

33. Origin 与 SigmaPlot 内置拟合函数功效测试一与 1stOpt 自定义函数拟合比较

33.1 引言

Origin和SigmaPlot是两款知名的科学绘图与数据分析软件，以易于使用、功能强大而闻名，国内外用户众多。两款软件的定位基本一致：高质量科学绘图+数据分析处理。而在数据分析功能中，非线性曲线拟合均是二款软件引以为傲的功能亮点，尤其是都提前内置（Built-in）了众多常用的拟合函数，相比自定义函数，选用内置函数最大的特点或益处就是用户不需要对未知参数人工赋值，而由软件本身自动确定，克服了盲目猜初值的“痛点”，Origin官方网页有这样的描述“Each built-in function includes automatic parameter initialization code that adjusts initial parameter values to your dataset(s), prior to fitting.”，意即每个内置函数都包含自动参数初始化代码，用于在拟合之前根据数据集调整确定合理参数初始值。

两款软件非线性拟合算法都是采用的经典局部最优算法，采用这类优化算法的优点是计算效率高，最大缺点则是计算是否收敛极度依赖参数初始值赋值质量的好坏，而根据前述，如果选用内置函数进行数据拟合计算，用户是无需提供或猜测参数初值就可以得到正确结果的，即使使用相同的局部最优算法，究其原因其实也不复杂，因为是内置函数，软件开发人员对这些函数已经有了充分的了解，软件本身提前“知道”每个内置函数中各个参数的实际几何物理意义，因此根据用户的实际数据在拟合计算之前就可以在后台估算出大概合理的参数初值，进而在此基础上迭代计算得到最终正确结果。而当选用自定义函数拟合时，即使自定义函数形式与内置函数完全相同，但因为“不知道”该自定义函数及各参数的几何意义，无法预判并得到合理的参数初始值，因此很难轻松得到最优解，需要多次手动调整参数初值才能保证迭代计算的收敛。

Origin内置了近200种各类常用函数，SigmaPlot相对少些。使用内置函数进行拟合计算，是否如软件介绍那样无需人工设置调配就可以得到最优结果？在此以实际数据计算验证，同时与1stOpt结果进行对比。

33.2 数据及模型

选取两组案例数据，如表33-1和表33-2，数据曲线图见图33-1和33-2。

表 33-1 案例数据 1

x	-6.8,-6.4,-6,-5.6,-5.2,-4.8,-4.4,-4,-3.6,-3.2,-2.8,-2.4,-2,-1.6,-1.2
y	-5.6121,-4.0471,-1.6874,1.9082,6.8139,12.3099,16.8705,18.8677,17.6083,13.8271,9.1697,5.1537,2.4853,0.1354,-1.9532

表33-2案例数据2

x	302.05,302.2,302.35,302.5,302.65,302.8,302.95,303.05,303.2,303.35,303.5,303.65,303.8,303.95,304.1,304.25,304.4,304.55,304.7,304.85,305,305.15,305.3,305.45,305.6,305.75,305.9,306.05,306.2,306.35,306.5,306.65,306.8,306.95,307.1,307.25,307.4,307.55,307.7,307.85,308,308.15,308.3,308.45,308.6,308.75,308.9,309.05,309.2,309.35,309.5,309.65,309.8,309.95,310
y	68,50,40,58,97,247,691,1254,2547,4282,6381,7936,9249,10106,10350,10296,9968,9232,9001,8224,7548,6928,6268,5700,4976,4667,4073,3742,3234,2876,2477,2235,2005,1777,1603,1377,1285,1058,1020,855,745,656,647,504,531,441,423,349,362,334,286,228,236,222,205

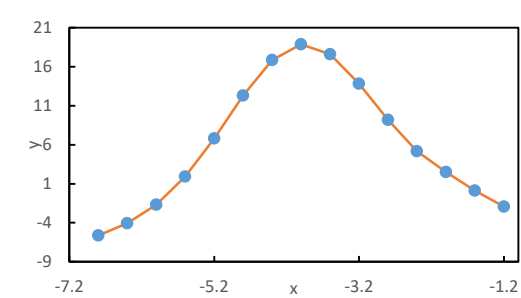


图 33-1 案例 1 数据图

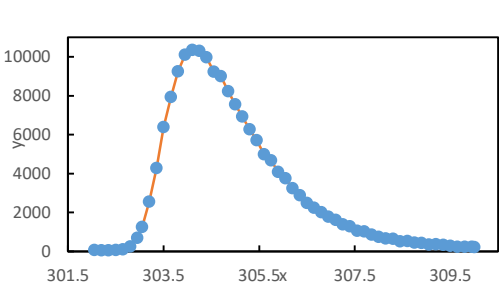


图 33-2 案例 2 数据图

参照上图，两组数据均类似于峰分布，因此两款软件均选取4种内置峰函数，Origin包括：Gaussian (4 Parameter)、Asym2Sig (6 Parameter)、Beta (6 Parameter)和Extreme (4 Parameter)，见表33-3；SigmaPlot包括：Gaussian (4 Parameter)、Modified Gaussian (5 Parameter)、Pseudo-Voigt (4 Parameter)和Pseudo-Voigt (5 Parameter)，见表33-4。

表33-3 Origin Pro选取的内置函数

函数名	模型公式
Gaussian (4 Parameter)	$y = y_0 + \left(\frac{a}{w \cdot \sqrt{\frac{\pi}{2}}} \right) \cdot \exp \left(-2 \cdot \left(\frac{x - xc}{w} \right)^2 \right)$
Asym2Sig (6 Parameter)	$y = y_0 + a \cdot \left(\frac{1}{1 + \exp \left(-\frac{x - xc + \frac{w_1}{2}}{w_2} \right)} \right) \cdot \left(1 - \frac{1}{1 + \exp \left(-\frac{x - xc - \frac{w_1}{2}}{w_3} \right)} \right)$
Beta (6 Parameter)	$y = y_0 + a \cdot \left(1 + \left(\frac{w_2 + w_3 - 2}{w_2 - 1} \right) \cdot \left(\frac{x - xc}{w_1} \right) \right)^{w_2 - 1} \cdot \left(1 + \left(\frac{w_2 + w_3 - 2}{w_3 - 1} \right) \cdot \left(\frac{x - xc}{w_1} \right) \right)^{w_3 - 1}$
Extreme (4 Parameter)	$y = y_0 + a \cdot \exp \left(-\exp \left(-\frac{x - xc}{w} \right) - \frac{x - xc}{w} + 1 \right)$

表33-4 SigmaPlot选取的内置函数

函数名	模型公式
Gaussian (4 Parameter)	$y = y_0 + a \cdot \exp \left(-.5 \cdot \left(\frac{x - x_0}{b} \right)^2 \right)$

Modified Gaussian (5 Parameter)	$y = y_0 + a \cdot \exp\left(-0.5 \cdot \left \frac{x - x_0}{b}\right ^c\right)$
Pseudo-Voigt (4 Parameter)	$y = a \cdot \left(c \cdot \left(\frac{1}{1 + \left(\frac{x - x_0}{b}\right)^2} \right) + (1 - c) \cdot \exp\left(-0.5 \cdot \left(\frac{x - x_0}{b}\right)^2\right) \right)$
Pseudo-Voigt (5 Parameter)	$y = y_0 + a \cdot \left(c \cdot \left(\frac{1}{1 + \left(\frac{x - x_0}{b}\right)^2} \right) + (1 - c) \cdot \exp\left(-0.5 \cdot \left(\frac{x - x_0}{b}\right)^2\right) \right)$

33.3 验证测试

采用Origin Pro和SigmaPlot，基于表33-1和表33-2两组数据，分别对应表33-3和表33-4所列内置模型公示，进行拟合计算。

Origin Pro内置函数拟合步骤：Analysis -> Fitting -> Single Peak Fit -> 内置函数选择，如图33-3示。

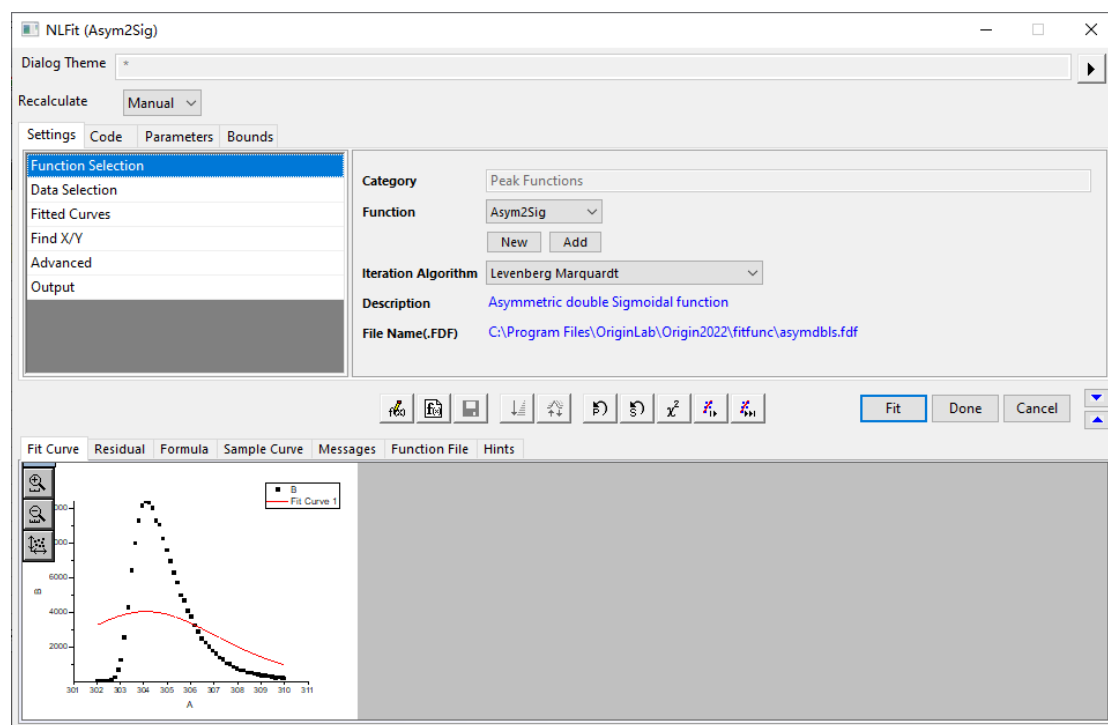


图33-3 Origin内置函数拟合界面

SigmaPlot内置函数拟合步骤：Analysis -> Global Curve Fit Wizard，如图33-4示。

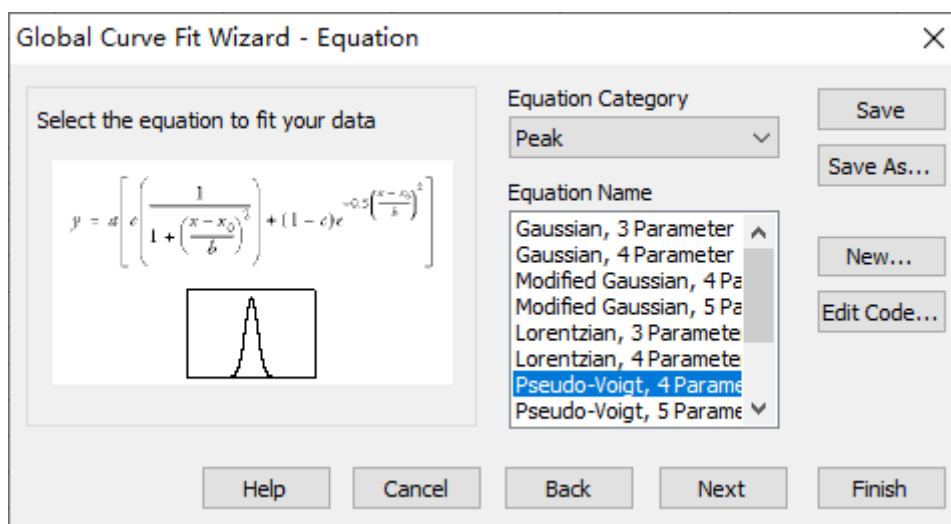


图33-4 SigmaPlot内置函数拟合界面

案例数据-1:

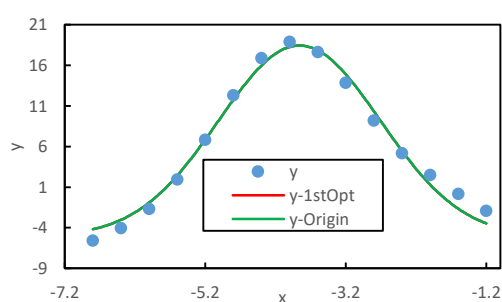
代码-1: 对应 Origin 内置函数的 1stOpt 计算代码（数据-1）

```
Parameter y0, xc, w, a;
//Parameter y0,xc=[-6,-1.2],a,w1,w2,w3;
Variable x, y;
Function y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2); //Gauss
//y=y0+A*(1/(1+exp(-(x-xc+w1/2)/w2)))*(1-1/(1+exp(-(x-xc-w1/2)/w3))); //Asym2Sig
//y=y0+A*(1+((w2+w3-2)/(w2-1))*((x-xc)/w1))^(w2-1)*(1-((w2+w3-2)/(w3-1))*((x-xc)/w1))^(w3-1);
//Beta
//y=y0+A*exp(-exp(-(x-xc)/w)-(x-xc)/w+1); //extreme;
Data;
x=-6.8,-6.4,-6,-5.6,-5.2,-4.8,-4.4,-4,-3.6,-3.2,-2.8,-2.4,-2,-1.6,-1.2;
y=-5.6121,-4.0471,-1.6874,1.9082,6.8139,12.3099,16.8705,18.8677,17.6083,13.8271,9.1697,5.1537,2.4853,
0.1354,-1.9532;
```

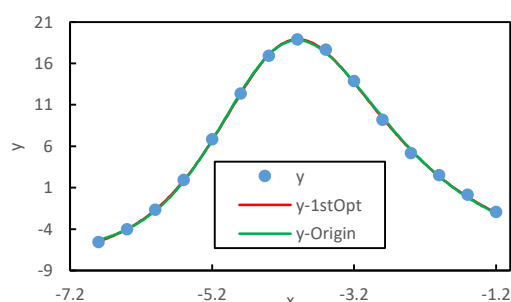
表33-5. Origin与1stOpt计算结果（数据-1）

函数	Origin Pro	1stOpt
Gaussian (4 Parameter)	Sum Squared Error (SSE): 14.84174 R-Square: 0.98442	Sum Squared Error (SSE): 14.84174068940 R-Square: 0.984416451518613
	y0 -5.10241	y0 -5.1024303157811
	xc -3.86027	xc -3.86026787366675
	w 2.30545	w 2.30545212552044
	a 67.99455	a 67.9947039628269
Asym2Sig (6 Parameter)	Sum Squared Error (SSE): 0.75558 R-Square: 0.99921	Sum Squared Error (SSE): 0.4380582393687 R-Square: 0.999540047090585
	y0 -6.82031	y0 -7.57686302372128
	xc -4.44732	xc -5.89402419336133
	a 93.86385	a 633.809689905272
	w1 3.57842E-13	w1 -3.25279043890732
	w2 0.58855	w2 0.537600593776992
Beta	w3 1.10881	w3 1.33833508956687
	Sum Squared Error (SSE): 858.04462	Sum Squared Error (SSE): 2.446563930284

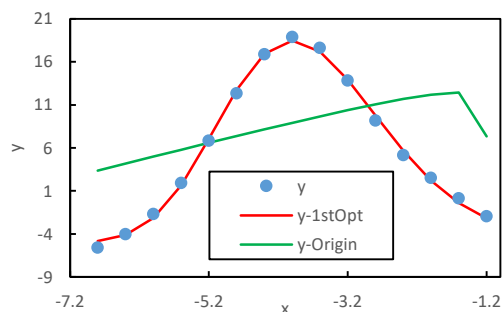
(6 Parameter)	R-Square: 0.09907 y0 -32.92192 xc -1.62111 a 45.35075 w1 26.19011 w2 2.22508 w3 1.02004	R-Square: 0.997431153904507 y0 -5.04665575921666 xc -3.99231524185906 a 23.5045055095231 w1 0.329349094529669 w2 -2084.59140661839 w3 2016.28410845371
Extreme (4 Parameter)	Sum Squared Error (SSE): 14.36745 R-Square 0.98491 y0 -4.93236 xc -4.12723 w 1.11056 a 23.32182	Sum Squared Error (SSE): 14.36744713416 R-Square 0.98491445082794 y0 -4.93237024016001 xc -4.12722939096263 w 1.11055900683535 a 23.3218268832349



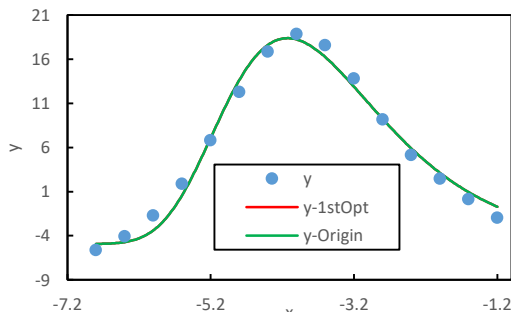
Gaussian



Asym2Sig



Beta



Extreme

图33-5 Origin与1stOpt计算对比图（数据-1）

代码-2: 对应 SigmaPlot 内置函数的 1stOpt 计算代码（数据-1）

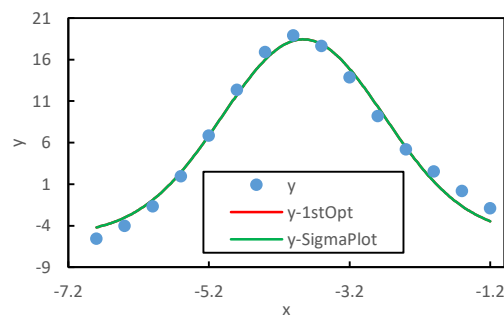
```

Parameter a,b,x0,y0;
//Parameter a,b,c,x0,y0;
Variable x, y;
Function y=y0+a*exp(-.5*((x-x0)/b)^2); //Peak, Gaussian, 4 Parameter
//y=y0+a*exp(-0.5*abs((x-x0)/b)^c); //Peak, Modified Gaussian, 5 Parameter
//y= a*(c*(1/(1+((x-x0)/b)^2)))+(1-c)*exp(-0.5*((x-x0)/b)^2); // Peak, Pseudo-Voigt, 4 Parameter
//y= y0+a*(c*(1/(1+((x-x0)/b)^2)))+(1-c)*exp(-0.5*((x-x0)/b)^2); //Peak, Pseudo-Voigt, 5 Parameter
Data;
x=-6.8,-6.4,-6,-5.6,-5.2,-4.8,-4.4,-4,-3.6,-3.2,-2.8,-2.4,-2,-1.6,-1.2;
y=-5.6121,-4.0471,-1.6874,1.9082,6.8139,12.3099,16.8705,18.8677,17.6083,13.8271,9.1697,5.1537,2.4853,
0.1354,-1.9532;

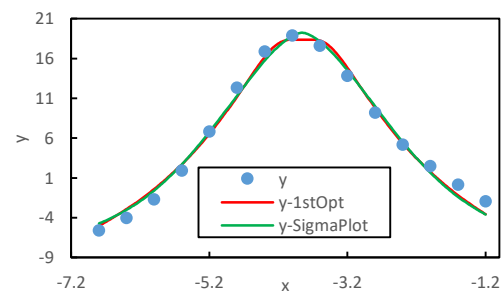
```

表33-6. SigmaPlot与1stOpt计算结果（数据-1）

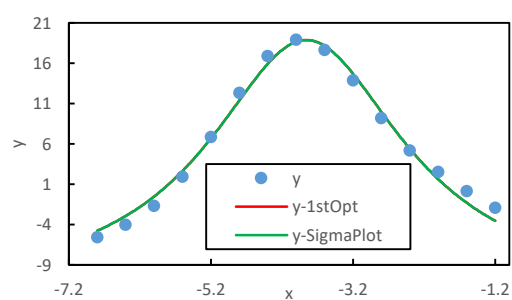
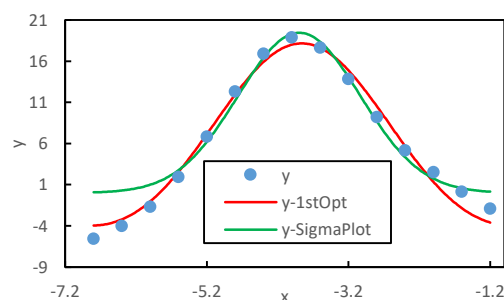
函数	Sigmaplot	1stOpt
Gaussian (4 Parameter)	Residual Sum of Squares = 14.8417 Rsqr = 0.9844 a 23.5320 b 1.1527 x0 -3.8603 y0 -5.1024	Sum Squared Error (SSE): 14.8417406894 R-Square: 0.9844164515186 a 23.5320108880111 b 1.15272606276159 x0 -3.86026787362344 y0 -5.10243031842668
Modified Gaussian (5 Parameter)	Residual Sum of Squares = 13.1869 Rsqr = 0.9862 a 26.6426 b 1.1641 c 1.6445 x0 -3.8579 y0 -7.3991	Sum Squared Error (SSE): 12.62504334979 R-Square: 0.98674394201877 a -45.901765278723 b -4.11862217349438 c -0.889534100154734 x0 -3.85697194553871 y0 18.3740980300299
Pseudo-Voigt (4 Parameter)	Residual Sum of Squares = 67.5850 Rsqr = 0.9290 a 19.4592 b 0.8625 c 1.0876E-08 x0 -3.8960	Sum Squared Error (SSE): 17.31978609101 R-Square: 0.981814920061235 a 18.1657608017856 b -3.12050513136682 c 7.68504552233671 x0 -3.86036737916031
Pseudo-Voigt (5 Parameter)	Residual Sum of Squares = 12.6859 Rsqr = 0.9867 a 31.2637 b 1.6724 c 0.9903 x0 -3.8585 y0 -12.4023	Sum Squared Error (SSE): 12.68585645340 R-Square: 0.986680089404155 a 31.2637604627974 b 1.67236223199068 c 0.990267094027557 x0 -3.85851764130709 y0 -12.4023600040049



Gaussian (4 Parameter)



Modified Gaussian (5 Parameter)



Pseudo-Voigt (4 Parameter)

Pseudo-Voigt (5 Parameter)

图33-6 SigmaPlot与1stOpt计算对比图（数据-1）

案例数据-2:

代码-3: 对应 Origin 内置函数的 1stOpt 计算代码（数据-2）

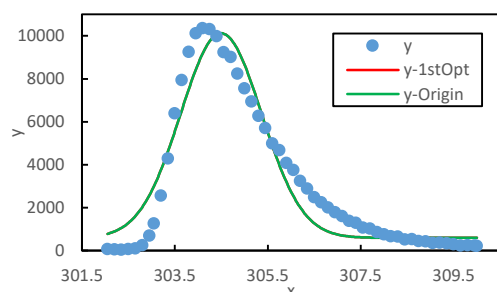
```
//Parameter y0,xc,w,a;
Parameter y0,xc=[302,310],a,w1,w2,w3;
Variable x,y;
Function y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2); //Gauss
//y=y0+A*(1/(1+exp(-(x-xc+w1/2)/w2)))*(1-1/(1+exp(-(x-xc-w1/2)/w3))); //Asym2Sig
//y=y0+A*(1+((w2+w3-2)/(w2-1))*((x-xc)/w1)^(w2-1)*(1-((w2+w3-2)/(w3-1))*((x-xc)/w1)^(w3-1));
//Beta
//y=y0+A*exp(-exp(-(x-xc)/w)-(x-xc)/w+1); //extreme;

Data;
x=302.05,302.2,302.35,302.5,302.65,302.8,302.95,303.05,303.2,303.35,303.5,303.65,303.8,303.95,304.1,304.2
5,304.4,304.55,304.7,304.85,305,305.15,305.3,305.45,305.6,305.75,305.9,306.05,306.2,306.35,306.5,306.65,3
06.8,306.95,307.1,307.25,307.4,307.55,307.7,307.85,308,308.15,308.3,308.45,308.6,308.75,308.9,309.05,309.
2,309.35,309.5,309.65,309.8,309.95,310;
y=68,50,40,58,97,247,691,1254,2547,4282,6381,7936,9249,10106,10350,10296,9968,9232,9001,8224,7548,69
28,6268,5700,4976,4667,4073,3742,3234,2876,2477,2235,2005,1777,1603,1377,1285,1058,1020,855,745,656,
647,504,531,441,423,349,362,334,286,228,236,222,205;
```

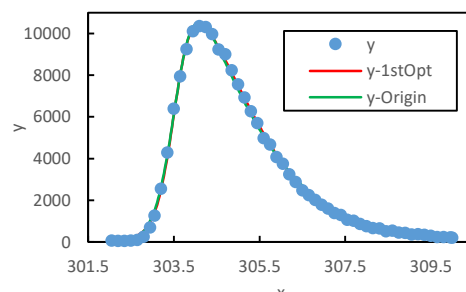
表33-7. Origin与1stOpt计算结果（数据-2）

函数	Origin Pro	1stOpt
Gaussian (4 Parameter)	Sum Squared Error (SSE): 4.66436E7 R-Square: 0.92596 y0 596.24426 xc 304.49553 w 1.74311 a 20803.8543	Sum Squared Error (SSE): 46643552.50536 R-Square: 0.925963584445763 y0 596.239707302723 xc 304.495535357821 w 1.74311222457526 a 20803.8922208817
Asym2Sig (6 Parameter)	Sum Squared Error (SSE): 1286725.85141 R-Square: 0.99796 y0 -113.96264 xc 303.69513 a 26577.32747 w1 0.23426 w2 0.2343 w3 1.25803	Sum Squared Error (SSE): 776671.9728105 R-Square: 0.998767203486018 y0 64.1547047392769 xc 304.156502783005 a 16739.6541093719 w1 1.24404355708866 w2 0.215319911000172 w3 1.00002452639898
Beta (6 Parameter)	Sum Squared Error (SSE): 3.50034E9 R-Square: 0.74161944 y0 10350 xc 304.1 a 1 w1 203.40886 w2 2 w3 101.70443	Sum Squared Error (SSE): 336095.9959348 R-Square: 0.99946652127712 y0 7.47745182391254 xc 304.170580157392 a 10344.3317087577 w1 -0.252264504706145 w2 59.5655627704939 w3 -64.5325301042246
Extreme (4 Parameter)	Sum Squared Error (SSE): 6162716.69976 R-Square: 0.99022	Sum Squared Error (SSE): 6162716.699718 R-Square: 0.990218038077806

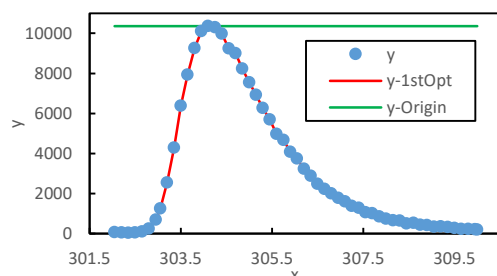
y0	279.82554	y0	279.826070609092
xc	304.27746	xc	304.277461649191
w	0.85648	w	0.856477737636556
a	10066.5658	a	10066.5661054463



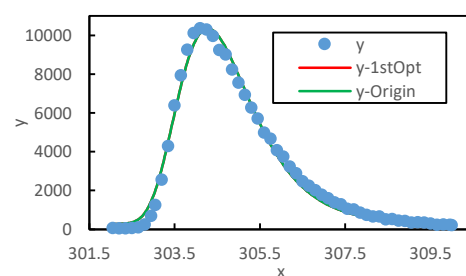
Gaussian



Asym2Sig



Beta



Extreme

图33-7 Origin与1stOpt计算对比图（数据-2）

代码-4： 对应 SigmaPlot 内置函数的 1stOpt 计算代码（数据-2）

```

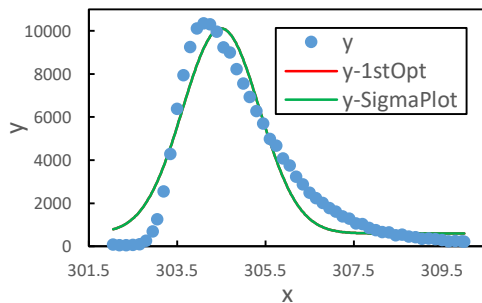
Parameter a,b,x0,y0;
//Parameter a,b,c,x0,y0;
//Parameter a,b,c,x0;
//Parameter a,b,c,x0,y0;
Variable x,y;
Function y=y0+a*exp(-.5*((x-x0)/b)^2); //Peak, Gaussian, 4 Parameter
//y=y0+a*exp(-0.5*abs((x-x0)/b)^c); //Peak, Modified Gaussian, 5 Parameter
//y= a*(c*(1/(1+((x-x0)/b)^2)))+(1-c)*exp(-0.5*((x-x0)/b)^2); // Peak, Pseudo-Voigt, 4 Parameter
//y= y0+a*(c*(1/(1+((x-x0)/b)^2)))+(1-c)*exp(-0.5*((x-x0)/b)^2); //Peak, Pseudo-Voigt, 5 Parameter
Data;
x=302.05,302.2,302.35,302.5,302.65,302.8,302.95,303.05,303.2,303.35,303.5,303.65,303.8,303.95,304.1,304.2
5,304.4,304.55,304.7,304.85,305,305.15,305.3,305.45,305.6,305.75,305.9,306.05,306.2,306.35,306.5,306.65,3
06.8,306.95,307.1,307.25,307.4,307.55,307.7,307.85,308,308.15,308.3,308.45,308.6,308.75,308.9,309.05,309.
2,309.35,309.5,309.65,309.8,309.95,310;
y=68,50,40,58,97,247,691,1254,2547,4282,6381,7936,9249,10106,10350,10296,9968,9232,9001,8224,7548,69
28,6268,5700,4976,4667,4073,3742,3234,2876,2477,2235,2005,1777,1603,1377,1285,1058,1020,855,745,656,
647,504,531,441,423,349,362,334,286,228,236,222,205;

```

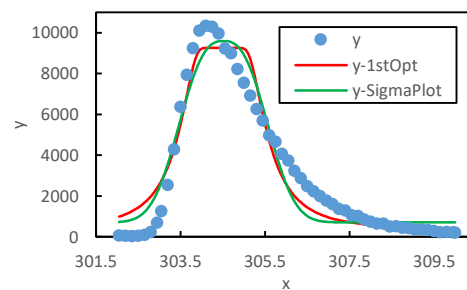
表33-8. SigmaPlot数据-2结果

函数	Sigmaplot	1stOpt
Gaussian (4 Parameter)	Sum Squared Error (SSE): 46643552.59 R-Square: 0.9260	Sum Squared Error (SSE): 46643552.50536 R-Square: 0.925963584445763

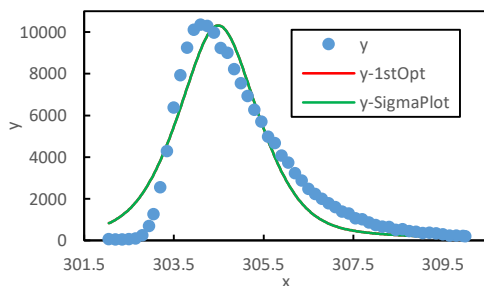
	a 9522.6801 b 0.8716 x0 304.4955 y0 596.2373	a 9522.68255380699 b 0.871556115053904 x0 304.4955358841 y0 596.239712548324
Modified Gaussian (5 Parameter)	Sum Squared Error (SSE): 44484488.859 R-Square: 0.9294 a 8885.8192 b 0.9679 c 2.6547 x0 304.5163 y0 710.3135	Sum Squared Error (SSE): 43843032.54644 R-Square: 0.930408796019713 a -8921.72424798327 b 1.22596024149766 c -2.71246741545735 x0 304.501252662689 y0 9253.99075620173
Pseudo-Voigt (4 Parameter)	Sum Squared Error (SSE): 50572495.6443 R-Square: 0.9197 a 10315.7236 b 0.9459 c 0.4670 x0 304.4908	Sum Squared Error (SSE): 50572495.63880 R-Square: 0.920981784897036 a 10315.7086087983 b 0.945945011454401 c 0.46699410588109 x0 304.490813494788
Pseudo-Voigt (5 Parameter)	Sum Squared Error (SSE): 46643552.5128 R-Square: 0.9260 a 9522.6838 b 0.8716 c 1.9574E-09 x0 304.4955 y0 596.2410	Sum Squared Error (SSE): 29716295.15373 R-Square: 0.952831895116033 a 22156.5324096902 b 1.2225864853992 c 5.23158759241729 x0 301.209835061922 y0 -2695.52974668904



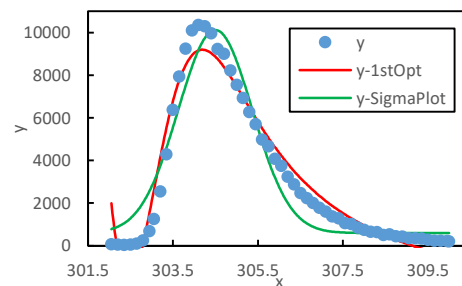
Gaussian



Modified Gaussian



Pseudo-Voigt



Pseudo-Voigt (5 Parameter)

图33-8 SigmaPlot与1stOpt计算对比图（数据-2）

详细计算结果参见前述表33-5至表33-8。拟合计算结果是否是最优解，只需参考各自计算的最小二乘目标函数值SSE（Sum Squared Error）即可，该值越小结果也越好。最终结果归纳如下表33-9，同一案例同一函数SSE最小者为最优解，用“✓”表示，反之为局部最优解或错误结果，用“✗”表示。

表33-9 计算结果汇总

内置函数		SSE (数据-1)	SSE (数据-2)	内置函数		数据-1	数据-2
Gaussian (4 Par)	Origin	14.84174 ✓	4.66436E7 ✓	Gaussian (4 Par)	SigmaPlot	14.8417 ✓	46643552.59 ✓
	1stOpt	14.84174	4.66436E7		1stOpt	14.8417	46643552.505
Asym2Sig (6 Par)	Origin	0.755580 ✗	1286725.85 ✗	Modified Gaussian (5 Par)	SigmaPlot	13.1869 ✗	44484488.86 ✗
	1stOpt	0.438058	776671.97		1stOpt	12.6250	43843032.546
Beta (6 Par)	Origin	858.0446 ✗	3.50034E9 ✗	Pseudo-Voigt (4 Par)	SigmaPlot	67.5850 ✗	50572495.64 ✓
	1stOpt	2.446564	336095.995		1stOpt	17.3198	50572495.64
Extreme (4 Par)	Origin	14.3674 ✓	6162716.699 ✓	Pseudo-Voigt (5 Par)	SigmaPlot	12.6859 ✓	46643552.51 ✗
	1stOpt	14.3674	6162716.699		1stOpt	12.6859	29716295.15
正确率	50%			正确率	50%		

由上述计算结果看，两款软件采用内置函数拟合时无需人为猜参数初值，使用简单快捷，但仅50%的准确率还是有些出乎意料的，毕竟是两款知名度非常高的科学计算类软件。虽然各自都只测试了四种内置峰函数，小样本无法代表全体，但可以确定的是两款软件在内置函数拟合方面确实存在不足，需要进一步的改进和完善。

33.4 小结

基于实际案例数据对两款知名科学绘图及数据处理分析软件 Origin Pro 和 SigmaPlot 内置函数非线性拟合功能和效果进行了测试验证，结果表明这两款软件均无法保证内置拟合函数计算的正确性，所得结果最好再与 1stOpt 的计算结果核实验证后再决定是否应该采用，防止错误结果而引起的后续问题。