44. 曲线拟合的瑞士军刀 — 1stOpt 神经网络拟合特例演示之二

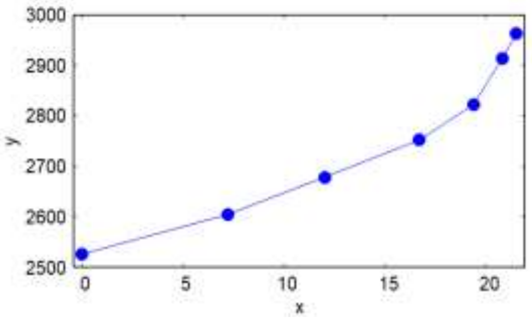
44.1 引言

在之前的文章“曲线拟合的瑞士军刀—1stOpt 神经网络拟合特例演示”中以实际案例演示了 1stOpt 神经网络拟合工具箱如何有效解决数据曲线形状特殊但模型公式未知的复杂拟合问题，1stOpt 的小巧但强大的“瑞士军刀”属性得到了很好的表现，不仅拟合效果优异同时还能给出具体模型表达式；那么在已知数据，拟合公式未知，要求拟合曲线通过每一个实际数据点，即完美拟合但又不同于插值，同时也必须给出具体模型表达式，这种情况，1stOpt 这把“瑞士军刀”是否有能力满足呢？在此以八个实际案例进行探讨。

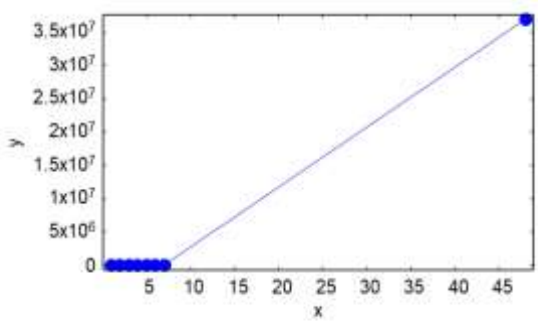
44.2 案例数据

表 44-1：案例数据

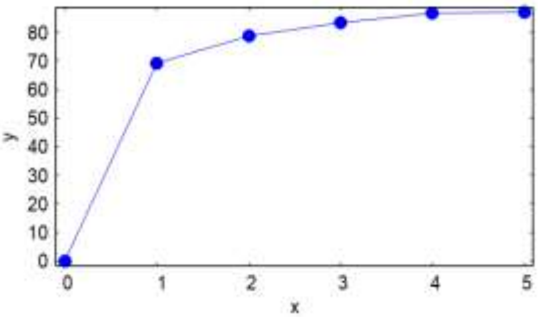
案例 1	x	0,7.2,12,16.7,19.4,20.8,21.5
	y	2526,2604,2678,2752,2822,2913,2963
案例 2	x	1,2,3,4,5,6,7,48
	y	119,163,240,395,617,1461,4310,36955464
案例 3	x	0,1,2,3,4,5
	y	0,69.18248,78.63425,83.30743,86.66291,87.06997
案例 4	x	177600,961200, 2504000, 4997000, 8884000
	y	6.754, 24.416, 58.622, 107.980, 154.507
案例 5	x	0,20,40,60,100,120,140,160
	y	1,2,3,4,10,11,12,13
案例 6	x	1,2,4,6,8,10,13,17,21,25
	y	0.2,0.5,1,2,4,7,10,14,18,22
案例 7	x1	200,400,1600,3200,6400,12800,25600,51200,102400
	x2	279,270,255,230,202,170,150,125,100
	y	169,160,140,112,90,79,55,51,49
案例 8	x	20,30,35,40,50,55,60,70,75,80
	y	0,6.25,58.82,58.82,82.35,93.75,93.75,100,250,250



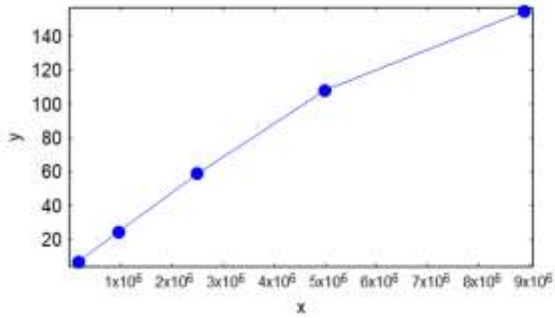
案例-1



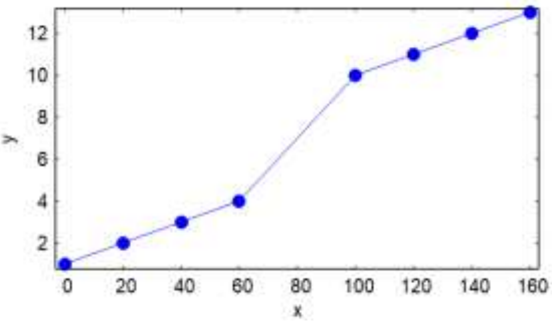
案例-2



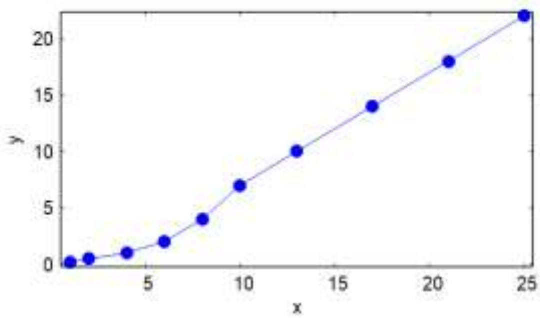
案例-3



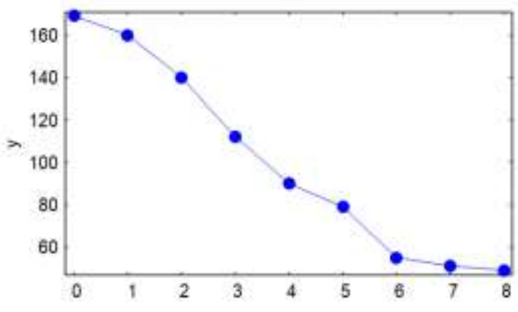
案例-4



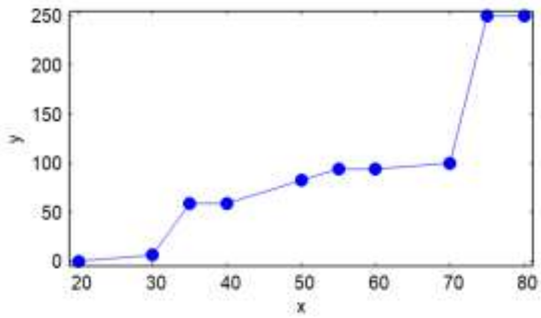
案例-5



案例-6



案例-7



案例-8

图 44-1 案例数据散点曲线图

44.3 神经网路结构

八个案例中的数据点从最少 5 个到最多 10 个。虽然数据点都不多，但拟合公式未知，要求拟合计算曲线要完美通过所有实际数据点，具体到数值评价指标就是最小二乘的目标函数值 SSE（Sum of Squared Error）小于 1E-10，无疑，这些看似简单的问题实则是非常棘手的事，首先要选择确定拟合模型公式，其次要保证计算拟合曲线必须通过每一个实际数据点，

再次，拟合模型公式的未知参数数目不能大于数据点数，否则会出现过拟合现象而失去意义。基于这些前提条件，确定合理的神经网路结构就成为第一步需要解决的问题。

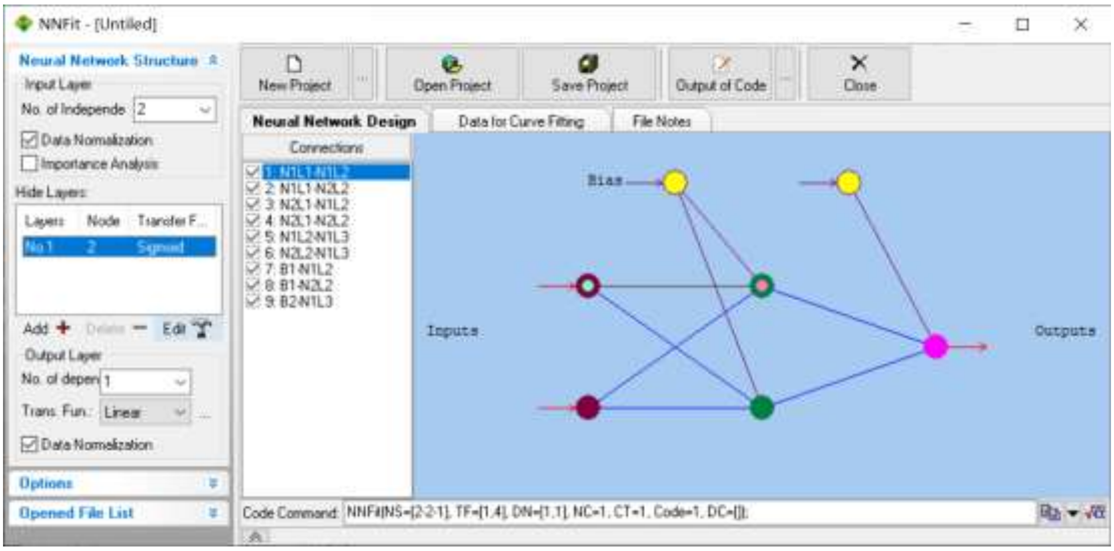


图 44-2 [2-2-1]神经网络结构

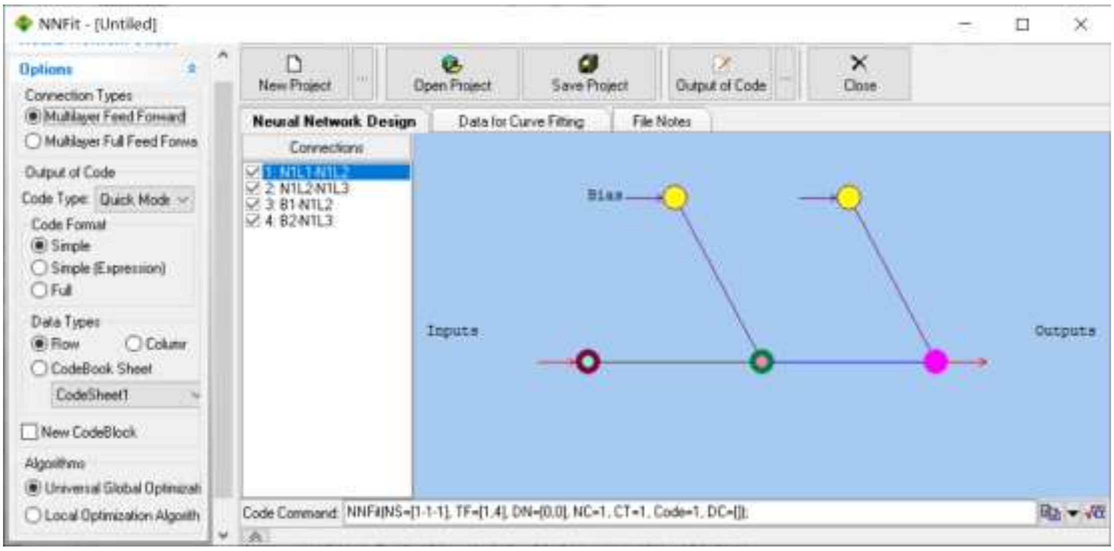


图 44-3 [1-1-1]神经网络结构

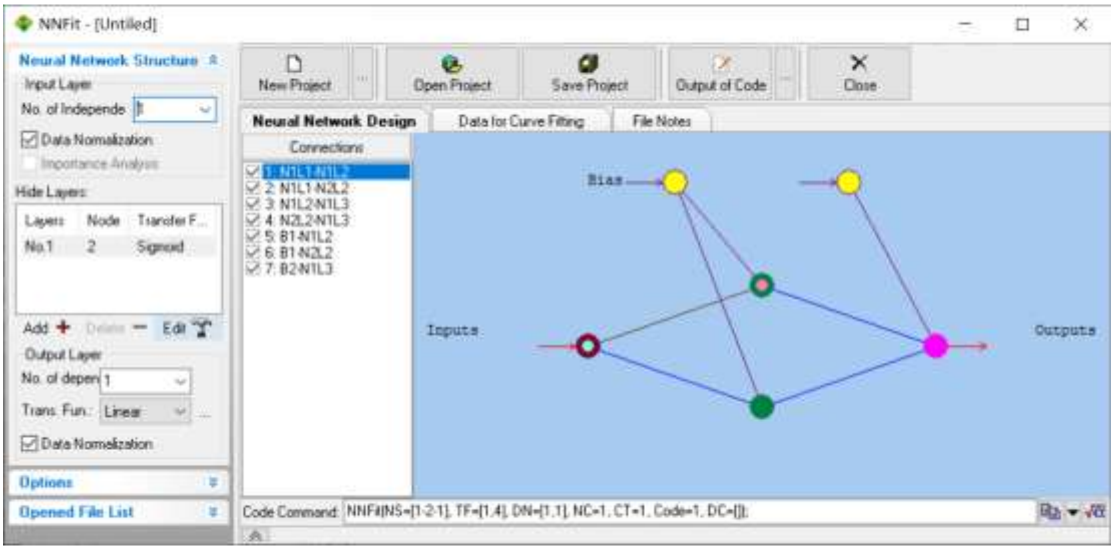


图 44-4　[1-2-1]神经网络结构

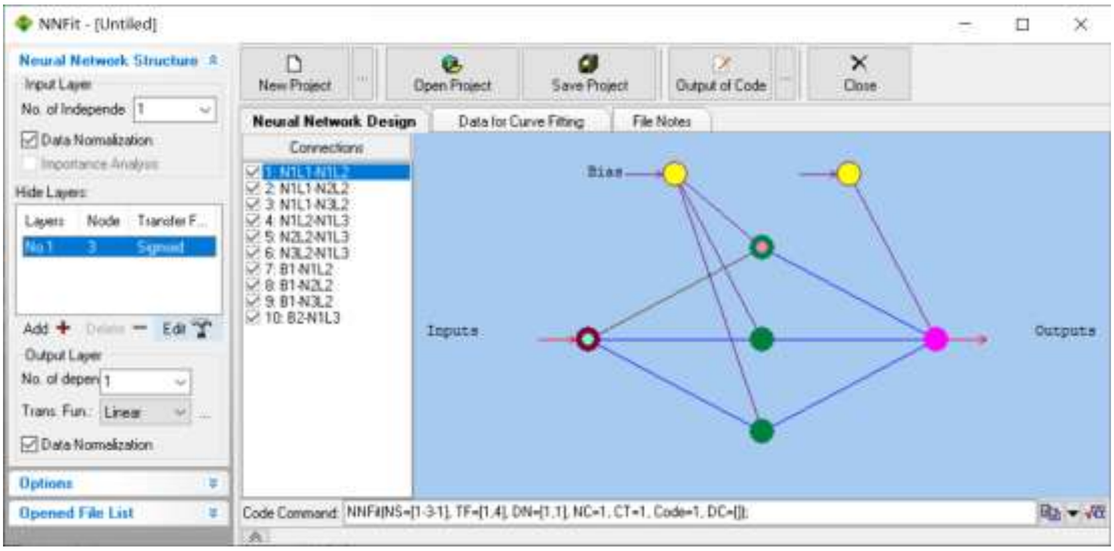


图 44-5　[1-3-1]神经网络结构

八个案例中除了第七个是两输入（两个自变量）一输出外，其余都是一输入一输出。对于前者（案例七），如图 44-2 示，具有一个含有两个神经元的隐含层恰好有 9 个参数，与拟合数据点数一致；而对于其它单一输入单一输出案例，经典网络结构有以下三种，均为一个隐含层但分别有 1、2 和 3 个神经元节点，如图 44-3、44-4 和 44-5 示，对应的参数数目分别为 4、7 和 10 个，如果数据点刚好为 4 或 7 或 10，则可分别采用这三种结构，但如果数据量有别于这个两个数，如案例-3 和案例-4 分别只有 6 个和 5 个数据点，这种情况该如何处理呢？如果神经网络模型参数数大于拟合数据点数，如案例-3，可以通过断开某神经元节点的链接从而减少模型参数，如图 44-6 示；而对于数据点数大于神经网络模型参数数，如案例-4，一是通过增加隐含层神经元节点数，二是将模型结构由“Multilayer Feed Forward”改为“Multilayer Full Feed Forward”，此结构改变了只有相邻层才能链接常规模式，增加了由输入层直接到输出层的链接，如图 44-7，达到了增加参数数的目的。

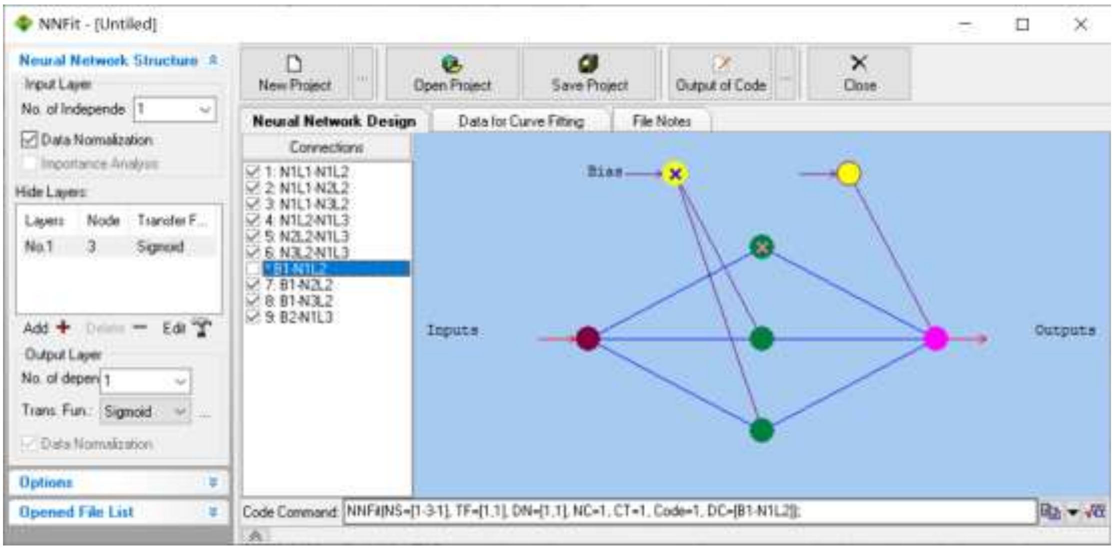


图 44-6　神经网络断开链接减少参数数

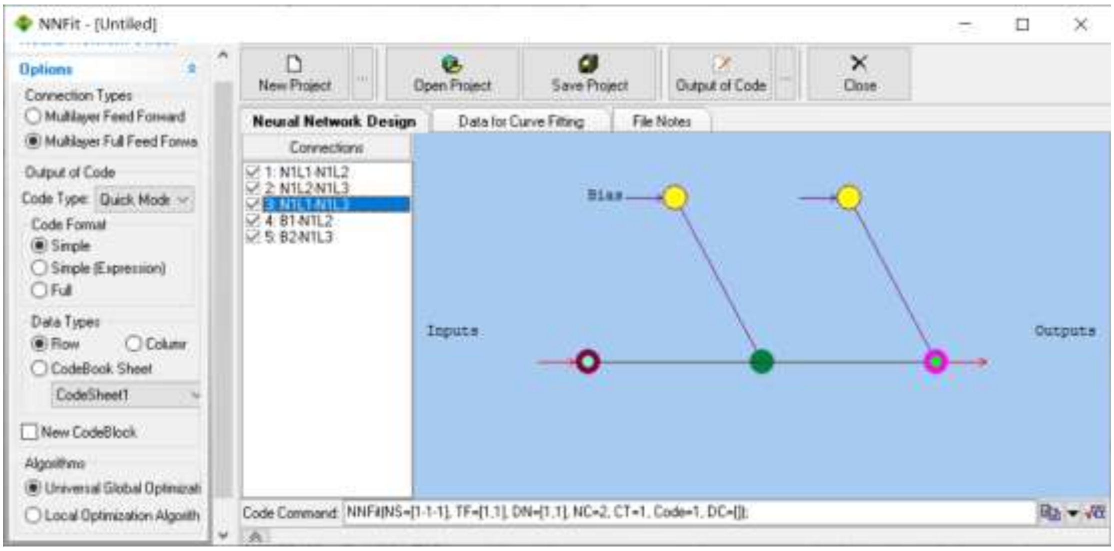


图 44-7　神经网络链接结构改变增加参数数

基于以上分析，8 个实际案例的神经网络结构及对应的命令和模型公式表达式小结列表如下。注意对应神经网络的模型公式表达式可以简单如下图直接获取 MathML 或 Latex 格式代码，建议 MathML 格式，其代码直接黏贴至 Word 中可直接自动转换为公式形式。

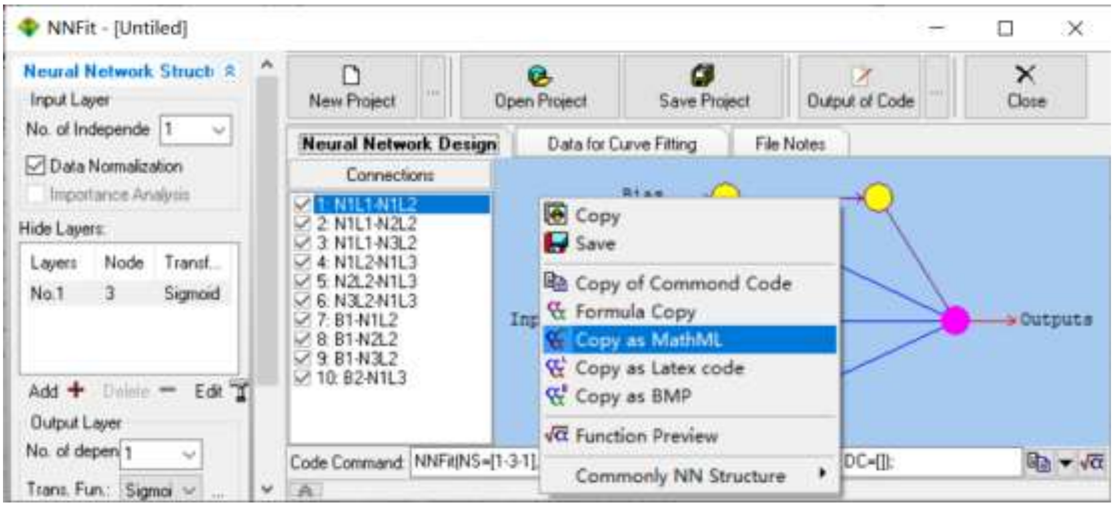
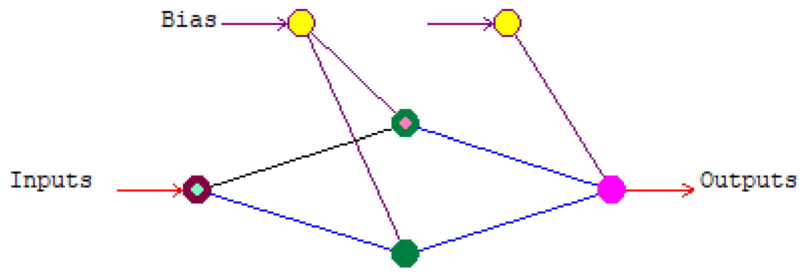
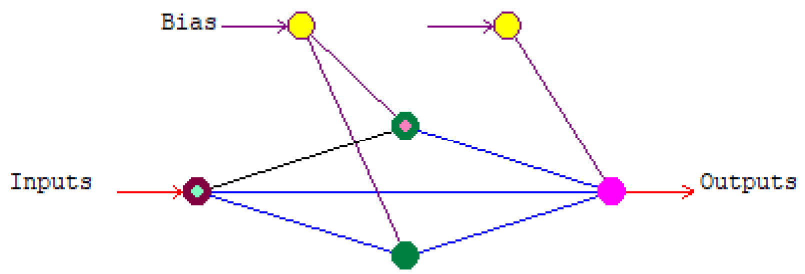
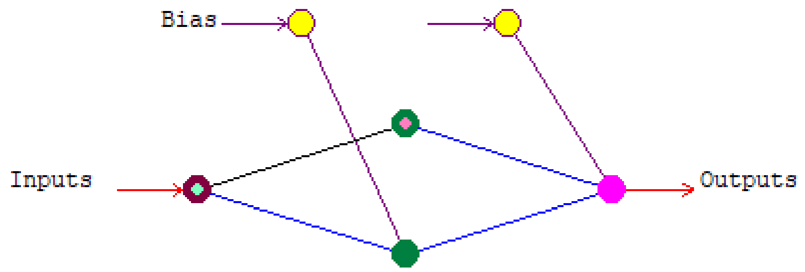
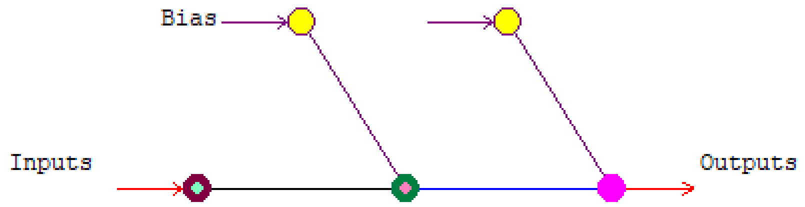
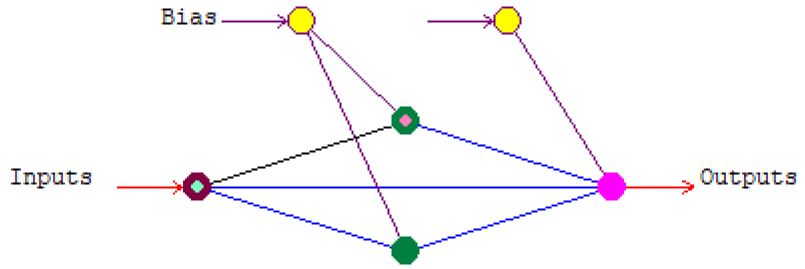
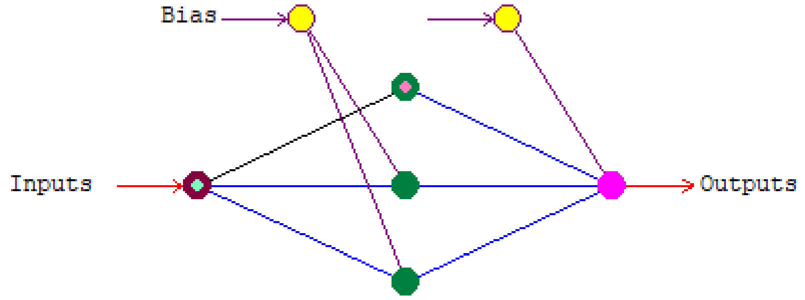
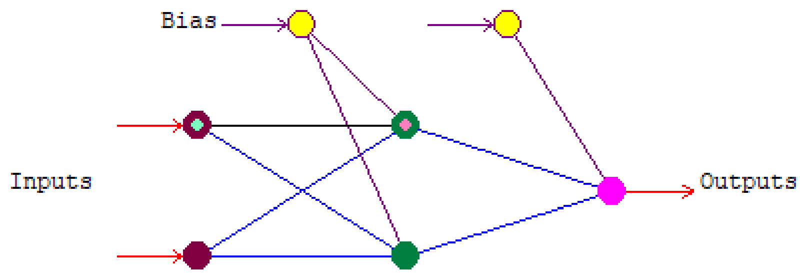
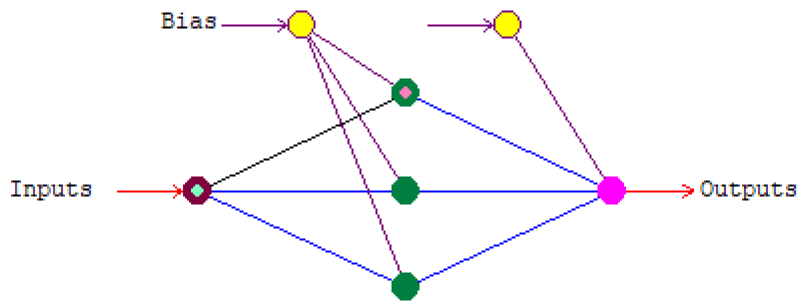


图 44-8　直接获取神经网络对应的模型公式表达式

表 44-1 各案例神经网络结构、对应命令及公式

案例	参数数/数据点数	神经网络结构、命令及对应公式
1	7	
		NNFit(NS=[1-2-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[]);
		$y=\frac{p_3}{1+\exp\left(-(p_1\cdot x+p_5)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot x+p_6)\right)}+p_7$
2	8	
		NNFit(NS=[1-2-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, DC=[])
		$y=\frac{p_3}{1+\exp\left(-(p_1\cdot x+p_6)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot x+p_7)\right)}+p_8+p_5\cdot x$

<table>
<tr><td rowspan="3">3</td><td rowspan="3">6</td><td>
</td></tr>
<tr><td>NNFit(NS=[1-2-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[B1-N1L2]);</td></tr>
<tr><td>$$y = \frac{p_3}{1 + \exp(-p_1 \cdot x)} + \frac{p_4}{1 + \exp\left(-(p_2 \cdot x + p_5)\right)} + p_6$$</td></tr>
<tr><td rowspan="3">4</td><td rowspan="3">5</td><td>
</td></tr>
<tr><td>NNFit(NS=[1-1-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, DC=[]);</td></tr>
<tr><td>$$y = \frac{p_2}{1 + \exp\left(-(p_1 \cdot x + p_4)\right)} + p_5 + p_3 \cdot x$$</td></tr>
<tr><td rowspan="3">5</td><td rowspan="3">8</td><td>
</td></tr>
<tr><td>NNFit(NS=[1-2-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, DC=[]);</td></tr>
<tr><td>$$y = \frac{p_3}{1 + \exp\left(-(p_1 \cdot x + p_6)\right)} + \frac{p_4}{1 + \exp\left(-(p_2 \cdot x + p_7)\right)} + p_8 + p_5 \cdot x$$</td></tr>
<tr><td rowspan="2">6</td><td rowspan="2">10</td><td>
</td></tr>
<tr><td>NNFit(NS=[1-3-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, DC=[B1-N1L2]);</td></tr>
</table>

<table>
<tr><td></td><td></td><td>$$y=\frac{p_4}{1+\exp(-p_1\cdot x)}+\frac{p_5}{1+\exp\left(-(p_2\cdot x+p_8)\right)}+\frac{p_6}{1+\exp\left(-(p_3\cdot x+p_9)\right)}+p_{10}+p_7\cdot x$$</td></tr>
<tr><td rowspan="3">7</td><td rowspan="3">9</td><td>
</td></tr>
<tr><td>NNFit(NS=[2-2-1], TF=[1,4], DN=[1,0], NC=1, CT=1, Code=1, DC=[]);</td></tr>
<tr><td>$$y=\frac{p_5}{1+\exp\left(-\left(p_1\cdot\left(-1+\frac{2\cdot(x_1-minx_1)}{maxx_1-minx_1}\right)+p_3\cdot\left(-1+\frac{2\cdot(x_2-minx_2)}{maxx_2-minx_2}\right)+p_7\right)\right)}+\frac{p_6}{1+\exp\left(-\left(p_2\cdot\left(-1+\frac{2\cdot(x_1-minx_1)}{maxx_1-minx_1}\right)+p_4\cdot\left(-1+\frac{2\cdot(x_2-minx_2)}{maxx_2-minx_2}\right)+p_8\right)\right)}+p_9$$</td></tr>
<tr><td rowspan="3">8</td><td rowspan="3">10</td><td>
</td></tr>
<tr><td>NNFit(NS=[1-3-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[]);</td></tr>
<tr><td>$$y=\frac{p_4}{1+\exp\left(-(p_1\cdot x+p_7)\right)}+\frac{p_5}{1+\exp\left(-(p_2\cdot x+p_8)\right)}+\frac{p_6}{1+\exp\left(-(p_3\cdot x+p_9)\right)}+p_{10}$$</td></tr>
</table>

44.4 计算代码及结果

各案例计算代码、计算结果及最终拟合结果对比图如下，可以看出拟合精度完全满足目标函数小于 1E-10 的要求，也即拟合计算值与实际值一致，或拟合完美通过每一个实际数据点。

案例-1代码

```
Function NNFit(NS=[1-2-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[]);
```

```
Data;
x=[0,7.2,12,16.7,19.4,20.8,21.5];
y=[2526,2604,2678,2752,2822,2913,2963];
```

案例-1结果

计算指标及参数值	实际 y 值	计算 y 值
Sum Squared Error (SSE): 6.05909798695093E-23	2526	2526
Root of Mean Square Error (RMSE): 2.94208332089232E-12	2604	2604
Correlation Coef. (R): 1	2678	2678
R-Square: 1	2752	2752
Adjusted R-Square: 1	2822	2822
Determination Coef. (DC): 1	2913	2913
Chi-Square: 1.08184078837433E-26	2963	2963
Parameter Best Estimate		
--------- -------------		
p1 1.16376405008171		
p2 0.156641107977491		
p3 223.945030823675		
p4 410.635844242334		
p5 -24.1872111480825		
p6 -1.86061665494952		
p7 2470.71560680971		

案例-2代码

```
Function NNFit(NS=[1-2-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, DC=[]);
Data;
x   = [1,2,3,4,5,6,7,48];
y   = [119,163,240,395,617,1461,4310,36955464];
```

案例-2结果

计算指标及参数值	实际 y 值	计算 y 值
Sum Squared Error (SSE): 5.26595234270244E-21	119	118.999999999994
Root of Mean Square Error (RMSE): 2.56562671259442E-11	163	163.000000000003
Correlation Coef. (R): 1	240	240.000000000067
R-Square: 1	395	394.999999999973
Adjusted R-Square: 1	617	617.000000000001
Determination Coef. (DC): 1	1461	1461
Chi-Square: 1.03813559410081E-23	4310	4310
F-Statistic: 0	36955464	36955464
Parameter Best Estimate		
--------- -------------		
p1 3.27295258314593		
p2 0.995083876555183		
p3 -457.161142818074		
p4 36954668.0526119		
p5 24.3751000475544		
p6 -16.5736267407347		
p7 -15.9760334259006		
p8 83.1037292497797		

案例-3代码

```
Function NNFit(NS=[1-2-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[B1-N1L2]);
Data;
x=[0,1,2,3,4,5];
y=[0,69.18248,78.63425,83.30743,86.66291,87.06997];
```

案例-3结果

计算指标及参数值	实际 y 值	计算 y 值
Sum Squared Error (SSE): 4.46323717196312E-22 Root of Mean Square Error (RMSE): 8.62480644416936E-12 Correlation Coef. (R): 1 R-Square: 1 Adjusted R-Square: 1 Determination Coef. (DC): 1 Chi-Square: -3.49587025993699E-12 F-Statistic: 0 Parameter Best Estimate --------- ------------- p1 2.74756994660354 p2 -2.68256752240245 p3 157.207098613986 p4 -8.50133405787532 p5 7.81229857889893 p6 -70.1056545738574	0 69.18248 78.63425 83.30743 86.66291 87.06997	-3.49587025993969E-12 69.1824799999952 78.6342500000166 83.3074300000043 86.6629100000016 87.0699699999892

案例-4代码

```
Function NNFit(NS=[1-1-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, DC=[]);
Data;
x = [177600,961200, 2504000, 4997000, 8884000];
y = [6.754, 24.416, 58.622, 107.980, 154.507];
```

案例-4结果

计算指标及参数值	实际 y 值	计算 y 值
Sum Squared Error (SSE): 1.75815086554508E-24 Root of Mean Square Error (RMSE): 5.92984125511818E-13 Correlation Coef. (R): 1 R-Square: 1 Adjusted R-Square: 1 Determination Coef. (DC): 1 Chi-Square: 1.44255704066553E-26 F-Statistic: 0 Parameter Best Estimate --------- ------------- p1 -8.19705898515556E-7 p2 63.9537766600794 p3 2.27589821043963E-5 p4 5.95127409341651 p5 -61.0498255724752	6.754 24.416 58.622 107.98 154.507	6.75400000000016 24.4160000000005 58.6220000000007 107.98 154.506999999999

案例-5代码

```
Function NNFit(NS=[1-2-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, DC=[]);
Data;
x=[0,20,40,60,100,120,140,160];
y=[1,2,3,4,10,11,12,13];
```

案例-5结果

计算指标及参数值	实际 y 值	计算 y 值
Root of Mean Square Error (RMSE): 0 Correlation Coef. (R): 1 R-Square: 1 Adjusted R-Square: 1 Determination Coef. (DC): 1	1 2 3 4 10	1 2 3 4 10

Chi-Square: 0 Parameter Best Estimate --------- ------------- p1 4.73917664887281 p2 1.08640413714859 p3 4 p4 8.17716097409907E-8 p5 0.05 p6 -334.390864473661 p7 113.885746228812 p8 0.99999991822839	11 12 13	11 12 13

案例-6代码

```
Function NNFit(NS=[1-3-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, DC=[B1-N1L2]);
Data;
x=[1,2,4,6,8,10,13,17,21,25];
y=[0.2,0.5,1,2,4,7,10,14,18,22];
```

案例-6结果

计算指标及参数值	实际 y 值	计算 y 值
Sum Squared Error (SSE): 5.0559071738991E-21 Root of Mean Square Error (RMSE): 2.24853445023622E-11 Correlation Coef. (R): 1 R-Square: 1 Adjusted R-Square: 1 Determination Coef. (DC): 1 Chi-Square: 2.81887624030795E-22 Parameter Best Estimate --------- ------------- p1 2.52972300746747 p2 -29.7485461313513 p3 -12.1001663698372 p4 -10.3716674357368 p5 -1.00000265445444 p6 2.43456760371176 p7 1.00000000000535 p8 250.833983137994 p9 48.0390969567133 p10 7.3716674356234	0.2 0.5 1 2 4 7 10 14 18 22	0.199999999999984 0.500000000000007 1 2.00000000000009 3.99999999999991 7.00000000004711 9.9999999999562 13.9999999999775 17.9999999999989 22.0000000000203

案例-7代码

```
Function NNFit(NS=[2-2-1], TF=[1,4], DN=[1,0], NC=1, CT=1, Code=1, DC=[]);
Data;
x1=[200,400,1600,3200,6400,12800,25600,51200,102400];
x2=[279,270,255,230,202,170,150,125,100];
y=[169,160,140,112,90,79,55,51,49];
```

案例-7结果

计算指标及参数值	实际 y 值	计算 y 值
Sum Squared Error (SSE): 6.98504146048273E-24 Root of Mean Square Error (RMSE): 8.8097430032403E-13 Correlation Coef. (R): 1 R-Square: 1 Adjusted R-Square: 1 Determination Coef. (DC): 1 Chi-Square: 3.49197406454923E-26 F-Statistic: 0	169 160 140 112 90 79 55 51	168.999999999999 159.999999999999 139.999999999999 112 90.0000000000014 79.0000000000011 54.9999999999999 51.0000000000008

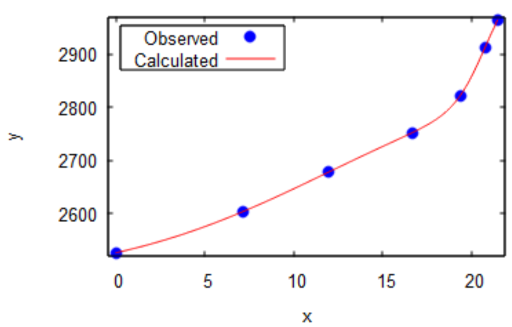
Parameter Best Estimate --------- ------------- p1 -3.32964494006522 p2 0.967623102512261 p3 1.67283764343845 p4 3.64460309502303 p5 417.891197143782 p6 -266.575989870856 p7 -3.51559408152574 p8 0.900189043235478 p9 87.4900151499586	49	48.9999999999998

案例-8代码

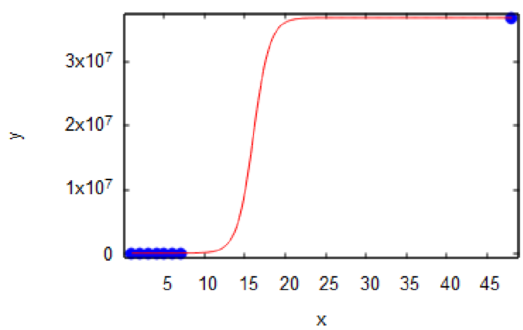
```
Hardness = 2;
Variable x,y;
Function NNFit(NS=[1-3-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[]);
Data;
x=20,30,35,40,50,55,60,70,75,80;
y=0,6.25,58.82,58.82,82.35,93.75,93.75,100,250,250;
```

案例-8结果

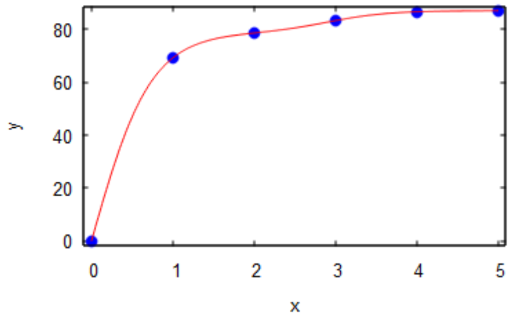
计算指标及参数值	实际 y 值	计算 y 值
Sum Squared Error (SSE): 6.06758475577719E-15 Root of Mean Square Error (RMSE): 2.46324679148826E-8 Correlation Coef. (R): 1 R-Square: 1 Adjusted R-Square: 1 Determination Coef. (DC): 1 Chi-Square: 1.31451620209484E-12 Parameter Best Estimate --------- ------------- p1 4.85018363957158 p2 5.32808449010718 p3 -6.87906048648328 p4 156.250000055077 p5 58.8200000006637 p6 -34.9299999993359 p7 -342.690908600726 p8 -161.972098854311 p9 343.228361476854 p10 34.9299999993372	0 6.25 58.82 58.82 82.35 93.75 93.75 100 250 250	1.31450406115619E-12 6.24999999999984 58.8199999993327 58.820000000665 82.3499999999995 93.7500000000009 93.7500000000009 100 249.999999944926 250.000000055077



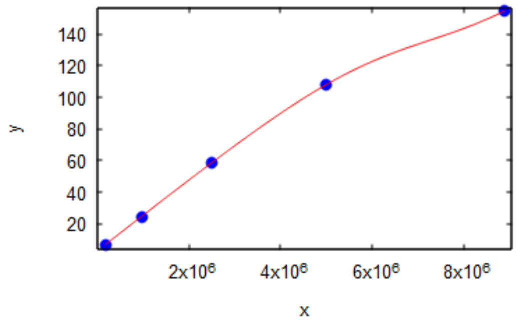
案例-1



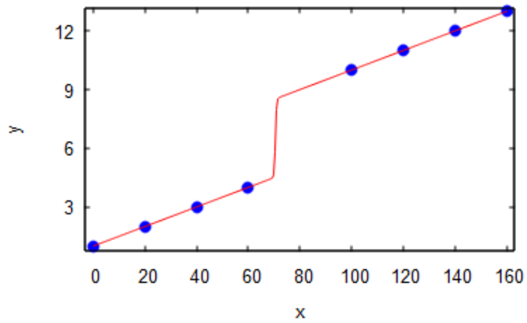
案例-2



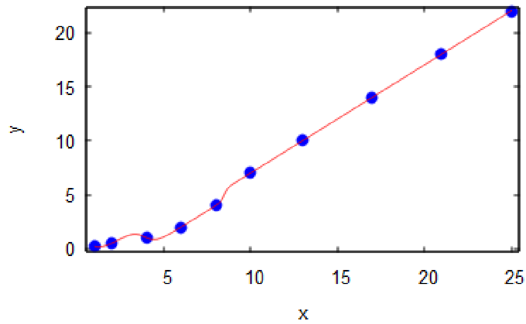
案例-3



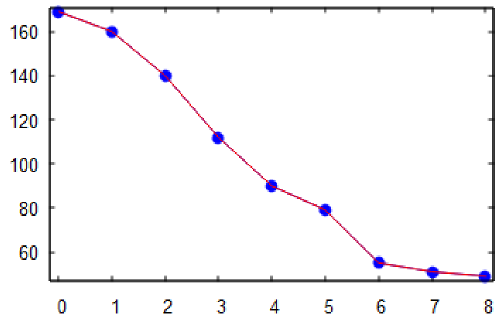
案例-4



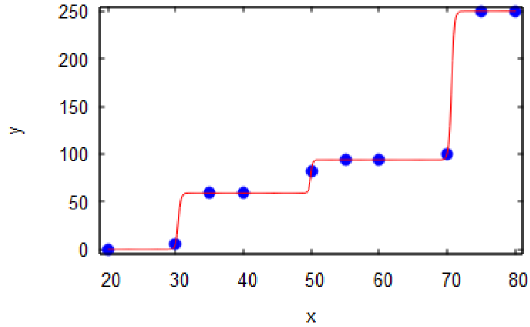
案例-5



案例-6



案例-7



案例-8

图 44-9　计算结果对比图

从上述八个案例详细计算结果看，计算曲线都几乎完美通过每一个实测点，完全满足最初的要求。

另外，所有案例的特点是参数数与数据量数一样，且要通过每一个实际点，当拟合公式确定后，这一情况也可等同视为求解非线性方程组问题，以案例-1 为例，其对应的模型拟合公式为：

$$y = \frac{p_3}{1+\exp\left(-(p_1 \cdot x + p_5)\right)} + \frac{p_4}{1+\exp\left(-(p_2 \cdot x + p_6)\right)} + p_7$$

相应非线性方程组、求解代码如下，计算结果与前面拟合计算一致。

$$
\begin{cases}
\frac{p_3}{1+\exp\left(-(p_1\cdot 0+p_5)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot 0+p_6)\right)}+p_7-2526=0\\
\frac{p_3}{1+\exp\left(-(p_1\cdot 7.2+p_5)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot 7.2+p_6)\right)}+p_7-2604=0\\
\frac{p_3}{1+\exp\left(-(p_1\cdot 12+p_5)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot 12+p_6)\right)}+p_7-2678=0\\
\frac{p_3}{1+\exp\left(-(p_1\cdot 16.7+p_5)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot 16.7+p_6)\right)}+p_7-2752=0\\
\frac{p_3}{1+\exp\left(-(p_1\cdot 19.4+p_5)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot 19.4+p6t)\right)}+p_7-2822=0\\
\frac{p_3}{1+\exp\left(-(p_1\cdot 20.8+p_5)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot 20.8+p_6)\right)}+p_7-2913=0\\
\frac{p_3}{1+\exp\left(-(p_1\cdot 21.5+p_5)\right)}+\frac{p_4}{1+\exp\left(-(p_2\cdot 21.5+p_6)\right)}+p_7-2963=0
\end{cases}
$$

案例-1非线性方程组及代码

```
Constant x=[0,7.2,12,16.7,19.4,20.8,21.5],y=[2526,2604,2678,2752,2822,2913,2963];
ConstStr f=p3/(1+exp(-(p1*x+p5)))+p4/(1+exp(-(p2*x+p6)))+p7;
Function For(x,y)(f-y=0);
```

结果：

```
Algorithms: Universal Global Optimization(UGO1)
Function Expression 1: ((p3/(1+exp(-(p1*0+p5)))+p4/(1+exp(-(p2*0+p6)))+p7))-2526-0 = -2.72848410531878E-12
2: ((p3/(1+exp(-(p1*7.2+p5)))+p4/(1+exp(-(p2*7.2+p6)))+p7))-2604-0 = 2.72848410531878E-12
3: ((p3/(1+exp(-(p1*12+p5)))+p4/(1+exp(-(p2*12+p6)))+p7))-2678-0 = -4.54747350886464E-12
4: ((p3/(1+exp(-(p1*16.7+p5)))+p4/(1+exp(-(p2*16.7+p6)))+p7))-2752-0 = -4.54747350886464E-13
5: ((p3/(1+exp(-(p1*19.4+p5)))+p4/(1+exp(-(p2*19.4+p6)))+p7))-2822-0 = 0
6: ((p3/(1+exp(-(p1*20.8+p5)))+p4/(1+exp(-(p2*20.8+p6)))+p7))-2913-0 = -3.63797880709171E-12
7: ((p3/(1+exp(-(p1*21.5+p5)))+p4/(1+exp(-(p2*21.5+p6)))+p7))-2963-0 = 5.45696821063757E-12
Objective Function (Min.): 7.87889533456759E-23
p3: 223.945030823597
p1: 1.16376405008207
p5: -24.1872111480897
p4: 410.635844242562
p2: 0.156641107977401
p6: -1.860616654949
p7: 2470.71560680965
```

44.5 小结

如何在要求拟合曲线必须通过每一个实际数据点的前提下确定拟合模型公式？1stOpt 的神经网络拟合工具箱再次展示了其瑞士军刀的优异特性，借助于独特且强大的全局优化计算功能，所有案例都获得了完美结果，也再次印证了 1stOpt 在优化计算领域的领先地步。当然也要注意，所有研究案例拟合数据点数都不多，数据点数越多，对应的神经网络结构会越复杂，待求参数数也会越多，相应求解难度趋于更高。