26. 1stOpt 神经网络拟合工具箱介绍与案例演示

26.1 简介

神经网络拟合工具箱NNFit是10.0版新增加的工具箱，不同于1stOpt已有的相对独立的神经网络工具箱NeuralPower，全新的神经网络拟合工具箱NNFit与1stOpt完全无缝融为一体，其可视化神经网络设计界面，不仅可帮助用户快速了解掌握该工具箱的使用方法和设计过程，还可以产生1stOpt标准运行代码，省时省力；通过产生的代码用户还可以清晰了解详细全面的计算流程甚至完整的拟合模型公式（虽然公式有时非常长），打破神经网络“黑箱”论的谬传，并且，拟合训练后的模型可方便迁移和再现，实用性显著增强。

在熟悉并掌握可视化设计后，仅用一句代码即可实现复杂神经网络拟合计算，再结合1stOpt特有的全局优化算法，在无预设拟合模型公式的情况下，几乎可以拟合任何复杂形式的数据并得到满意的结果。

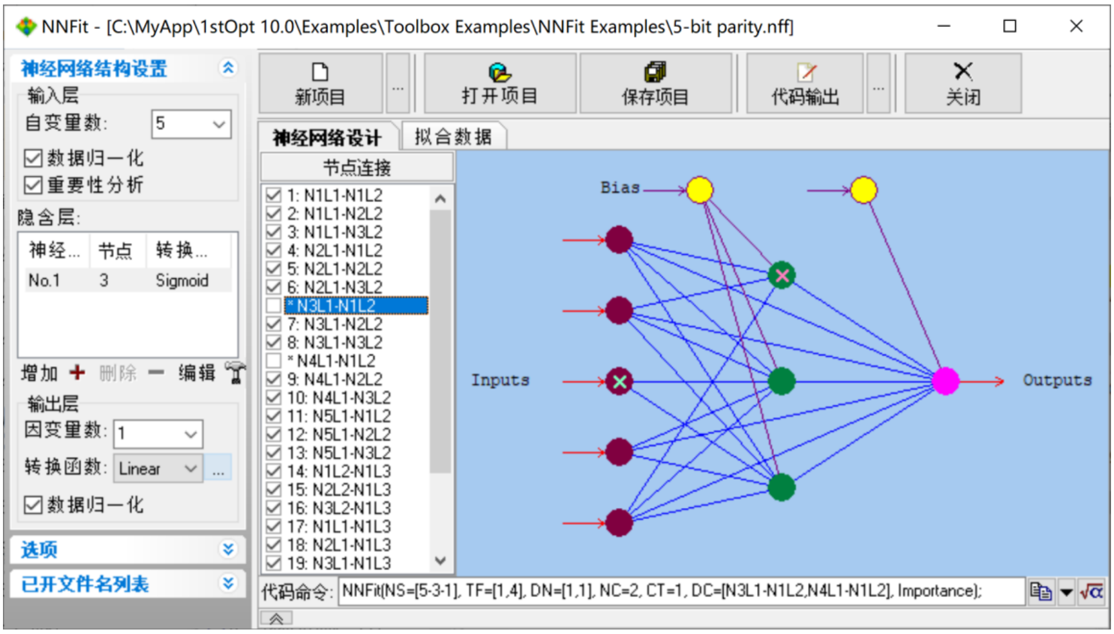


图 26.1 神经网络可视化设计

26.2 神经网络结构设计

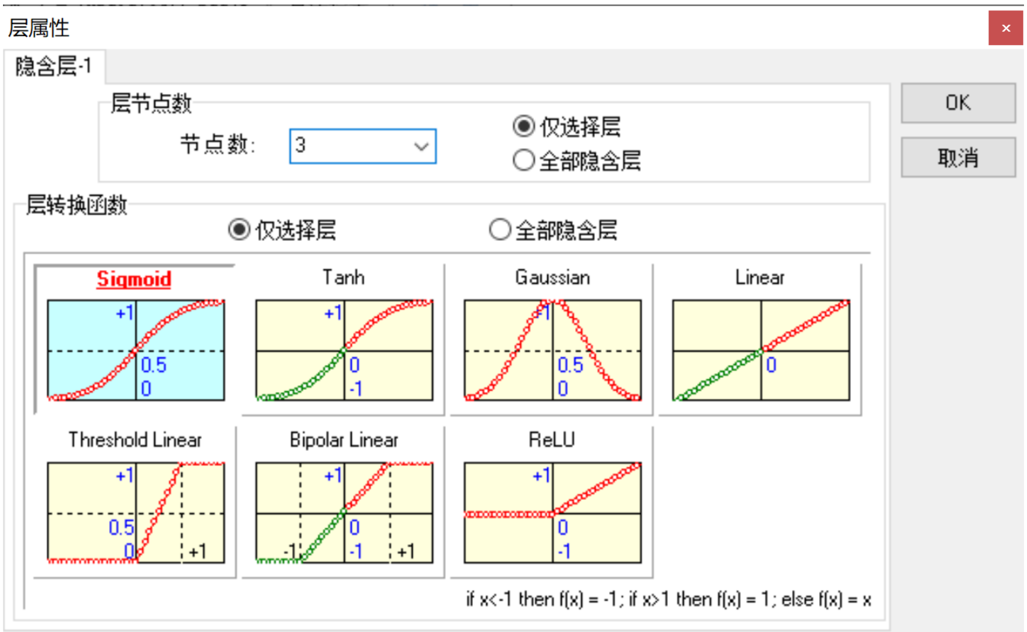


图 26.2. 神经网络转换（激活）函数

输入层：

1) 自变量数：等同于神经网络输入层节点数，根据问题实际情况输入具体值；
2) 数据归一化：缺省是将所有输入数据归一至[-1, 1]范围；
3) 重要性分析：当自变量数大于 1 时，可定性分析自变量的重要度。

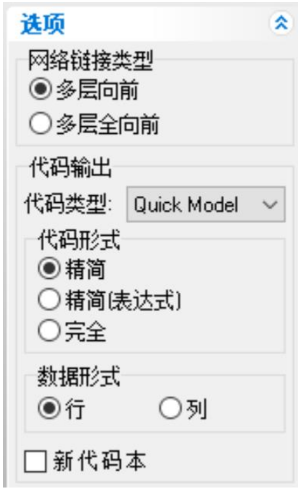
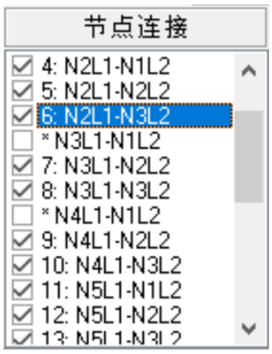
隐含层：

1) 确定有几个隐含层，每个隐含层有多少个神经元节点以及转换函数类型（激活函数），7 种类型转换函数，如图 26.2，可以任意修改。

   具体选几个隐含层？每个隐含层多少个节点？这些都没有固定的标准答案，得根据实际情况去确定，对一般拟合问题而言，一个隐含层或最多二个隐含层就足够了，节点数太多容易造成过拟合，并且计算量巨大。

输出层：

1) 因变量数：等同于输出层节点数，根据实际问题确定；
2) 转换函数：7 种类型可选，如图 26.2
3) 数据归一化：输出数据均匀化，只有选“Linear”或“ReLU”转换函数时，才可以选择数据不归一化。

<table>
<tr>
<td></td>
<td>网络链接类型：
1) 多层向前：一般至少包括一个隐含层，从隐含层到输出层，每层仅收到其紧邻上一层的输入，每层的输出仅对其紧邻下一层起作用，如图 26.3 示。
2) 多层全向前：每层的输出不仅至其紧邻下一层，还包括其所有的后续层，如图 26.4 示。
代码输出：
1) 代码类型：代码输出形式，包括快捷模式，Fortran，Pascal 或 Basic 编程模式；
2) 代码形式：精简模式，见图 26.5；精简（表达式）模式，见图 26.6；或完全模式，如图 26.7；三种模式运行效果一样，精简模式可以方便修改，精简（表达式）模式可以得到一个完整的模型公式，完全模式可以了解详细的计算步骤；
3) 数据形式：选择确定代码数据是以列还是行形式；
4) 新代码本：产生的代码是输出到在现有代码本，还是输出到一个新开的代码本。</td>
</tr>
<tr>
<td></td>
<td>任意控制不同层之间的神经元节点连接状态。</td>
</tr>
</table>

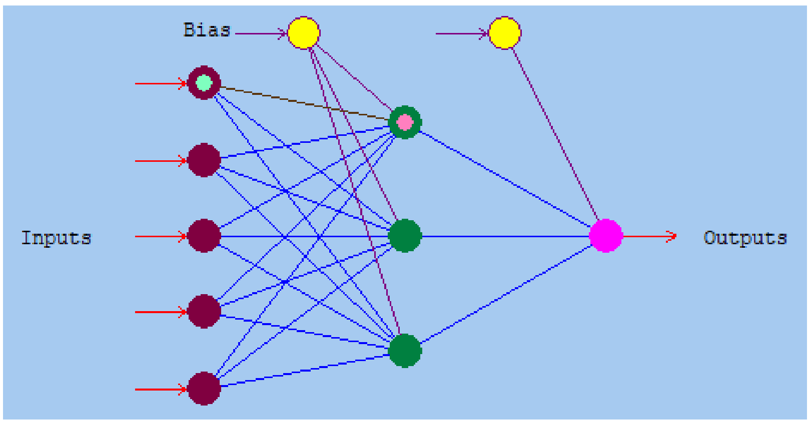


图 26.3 “5-3-1”结构多层向前

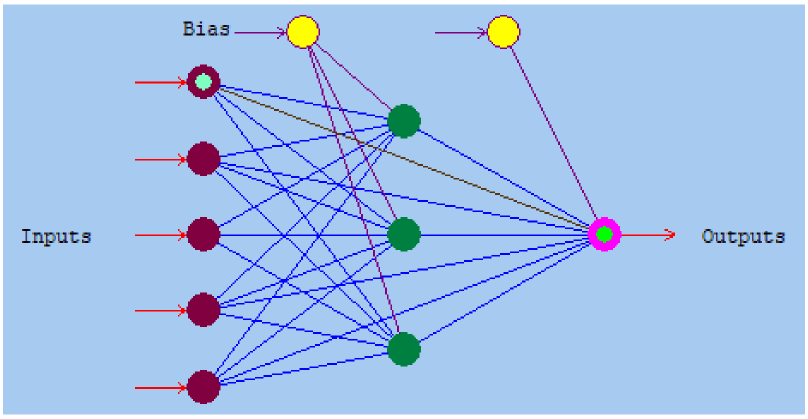


图 26.4“5-3-1”结构多层全向前

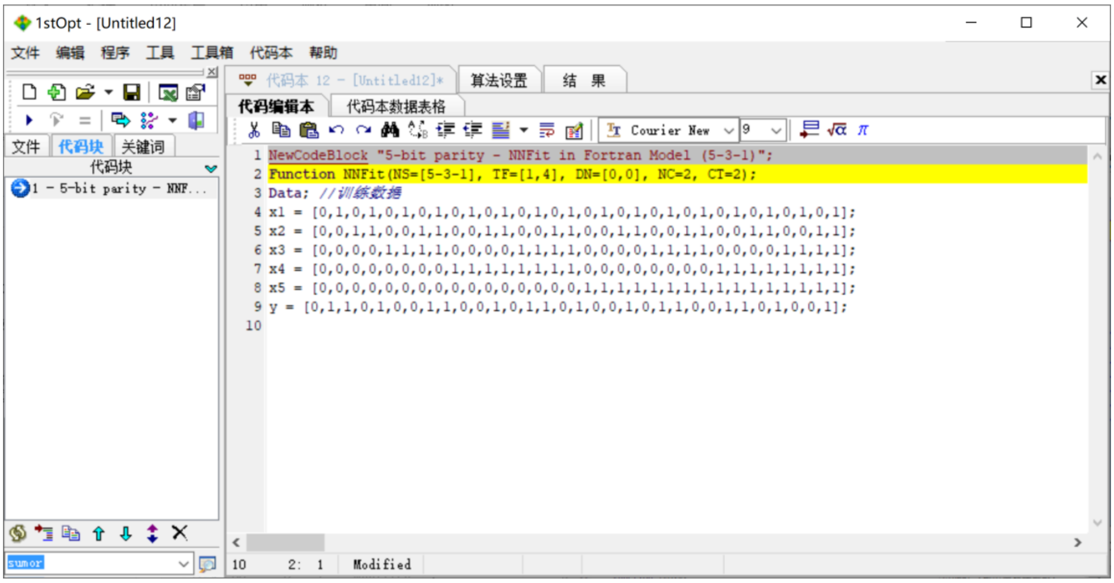


图 26.5 精简格式代码自动生成

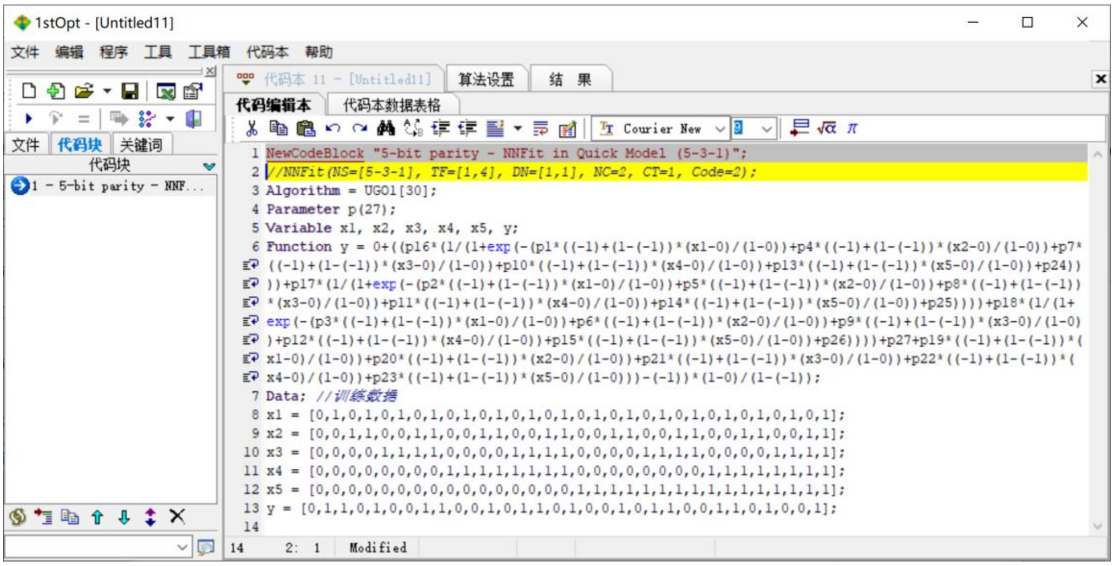


图 26.6 精简（表达式）格式代码自动生成

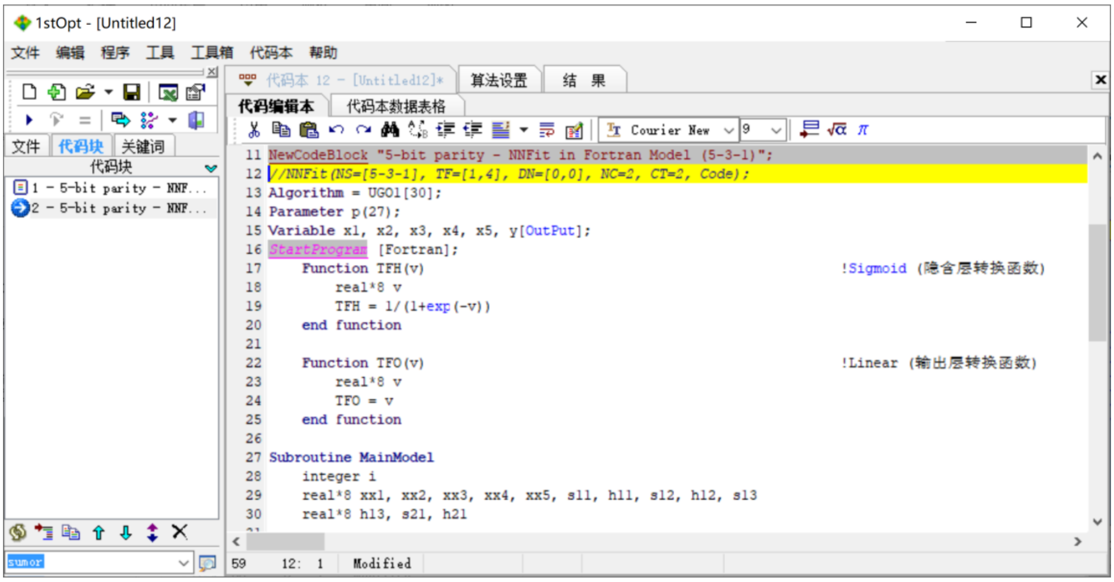


图 26.7 完全格式代码自动生成（Fortran 编程模式）

26.3 训练及验证数据

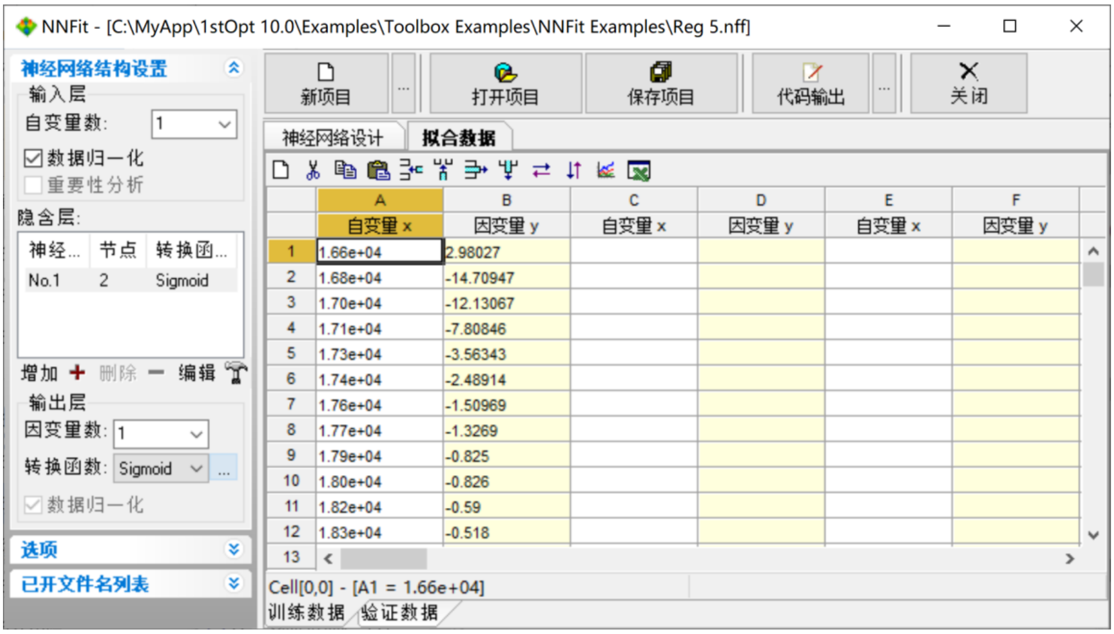


图 26.8 训练及验证数据

神经网络数据可直接在拟合数据表格录入，数据表格分为“训练数据”表格和“验证数据”表格，均可以录入多组数据。

验证数据将仅用于训练结果实时验证，对训练结果不起任何影响，主要通过关键字“DataFileWeight”控制，对应值为0的数据将被视为验证数据。图26.8案例产生代码如下图26.9：

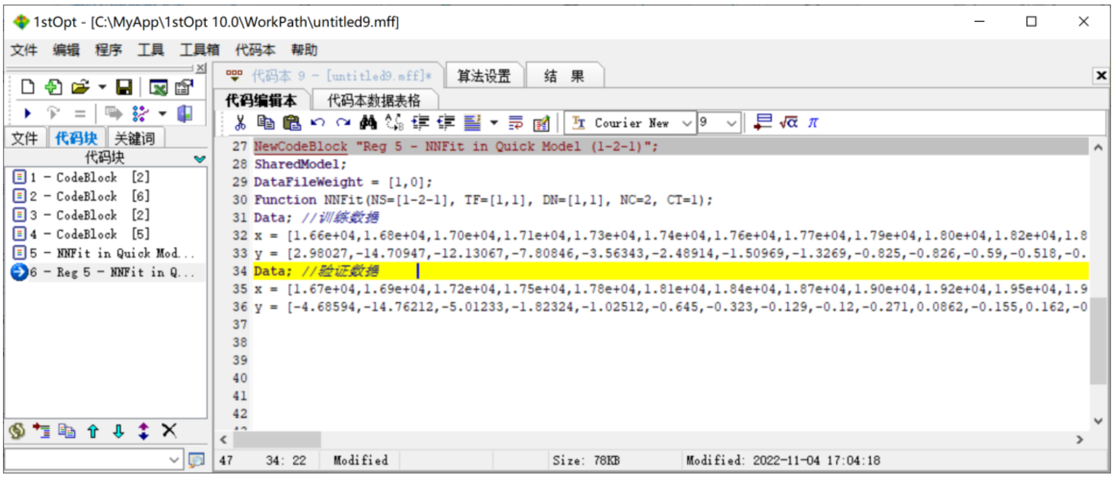


图 26.9 训练及验证数据

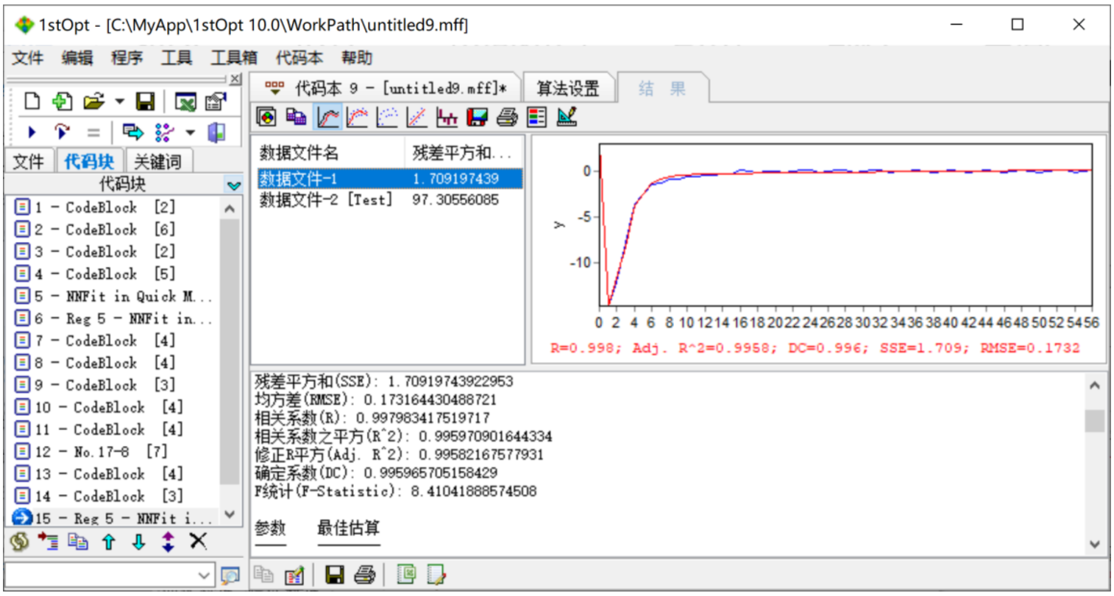


图 26.10 训练数据计算对比过程

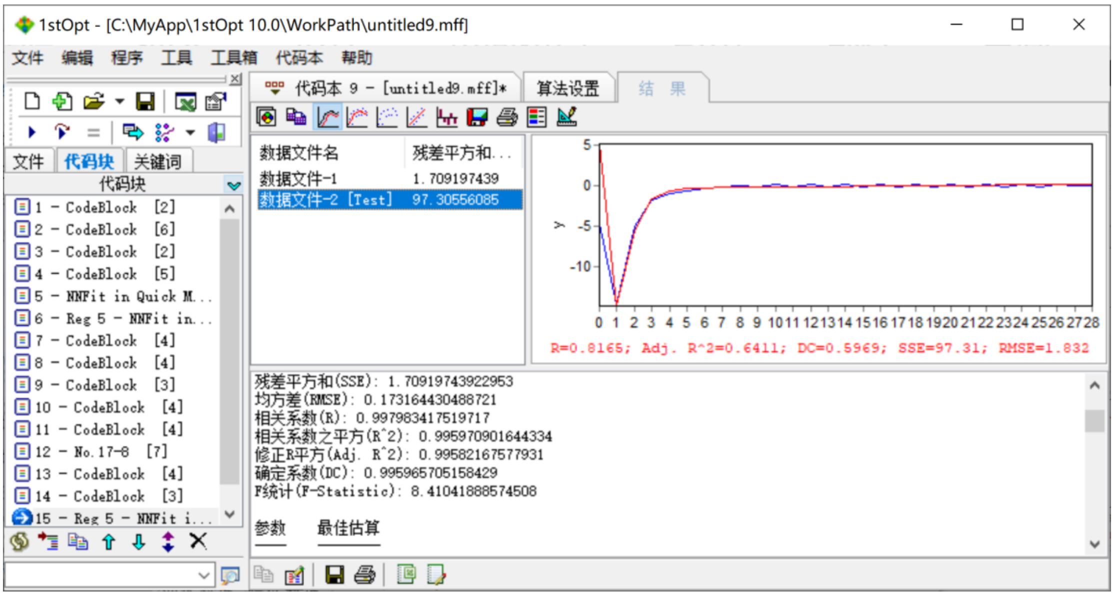


图 26.11 验证数据计算对比过程

26.4 神经网络拟合命令行代码及不同形式的公式复制

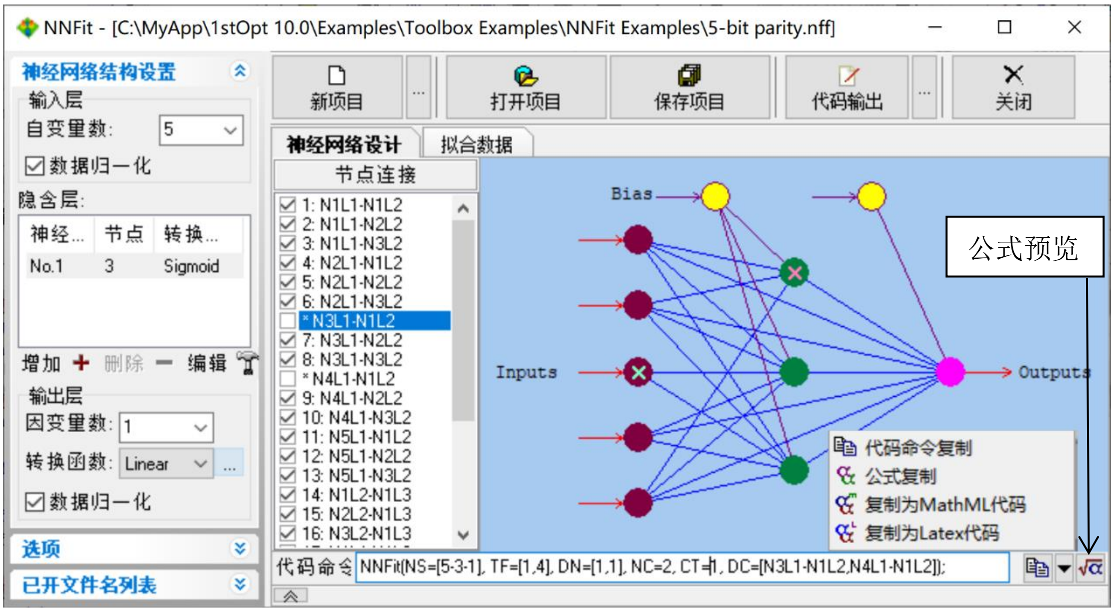


图 26.12 可视化设计：命令行代码及拟合模型公式

```
NewCodeBlock "xor - NNFit in Quick Model (2-1-1)";
Function NNFit(NS=[2-1-1], TF=[1,4], DN=[0,0], NC=2, CT=1);
Data; //训练数据
x1 = [0,0,1,1];
x2 = [0,1,0,1];
y = [0,1,1,0];
```

图 26.13 神经网络命令行代码

如图26.12和26.13，可视化设计界面对应有代码命令，该代码命令可直接用于1stOpt代码本作为拟合命令，当对该命令所代表的含义熟悉后，也可直接在代码本中通过组合键“Ctrl+k”选择“NNFit”直接输入神经网络拟合命令并可随意修改，省去可视化设计这一环节。

神经网络拟合命令以“NNFit”开始，缺省典型格式如下：

NNFit(NS=[1-3-1], TF=[1,1], DN=[1,1], NC=1, CT=1, Code=1, DC=[]);

其中含义主要包括：

1) NS=[1-3-1]：NS源自“Network Structure”，“1-3-1”表示是三层结构：输入层，含一个输入节点（一个自变量）；一个隐含层，含三个节点；输出层，含一个输出节点（一个因变量），见图26.14。

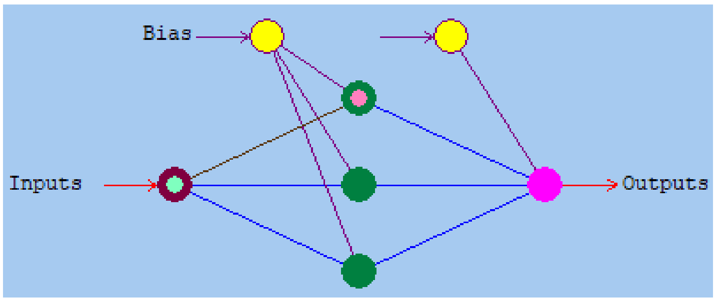


图26.14 “1-3-1”神经网络结构

例：NS=[2-1-1]：二个自变量的输入层，一个隐含层含1个节点，一个因变量的输出层。

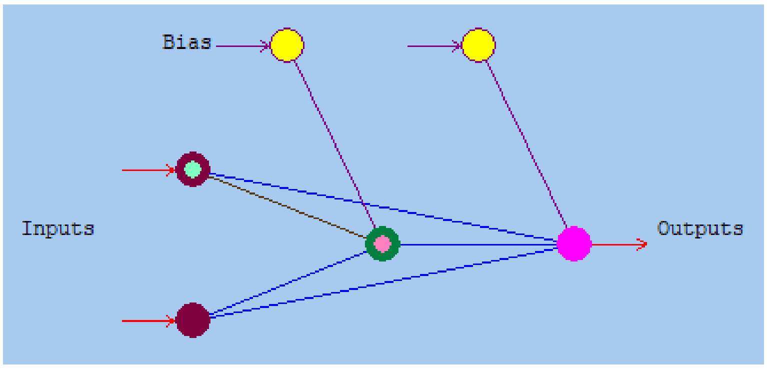


图26.15 “2-1-1”神经网络结构

例：NS=[5-6-3-2]：五个自变量的输入层，两个隐含层，神经元节点分别为6和3，两个个因变量的输出层。

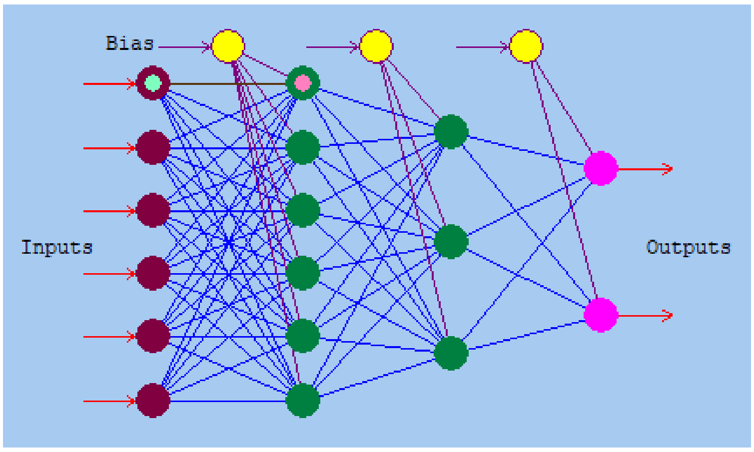


图26.16 “5-6-3-2”神经网络结构

2) TF=[1,4]，TF源自“Transfer Function”，也称之为激活函数（Activate Function），表示各隐含层及输出层的转换函数，参考前面图26.2，不同数字对应的转换函数如下：
1：Sigmoid函数；2：Tanh函数；3：Gaussian函数；4：Linear函数；5：Threshold Linear函数；6：Bipolar Linear函数；7：ReLU函数。
注意，激活函数仅存在于隐含层和输出层，输入层是没有的。
例：NS=[2-1-1], TF=[1,2]：三层结构，隐含层转换函数是Sigmoid，输出层转换函数为Tanh；
例：NS=[5-6-3-2], TF=[1,2,4]：四层结构，隐含层1转换函数为Sigmoid函数，隐含层2转换函数为Tanh函数，输出层转换函数Linear函数。

3) DN=[1,1]：DN意指“Data Nomalization”，数据均一化，仅对输入层和输出层，“1”表示数据均一化，“0”则表示不均一化，即保持原始数据规模；对于输入层，如果选择均一化，输入数据会自动均一化至范围[-1, 1]；对于输出层，仅当输出层转换函数为Linear或ReLU时，方可选择不均匀化，其它则必须均匀化。不同输出层转换函数对应的均一化数据范围：
   - Sigmoid：[0.1,0.9]；
   - Tanh：[-0.9,0.9]；
   - Gauissian：[0.1,0.9]；
   - Linear：[-1,1]；
   - Threshold Linear：[0.1,0.9]；
   - Bipolar Linear：[-0.9, 0.9]；
   - ReLU：[0.1,1.0]；

4) NC=2：NC指“Network Connection”，取值1或2，”1”代表多层向前网络，参照图26.3，”2”代表多层全向前，见图26.4；

5) CT=1：CT即产生的代码类型：1：快捷模式代码（Quick Model），2：Fortran编程模式代码，3：Pascal编程模式代码，4：Basic编程模式代码；

6) Code=1：产生的代码形式：1：精简模式，2：精简（表达式）模式，3：完全模式；

如前图26.15所示“2-1-1”神经网络结构，其对应自动产生的三种代码形式：

精简模式	Function NNFit(NS=[2-1-1], TF=[1,1], DN=[1,1], NC=2, CT=1, Code=1); Data;
精简（表达式）模式	Algorithm = UGO1[30]; Constant Minx1 = MinVariable(x1), Maxx1 = MaxVariable(x1), Minx2 = MinVariable(x2), Maxx2 = MaxVariable(x2), Miny = MinVariable(y), Maxy = MaxVariable(y); Parameter p(7); Variable x1, x2, y; Function y = miny+((1/(1+exp(-(p3*(1/(1+exp(-(p1*((-1)+(1-(-1))*(x1-minx1)/(maxx1-minx1))+p2*((-1)+(1-(-1))*(x2-minx2)/(maxx2-minx2))+p6))))+p7+p4*((-1)+(1-(-1))*(x1-minx1)/(maxx1-minx1))+p5*((-1)+(1-(-1))*(x2-minx2)/(maxx2-minx2))))))-0.1)*(maxy-miny)/(0.9-0.1); Data;
完全模式	Algorithm = UGO1[30]; Constant RMin = -1.0, RMax = 1.0, SMin = 0.1, SMax = 0.9, Minx1 = MinVariable(x1), Maxx1 = MaxVariable(x1), Minx2 = MinVariable(x2), Maxx2 = MaxVariable(x2), Miny = MinVariable(y), Maxy = MaxVariable(y); ConstStr TFH(v) = 1/(1+exp(-v)), TFO(v) = 1/(1+exp(-v)), xx1 = RMin+(RMax-RMin)*(x1-Minx1)/(Maxx1-Minx1), xx2 = RMin+(RMax-RMin)*(x2-Minx2)/(Maxx2-Minx2), s11 = p1*xx1+p2*xx2+p6, h11 = TFH(s11), s21 = p3*h11+p7+p4*xx1+p5*xx2, h21 = TFO(s21); Parameter p(7); Variable x1, x2, y; Function y = Miny+(h21-SMin)*(Maxy-Miny)/(SMax-SMin); Data;

7) DC=[N3L1-N3L2]：DC=DisConnection：不同层节点是否连接；N3L1-N3L2：N表示节点，L表示层，“N3L1”表示第一层（也即输入层）第三个节点，“N3L2”，第二层（第一隐含层）第三各节点；
8) Importance：是否进行输入因子重要性分析，仅对多输入（大于一个自变量）有效

在可视化设计界面，还可以直接复制神经网络拟合公式至三种形式：一般公式表达式形式，MathML形式和Latex形式。

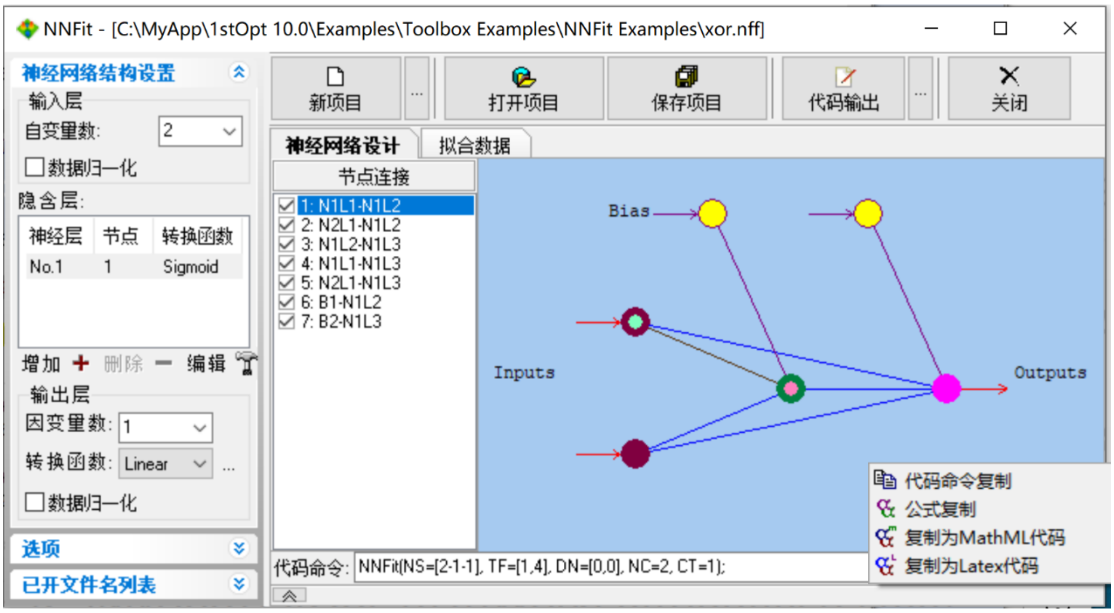


图26.17 XOR问题："2-1-1"神经网络结构

如图26.17，代码命令：NNFit(NS=[2-1-1], TF=[1,4], DN=[0,0], NC=2, CT=1);

✧ 复制为公式表达式：

y = p3*(1/(1+exp(-(p1*x1+p2*x2+p6))))+p7+p4*x1+p5*x2;

✧ 复制为MathML：MathML格式可以被Word软件自动识别，因此可以直接黏贴至Word文档中，成为可编辑的公式形式

$$y = p_3 \cdot \left(\frac{1}{1 + \exp\left(-\left(p_1 \cdot x_1 + p_2 \cdot x_2 + p_6 \right) \right)} \right) + p_7 + p_4 \cdot x_1 + p_5 \cdot x_2$$

✧ 复制为Latex形式：直接生成Latex格式，如想显示为数学公式形式，有很多在线网站可完成此项工作，如：https://quicklatex.com，https://latex.codecogs.com，https://www.latexlive.com，黏贴至这些网站相应位置即可获得精美公式

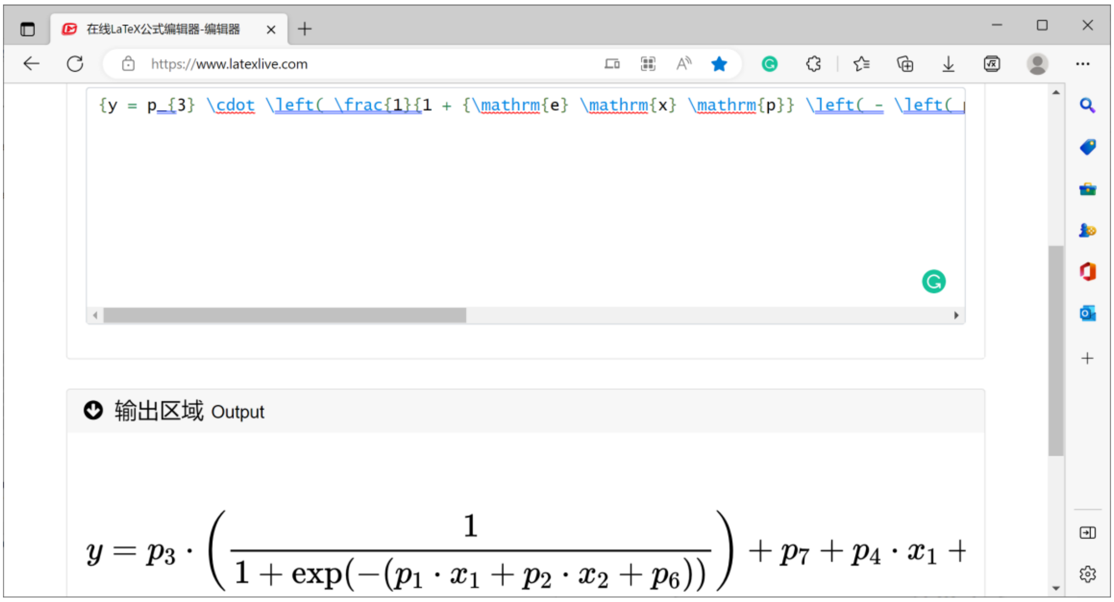


图26.18 Latex公式展示

26.5 案例应用

案例1. 复杂数据拟合

数据如下，一个自变量一个因变量，模型公式未知，通过神经网络进行拟合。

表26.1 案例数据

x	-40,-39,-38,-37,-36,-35,-34,-33,-32,-31,-30,-29,-28,-27,-26,-25,-24,-23,-22,-21,-20,-19,-18,-17,-16,-15,-14,-13,-12,-11,-10,-9,-8,-7,-6,-5,-4,-3,-2,-1,0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39
y	242.1186,242.7174,239.5974,236.1497,241.2914,243.7892,244.7427,237.2906,239.8566,236.1128,233.3459,235.1544,233.2103,235.4884,230.7748,237.7389,237.0666,242.9973,241.4185,243.022,251.0804,255.72,257.3275,255.2987,257.2623,259.7563,260.1721,261.7386,262.4231,269.2953,266.7079,263.9616,263.2913,267.5524,266.5403,272.3949,266.5601,265.9458,269.3813,269.7026,276.3673,277.9156,274.8442,274.4397,274.654,277.0243,277.7825,278.8895,280.7603,281.655,279.3137,278.8639,277.4572,275.9028,274.0923,273.4314,263.0251,255.0052,254.0972,255.0551,243.9512,236.6583,244.1018,240.4926,245.8669,239.2998,233.2845,234.9251,246.9335,231.857,238.8566,234.9202,232.5618,242.4568,237.2969,235.6021,246.2383,240.7228,256.4141,243.881

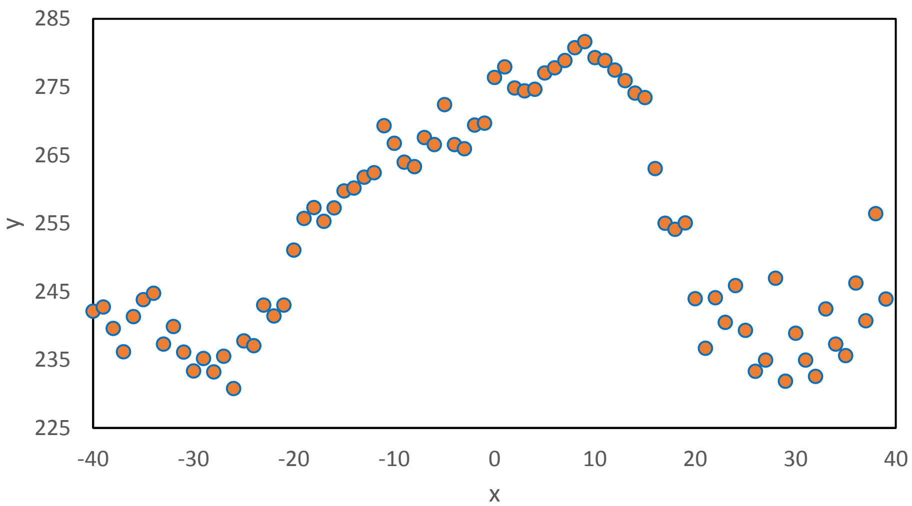


图26.19 神经网络拟合案例数据图

测试两种结构：“1-3-1”及“1-5-1”，均为多层全向前结构，如图26.20和图26.21

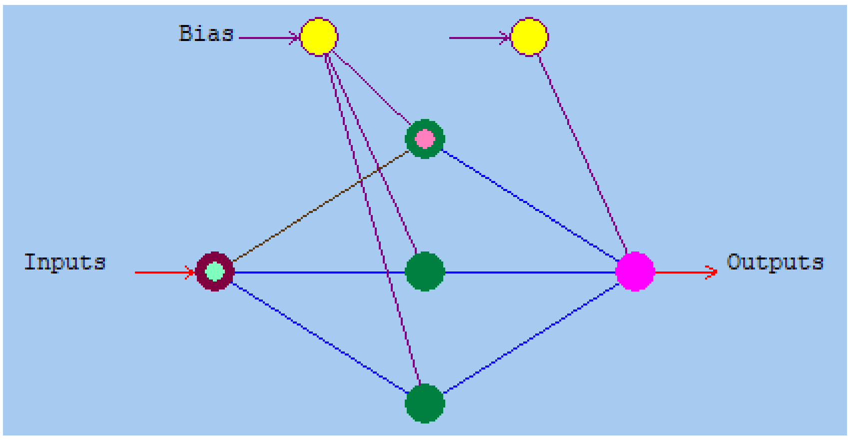


图26.20 案例神经网络拟合：“1-3-1”结构

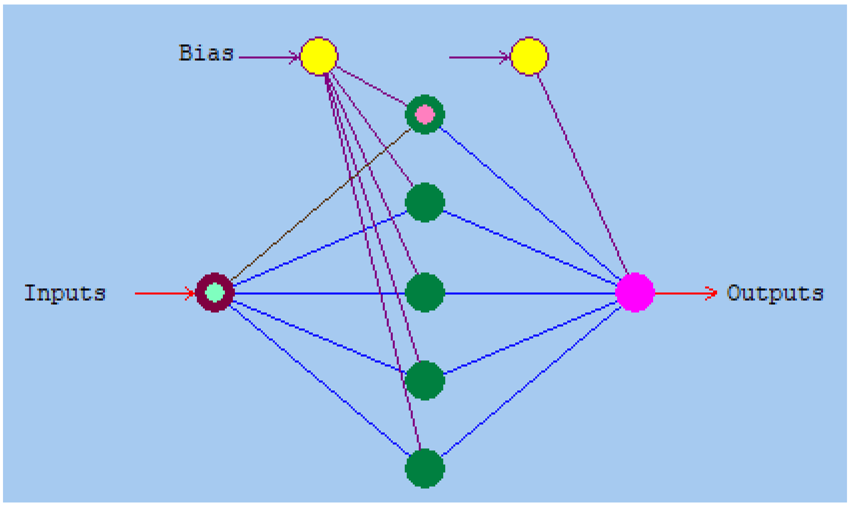


图26.21 案例神经网络拟合："1-5-1"结构

代码：

```
Function NNFit(NS=[1-3-1], TF=[1,4], DN=[1,1], NC=2, CT=2, Code=1);      //1-3-1结构
            //NNFit(NS=[1-5-1], TF=[1,4], DN=[1,1], NC=2, CT=2, Code=1);    //1-5-1结构
Data;
x=-40,-39,-38,-37,-36,-35,-34,-33,-32,-31,-30,-29,-28,-27,-26,-25,-24,-23,-22,-21,-20,-19,-18,-17,-16,-15,-14,-13,-12,-11,-10,-9,-8,-7,-6,-5,-4,-3,-2,-1,0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36,37,38,39;
y=242.1186,242.7174,239.5974,236.1497,241.2914,243.7892,244.7427,237.2906,239.8566,236.1128,233.3459,235.1544,233.2103,235.4884,230.7748,237.7389,237.0666,242.9973,241.4185,243.022,251.0804,255.72,257.3275,255.2987,257.2623,259.7563,260.1721,261.7386,262.4231,269.2953,266.7079,263.9616,263.2913,267.5524,266.5403,272.3949,266.5601,265.9458,269.3813,269.7026,276.3673,277.9156,274.8442,274.4397,274.654,277.0243,277.7825,278.8895,280.7603,281.655,279.3137,278.8639,277.4572,275.9028,274.0923,273.4314,263.0251,255.0052,254.0972,255.0551,243.9512,236.6583,244.1018,240.4926,245.8669,239.2998,233.2845,234.9251,246.9335,231.857,238.8566,234.9202,232.5618,242.4568,237.2969,235.6021,246.2383,240.7228,256.4141,243.881;
```

计算结果：

"1-3-1" 结构	"1-5-1" 结构
残差平方和(SSE): 931.576981042265	残差平方和(SSE): 750.571187411071
均方差(RMSE): 3.41243494634378	均方差(RMSE): 3.06302788799553
相关系数(R): 0.976919416755453	相关系数(R): 0.981446470369486
相关系数之平方(R^2): 0.954371546833814	相关系数之平方(R^2): 0.963237174200722
修正R平方(Adj. R^2): 0.95318639220612	修正R平方(Adj. R^2): 0.962282295608533
确定系数(DC): 0.954371546833813	确定系数(DC): 0.963237174200721
卡方系数(Chi-Square): 1.88285736536113	卡方系数(Chi-Square): 1.51167290951563
F统计(F-Statistic): 144.321432066418	F统计(F-Statistic): 103.167977257229
参数 最佳估算	参数 最佳估算
---- --------	---- --------
p1 -34.2404429558967	p1 -18.3132956755537
p2 -14.102131295434	p2 1.33517503223536
p3 85.7432968746746	p3 38.7011027808537
p4 0.64780810410262	p4 -14.5222877101718
p5 2.55067090259566	p5 -165.49775276136
p6 0.515330123269865	p6 2.09361880302847
p7 1.47347827445446	p7 45.7333860780319

p8	-27.3666481097588	p8	0.849726600471073
p9	6.43642610762824	p9	-1.71120850519916
p10	43.285236259544	p10	-0.513163853132785
p11	-2.39995767090118	p11	-13.6518228062864
		p12	7.88057824168973
		p13	-0.1920121579672 7
		p14	-35.731897219505
		p15	-7.72172896049439
		p16	-149.155741776429
		p17	-22.1484011690135

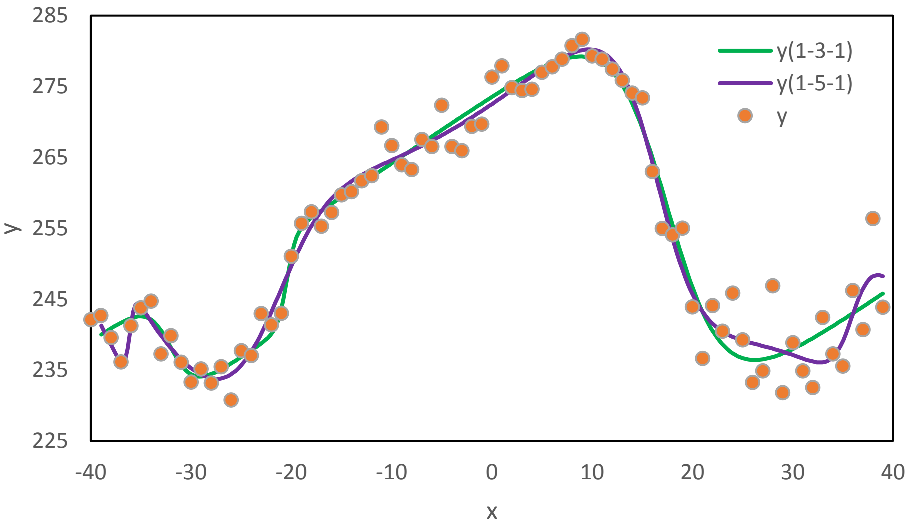


图26.22 案例拟合对比结果

从计算拟合指标看,"1-5-1"与"1-3-1"结构的残差平方和SSE分别为750.571和931.576,前者结果明显好于后者，但从图26.22拟合对比图看，"1-5-1"结构明显存在过拟合，"1-3-1"结构结果更加合理。

案例2：Iris鸢尾花卉分类问题

Iris鸢尾花卉数据集是经典的分类问题，该数据集包含150组数据，分为3类，每类50个样本数据，每个数据包含4个属性，即花萼长度（x1）、花萼宽度（x2）、花瓣长度（x3）和花瓣宽度（x4）共4个属性预测鸢尾花卉属于Setosa、Versicolour和Virginica三个种类中的哪一类。全部150组数据中105组用于训练，其余45组用于验证。

表26.2 Iris训练数据集（105组）

x1	4.7,4.6,5.0,5.4,4.6,4.4,5.4,4.8,4.3,5.8,5.7,5.4,5.1,5.1,5.4,5.1,4.8,5.0,5.2,5.2,4.7,4.8,5.2,5.5,5.1,4.5,4.4,5.0,5.1,4.8,5.1,4.6,5.3,5.0,6.4,6.9,6.5,5.7,6.3,6.6,5.2,5.0,5.9,6.0,6.1,5.6,5.8,6.2,5.9,6.1,6.3,6.1,6.6,6.8,6.7,6.0,5.7,5.5,5.5,5.8,6.0,5.6,5.5,5.5,6.1,5.8,5.6,5.7,5.1,5.7,6.3,5.8,7.1,6.3,7.6,4.9,7.3,6.7,6.5,6.4,6.8,5.8,6.5,7.7,7.7,6.9,5.6,6.3,6.1,7.2,7.4,7.9,6.3,7.7,6.4,6.0,6.9,6.7,5.8,6.8,6.7,6.7,6.3,6.5,6.2
x2	3.2,3.1,3.6,3.9,3.4,2.9,3.7,3.0,3.0,4.0,4.4,3.9,3.5,3.8,3.4,3.7,3.4,3.4,3.5,3.4,3.2,3.1,4.1,3.5,3.4,2.3,3.2,3.5,3.8,3.0,3.8,3.2,3.7,3.3,3.2,3.1,2.8,2.8,3.3,2.9,2.7,2.0,3.0,2.2,2.9,3.0,2.7,2.2,3.2,2.8,2.5,2.8,3.0,2.8,3.0,2.9,2.6,2.4,2.4,2.7,3.4,3.0,2.5,2.6,3.0,2.6,2.7,2.9,2.5,2.8,3.3,2.7,3.0,2.9,3.0,2.5,2.9,2.5,3.2,2.7,3.0,2.8,3.0,3.8,2.6,3.2,2.8,2.7,3.0,3.0,2.8,3.8,2.8,3.0,3.1,3.0,3.1,3.1,2.7,3.2,3.3,3.0,2.5,3.0,3.4
x3	1.3,1.5,1.4,1.7,1.4,1.4,1.5,1.4,1.1,1.2,1.5,1.3,1.4,1.5,1.7,1.5,1.9,1.6,1.5,1.4,1.6,1.6,1.5,1.3,1.5,1.3,1.3,1.6,1.9,1.4,1.6,1.4,1.5,1.4,4.5,4.9,4.6,4.5,4.7,4.6,3.9,3.5,4.2,4.0,4.7,4.5,4.1,4.5,4.8,4.0,4.9,4.7,4.4,4.8,5.0,4.5,3.5,3.8,3.7,3.9,4.5,4.1,4.0,4.4,4.6,4.0,4.2,4.2,3.0,4.1,6.0,5.1,5.9,5.6,6.6,4.5,6.3,5.8,5.1,5.3,5.5,5.1,5.5,6.7,6.9

	,5.7,4.9,4.9,4.9,5.8,6.1,6.4,5.1,6.1,5.5,4.8,5.4,5.6,5.1,5.9,5.7,5.2,5.0,5.2,5.4
x4	0.2,0.2,0.2,0.4,0.3,0.2,0.2,0.1,0.1,0.2,0.4,0.4,0.3,0.3,0.2,0.4,0.2,0.4,0.2,0.2,0.2,0.2,0.1,0.2,0.2,0.3,0.2,0.6,0.4,0.3,0.2,0.2,0.2,0.2,1.5,1.5,1.5,1.3,1.6,1.3,1.4,1.0,1.5,1.0,1.4,1.5,1.0,1.5,1.8,1.3,1.5,1.2,1.4,1.4,1.7,1.5,1.0,1.1,1.0,1.2,1.6,1.3,1.3,1.2,1.4,1.2,1.3,1.3,1.1,1.3,2.5,1.9,2.1,1.8,2.1,1.7,1.8,1.8,2.0,1.9,2.1,2.4,1.8,2.2,2.3,2.3,2.0,1.8,1.8,1.6,1.9,2.0,1.5,2.3,1.8,1.8,2.1,2.4,1.9,2.3,2.5,2.3,1.9,2.0,2.3
y	1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3

表26.3 Iris验证数据集（45组）

x1	5.1,4.9,5.0,4.9,4.8,5.7,4.6,5.1,5.0,5.4,5.5,4.9,5.0,4.9,4.4,5.0,7.0,5.5,4.9,5.6,6.7,5.6,6.4,6.0,5.4,6.7,6.3,5.0,5.7,6.2,6.5,7.2,5.7,6.4,6.0,7.7,6.7,7.2,6.2,6.4,6.4,6.1,6.3,6.9,5.9
x2	3.5,3.0,3.4,3.1,3.4,3.8,3.6,3.3,3.0,3.4,4.2,3.1,3.2,3.1,3.0,3.5,3.2,2.3,2.4,2.9,3.1,2.5,2.9,2.7,3.0,3.1,2.3,2.3,3.0,2.9,3.0,3.6,2.5,3.2,2.2,2.8,3.3,3.2,2.8,2.8,2.8,2.6,3.4,3.1,3.0
x3	1.4,1.4,1.5,1.5,1.6,1.7,1.0,1.7,1.6,1.5,1.4,1.5,1.2,1.5,1.3,1.3,4.7,4.0,3.3,3.6,4.4,3.9,4.3,5.1,4.5,4.7,4.4,3.3,4.2,4.3,5.8,6.1,5.0,5.3,5.0,6.7,5.7,6.0,4.8,5.6,5.6,5.6,5.6,5.1,5.1
x4	0.2,0.2,0.2,0.1,0.2,0.3,0.2,0.5,0.2,0.4,0.2,0.1,0.2,0.1,0.2,0.3,1.4,1.3,1.0,1.3,1.4,1.1,1.3,1.6,1.5,1.5,1.3,1.0,1.2,1.3,2.2,2.5,2.0,2.3,1.5,2.0,2.1,1.8,1.8,2.1,2.2,1.4,2.4,2.3,1.8
y	1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,2,2,2,2,2,2,2,2,2,2,2,2,2,2,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3

测试两种神经网络结构如下

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

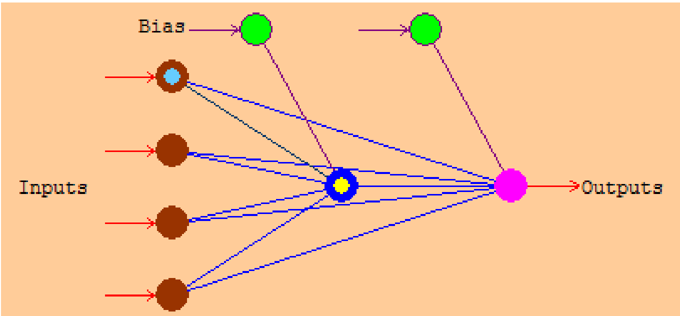


图26.23 “4-1-1”结构

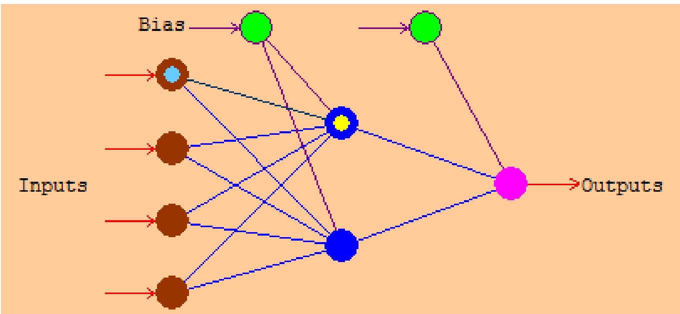


图26.23 “4-2-1”结构

自动产生精简模式求解代码

```
SharedModel;
DataFileWeight = [1,0];
Function NNFit(NS=[4-2-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, Importance);    //"4-2-1"结构
//Function NNFit(NS=[4-1-1], TF=[1,4], DN=[0,0], NC=2, CT=1, Code=1, Importance); //"4-1-1"结构
Data; //Training Data
x1 =[4.7,4.6,5.0,5.4,4.6,4.4,5.4,4.8,4.3,5.8,5.7,5.4,5.1,5.1,5.4,5.1,4.8,5.0,5.2,5.2,4.7,4.8,5.2,5.5,5.1,4.5,4.4,5.0,
```

```
5.1,4.8,5.1,4.6,5.3,5.0,6.4,6.9,6.5,5.7,6.3,6.6,5.2,5.0,5.9,6.0,6.1,5.6,5.8,6.2,5.9,6.1,6.3,6.1,6.6,6.8,6.7,6.0,5.7,5.5
,5.5,5.8,6.0,5.6,5.5,5.5,6.1,5.8,5.6,5.7,5.1,5.7,6.3,5.8,7.1,6.3,7.6,4.9,7.3,6.7,6.5,6.4,6.8,5.8,6.5,7.7,7.7,6.9,5.6,6.
3,6.1,7.2,7.4,7.9,6.3,7.7,6.4,6.0,6.9,6.7,5.8,6.8,6.7,6.7,6.3,6.5,6.2];
x2 =[3.2,3.1,3.6,3.9,3.4,2.9,3.7,3.0,3.0,4.0,4.4,3.9,3.5,3.8,3.4,3.7,3.4,3.4,3.5,3.4,3.2,3.1,4.1,3.5,3.4,2.3,3.2,3.5,
3.8,3.0,3.8,3.2,3.7,3.3,3.2,3.1,2.8,2.8,3.3,2.9,2.7,2.0,3.0,2.2,2.9,3.0,2.7,2.2,3.2,2.8,2.5,2.8,3.0,2.8,3.0,2.9,2.6,2.4
,2.4,2.7,3.4,3.0,2.5,2.6,3.0,2.6,2.7,2.9,2.5,2.8,3.3,2.7,3.0,2.9,3.0,2.5,2.9,2.5,3.2,2.7,3.0,2.8,3.0,3.8,2.6,3.2,2.8,2.
7,3.0,3.0,2.8,3.8,2.8,3.0,3.1,3.0,3.1,3.1,2.7,3.2,3.3,3.0,2.5,3.0,3.4];
x3 =[1.3,1.5,1.4,1.7,1.4,1.4,1.5,1.4,1.1,1.2,1.5,1.3,1.4,1.5,1.7,1.5,1.9,1.6,1.5,1.4,1.6,1.6,1.5,1.3,1.5,1.3,1.3,1.6,
1.9,1.4,1.6,1.4,1.5,1.4,4.5,4.9,4.6,4.5,4.7,4.6,3.9,3.5,4.2,4.0,4.7,4.5,4.1,4.5,4.8,4.0,4.9,4.7,4.4,4.8,5.0,4.5,3.5,3.8
,3.7,3.9,4.5,4.1,4.0,4.4,4.6,4.0,4.2,4.2,3.0,4.1,6.0,5.1,5.9,5.6,6.6,4.5,6.3,5.8,5.1,5.3,5.5,5.1,5.5,6.7,6.9,5.7,4.9,4.
9,4.9,5.8,6.1,6.4,5.1,6.1,5.5,4.8,5.4,5.6,5.1,5.9,5.7,5.2,5.0,5.2,5.4];
x4 =[0.2,0.2,0.2,0.4,0.3,0.2,0.2,0.1,0.1,0.2,0.4,0.4,0.3,0.3,0.2,0.4,0.2,0.4,0.2,0.2,0.2,0.2,0.1,0.2,0.2,0.3,0.2,0.6,
0.4,0.3,0.2,0.2,0.2,0.2,1.5,1.5,1.5,1.3,1.6,1.3,1.4,1.0,1.5,1.0,1.4,1.5,1.0,1.5,1.8,1.3,1.5,1.2,1.4,1.4,1.7,1.5,1.0,1.1
,1.0,1.2,1.6,1.3,1.3,1.2,1.4,1.2,1.3,1.3,1.1,1.3,2.5,1.9,2.1,1.8,2.1,1.7,1.8,1.8,2.0,1.9,2.1,2.4,1.8,2.2,2.3,2.3,2.0,1.
8,1.8,1.6,1.9,2.0,1.5,2.3,1.8,1.8,2.1,2.4,1.9,2.3,2.5,2.3,1.9,2.0,2.3];
y =[1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,
2,2,2,2,2,2,2,2,2,2,2,2,2,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3];
Data; //Verification Data
x1 =[5.1,4.9,5.0,4.9,4.8,5.7,4.6,5.1,5.0,5.4,5.5,4.9,5.0,4.9,4.4,5.0,7.0,5.5,4.9,5.6,6.7,5.6,6.4,6.0,5.4,6.7,6.3,5.0,
5.7,6.2,6.5,7.2,5.7,6.4,6.0,7.7,6.7,7.2,6.2,6.4,6.4,6.1,6.3,6.9,5.9];
x2 = [3.5,3.0,3.4,3.1,3.4,3.8,3.6,3.3,3.0,3.4,4.2,3.1,3.2,3.1,3.0,3.5,3.2,2.3,2.4,2.9,3.1,2.5,2.9,2.7,3.0,3.1,2.3,2.3,
3.0,2.9,3.0,3.6,2.5,3.2,2.2,2.8,3.3,3.2,2.8,2.8,2.8,2.6,3.4,3.1,3.0];
x3 = [1.4,1.4,1.5,1.5,1.6,1.7,1.0,1.7,1.6,1.5,1.4,1.5,1.2,1.5,1.3,1.3,4.7,4.0,3.3,3.6,4.4,3.9,4.3,5.1,4.5,4.7,4.4,3.3,
4.2,4.3,5.8,6.1,5.0,5.3,5.0,6.7,5.7,6.0,4.8,5.6,5.6,5.6,5.6,5.1,5.1];
x4 = [0.2,0.2,0.2,0.1,0.2,0.3,0.2,0.5,0.2,0.4,0.2,0.1,0.2,0.1,0.2,0.3,1.4,1.3,1.0,1.3,1.4,1.1,1.3,1.6,1.5,1.5,1.3,1.0,
1.2,1.3,2.2,2.5,2.0,2.3,1.5,2.0,2.1,1.8,1.8,2.1,2.2,1.4,2.4,2.3,1.8];
y = [1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,2,2,2,2,2,2,2,2,2,2,2,2,2,2,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3];
```

结果：

“4-2-1”结构	“4-1-1”结构
Sum Squared Error (SSE): 2.01209908589975E-8	Sum Squared Error (SSE): 1.0812715929826
Root of Mean Square Error (RMSE): 1.38429940537228E-5	Root of Mean Square Error (RMSE): 0.101478198126851
Correlation Coef. (R): 0.999999999854177	Correlation Coef. (R): 0.992132669530855
R-Square: 0.999999999708354	R-Square: 0.984327233950422
Adjusted R-Square: 0.999999999693624	Adjusted R-Square: 0.983535680109534
Determination Coef. (DC): 0.999999999708351	Determination Coef. (DC): 0.984327233950418
Chi-Square: 4.18142237932451E-9	Chi-Square: 0.313610610190872
F-Statistic: 26287322978.712	F-Statistic: 590.366539766407
Parameter Best Estimate	Parameter Best Estimate
--------- -------------	--------- -------------
p1 114.207580409608	p1 207.825569158689
p2 -122.523901702517	p2 194.766315283213
p3 151.179491798249	p3 -390.856116512175
p4 -84.9193198805805	p4 -310.370179844676
p5 -323.575020620672	p5 -0.667021684228522
p6 137.954212993959	p6 -0.0842916315484619
p7 -309.134449824631	p7 -0.168819709945963
p8 488.929100087276	p8 0.230681604748573
p9 -1.00000814053885	p9 0.234766655439116
p10 0.999996010956135	p10 594.326602425148
p11 961.429116156488	p11 2.30365798044574
p12 132.3849479961	
p13 2.00000813617098	PassParameter:
	important_x1: 0.176941419949143

PassParameter: important_x1: 0.141776778069183 important_x2: 0.0942652508716834 important_x3: 0.445321633124792 important_x4: 0.318636337934342	important_x2: 0.110599530817723 important_x3: 0.536232422084661 important_x4: 0.176226627148473

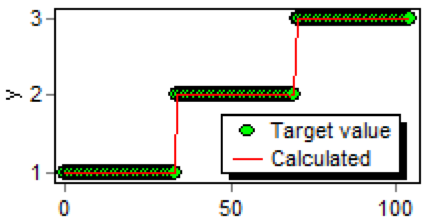
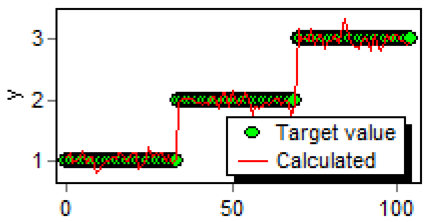
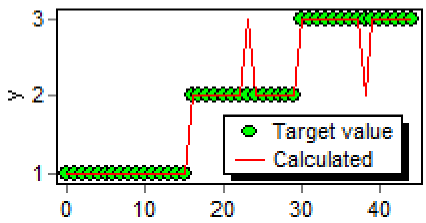
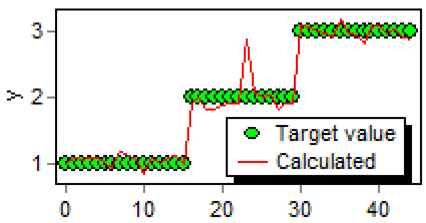
	“4-2-1”结构	“4-1-1”结构
训练		
验证		

图26.24不同结构训练与验证结果对比图

两种结构的训练结果精度都可达100%，验证结果也均高于90%。

案例3. 复杂峰数据拟合

数据如下，一个自变量一个因变量，模型公式未知，通过神经网络进行拟合。

表26.4 案例数据

x	0,0.01,0.02,0.03,0.04,0.05,0.06,0.07,0.08,0.09,0.1,0.11,0.12,0.13,0.14,0.15,0.16,0.17,0.18,0.19,0.2,0.21,0.22,0.23,0.24,0.25,0.26,0.27,0.28,0.29,0.3,0.31,0.32,0.33,0.34,0.35,0.36,0.37,0.38,0.39,0.4,0.41,0.42,0.43,0.44,0.45,0.46,0.47,0.48,0.49,0.5,0.51,0.52,0.53,0.54,0.55,0.56,0.57,0.58,0.59,0.6,0.61,0.62,0.63,0.64,0.65,0.66,0.67,0.68,0.69,0.7,0.71,0.72,0.73,0.74,0.75,0.76,0.77,0.78,0.79,0.8,0.81,0.82,0.83,0.84,0.85,0.86,0.87,0.88,0.89,0.9,0.91,0.92,0.93,0.94,0.95,0.96,0.97,0.98,0.99,1
y	0.726,0.801,0.861,0.879,0.947,0.945,1.035,1.022,1.017,0.944,0.945,0.914,0.935,0.843,0.799,0.712,0.656,0.614,0.532,0.424,0.348,0.275,0.176,0.077,-0.016,-0.062,0.106,0.695,1.388,1.351,0.547,-0.264,-0.611,-0.801,-0.852,-0.844,-0.958,-1.000,-0.946,-0.989,-0.963,-0.993,-1.012,-0.953,-0.897,-0.936,-0.862,-0.800,-0.732,-0.668,-0.574,-0.528,-0.405,-0.324,-0.242,-0.150,-0.049,0.049,0.141,0.246,0.326,0.411,0.490,0.583,0.630,0.761,0.815,0.854,0.891,0.916,0.942,0.972,1.041,1.008,1.037,0.949,0.913,0.899,0.871,0.865,0.792,0.715,0.672,0.573,0.463,0.378,0.303,0.215,0.117,0.022,-0.071,-0.174,-0.269,-0.343,-0.459,-0.525,-0.601,-0.675,-0.761,-0.791,-0.878

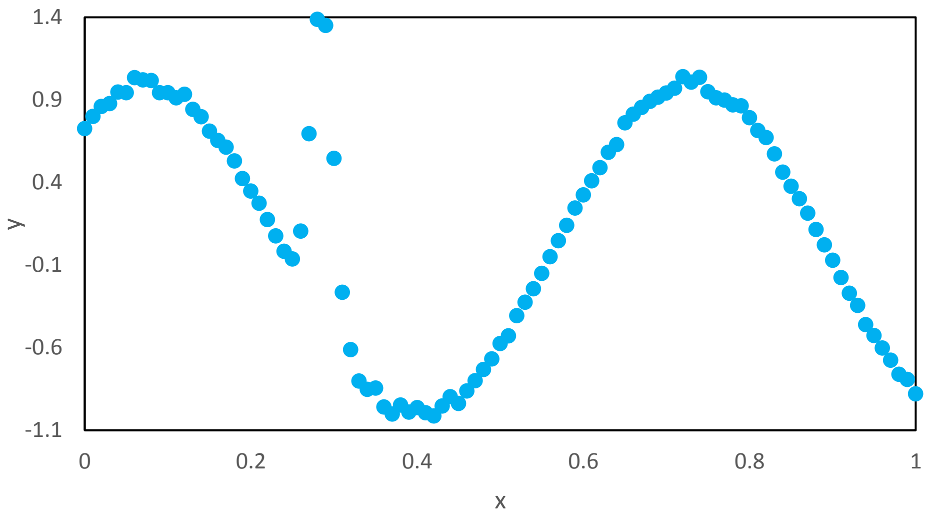


图26.25 神经网络拟合案例数据图

由图6.25中间的峰点数少，拟合难度较大，在此直接采用“1-5-1”结构，隐含层及输出层分别采用Sigmoid和Linear函数，其对应的具体拟合公式和代码如下。

$$
\begin{aligned}
y = p_6 \cdot \left(\frac{1}{1+\exp\big(-(p_1\cdot(-1+2\cdot x)+p_{11})\big)}\right) + \\
p_7 \cdot \left(\frac{1}{1+\exp\big(-(p_2\cdot(-1+2\cdot x)+p_{12})\big)}\right) + \\
p_8 \cdot \left(\frac{1}{1+\exp\big(-(p_3\cdot(-1+2\cdot x)+p_{13})\big)}\right) + \\
p_9 \cdot \left(\frac{1}{1+\exp\big(-(p_4\cdot(-1+2\cdot x)+p_{14})\big)}\right) + \\
p_{10} \cdot \left(\frac{1}{1+\exp\big(-(p_5\cdot(-1+2\cdot x)+p_{15})\big)}\right) + p_{16}
\end{aligned}
$$

多峰函数神经网络拟合求解代码

```
Function NNFit(NS=[1-5-1], TF=[1,4], DN=[1,0], NC=1, CT=1, Code=1);
Data;
x=0,0.01,0.02,0.03,0.04,0.05,0.06,0.07,0.08,0.09,0.1,0.11,0.12,0.13,0.14,0.15,0.16,0.17,0.18,0.19,0.2,0.21,0.22,
0.23,0.24,0.25,0.26,0.27,0.28,0.29,0.3,0.31,0.32,0.33,0.34,0.35,0.36,0.37,0.38,0.39,0.4,0.41,0.42,0.43,0.44,0.45
,0.46,0.47,0.48,0.49,0.5,0.51,0.52,0.53,0.54,0.55,0.56,0.57,0.58,0.59,0.6,0.61,0.62,0.63,0.64,0.65,0.66,0.67,0.6
8,0.69,0.7,0.71,0.72,0.73,0.74,0.75,0.76,0.77,0.78,0.79,0.8,0.81,0.82,0.83,0.84,0.85,0.86,0.87,0.88,0.89,0.9,0.9
1,0.92,0.93,0.94,0.95,0.96,0.97,0.98,0.99,1;
y=0.726,0.801,0.861,0.879,0.947,0.945,1.035,1.022,1.017,0.944,0.945,0.914,0.935,0.843,0.799,0.712,0.656,0.6
14,0.532,0.424,0.348,0.275,0.176,0.077,-0.016,-0.062,0.106,0.695,1.388,1.351,0.547,-0.264,-0.611,-0.801,-
0.852,-0.844,-0.958,-1.000,-0.946,-0.989,-0.963,-0.993,-1.012,-0.953,-0.897,-0.936,-0.862,-0.800,-0.732,-
0.668,-0.574,-0.528,-0.405,-0.324,-0.242,-0.150,-
0.049,0.049,0.141,0.246,0.326,0.411,0.490,0.583,0.630,0.761,0.815,0.854,0.891,0.916,0.942,0.972,1.041,1.008
,1.037,0.949,0.913,0.899,0.871,0.865,0.792,0.715,0.672,0.573,0.463,0.378,0.303,0.215,0.117,0.022,-0.071,-
0.174,-0.269,-0.343,-0.459,-0.525,-0.601,-0.675,-0.761,-0.791,-0.878;
```

结果

```
Sum Squared Error (SSE): 0.0407072822486642
Root of Mean Square Error (RMSE): 0.0200759158820121
Correlation Coef. (R): 0.999599017851086
R-Square: 0.999198196488855
```

Adjusted R-Square: 0.991818833151893
Determination Coef. (DC): 0.999198196485407
Chi-Square: -0.0114919532739429
F-Statistic: 7061.70804866807

Parameter	Best Estimate
---------	-------------
p1	81.5394604160107
p2	0.942311645028003
p3	76.3823482929839
p4	-2.38231303180257
p5	-1.69183932579666
p6	2.38826618297683
p7	469.566951648608
p8	-2.45223255233963
p9	-256.840131958998
p10	611.49700128708
p11	37.1863263888478
p12	-0.218408860942527
p13	30.6529421753032
p14	0.346813384997559
p15	0.272725697130809
p16	-406.485976579266

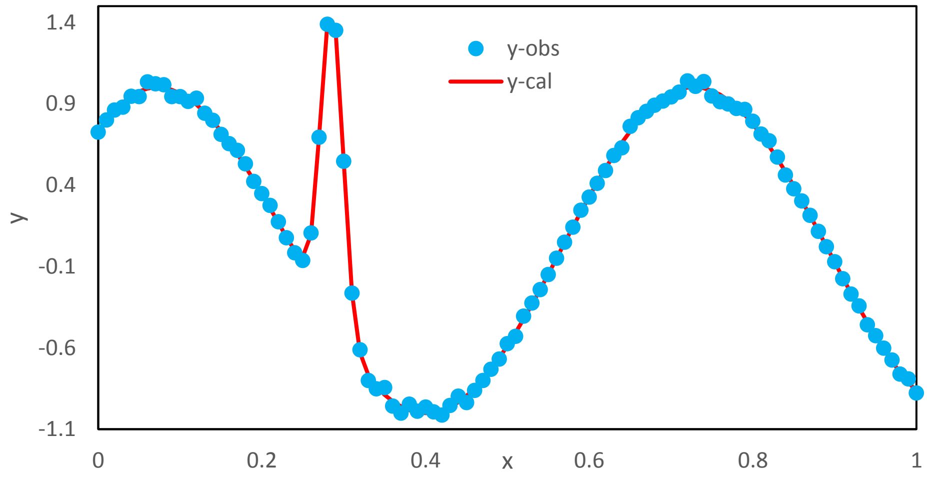


图26.26 神经网络拟合结果对比图

拟合结果非常完美。

26.6 小结

神经网络拟合工具箱NNFit具有极其强大的拟合计算功能，同时还能给出具体单一的神经网络拟合公式，如果需要，也能得到详细的中间计算过程，极大满足用户迁移扩展模型的特殊需求。