| X-Y Data                       |            |                    |               |               |   |               |                   |             |   |   |
| Cell[3,0] - [D1 = Integration] |            |                    |               |               |   |               |                   |             |   |   |

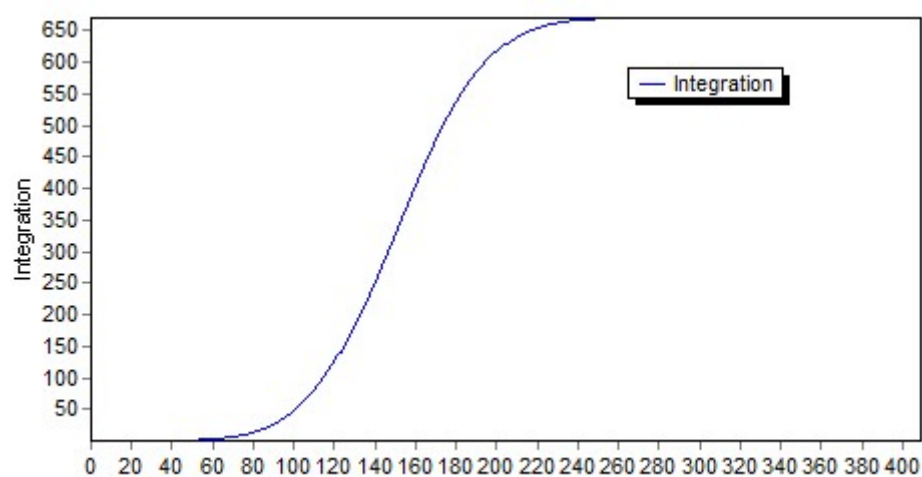
由上述计算所得面积变化数据值，可得到整体及每个单峰面积变化图。  
整体复合峰面积变化图：



单峰一面积变化图：

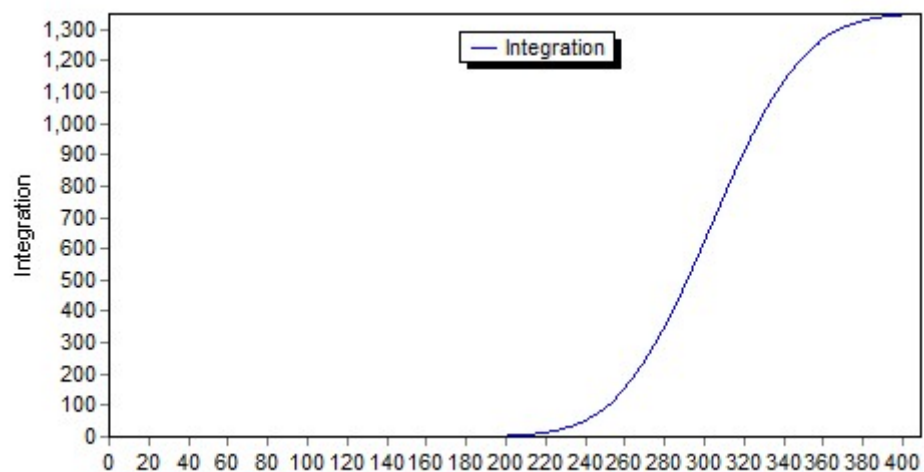


单峰二面积变化图：

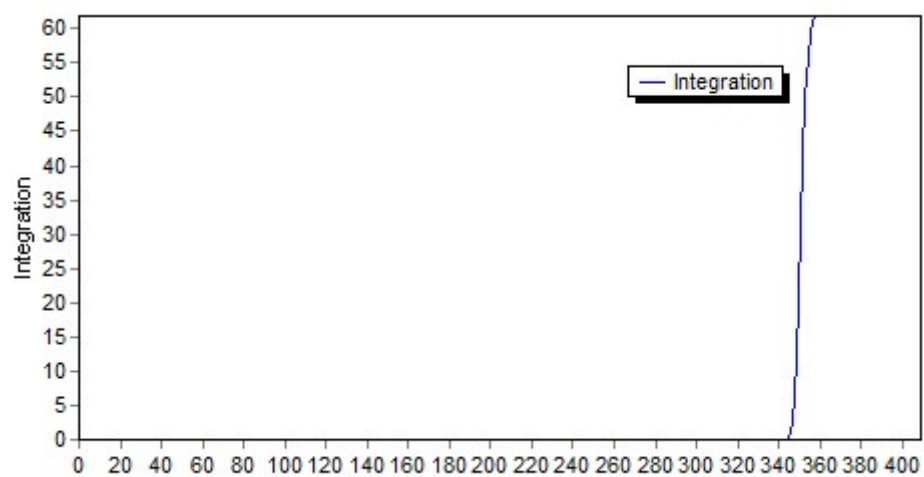


单峰三面积变化图：





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。