37. 1stOpt 多峰函数拟合技巧－全局与局部优化算法协同

37.1 引言

多峰函数拟合具有一定的难度，即使知道峰函数中各个参数的实际几何意义，也无法保证拟合计算结果符合要求，尤其是当“峰”数较多时，相应需求解的未知参数数与“峰”数成正比而成倍增加，求解难度及计算时间随之指数增加。

1stOpt的优化算法既包括独有的通用全局优化算法，也包含经典的局部最优算法，前者在理论上具有无需初值既能得到全局最优解的特性，但实际当中，当参数数较多时也不易短时间内获得理想结果；而后者局部最优算法的最大优点是计算速度快，当然前提是赋予的参数初值合理正确，而如何猜测并给出合理的参数初值却是公认的难点，尤其对普通用户而言更无异于噩梦。那么有无好的方法将全局与局部两种优化算法进行合理组合，充分发挥各自的优势特长，从而对多参数的拟合问题进行高效且正确的求解？下面以多峰函数拟合为例给予展示。

37.2 案例

选择了两个实际案例。案例1参见表37-1数据及图37.1和图37.2，共有6个峰，因为是对称的峰，因此需要用Gauss（高斯）函数去拟合，拟合模型如下公式（37-1），共有19个待求参数；案例2见表37-2数据及图37.3和图37.4，峰函数类型为非对称的Asym2Sig函数，其特点是峰左侧陡峭而右侧平缓，具体表达式见公式（37-2），共有31个未知参数。

$$y = y_0 + \sum_{i=1}^{6}\left(a_i \exp\left(b_i (x - c_i)^2\right)\right) \tag{37-1}$$

$$y = y_0 + \sum_{i=1}^{6}\left(a_i \left(\frac{1}{1+\exp\left(c_i (x - b_i + w_i)\right)}\right)\left(1 - \frac{1}{1+\exp\left(d_i (x - b_i - w_i)\right)}\right)\right) \tag{37-2}$$

表 37-1 案例数据 1

x	0.000,0.286,0.571,0.857,1.143,1.429,1.714,2.000,2.286,2.571,2.857,3.143,3.429,3.714,4.000,4.286,4.571,4.857,5.143,5.429,5.714,6.000,6.286,6.571,6.857,7.143,7.429,7.714,8.000,8.286,8.571,8.857,9.143,9.429,9.714,10.000,10.286,10.571,10.857,11.143,11.429,11.714,12.000,12.286,12.571,12.857,13.143,13.429,13.714,14.000,14.286,14.571,14.857,15.143,15.429,15.714,16.000,16.286,16.571,16.857,17.143,17.429,17.714,18.000,18.286,18.571,18.857,19.143,19.429,19.714,20.000,20.286,20.571,20.857,21.143,21.429,21.714,22.000,22.286,22.571,22.857,23.143,23.429,23.714,24.000,24.286,24.571,24.857,25.143,25.429,25.714,26.000,26.286,26.571,26.857,27.143,27.429,27.714,28.000,28.286,28.571,28.857,29.143,29.429,29.714,30.000,30.286,30.571,30.857,31.143,31.429,31.714,32.000,32.286,32.571,32.857,33.143,33.429,33.714,34.000,34.286,34.571,34.857,35.143,35.429,35.714,36.000,36.286,36.571,36.857,37.143,37.429,37.714,38.000,38.286,38.571,38.857,39.143,39.429,39.714,40.000

y	0.017,0.029,0.054,0.083,0.177,0.301,0.482,0.891,1.467,2.609,3.949,6.186,10.285,14.197,20.815,27.962,34.189,50.994,52.890,74.715,78.274,94.834,97.191,106.907,110.576,99.709,95.237,100.980,95.305,84.724,72.503,63.761,53.869,45.343,47.687,39.261,41.260,38.483,41.061,42.872,52.425,54.631,58.566,57.691,62.233,63.660,74.559,76.366,76.834,76.417,73.934,83.633,79.573,77.333,82.758,74.844,70.299,69.107,62.965,63.991,63.361,54.334,70.000,100.000,80.000,50.000,37.315,35.473,31.401,31.614,29.318,29.209,25.646,23.543,21.643,20.547,21.038,23.023,23.379,22.613,28.586,29.229,34.625,40.524,43.533,44.408,55.342,63.879,70.384,64.793,84.106,85.235,96.396,101.507,101.564,125.477,123.029,116.855,132.579,146.072,152.345,149.528,149.292,167.817,140.396,146.256,140.288,150.331,151.084,135.049,124.152,128.279,121.819,127.717,109.324,98.865,101.041,95.462,82.976,108.280,173.023,125.904,55.389,48.475,40.554,32.513,30.720,26.072,35.330,58.550,42.860,23.900,11.696,8.861,7.205,6.087,5.144,4.176,3.048,2.764,2.108

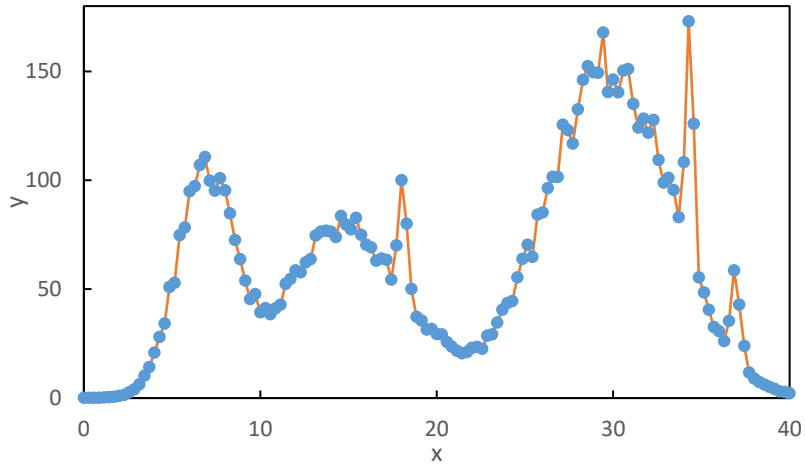


图37.1 案例1多峰示意图（自变量x作为横轴）

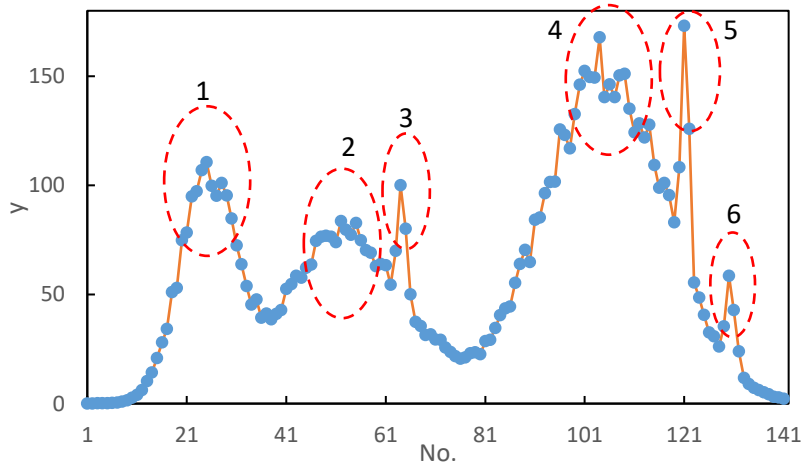


图37.2 案例1多峰示意图（数据序号作为横轴）

表 37-2 案例数据 2

x	301.2,301.5,301.8,302.1,302.4,302.7,303,303.3,303.6,303.9,304.2,304.5,304.8,305.1,305.4,305.7,306,306.3,306.6,306.9,307.2,307.5,307.8,308.1,308.4,308.7,309,309.3,309.6,309.9,310.2,310.5,310.8,311.1,311.4,311.7,312,312.3,312.6,312.9,313.2,313.5,313.8,314.1,314.4,314.7,315,315.3,315.6,315.9,316.2,316.5,316.8,317.1,317.4,317.7,318,318.3,318.6,318.9,319.2,319.5,319.8,320.1,320.4,320.7,321,321.3,321.6,321.9,322.2,322.5,322.8,323.1,323.4,323.7,324,324.3,324.6,324.9,325.2,325.5,325.8,326.1,326.4,326.7,327,327.3,327.6,327.9,328.2,328.5,328.8,329.1,329.4,329.7,330,330.3,330.6,330.9,331.2,331.5,331.8,332.1,332.4,332.7,333,333.3,333.6,333.9,334.2,334.5,334.8,335.1,335.4,335.7,336,336.3,336.6,336.9,337.2,337.5,337.8,338.1,338.4,338.7,339,339.3,339.6,339.9,340.2,340.5,340.8,341.1,341.4,

	341.7,342,342.3,342.6,342.9,343.2,343.5,343.8,344.1,344.4,344.7,345,345.3,345.6,345.9,346.2,346.5,346.8,347.1,347.4,347.7,348,348.3,348.6,348.9,349.2,349.5,349.8,350.1,350.4,350.7,351,351.3,351.6,351.9,352.2,352.5,352.8,353.1,353.4,353.7,354,354.3,354.6,354.9,355.2,355.5,355.8,356.1,356.4,356.7,357,357.3,357.6,357.9,358.2,358.5,358.8,359.1,359.4,359.7,360
y	55,60,61,54,52,117,929,3708,7538,9664,10098,9580,8381,7142,5921,4703,3695,2979,2426,1864,1432,1182,912,678,576,488,400,290,266,199,152,151,122,137,98,100,86,65,75,257,2773,12279,24914,30511,27803,21832,16093,12046,8874,6612,4905,3610,2736,2075,1581,1174,828,696,516,406,337,248,199,164,163,126,101,97,89,65,79,58,295,2912,12557,25807,31309,27652,21437,15760,11659,8602,6426,4792,3432,2665,1980,1577,1130,811,662,515,402,329,290,182,174,154,126,100,69,88,80,60,63,97,822,5067,14735,22983,25040,22412,18140,14082,10632,8058,6026,4553,3457,2615,1980,1538,1089,879,719,493,423,343,250,204,197,121,117,141,91,82,77,71,84,502,3616,11538,19597,22048,19365,15128,11681,9282,7267,5746,4017,2873,2160,1587,1169,923,712,545,439,372,326,232,203,163,134,137,135,101,105,70,85,81,365,2295,7080,12381,14780,13943,11824,9431,8293,7019,5660,4306,3050,2112,1623,1296,957,722,607,527,373,352,283,280,220

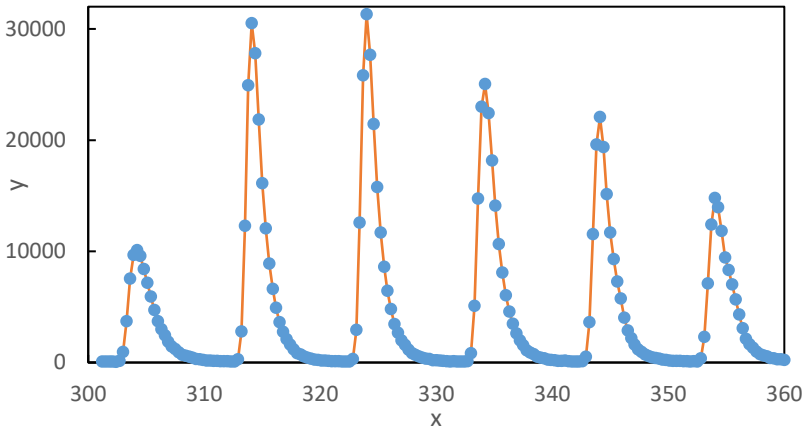


图37.3 案例2多峰示意图（自变量x作为横轴）

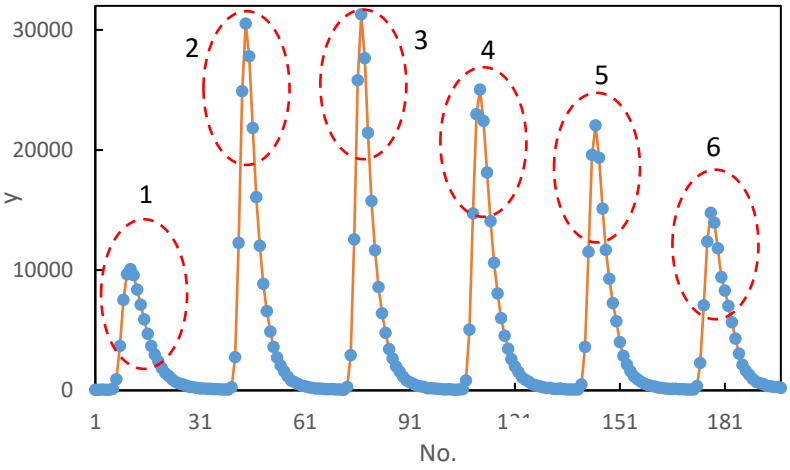


图37.4 案例2多峰示意图（数据序号作为横轴）

37.3 模型分析及求解

两个案例均是6个峰（实际可以有更多）的叠加组合，单峰函数形式分别为Gauss和Asym2Sig函数。如果按常规方式直接采用缺省的通用全局优化算法进行拟合计算，因为参数数分别达到了19和31个，同时数据量也不少，将会出现两个问题，一是计算时间过长，二

是无法保证计算收敛并得到完美的峰拟合结果。

多峰函数的拟合有一个特点，即分别对单个峰进行拟合计算，其计算出的参数值与多峰整体同时拟合所计算得出的对应的峰的参数值虽不完全相同但却是趋同接近的。基于这一特性，可以先将多峰数据分解成单峰数据，再采用求解效果好的全局优化算法，对单峰数据逐一进行拟合计算，计算完成后，因为第一个参数y0是各单峰共享的，取其平均值，其余所有单峰的参数值（除y0）按峰的顺序与y0的平均值组合成一组新的数据，将该组数据作为多峰整体同时拟合计算时各参数的初值，采用效率高的经典局部最优算法（如Levenberg-Marquardt算法），即可快速得到满意的多峰函数拟合结果。

由上分析，求解思路是先将多峰分解成单峰，用全局优化算法分别求解，其结果再作为多峰整体同时求解的参数初值，再用经典局部最优算法进行快速求解，最终获得多峰拟合的最优解，这样充分利用全局与局部最优算法各自的优点，快速并准确地求出模型参数值。

多峰分解成单峰是以数据序号进行划分的，相对比较简单，如对案例-1，参考图37.2，第一个峰在[1, 38]之间，第二个峰在[39, 62]之间，同理其余4个峰数据区间分别为[62, 76]、[76, 118]、[119, 128]和[128,136]，注意分峰区间没有那么苛刻，大概即可，可以有部分重叠，也可以不连续。同理，参考图37.4，案例-2的6个峰区间分别为：[1, 35]、[36, 68]、[69, 100]、[101, 135]、[136, 170]和[171, 197]；

分峰点确定后，是否就需要将全部数据分解成独立的子数据集，再分别进行拟合计算？虽然按常规是应该这样处理，但对单峰数据一个个分别进行独立计算还是稍显繁琐。在1stOpt中有更高效快捷的处理方式，主要涉及到两个关键字的使用，既“RegStartP”和“RegEndP”。

1) RegStartP 定义拟合起始数据点，缺省为 1
2) RegEndP 定义拟合终止数据点，缺省为拟合数据长度

“RegStartP”和“RegEndP”批量定义拟合数据起始及终止数据点，这样在确定完各单峰的起始终止点后，通过这两个关键字，无需分解成独立的数据，1stOpt可以基于全部整体数据自动批量拟合，方便、快捷、高效。

对案例1，起始及终止数据点集为：

RegStartP = [1,39,62,76,119,128];

RegEndP = [38,62,76,118,128,136];

对案例2，则为：

RegStartP = [1,36,69,101,136,171];

RegEndP = [35,68,100,135,170,197];

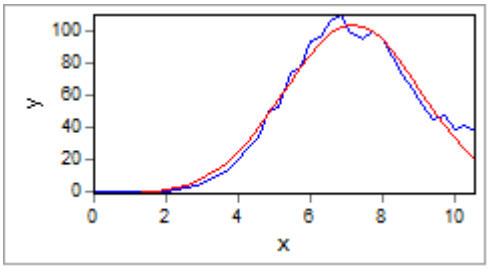
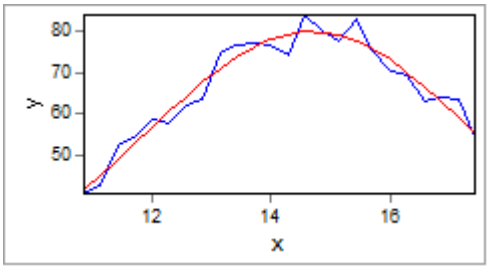
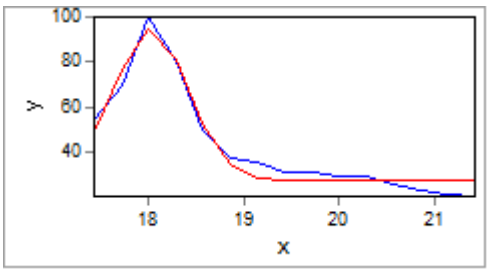
案例1各单峰批量自动拟合代码：

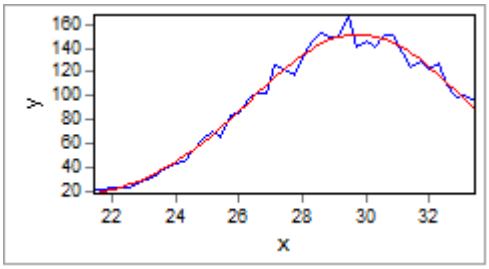
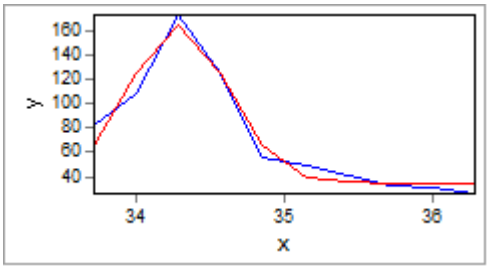
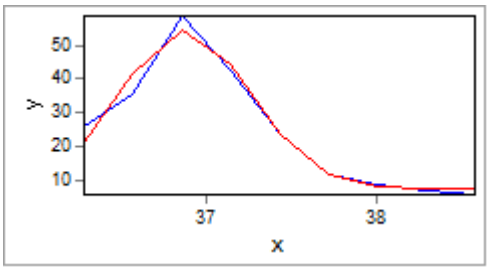
```
RegStartP = [1,39,62,76,119,128];
RegEndP = [38,62,76,118,128,136];
Variable x,y;
Function y=y0+a*exp(b*(x-c)^2);
Data;
```

x=[0.000,0.286,0.571,0.857,1.143,1.429,1.714,2.000,2.286,2.571,2.857,3.143,3.429,3.714,4.000,4.286,4.571,4.857,5.143,5.429,5.714,6.000,6.286,6.571,6.857,7.143,7.429,7.714,8.000,8.286,8.571,8.857,9.143,9.429,9.714,10.000,10.286,10.571,10.857,11.143,11.429,11.714,12.000,12.286,12.571,12.857,13.143,13.429,13.714,14.000,14.286,14.571,14.857,15.143,15.429,15.714,16.000,16.286,16.571,16.857,17.143,17.429,17.714,18.000,18.286,18.571,18.857,19.143,19.429,19.714,20.000,20.286,20.571,20.857,21.143,21.429,21.714,22.000,22.286,22.571,22.857,23.143,23.429,23.714,24.000,24.286,24.571,24.857,25.143,25.429,25.714,26.000,26.286,26.571,26.857,27.143,27.429,27.714,28.000,28.286,28.571,28.857,29.143,29.429,29.714,30.000,30.286,30.571,30.857,31.143,31.429,31.714,32.000,32.286,32.571,32.857,33.143,33.429,33.714,34.000,34.286,34.571,34.857,35.143,35.429,35.714,36.000,36.286,36.571,36.857,37.143,37.429,37.714,38.000,38.286,38.571,38.857,39.143,39.429,39.714,40.000];

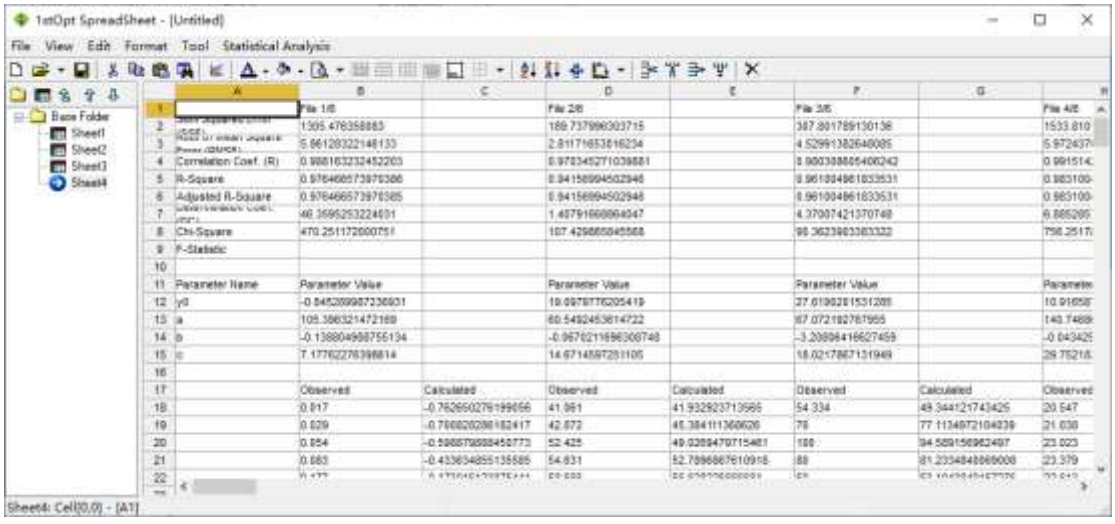
y=[0.017,0.029,0.054,0.083,0.177,0.301,0.482,0.891,1.467,2.609,3.949,6.186,10.285,14.197,20.815,27.962,34.189,50.994,52.890,74.715,78.274,94.834,97.191,106.907,110.576,99.709,95.237,100.980,95.305,84.724,72.503,63.761,53.869,45.343,47.687,39.261,41.260,38.483,41.061,42.872,52.425,54.631,58.566,57.691,62.233,63.660,74.559,76.366,76.834,76.417,73.934,83.633,79.573,77.333,82.758,74.844,70.299,69.107,62.965,63.991,63.361,54.334,70.000,100.000,80.000,50.000,37.315,35.473,31.401,31.614,29.318,29.209,25.646,23.543,21.643,20.547,21.038,23.023,23.379,22.613,28.586,29.229,34.625,40.524,43.533,44.408,55.342,63.879,70.384,64.793,84.106,85.235,96.396,101.507,101.564,125.477,123.029,116.855,132.579,146.072,152.345,149.528,149.292,167.817,140.396,146.256,140.288,150.331,151.084,135.049,124.152,128.279,121.819,127.717,109.324,98.865,101.041,95.462,82.976,108.280,173.023,125.904,55.389,48.475,40.554,32.513,30.720,26.072,35.330,58.550,42.860,23.900,11.696,8.861,7.205,6.087,5.144,4.176,3.048,2.764,2.108];

运行上述代码可自动对6个单峰分别进行拟合计算，结果如下：

峰	拟合对比图形	拟合结果
1		Sum Squared Error (SSE): 1305.476358083 Root of Mean Square Error (RMSE): 5.86128322146133 Correlation Coef. (R): 0.988163232452203 R-Square: 0.976466573970386 Parameter Best Estimate --------- ------------- y0 -0.845289987236931 a 105.396321472169 b -0.138804988755134 c 7.17762276398614
2		Sum Squared Error (SSE): 189.737996303715 Root of Mean Square Error (RMSE): 2.81171653016234 Correlation Coef. (R): 0.970345271039881 R-Square: 0.94156994502946 Parameter Best Estimate --------- ------------- y0 19.0979776205419 a 60.5492453614722 b -0.0670211696308748 c 14.6714597251105
3		Sum Squared Error (SSE): 307.801789130136 Root of Mean Square Error (RMSE): 4.52991382648085 Correlation Coef. (R): 0.980308605406242 R-Square: 0.961004961833531 Parameter Best Estimate --------- ------------- y0 27.6190201531285 a 67.072192767955 b -3.20806416627459 c 18.0217867131949

4		Sum Squared Error (SSE): 1533.81019322287 Root of Mean Square Error (RMSE): 5.97243706484674 Correlation Coef. (R): 0.991514226677208 R-Square: 0.983100461703301 Parameter Best Estimate --------- ------------- y0 10.916587018463 a 140.746864953954 b -0.0434299207545469 c 29.7521830258852
5		Sum Squared Error (SSE): 971.332401907046 Root of Mean Square Error (RMSE): 9.85561972636448 Correlation Coef. (R): 0.977402160483887 R-Square: 0.95531498331857 Parameter Best Estimate --------- ------------- y0 34.8592029564139 a 129.565160159349 b -4.46245241884037 c 34.2864781166397
6		Sum Squared Error (SSE): 79.9857208930875 Root of Mean Square Error (RMSE): 2.98115788267817 Correlation Coef. (R): 0.984869181355317 R-Square: 0.969967304383491 Parameter Best Estimate --------- ------------- y0 7.58938127041431 a 46.9269847502386 b -3.48791254786636 c 36.8807565621267

计算完成后，在结果页面点击“结果报表”按钮，可得如下包括参数归纳好的表格内容：



基于该表格计算所得参数数据值结果，将对应6个峰拟合结果的y0取其平均值（在此为16.539479），其余参数按顺序，组成下列数据：

初值数据	16.5394797042626,105.396321473274,-0.138804988754255,7.17762276398742, 60.5492461073039,-0.0670211685352409,14.6714597230363,67.0721927729719, -3.20806417780258,18.0217867137152,140.746865023201,-0.0434299207346127, 29.7521830255649,129.565160431081,-4.46245241848968,34.2864781169989, 46.9269846726549,-3.48791258537038,36.8807565611257

对应参数	y0,a1,b1,c1,a2,b2,c2,a3,b3,c3,a4,b4,c4,a5,b5,c5,a6,b6,c6

以上述数据作为初值，并采用局部经典优化算法Levenberg-Marquardt算法（对应CLO1），对全部峰数据进行整体拟合计算。设定初值时用关键字“StartValue”。

1stOpt代码：

```
Constant n=6;
Algorithm = CLO1;
StartValue = [16.5394797042626,105.396321473274,-0.138804988754255,7.17762276398742,
60.5492461073039,-0.0670211685352409,14.6714597230363,67.0721927729719,-3.20806417780258,
18.0217867137152,140.746865023201,-0.0434299207346127,29.7521830255649,129.565160431081,
-4.46245241848968,34.2864781169989,46.9269846726549,-3.48791258537038,36.8807565611257];
Variable x,y;
Function y=y0+Sum(n,a,b,c)(a*exp(b*(x-c)^2));Data;
x=[0.000,0.286,0.571,0.857,1.143,1.429,1.714,2.000,2.286,2.571,2.857,3.143,3.429,3.714,4.000,4.286,4.571
,4.857,5.143,5.429,5.714,6.000,6.286,6.571,6.857,7.143,7.429,7.714,8.000,8.286,8.571,8.857,9.143,9.429,9.
714,10.000,10.286,10.571,10.857,11.143,11.429,11.714,12.000,12.286,12.571,12.857,13.143,13.429,13.714,
14.000,14.286,14.571,14.857,15.143,15.429,15.714,16.000,16.286,16.571,16.857,17.143,17.429,17.714,18.
000,18.286,18.571,18.857,19.143,19.429,19.714,20.000,20.286,20.571,20.857,21.143,21.429,21.714,22.000
,22.286,22.571,22.857,23.143,23.429,23.714,24.000,24.286,24.571,24.857,25.143,25.429,25.714,26.000,26.
286,26.571,26.857,27.143,27.429,27.714,28.000,28.286,28.571,28.857,29.143,29.429,29.714,30.000,30.286
,30.571,30.857,31.143,31.429,31.714,32.000,32.286,32.571,32.857,33.143,33.429,33.714,34.000,34.286,34.
571,34.857,35.143,35.429,35.714,36.000,36.286,36.571,36.857,37.143,37.429,37.714,38.000,38.286,38.571
,38.857,39.143,39.429,39.714,40.000];
y=[0.017,0.029,0.054,0.083,0.177,0.301,0.482,0.891,1.467,2.609,3.949,6.186,10.285,14.197,20.815,27.962,
34.189,50.994,52.890,74.715,78.274,94.834,97.191,106.907,110.576,99.709,95.237,100.980,95.305,84.724,
72.503,63.761,53.869,45.343,47.687,39.261,41.260,38.483,41.061,42.872,52.425,54.631,58.566,57.691,62.
233,63.660,74.559,76.366,76.834,76.417,73.934,83.633,79.573,77.333,82.758,74.844,70.299,69.107,62.965
,63.991,63.361,54.334,70.000,100.000,80.000,50.000,37.315,35.473,31.401,31.614,29.318,29.209,25.646,2
3.543,21.643,20.547,21.038,23.023,23.379,22.613,28.586,29.229,34.625,40.524,43.533,44.408,55.342,63.8
79,70.384,64.793,84.106,85.235,96.396,101.507,101.564,125.477,123.029,116.855,132.579,146.072,152.34
5,149.528,149.292,167.817,140.396,146.256,140.288,150.331,151.084,135.049,124.152,128.279,121.819,1
27.717,109.324,98.865,101.041,95.462,82.976,108.280,173.023,125.904,55.389,48.475,40.554,32.513,30.7
20,26.072,35.330,58.550,42.860,23.900,11.696,8.861,7.205,6.087,5.144,4.176,3.048,2.764,2.108];
```

运行上述代码可以秒得如下结果：

```
Iterations: 12
Elapsed Time (Hr:Min:Sec:Msec): 00:00:00:344
Algorithms: Levenberg-Marquardt (CLO1)
Stop Reason of Computation: Convergence tolerance reached
Sum Squared Error (SSE): 2252.44866181742
Root of Mean Square Error (RMSE): 3.99685041055815
Correlation Coef. (R): 0.995896671819255
R-Square: 0.991810180940669
Adjusted R-Square: 0.991691487910824
Determination Coef. (DC): 0.991810180939982
Chi-Square: 11.6975167490019
F-Statistic: 820.806634510175

Parameter  Initial Value        Final Estimate
---------  -------------  --------------
y0         16.5394797042626    -0.235181429275068
a1         105.396321473274    102.986793161424
b1         -0.138804988754255  -0.19998587385328
c1         7.17762276398742    6.86090278586939
a2         60.5492461073039    78.8430443771243
b2         -0.0670211685352409 -0.0442818031399889
c2         14.6714597230363    14.7884561034406
a3         67.0721927729719    51.9804931939337
b3         -3.20806417780258   -9.33708069421343
c3         18.0217867137152    18.0746915036115
a4         140.746865023201    151.811599999107
b4         -0.0434299207346127 -0.0396178798530483
c4         29.7521830255649    29.7225064920334
a5         129.565160431081    111.05317295218
```

b5	-4.46245241848968	-10.2012057289766
c5	34.2864781169989	34.3406093055573
a6	46.9269846726549	39.2170205322283
b6	-3.48791258537038	-8.09272767739871
c6	36.8807565611257	36.9415147484608

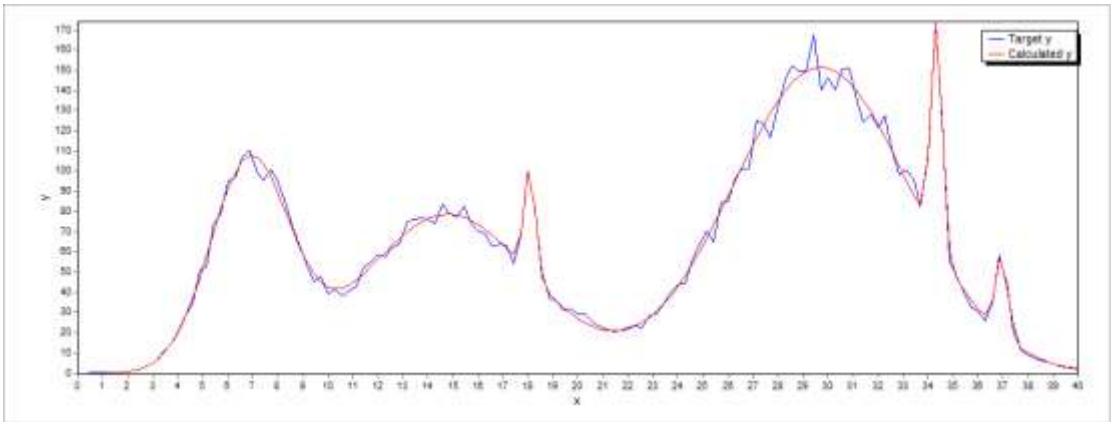


图37.5 案例1多峰整体拟合计算结果示意图

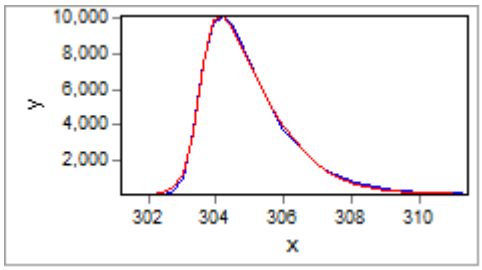
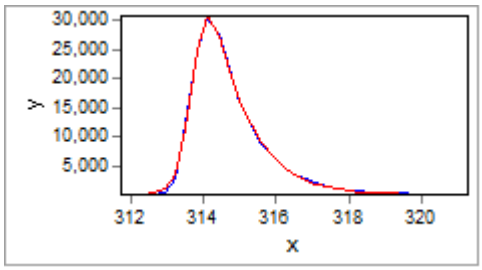
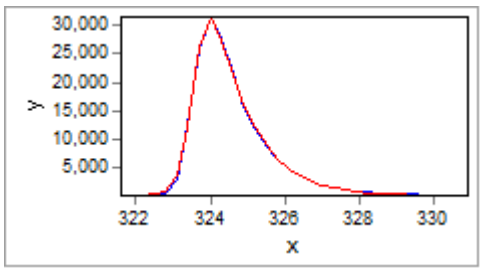
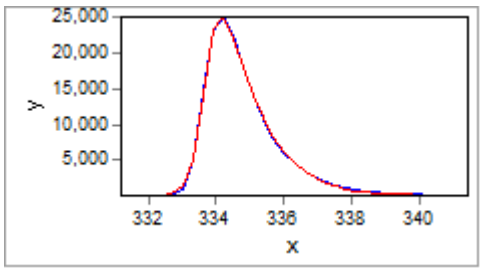
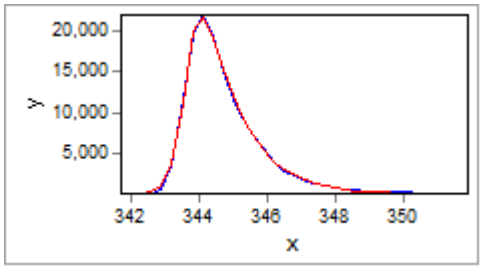
对案例 2 采用相同的处理方式。

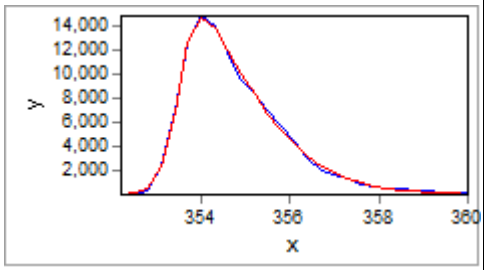
案例2各单峰批量自动拟合代码：

```
RegStartP = [1,36,69,101,136,171];
RegEndP = [35,68,100,135,170,197];
Variable x,y;
Function y=y0+a*(1/(1+exp(c*(x-b+w))))*(1-1/(1+exp(d*(x-b-w))));
Data;
x=[301.2,301.5,301.8,302.1,302.4,302.7,303,303.3,303.6,303.9,304.2,304.5,304.8,305.1,305.4,305.7,306,306.3,
306.6,306.9,307.2,307.5,307.8,308.1,308.4,308.7,309,309.3,309.6,309.9,310.2,310.5,310.8,311.1,311.4,311.7,3
12,312.3,312.6,312.9,313.2,313.5,313.8,314.1,314.4,314.7,315,315.3,315.6,315.9,316.2,316.5,316.8,317.1,317.
4,317.7,318,318.3,318.6,318.9,319.2,319.5,319.8,320.1,320.4,320.7,321,321.3,321.6,321.9,322.2,322.5,322.8,3
23.1,323.4,323.7,324,324.3,324.6,324.9,325.2,325.5,325.8,326.1,326.4,326.7,327,327.3,327.6,327.9,328.2,328.
5,328.8,329.1,329.4,329.7,330,330.3,330.6,330.9,331.2,331.5,331.8,332.1,332.4,332.7,333,333.3,333.6,333.9,3
34.2,334.5,334.8,335.1,335.4,335.7,336,336.3,336.6,336.9,337.2,337.5,337.8,338.1,338.4,338.7,339,339.3,339.
6,339.9,340.2,340.5,340.8,341.1,341.4,341.7,342,342.3,342.6,342.9,343.2,343.5,343.8,344.1,344.4,344.7,345,3
45.3,345.6,345.9,346.2,346.5,346.8,347.1,347.4,347.7,348,348.3,348.6,348.9,349.2,349.5,349.8,350.1,350.4,35
0.7,351,351.3,351.6,351.9,352.2,352.5,352.8,353.1,353.4,353.7,354,354.3,354.6,354.9,355.2,355.5,355.8,356.1
,356.4,356.7,357,357.3,357.6,357.9,358.2,358.5,358.8,359.1,359.4,359.7,360];
y=[55,60,61,54,52,117,929,3708,7538,9664,10098,9580,8381,7142,5921,4703,3695,2979,2426,1864,1432,118
2,912,678,576,488,400,290,266,199,152,151,122,137,98,100,86,65,75,257,2773,12279,24914,30511,27803,21
832,16093,12046,8874,6612,4905,3610,2736,2075,1581,1174,828,696,516,406,337,248,199,164,163,126,101,
97,89,65,79,58,295,2912,12557,25807,31309,27652,21437,15760,11659,8602,6426,4792,3432,2665,1980,157
7,1130,811,662,515,402,329,290,182,174,154,126,100,69,88,80,60,63,97,822,5067,14735,22983,25040,22412,
18140,14082,10632,8058,6026,4553,3457,2615,1980,1538,1089,879,719,493,423,343,250,204,197,121,117,14
1,91,82,77,71,84,502,3616,11538,19597,22048,19365,15128,11681,9282,7267,5746,4017,2873,2160,1587,116
9,923,712,545,439,372,326,232,203,163,134,137,135,101,105,70,85,81,365,2295,7080,12381,14780,13943,11
824,9431,8293,7019,5660,4306,3050,2112,1623,1296,957,722,607,527,373,352,283,280,220];
```

运行上述代码自动对6个单峰分别进行拟合计算，结果如下：

峰	拟合对比图形	拟合结果

1		Sum Squared Error (SSE): 440469.055914927 Root of Mean Square Error (RMSE): 112.182129454731 Correlation Coef. (R): 0.999392796305046 R-Square: 0.998785961306418 Parameter Best Estimate --------- ------------- y0 76.986944800012 a 15479.7045278679 c -4.71538636062849 b 304.215124028422 w 0.700036886171906 d -1.03063656785765
2		Sum Squared Error (SSE): 2467958.79155356 Root of Mean Square Error (RMSE): 273.471442836501 Correlation Coef. (R): 0.99950863838028 R-Square: 0.999017518196802 Parameter Best Estimate --------- ------------- y0 67.7531457631696 a 114286.576638681 c -5.18590118141677 b 313.573711201063 w -0.177330471910741 d -1.1146330811688
3		Sum Squared Error (SSE): 1887521.74716656 Root of Mean Square Error (RMSE): 242.868389460125 Correlation Coef. (R): 0.999626803798998 R-Square: 0.999253746873401 Parameter Best Estimate --------- ------------- y0 65.6885207855359 a 150107.10792265 c -5.32635172695292 b 323.305033280354 w -0.346910273514656 d -1.09565086849451
4		Sum Squared Error (SSE): 1680630.86806676 Root of Mean Square Error (RMSE): 219.130154935161 Correlation Coef. (R): 0.999554939152299 R-Square: 0.999110076383755 Parameter Best Estimate --------- ------------- y0 84.6264976395272 a 56577.0160295968 c -4.95283031355359 b 333.903975100034 w 0.213183907073635 d -1.12206786568083
5		Sum Squared Error (SSE): 1246918.19630452 Root of Mean Square Error (RMSE): 188.749130276484 Correlation Coef. (R): 0.999549450087297 R-Square: 0.999099103169818 Parameter Best Estimate --------- ------------- y0 32.1009057122061 a 69846.812040843 c -5.10135277700944 b 343.556315519642 w -0.0886647329841992 d -1.02500227487634

6		Sum Squared Error (SSE): 1212863.69574776 Root of Mean Square Error (RMSE): 211.945459069751 Correlation Coef. (R): 0.998975067805045 R-Square: 0.997951186096094 Parameter Best Estimate --------- ------------- y0 15.7033340560961 a 26357.5269639721 c 1.00747016706865 b 353.969718926859 w -0.449659355395154 d 4.98286248595039

将对应6个峰拟合结果的y0取其平均值（在此为57.14322），其余参数按顺序，组成下列数据：

初值数据	57.1432222954798,15479.7044139651,-4.71538637853395,304.215124034521, 0.700036893506538,-1.03063657313005,114286.575826879,-5.18590116993403, 313.573711210966,-0.177330463554913,-1.11463308766114,150107.112395599, -5.32635175497505,323.305033257467,-0.346910296941534,-1.09565085971277, 56577.0164858569,-4.95283029316326,333.903975094996,0.213183901116798, -1.12206786370693,69846.8120074951,1.02500227517689,343.556315520649, 0.0886647322702762,5.1013527619182,26357.5276301849,1.00747015642183, 353.969718907557,-0.44965933139946,4.98286242616802
对应参数	y0,a1,c1,b1,w1,d1,a2,c2,b2,w2,d2,a3,c3,b3,w3,d3,a4,c4,b4,w4,d4,a5,c5,b5,w5,d5,a6,c6,b6,w6,d6

同样以上述数据作为初值，并采用局部经典优化算法Levenberg-Marquardt算法（对应CLO1），对全部峰数据进行整体拟合计算。

1stOpt代码：

```
Algorithm = CLO1;
StartValue = [57.1432222954798,15479.7044139651,-4.71538637853395,304.215124034521,
0.700036893506538,-1.03063657313005,114286.575826879,-5.18590116993403,313.573711210966,
-0.177330463554913,-1.11463308766114,150107.112395599,-5.32635175497505,323.305033257467,
-0.346910296941534,-1.09565085971277,56577.0164858569,-4.95283029316326,333.903975094996,
0.213183901116798,-1.12206786370693,69846.8120074951, 1.02500227517689,343.556315520649,
0.0886647322702762,5.1013527619182,26357.5276301849,1.00747015642183,353.969718907557,
-0.44965933139946,4.98286242616802];
Variable x,y;
Function y=y0+Sum(6,a,b,w,c,d)(a*(1/(1+exp(c*(x-b+w))))*(1-1/(1+exp(d*(x-b-w)))));
Data;
x=[301.2,301.5,301.8,302.1,302.4,302.7,303,303.3,303.6,303.9,304.2,304.5,304.8,305.1,305.4,305.7,306,30
6.3,306.6,306.9,307.2,307.5,307.8,308.1,308.4,308.7,309,309.3,309.6,309.9,310.2,310.5,310.8,311.1,311.4,3
11.7,312,312.3,312.6,312.9,313.2,313.5,313.8,314.1,314.4,314.7,315,315.3,315.6,315.9,316.2,316.5,316.8,3
17.1,317.4,317.7,318,318.3,318.6,318.9,319.2,319.5,319.8,320.1,320.4,320.7,321,321.3,321.6,321.9,322.2,3
22.5,322.8,323.1,323.4,323.7,324,324.3,324.6,324.9,325.2,325.5,325.8,326.1,326.4,326.7,327,327.3,327.6,3
27.9,328.2,328.5,328.8,329.1,329.4,329.7,330,330.3,330.6,330.9,331.2,331.5,331.8,332.1,332.4,332.7,333,3
33.3,333.6,333.9,334.2,334.5,334.8,335.1,335.4,335.7,336,336.3,336.6,336.9,337.2,337.5,337.8,338.1,338.4
,338.7,339,339.3,339.6,339.9,340.2,340.5,340.8,341.1,341.4,341.7,342,342.3,342.6,342.9,343.2,343.5,343.8
,344.1,344.4,344.7,345,345.3,345.6,345.9,346.2,346.5,346.8,347.1,347.4,347.7,348,348.3,348.6,348.9,349.2
,349.5,349.8,350.1,350.4,350.7,351,351.3,351.6,351.9,352.2,352.5,352.8,353.1,353.4,353.7,354,354.3,354.6
,354.9,355.2,355.5,355.8,356.1,356.4,356.7,357,357.3,357.6,357.9,358.2,358.5,358.8,359.1,359.4,359.7,360
];
y=[55,60,61,54,52,117,929,3708,7538,9664,10098,9580,8381,7142,5921,4703,3695,2979,2426,1864,1432,1
182,912,678,576,488,400,290,266,199,152,151,122,137,98,100,86,65,75,257,2773,12279,24914,30511,2780
3,21832,16093,12046,8874,6612,4905,3610,2736,2075,1581,1174,828,696,516,406,337,248,199,164,163,12
6,101,97,89,65,79,58,295,2912,12557,25807,31309,27652,21437,15760,11659,8602,6426,4792,3432,2665,1
980,1577,1130,811,662,515,402,329,290,182,174,154,126,100,69,88,80,60,63,97,822,5067,14735,22983,25
040,22412,18140,14082,10632,8058,6026,4553,3457,2615,1980,1538,1089,879,719,493,423,343,250,204,1
97,121,117,141,91,82,77,71,84,502,3616,11538,19597,22048,19365,15128,11681,9282,7267,5746,4017,287
3,2160,1587,1169,923,712,545,439,372,326,232,203,163,134,137,135,101,105,70,85,81,365,2295,7080,123
81,14780,13943,11824,9431,8293,7019,5660,4306,3050,2112,1623,1296,957,722,607,527,373,352,283,280,
220];
```

运行上述代码，虽然有多达 31 个未知参数及近 200 组数据，仍可快速得到如下结果：

```
Iterations: 16
Elapsed Time (Hr:Min:Sec:Msec): 00:00:01:437
Algorithms: Levenberg-Marquardt (CLO1)
Stop Reason of Computation: Convergence tolerance reached
Sum Squared Error (SSE): 9001175.76912437
Root of Mean Square Error (RMSE): 213.75511118803
Correlation Coef. (R): 0.999526977343484
R-Square: 0.999054178437402
Adjusted R-Square: 0.999044427699643
Determination Coef. (DC): 0.999054178436869
Chi-Square: 3143.41788138859
F-Statistic: 5844.75250012062
```

Parameter	Initial Value	Final Estimate
y0	57.1432222954798	59.1907818150037
a1	15479.7044139651	15687.1119151793
c1	-4.71538637853395	-4.6846796169932
b1	304.215124034521	304.204773646841
w1	0.700036893506538	0.688186730791046
d1	-1.03063657313005	-1.01957266937032
a2	114286.575826879	115408.095015007
c2	-5.18590116993403	-5.18430258801988
b2	313.573711210966	313.567167726601
w2	-0.177330463554913	-0.18429232102113
d2	-1.11463308766114	-1.11206361760802
a3	150107.112395599	151635.627750713
c3	-5.32635175497505	-5.32540954334395
b3	323.305033257467	323.298460395154
w3	-0.346910296941534	-0.35379349629001
d3	-1.09565085971277	-1.09371161696789
a4	56577.0164858569	57924.7310530061
c4	-4.95283029316326	-4.93477416158312
b4	333.903975094996	333.887077797883
w4	0.213183901116798	0.194090193436715
d4	-1.12206786370693	-1.11145469913547
a5	69846.8120074951	66436.6703374719
c5	1.02500227517689	1.03829102253651
b5	343.556315520649	343.592966302127
w5	0.0886647322702762	0.0489734687127772
d5	5.1013527619182	5.12396107134824
a6	26357.5276301849	25380.784406928
c6	1.00747015642183	1.03046762946505
b6	353.969718907557	354.000722056015
w6	-0.44965933139946	-0.484310433236869
d6	4.98286242616802	5.04376493385273

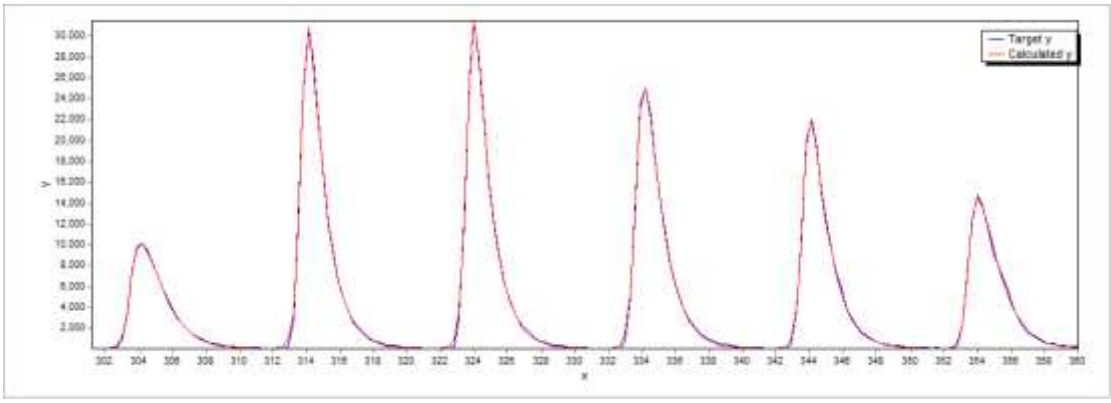


图37.6 案例2多峰整体拟合计算结果示意图

参考图37.5和图37.6，两个案例的最终计算结果都是非常令人满意的，说明本文采用的方法是合理可行的。

37.4 小结

根据峰函数的特性，在充分考虑全局与局部最优算法优缺点的基础上，提出了1stOpt软件对多峰函数拟合计算的有效方法及流程，实际案例计算结果也表明了该方法的现实可行性和高效性。此外也演示了1stOpt中关键字“RegStartP”、“RegEndP”和“StartValue”的使用场景和方式。