# 30. 神经网络是通用万能拟合器吗？-1stOpt 神经网络拟合工具箱实战测试

## 30.1 引言

神经网络是现代深度学习和人工智能的基础，应用极其广泛，目前火爆的ChatGPT背后，其技术支撑也有神经网络。具体到非线性曲线拟合领域，对神经网络则存在两种观点相左的流派，乐观积极派认为神经网络可以拟合任意类型的数据关系，是通用万能的拟合工具，大有神经网络一统天下，舍“神经网络”其谁的感觉；悲观消极派则视神经网络是个“黑箱”工具，无法知道也无法掌控详细计算过程，具体的拟合模型公式也无法获取，泛化外延能力弱，不到万不得已不推荐使用。两种观点孰是孰非？神经网络是否可作为通用万能拟合器？通过下面五个实际案例进行测试验证。所有案例都是已知自变量（输入）和因变量（输出）数据而不知或没有指定拟合的具体模型公式，如果拟合模型公式已确定，则就和神经网络拟合无关了。

## 30.2 案例

案例数据见表30.1至表30.5，对应散点图形见图30-1至图30-6。

表 30.1 案例.1 数据

| | |
|---|---|
| x | 1,2,3,4,5,5.85,5.93,6,6.06,6.2,7,8,9,10 |
| y | 9,7,6,3,-1,-3.8,-1.5,2,4.5,7.8,5,7,20,50 |

表 30.2 案例.2 数据

| | |
|---|---|
| x | 9.97E+03,1.37E+04,1.76E+04,2.16E+04,2.56E+04,2.96E+04,3.36E+04,3.76E+04,4.15E+04,4.55E+04,4.95E+04,5.35E+04,5.75E+04,6.15E+04,6.54E+04,6.94E+04,7.34E+04,7.74E+04,8.14E+04,8.54E+04,8.67E+04,8.68E+04,8.68E+04,8.69E+04,8.69E+04,8.69E+04,8.69E+04,8.70E+04,8.70E+04,8.70E+04,8.70E+04,8.70E+04,8.71E+04,8.71E+04,8.71E+04,8.71E+04,8.72E+04,8.72E+04,8.72E+04,8.72E+04,8.77E+04,8.90E+04,9.30E+04,9.70E+04,1.01E+05,1.05E+05,1.09E+05,1.13E+05,1.17E+05,1.21E+05,1.25E+05,1.29E+05,1.33E+05,1.37E+05,1.41E+05,1.45E+05,1.49E+05,1.53E+05,1.57E+05,1.61E+05,1.65E+05,1.69E+05,1.73E+05,1.77E+05,1.81E+05 |
| y | 20.9,11.4,9.07,7.42,6.14,5.46,4.66,4.07,3.55,3.22,2.87,2.64,2.43,2.23,2.05,1.94,1.82,1.71,1.59,1.52,1.52,1.2,1.12,1.08,1.06,1.03,1.01,0.979,0.958,0.958,0.928,0.928,0.909,0.899,0.871,0.881,0.862,0.871,0.862,0.844,0.784,0.713,0.635,0.615,0.596,0.571,0.542,0.525,0.509,0.503,0.488,0.468,0.473,0.463,0.444,0.434,0.425,0.416,0.403,0.395,0.395,0.387,0.375,0.371,0.359 |

表 30-3 案例.3 数据

| | |
|---|---|
| x | 0,5,10,15,20,25,30,35,40,45,50,55,60,65,70,75,80,85,90,95,100,105,110,115,120,125,130,135,140,145,150,155,160,165,170,175,180,185,190,195,200,205,210,215,220,225,230,235,240,245,250,255,260,265,270,275,280,285,290,295,300 |
| y | 0.2,1.049,1.142,1.201,1.245,1.28,1.31,1.336,1.359,1.38,1.399,1.416,1.432,1.447,1.461,1.474,1.486,1.498, |

| | |
|---|---|
| | 1.509,1.52,1.53,2.189,2.291,2.359,2.412,2.456,2.494,2.528,2.558,2.586,2.612,2.637,2.659,2.681,2.701,2.721,2.739,2.757,2.774,2.79,2.806,2.13,2.022,1.949,1.891,1.842,1.799,1.76,1.725,1.692,1.661,1.633,1.605,1.58,1.555,1.531,1.509,1.487,1.466,1.445,1.425 |

表 30-4 案例.4 数据

| | |
|---|---|
| x | 0,0.05,0.1,0.15,0.2,0.25,0.3,0.35,0.4,0.45,0.5,0.55,0.6,0.65,0.7,0.75,0.8,0.85,0.9,0.95,1 |
| $y_1$ | 0.1,0.09363,0.08765,0.08206,0.07682,0.07191,0.06733,0.06305,0.0592,0.05654,0.06111,0.12197,0.57603,2.31729,4.59434,5.90324,6.28589,6.08804,5.54222,4.78943,3.91983 |
| $y_2$ | 0.001845,0.001732,0.001625,0.001524,0.001429,0.001337,0.001242,0.001102,0.000652,-0.001978,-0.021728,-0.181354,-1.205571,-3.756468,-4.89856,-4.683934,-4.279801,-3.935516,-3.658357,-3.424578,-3.212917 |
| $y_3$ | -0.013171,-0.012338,-0.011557,-0.010825,-0.010138,-0.009491,-0.008869,-0.0082,-0.007042,-0.002252,0.03123,0.297614,1.911671,4.766427,3.751245,1.565312,0.086857,-0.802556,-1.3351,-1.646745,-1.811243 |
| $y_4$ | -0.000292875,-0.00027575,-0.0002595,-0.0002445,-0.000231875,-0.000227125,-0.000261,-0.000519,-0.002252875,-0.014937875,-0.1176755,-0.936735125,-4.887517,-5.808778,-0.399008375,0.99239425,0.956371375,0.7678885,0.62863025,0.549160375,0.515598875 |
| $y_5$ | -0.005016,-0.004707,-0.004417,-0.004143,-0.003885,-0.003637,-0.003378,-0.002996,-0.001775,0.005381,0.059069,0.491166,3.174846,8.754624,9.109239,6.83957,4.995247,3.741764,2.877479,2.256777,1.793657 |

表 30-5 案例.5 数据

| | |
|---|---|
| $x_1$ | 200,200,200,200,200,200,200,200,300,300,300,300,300,300,300,300,300,300,300,300,300,400,400,400,400,400,400,400,400,400,400,400,400,500,500,500,500,500,500,500,500,500,500,500,600,600,600,600,600,600,600,600,600,600,600,600,700,700,700,700,700,700,700,700,700,700,700,800,800,800,800,800,800,800,800,800,800,800,800,900,900,900,900,900,900,900,900,900,900,900,900,1000,1000,1000,1000,1000,1000,1000,1000,1000,1000,1000,1000; |
| $x_2$ | 0.28,0.4,0.52,0.64,0.76,0.79,0.82,0.85,0.1,0.34,0.46,0.55,0.58,0.61,0.64,0.67,0.7,0.73,0.76,0.79,0.82,0.2,0.32,0.44,0.5,0.53,0.56,0.59,0.62,0.65,0.68,0.71,0.74,0.13,0.19,0.31,0.43,0.49,0.52,0.55,0.58,0.61,0.64,0.67,0.7,0.15,0.27,0.39,0.42,0.45,0.48,0.51,0.54,0.57,0.6,0.63,0.66,0.13,0.19,0.25,0.31,0.37,0.4,0.43,0.46,0.49,0.52,0.55,0.58,0.13,0.19,0.25,0.31,0.37,0.4,0.43,0.46,0.49,0.52,0.55,0.58,0.13,0.19,0.25,0.31,0.34,0.37,0.4,0.43,0.46,0.49,0.52,0.55,0.13,0.19,0.25,0.31,0.34,0.37,0.4,0.43,0.46,0.49,0.52,0.55; |
| y | 0.03,0.04,0.124,0.508,3.411,8.712,19.975,260.5,0.024,0.094,0.287,1,2.058,3.443,5.9,15.237,29.012,77.895,268.266,926.133,3226.499,0.069,0.19,0.886,1.861,2.966,5.848,12.202,32.432,91.408,161.481,705.156,2118.492,0.065,0.104,0.315,1.929,5.122,10.026,22.473,70.457,150.428,330.854,1287.065,4971.452,0.07,0.339,1.817,3.477,5.458,11.003,26.776,50.797,173.851,515.246,1205.304,5192.83,0.111,0.163,0.486,1.019,2.607,4.663,8.554,17.711,37.202,109.288,266.517,801.336,0.125,0.304,0.517,1.146,4.362,8.469,19.19,42.242,100.535,269.473,797.309,1782.525,0.153,0.393,0.933,2.447,3.752,7.959,15.92,33.265,101.495,185.408,733.459,2062.239,0.192,0.535,1.208,3.55,7.758,13.881,27.788,68.756,186.803,394.723,1358.639,3983.95; |

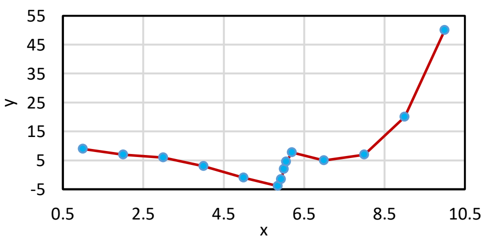


图 30-1 案例 1 图

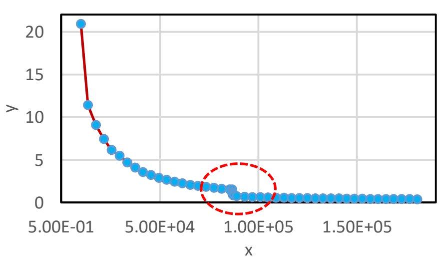


图 30-2 案例 2 图

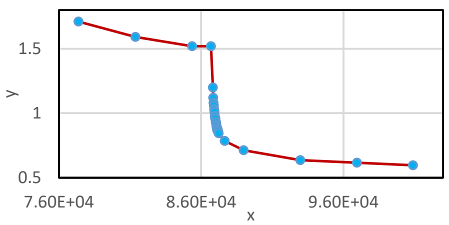


图 30-3 案例 2 局部放大图

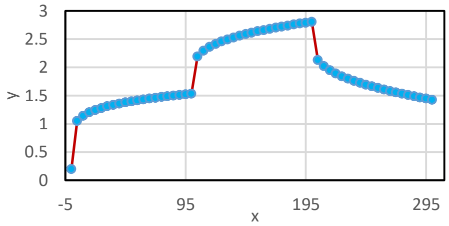


图 30-4 案例 3 图

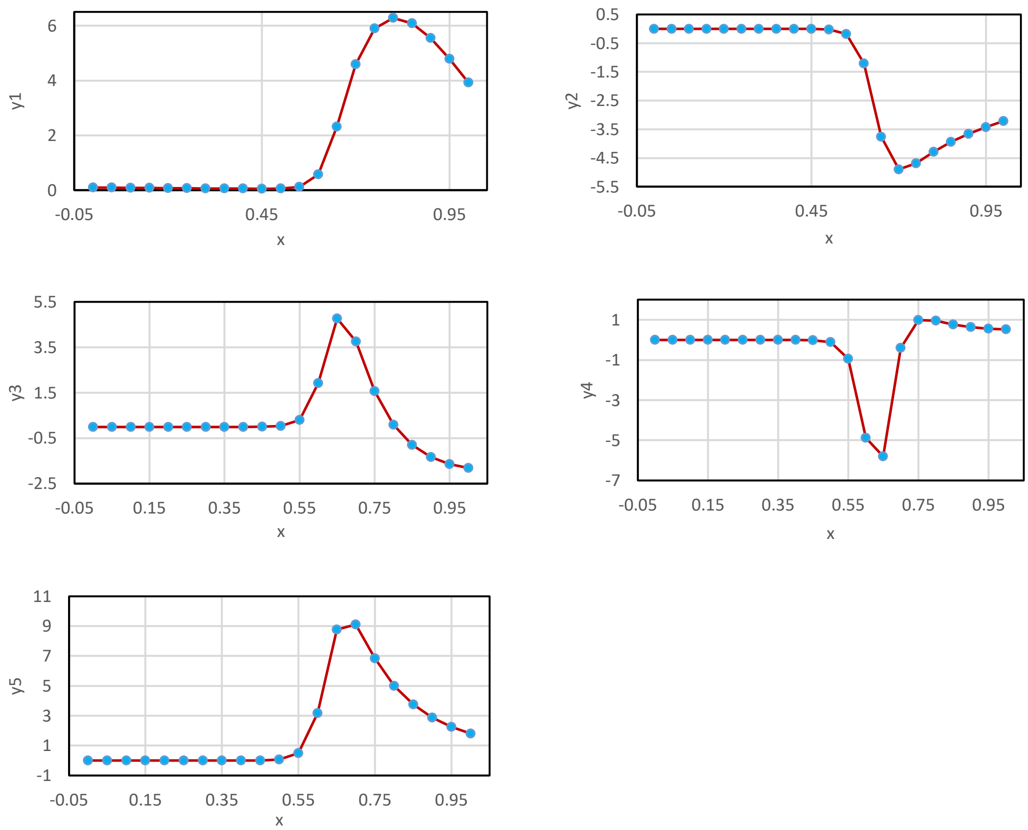


图 30-5 案例 4 多因变量系列图

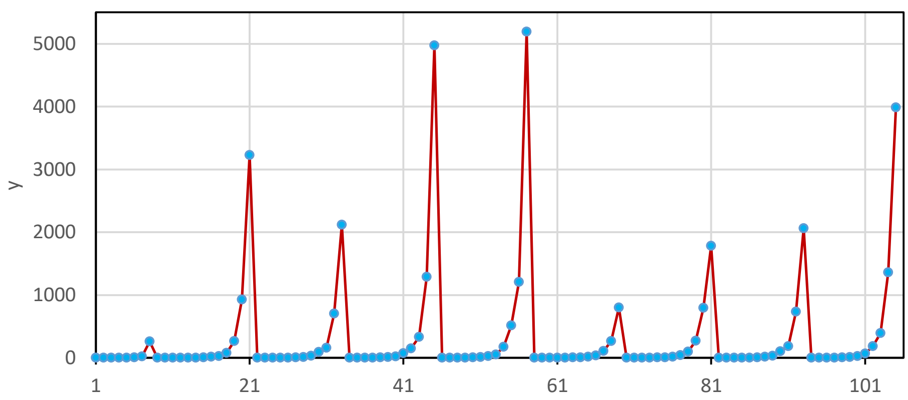


图30-6 案例5因变量散点图

案例1至案例3，均只有一个自变量（输入）和一个因变量（输出），从其数据散点图上可以看出，都有一个或两个突变点，要求用一个不含分段函数的拟合公式进行拟合计算，该如何确定相应的模型公式会成为一个较难的问题。虽然1stOpt有一个快速公式搜索工具，可以根据数据自动搜索最佳匹配公式，但对于这些有突变点的数据也是很难找到吻合较好的模型公式，比如对案例.1数据通过“快速公式拟合搜索”工具箱进行数据公式自动匹配计算，得到如下公式及计算结果如图30-7，虽然从总体上看拟合效果也不错，但突变点完全没有得到体现，无法视为成功的拟合。案例2和案例3数据图形显得更为复杂，想快速找到匹配良好的模型公式无疑难度更高。

$$y = \frac{p_1}{x} + p_2 \cdot x^{p_3}$$

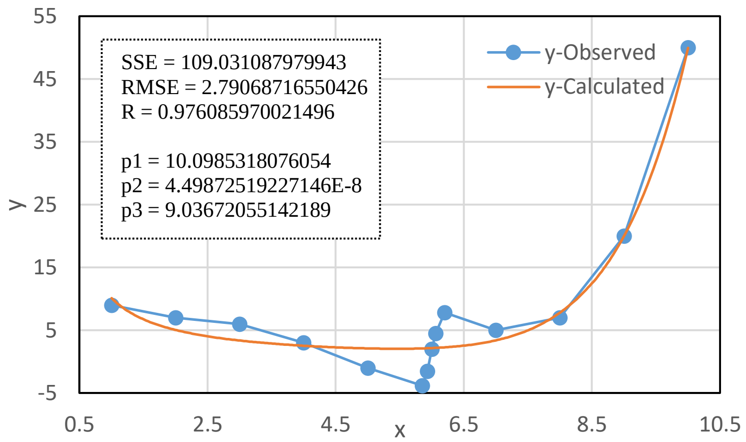


图30-7 快速拟合自动搜索匹配公式对比

案例4有一个自变量（输入）和五个因变量（输出），相应的需要确定五个模型公式，要求公式形式一样且有参数共享。如果说案例1至案例3还有其它方式可以解决的话，案例4这种情况应该说是非神经网络莫属了，主要因为神经网络对多输入（自变量）多输出（因变量）、单输入（自变量）多输出（因变量）和多输入（自变量）单输出（因变量）都可以非常容易处理，因此目前为止，神经网络是该问题的最佳选择。

案例5有两个自变量（输入）和一个因变量（输出），从图30-6因变量数据图形可看出，其由九段单调上升的曲线组合而成，在缺乏数据物理背景的前提下，想确定一个单一的模型公式去描述该三维曲线无疑难度极高，神经网络值得一试。

## 30.3 神经网络解决方案

1stOpt的神经网络拟合工具箱是一个可视化设计界面，对神经网络的初学者有很好的指导和帮助作用，其最终输出也是帮助用户产生1stOpt可运行的代码，当对神经网络拟合命令代码熟悉后也可以直接通过快捷键“Ctrl+k”直接输入相关命令，并根据拟合数据实际情况对代码进行相应修改，更为方便快捷。

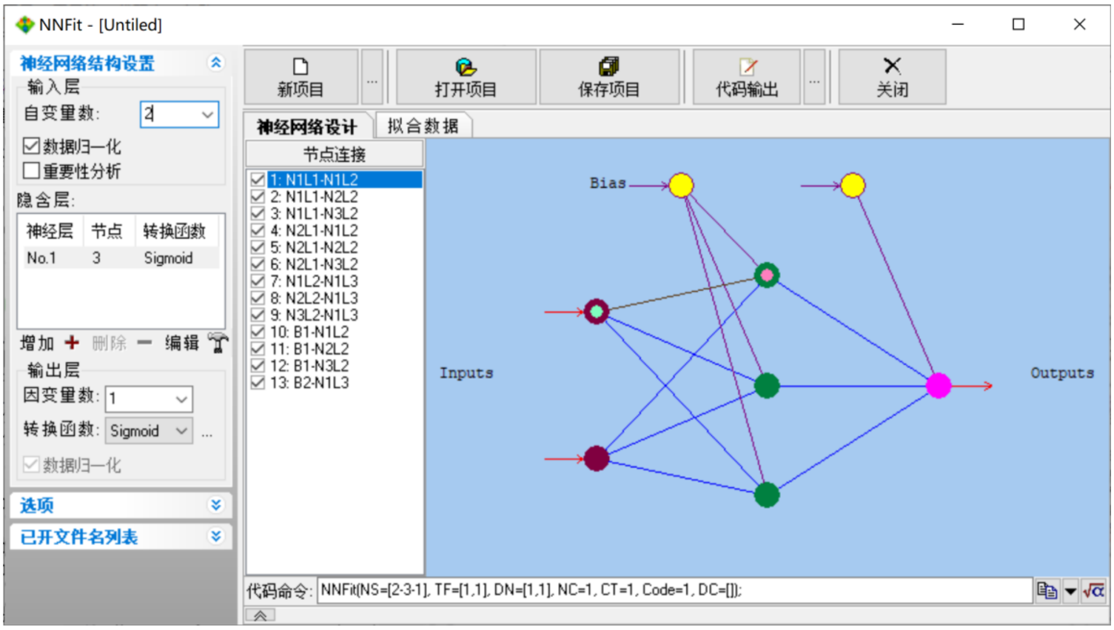

图30-8 神经网络拟合工具箱设计界面之一

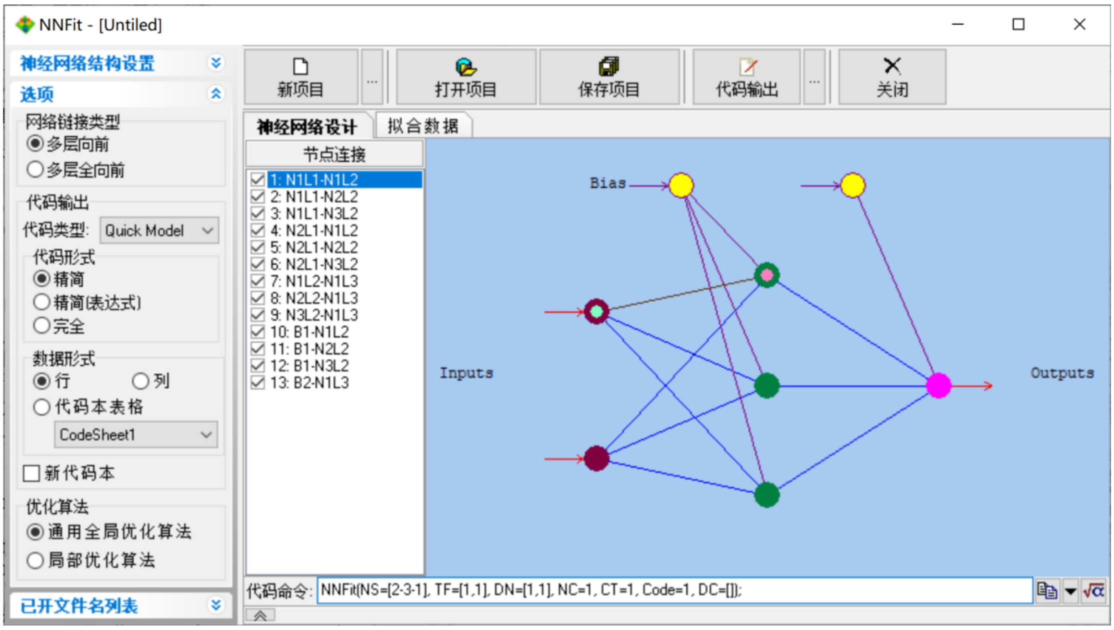

图30-9 神经网络拟合工具箱设计界面之二

图30-8和图30-9是神经网络拟合工具箱的主要设计界面，非常方便可视化设计神经网络的所有要素如隐含层数、各隐含层神经元节点数、隐含层及输出层激活转换函数、输入输出数据是否归一化处理、代码输出形式等等，而所有这些设计或设定除了都包含在输出代码里之外，也可以在“代码命令”栏里得到具体体现，也即可以用“代码命令”栏里的一句命令代码去描述整个神经网络拟合问题。通用的神经网络拟合代码命令“NNFit”已经集成在关键字集合中，在代码本中通过快捷键 “Ctrl+k” 激活选择，或通过关键字导航栏选择，如图30-10所示：

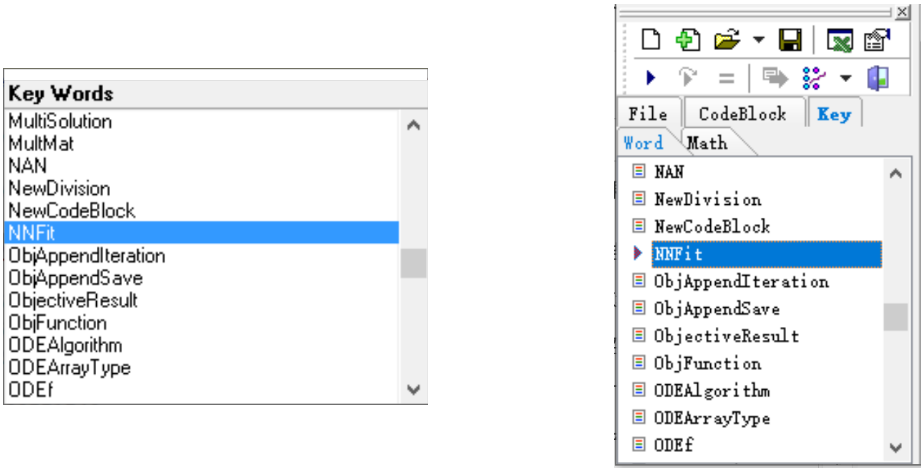


图30-10 神经网络拟合快捷命令

选择该关键字输入的缺省格式为：

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

其中：

1) NS=[1-3-1]：神经网络结构，一个输入层（含一个神经元节点）、一个隐含层（含三个神经元节点）和一个输出层（含一个神经元节点），可以自行修改，如“NS=[3-5-3-2]”则表示有一个3节点输入层、一个2节点输出层及两个隐含层，分别有5和3个神经元节点；
2) TF=[1,1]：隐含层及输出层激活或转换函数，对应1）设定的神经网络结构，共有7种类型的激活函数：1：Sigmoid，2：Tanh，3：Gaussian，4：Linear，5：Threshold Linear，6：Bipolar Linear，7：ReLU，注意只有隐含层和输出层才有激活函数，输入层是不需要的，比如有两个隐含层（对应NS=[3-5-3-2]），则有“TF=[1,1,1]”；
3) DN=[1,1]：对应输入及输出层数据是否要归一化处理，“1”表示要归一化处理，“0”表示不处理；注意对输入层数据的归一化处理，任何时候都是可选项，但对输出层还有要取决于输出层激活函数类型，只有当输出层激活函数为4（linear）和5（ReLU）时才可以选择不对输出数据做归一化处理，选择其它激活函数时必须进行归一化处理（即使选择不归一化处理，程序后台也会自动强制归一化处理）；
4) NC=1：网络连接方式，“1”表示多层向即每层的输出仅对其紧邻下一层起作用，“2”表示多层全向前连接，即每层的输出不仅至其紧邻下一层，还包括其所有的后续层；
5) CT=1：输出代码类型，“1“表示快捷模式代码（Quick Model），“2”表示Fortran编程模式代码，“3”表示Pascal编程模式代码，“4”表示Basic编程模式代码；
6) Code=1：产生的代码形式，“1”不是精简模式，“2”不是精简（表达式）模式，“3”表示完全模式；
7) DC=[]：连接是否断开，比如“DC=[N2L2-N1L3]”表示第二层第二个节点与第三层第一个节点的连接是断开的。

使用神经网络进行数据拟合，如何确定神经网络的主要基本结构，即使用几个隐含层，

每个隐含层又用多少个神经元节点？这些是非常重要但又是比较困难的事，没有确定的规则可循，得根据拟合数据的特性进行尝试。一般而言，一个或最多二个隐含层就可以满足绝大多数拟合问题，每个隐含层的神经元节点数应该由少到多进行尝试，理论上隐含层神经元节点数越多，待求未知参数也越多，虽然拟合的精度会更高，但计算时间需求高，不易获得最优解，同时还可能出现过拟合现象。神经网络待求的优化参数数不多于拟合数据的总量可以视为基本准则之一。

案例1设定一个含3个神经元节点的隐含层，输出层激活函数由缺省的1（Sigmoid）改为4（Linear），输入输出数据均不进行归一化处理；案例2与案例1完全一致；案例3隐含层含有7个神经元节点，其余与案例1一样；案例4有两个隐含层，分别有2和4个神经元节点，对应5个因变量，输出层有5个神经元节点；案例5也有两个隐含层，每个隐含层都有3个神经元节点，对应2个自变量，输入层有2个神经元节点。五个案例神经网络结构、计算代码、计算结果及对比图见下，此外还可输出每个案例对应的具体模型公式。

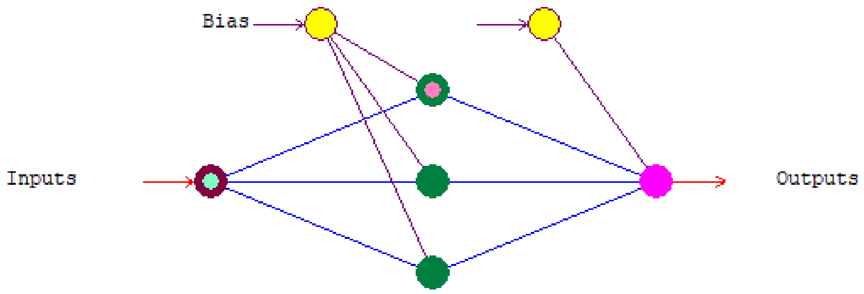


图 30-11 案例 1、2 神经网络结构

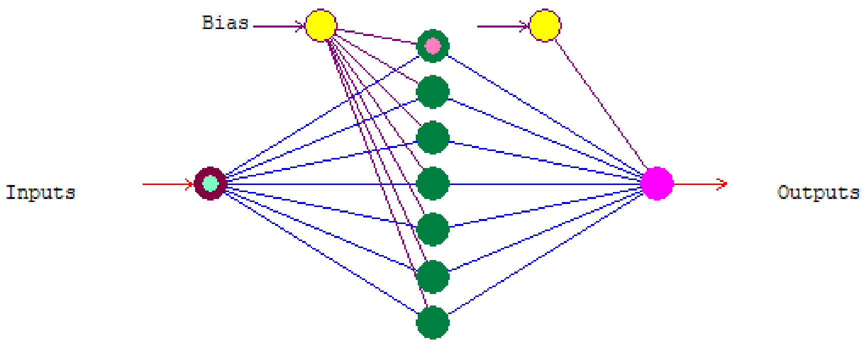


图 30-12 案例 3 神经网络结构

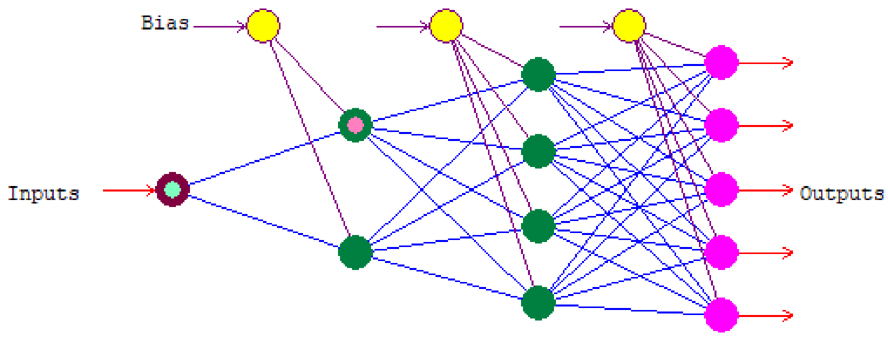


图 30-13 案例 4 神经网络结构

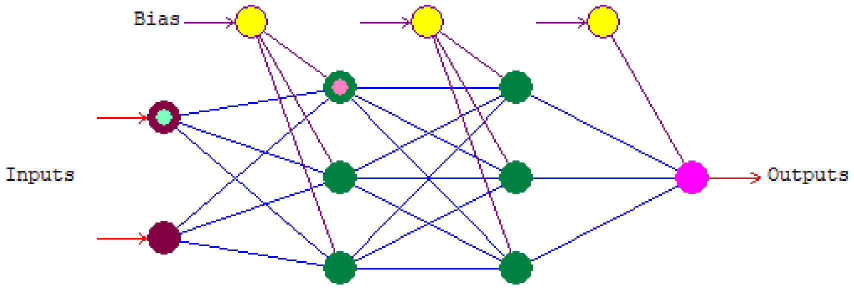


图 30-14 案例 5 神经网络结构

对应的拟合公式可从对应的代码段里按组合键“Ctrl+t”，激活公式编辑器查看，可以直接复制成MathML或Latex格式，前者又可以直接黏贴至Word自动生产可编辑的公式形式，此外拟合公式的文本形式计算完成后也可在结果输出页面直接给出。

案例 1 和案例 2 对应模型公式：

$$y=\frac{p_4}{1+\exp\left(-(p_1x+p_7)\right)}+\frac{p_5}{1+\exp\left(-(p_2x+p_8)\right)}+\frac{p_6}{1+\exp\left(-(p_3x+p_9)\right)}+p_{10}$$

案例 3 对应模型公式：

$$y=\frac{p_8}{1+\exp\left(-(p_1x+p_{15})\right)}+\frac{p_9}{1+\exp\left(-(p_2x+p_{16})\right)}+\frac{p_{10}}{1+\exp\left(-(p_3x+p_{17})\right)}+\frac{p_{11}}{1+\exp\left(-(p_4x+p_{18})\right)}$$
$$+\frac{p_{12}}{1+\exp\left(-(p_5x+p_{19})\right)}+\frac{p_{13}}{1+\exp\left(-(p_6x+p_{20})\right)}+\frac{p_{14}}{1+\exp\left(-(p_7x+p_{21})\right)}+p_{22}$$

案例 4 对应模型公式：

$$y_1=\frac{p_{11}}{1+\exp\left(-\left(\frac{p_3}{1+\exp\left(-(p_1x+p_{31})\right)}+\frac{p_7}{1+\exp\left(-(p_2x+p_{32})\right)}+p_{33}\right)\right)}+$$
$$\frac{p_{16}}{1+\exp\left(-\left(\frac{p_4}{1+\exp\left(-(p_1x+p_{31})\right)}+\frac{p_8}{1+\exp\left(-(p_2x+p_{32})\right)}+p_{34}\right)\right)}+$$
$$\frac{p_{21}}{1+\exp\left(-\left(\frac{p_5}{1+\exp\left(-(p_1x+p_{31})\right)}+\frac{p_9}{1+\exp\left(-(p_2x+p_{32})\right)}+p_{35}\right)\right)}+$$
$$\frac{p_{26}}{1+\exp\left(-\left(\frac{p_6}{1+\exp\left(-(p_1x+p_{31})\right)}+\frac{p_{10}}{1+\exp\left(-(p_2x+p_{32})\right)}+p_{36}\right)\right)}+p_{37}$$
$$y_2=\frac{p_{12}}{1+\exp\left(-\left(\frac{p_3}{1+\exp\left(-(p_1x+p_{31})\right)}+\frac{p_7}{1+\exp\left(-(p_2x+p_{32})\right)}+p_{33}\right)\right)}+$$
$$\frac{p_{17}}{1+\exp\left(-\left(\frac{p_4}{1+\exp\left(-(p_1x+p_{31})\right)}+\frac{p_8}{1+\exp\left(-(p_2x+p_{32})\right)}+p_{34}\right)\right)}+$$
$$\frac{p_{22}}{1+\exp\left(-\left(\frac{p_5}{1+\exp\left(-(p_1x+p_{31})\right)}+\frac{p_9}{1+\exp\left(-(p_2x+p_{32})\right)}+p_{35}\right)\right)}+$$

$$\frac{p_{27}}{1+\exp\left(-\left(\frac{p_6}{1+\exp(-(p_1x+p_{31}))}+\frac{p_{10}}{1+\exp(-(p_2x+p_{32}))}+p_{36}\right)\right)}+p_{38}$$

$$y_3=\frac{p_{13}}{1+\exp\left(-\left(\frac{p_3}{1+\exp(-(p_1x+p_{31}))}+\frac{p_7}{1+\exp(-(p_2x+p_{32}))}+p_{33}\right)\right)}+$$

$$\frac{p_{18}}{1+\exp\left(-\left(\frac{p_4}{1+\exp(-(p_1x+p_{31}))}+\frac{p_8}{1+\exp(-(p_2x+p_{32}))}+p_{34}\right)\right)}+$$

$$\frac{p_{23}}{1+\exp\left(-\left(\frac{p_5}{1+\exp(-(p_1x+p_{31}))}+\frac{p_9}{1+\exp(-(p_2x+p_{32}))}+p_{35}\right)\right)}+$$

$$\frac{p_{28}}{1+\exp\left(-\left(\frac{p_6}{1+\exp(-(p_1x+p_{31}))}+\frac{p_{10}}{1+\exp(-(p_2x+p_{32}))}+p_{36}\right)\right)}+p_{39}$$

$$y_4=\frac{p_{14}}{1+\exp\left(-\left(\frac{p_3}{1+\exp(-(p_1x+p_{31}))}+\frac{p_7}{1+\exp(-(p_2x+p_{32}))}+p_{33}\right)\right)}+$$

$$\frac{p_{19}}{1+\exp\left(-\left(\frac{p_4}{1+\exp(-(p_1x+p_{31}))}+\frac{p_8}{1+\exp(-(p_2x+p_{32}))}+p_{34}\right)\right)}+$$

$$\frac{p_{24}}{1+\exp\left(-\left(\frac{p_5}{1+\exp(-(p_1x+p_{31}))}+\frac{p_9}{1+\exp(-(p_2x+p_{32}))}+p_{35}\right)\right)}+$$

$$\frac{p_{29}}{1+\exp\left(-\left(\frac{p_6}{1+\exp(-(p_1x+p_{31}))}+\frac{p_{10}}{1+\exp(-(p_2x+p_{32}))}+p_{36}\right)\right)}+p_{40}$$

$$y_5=\frac{p_{15}}{1+\exp\left(-\left(\frac{p_3}{1+\exp(-(p_1x+p_{31}))}+\frac{p_7}{1+\exp(-(p_2x+p_{32}))}+p_{33}\right)\right)}+$$

$$\frac{p_{20}}{1+\exp\left(-\left(\frac{p_4}{1+\exp(-(p_1x+p_{31}))}+\frac{p_8}{1+\exp(-(p_2x+p_{32}))}+p_{34}\right)\right)}+$$

$$\frac{p_{25}}{1+\exp\left(-\left(\frac{p_5}{1+\exp(-(p_1x+p_{31}))}+\frac{p_9}{1+\exp(-(p_2x+p_{32}))}+p_{35}\right)\right)}+$$

$$\frac{p_{30}}{1+\exp\left(-\left(\frac{p_6}{1+\exp(-(p_1x+p_{31}))}+\frac{p_{10}}{1+\exp(-(p_2x+p_{32}))}+p_{36}\right)\right)}+p_{41}$$

案例 5 对应模型公式：

$y=$

$$\frac{p_{16}}{1+\exp\left(-\left(\frac{p_7}{1+\exp(-(p_1x_1+p_4x_2+p_{19}))}+\frac{p_{10}}{1+\exp(-(p_2x_1+p_5x_2+p_{20}))}+\frac{p_{13}}{1+\exp(-(p_3x_1+p_6x_2+p_{21}))}+p_{22}\right)\right)}$$

$$+\frac{p_{17}}{1+\exp\left(-\left(\frac{p_8}{1+\exp(-(p_1x_1+p_4x_2+p_{19}))}+\frac{p_{11}}{1+\exp(-(p_2x_1+p_5x_2+p_{20}))}+\frac{p_{14}}{1+\exp(-(p_3x_1+p_6x_2+p_{21}))}+p_{23}\right)\right)}$$

$$+\frac{p_{18}}{1+\exp\left(-\left(\frac{p_9}{1+\exp(-(p_1x_1+p_4x_2+p_{19}))}+\frac{p_{12}}{1+\exp(-(p_2x_1+p_5x_2+p_{20}))}+\frac{p_{15}}{1+\exp(-(p_3x_1+p_6x_2+p_{21}))}+p_{24}\right)\right)}$$

$$+p_{25}$$

案例 1 代码

```
Function NNFit(NS=[1-3-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[]);
Data;
x=[1 2 3 4 5 5.85 5.93 6 6.06 6.2 7 8 9 10];
y=[9 7 6 3 -1 -3.8 -1.5 2 4.5 7.8 5 7 20 50];
```

案例 1 计算结果

```
Sum Squared Error (SSE): 0.758235614615373
Root of Mean Square Error (RMSE): 0.232722338330984
Correlation Coef. (R): 0.999835662581801
R-Square: 0.999671352170389
Adjusted R-Square: 0.99961159801955
Determination Coef. (DC): 0.999671352170389
Chi-Square: 0.0552176867177578
F-Statistic: 1351.89810954295

Parameter   Best Estimate
---------   -------------
p1          -0.583228236179482
p2          15.0506550612493
p3          0.602359725586618
p4          122.757261692124
p5          15.1969191320489
p6          413.810166204637
p7          4.5965809701182
p8          -90.2287385650367
p9          -6.92097341168258
p10         -112.683154949073
```

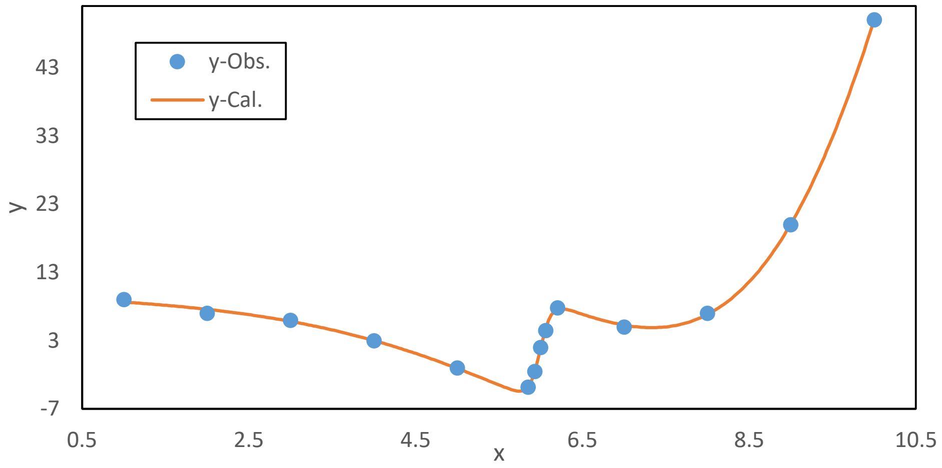


图30-15  案例1计算结果对比图

案例 2 代码

```
Function NNFit(NS=[1-3-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[]);
Data;
x=9.968e+03,1.365e+04,1.763e+04,2.162e+04,2.560e+04,2.958e+04,3.357e+04,3.755e+04,4.153e+04,4.552e+04,4.950e+04,5.348e+04,5.747e+04,6.145e+04,6.543e+04,6.942e+04,7.340e+04,7.738e+04,8.137e+04,8.535e+04,8.668e+04,8.682e+04,8.684e+04,8.686e+04,8.688e+04,8.691e+04,8.693e+04,8.695e+04,8.697e+04,8.700e+04,8.702e+04,8.704e+04,8.706e+04,8.708e+04,8.711e+04,8.713e+04,8.715e+04,8.717e+04,8.719e+04,8.722e+04,8.765e+04,8.898e+04,9.296e+04,9.695e+04,1.009e+05,1.049e+05,1.089e+05,1.129e+05,1.169e+05,1.208e+05,1.248e+05,1.288e+05,1.328e+05,1.368e+05,1.408e+05,1.447e+05,1.487e+05,1.527e+05,1.567e+05,1.607e+05,1.647e+05,1.686e+05,1.726e+05,1.766e+05,1.806e+05;
y=20.9,11.4,9.07,7.42,6.14,5.46,4.66,4.07,3.55,3.22,2.87,2.64,2.43,2.23,2.05,1.94,1.82,1.71,1.59,1.52,1.52,1.2,1.12,1.08,1.06,1.03,1.01,0.979,0.958,0.958,0.928,0.928,0.909,0.899,0.871,0.881,0.862,0.871,0.862,0.844,0.784,0.713,0.635,0.615,0.596,0.571,0.542,0.525,0.509,0.503,0.488,0.468,0.473,0.463,0.444,0.434,0.425,0.416,0.403,0.395,0.395,0.387,0.375,0.371,0.359;
```

案例 2 计算结果

```
Sum Squared Error (SSE): 0.21502928085557
Root of Mean Square Error (RMSE): 0.0575164566223737
Correlation Coef. (R): 0.99983440356436
R-Square: 0.999668834550899
Adjusted R-Square: 0.999658151794476
Determination Coef. (DC): 0.999668834550893
Chi-Square: 0.0837484667109559
F-Statistic: 18447.2333272351

Parameter  Best Estimate
---------  -------------
p1         -0.0053368738370459
p2         -4.94707202413304E-5
p3         0.000571359726528994
p4         0.893583645868982
p5         87729.7821315783
p6         -6242.61730746198
p7         463.579965097663
p8         -8.50421815726059
p9         0.87761172618996
p10        6243.05381603183
```

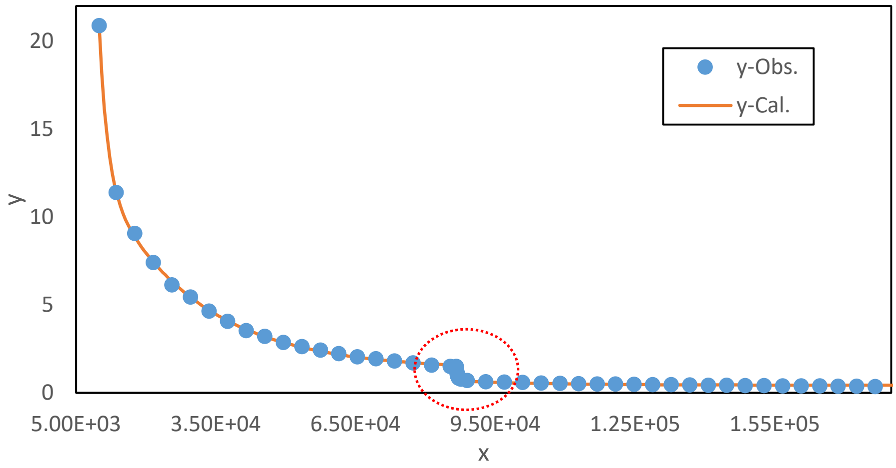


图30-16 案例2计算结果对比图

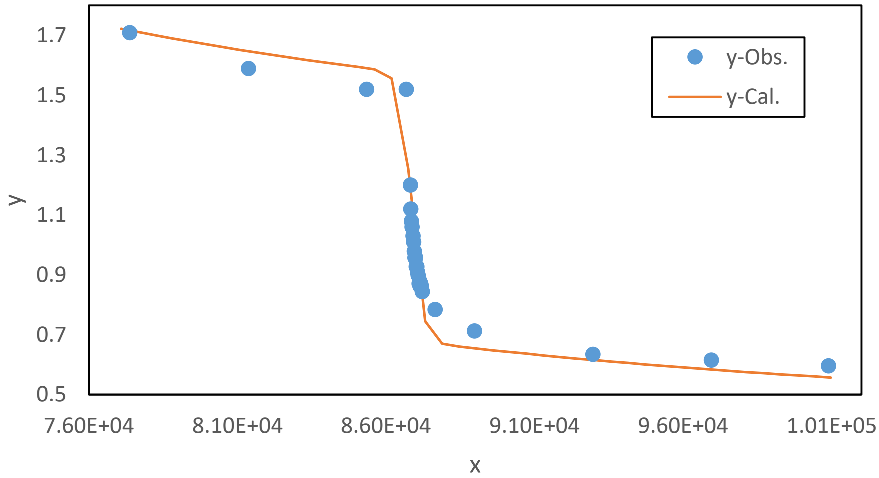


图30-17 案例2中部放大计算结果对比图

案例 3 代码

```
Function NNFit(NS=[1-7-1], TF=[1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[]);
Data;
0,5,10,15,20,25,30,35,40,45,50,55,60,65,70,75,80,85,90,95,100,105,110,115,120,125,130,135,140,145,150,155,
160,165,170,175,180,185,190,195,200,205,210,215,220,225,230,235,240,245,250,255,260,265,270,275,280,28
5,290,295,300;
0.200,1.049,1.142,1.201,1.245,1.280,1.310,1.336,1.359,1.380,1.399,1.416,1.432,1.447,1.461,1.474,1.486,1.498
,1.509,1.520,1.530,2.189,2.291,2.359,2.412,2.456,2.494,2.528,2.558,2.586,2.612,2.637,2.659,2.681,2.701,2.72
1,2.739,2.757,2.774,2.790,2.806,2.130,2.022,1.949,1.891,1.842,1.799,1.760,1.725,1.692,1.661,1.633,1.605,1.5
80,1.555,1.531,1.509,1.487,1.466,1.445,1.425;
```

案例 3 计算结果

```
Sum Squared Error (SSE): 0.00612943622532886
Root of Mean Square Error (RMSE): 0.010024099015421
Correlation Coef. (R): 0.999849581641433
R-Square: 0.999699185908548
Adjusted R-Square: 0.999688813008843
Determination Coef. (DC): 0.999699185908549
Chi-Square: 0.00154364360088917
F-Statistic: 6171.865800694
```

| Parameter | Best Estimate |
| --- | --- |
| p1 | 0.526597986694299 |
| p2 | -0.102726481917293 |
| p3 | -3.02476958011251 |
| p4 | -3.16980834132475 |
| p5 | 0.0429028199158662 |
| p6 | 0.0235002483915679 |
| p7 | -0.0174817749873293 |
| p8 | 842.721211223321 |
| p9 | -0.588553114613591 |
| p10 | -0.712479240444775 |
| p11 | 0.73850937426005 |
| p12 | 2.76888524234888 |
| p13 | -4.31115297237267 |
| p14 | -3.06494501407944 |
| p15 | 6.8854983426218 |
| p16 | 18.824237157824 |
| p17 | 315.746783471888 |
| p18 | 648.038841554859 |
| p19 | -5.68686914565436 |
| p20 | -3.50923712926971 |
| p21 | -0.533875492113382 |
| p22 | -839.84910481652 |

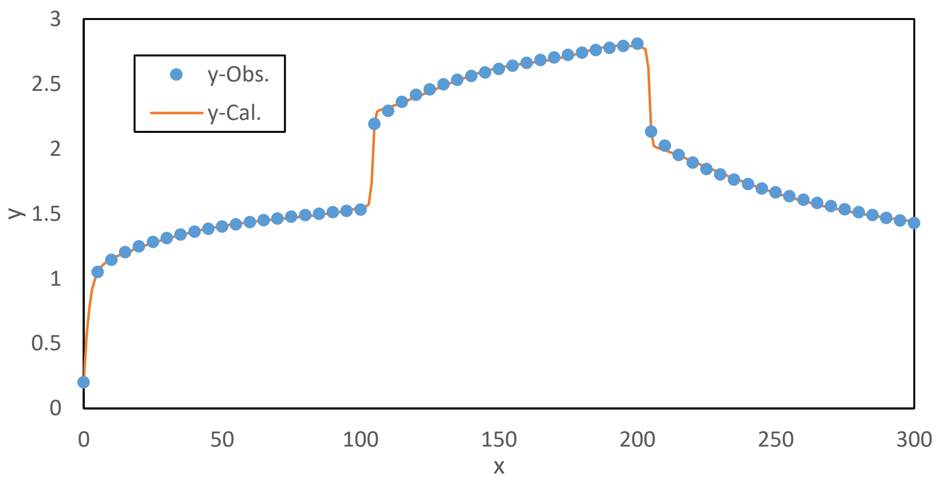


图30-18 案例3计算结果对比图

案例 4 代码

```
MaxIteration = 5000;
Algorithm = CLO3[10];// UGO1[5];
Function NNFit(NS=[1-2-4-5], TF=[1,1,4], DN=[0,0], NC=1, CT=1, Code=1, DC=[]); //NS: Network Structure; TF: Transfer Fun.; DN: Data Normalization; NC: Network Connetion; CT: Code Type
Data;
x=0,0.05,0.1,0.15,0.2,0.25,0.3,0.35,0.4,0.45,0.5,0.55,0.6,0.65,0.7,0.75,0.8,0.85,0.9,0.95,1;
y1=0.1,0.09363,0.08765,0.08206,0.07682,0.07191,0.06733,0.06305,0.0592,0.05654,0.06111,0.12197,0.57603,2.31729,4.59434,5.90324,6.28589,6.08804,5.54222,4.78943,3.91983;
y2=0.001845,0.001732,0.001625,0.001524,0.001429,0.001337,0.001242,0.001102,0.000652,-0.001978,-0.021728,-0.181354,-1.205571,-3.756468,-4.89856,-4.683934,-4.279801,-3.935516,-3.658357,-3.424578,-3.212917;
```

y3=-0.013171,-0.012338,-0.011557,-0.010825,-0.010138,-0.009491,-0.008869,-0.0082,-0.007042,-0.002252,0.03123,0.297614,1.911671,4.766427,3.751245,1.565312,0.086857,-0.802556,-1.3351,-1.646745,-1.811243;
y4=-0.000292875,-0.00027575,-0.0002595,-0.0002445,-0.000231875,-0.000227125,-0.000261,-0.000519,-0.002252875,-0.014937875,-0.1176755,-0.936735125,-4.887517,-5.808778,-0.399008375,0.99239425,0.956371375,0.7678885,0.62863025,0.549160375,0.515598875;
y5=-0.005016,-0.004707,-0.004417,-0.004143,-0.003885,-0.003637,-0.003378,-0.002996,-0.001775,0.005381,0.059069,0.491166,3.174846,8.754624,9.109239,6.83957,4.995247,3.741764,2.877479,2.256777,1.793657;

案例 4 计算结果

Sum Squared Error (SSE): 0.00364746082305389
Root of Mean Square Error (RMSE): 0.00589387157345007
Correlation Coef. (R): 0.999996278046376
R-Square: 0.999992556106604
Adjusted R-Square: 0.999989365883879
Determination Coef. (DC): 0.999992556118714
F-Statistic: -25444.8425310123

| Parameter | Best Estimate |
|---|---|
| p1 | -12.3849098241499 |
| p2 | 4.93969817528999 |
| p3 | 14.1489042008414 |
| p4 | -11.5591727947315 |
| p5 | -17.3481525780038 |
| p6 | -52.2975614042363 |
| p7 | -7.2407545766792 |
| p8 | 19.4851348469939 |
| p9 | 14.5075646217547 |
| p10 | 3.57228460304124 |
| p11 | -16.6600876090188 |
| p12 | -15.3099275490999 |
| p13 | 48.0988337665421 |
| p14 | 24.8774775617639 |
| p15 | 61.7427359568818 |
| p16 | -9.99116070624638 |
| p17 | -16.7580246841858 |
| p18 | 45.674498431996 |
| p19 | -25.5687493717376 |
| p20 | 61.4334019747605 |
| p21 | 0.85177935089539 |
| p22 | -2.19120297971707 |
| p23 | 0.100221853309021 |
| p24 | 50.5815703460753 |
| p25 | 2.37659203445402 |
| p26 | -47.6916951480172 |
| p27 | 7.2807900497889 |
| p28 | 2.19951602681378 |
| p29 | 2.80599100014001 |
| p30 | -9.85045179731635 |
| p31 | 6.40184801954178 |
| p32 | -4.68040761552348 |
| p33 | -0.823898455647637 |
| p34 | -1.36311675247959 |
| p35 | -0.225614623402655 |
| p36 | -4.40574739607399 |

| | |
|---|---|
| p37 | 16.7336576182532 |
| p38 | 15.3097944091464 |
| p39 | -48.1105575770445 |
| p40 | -24.8779481119334 |
| p41 | -61.7469694690291 |

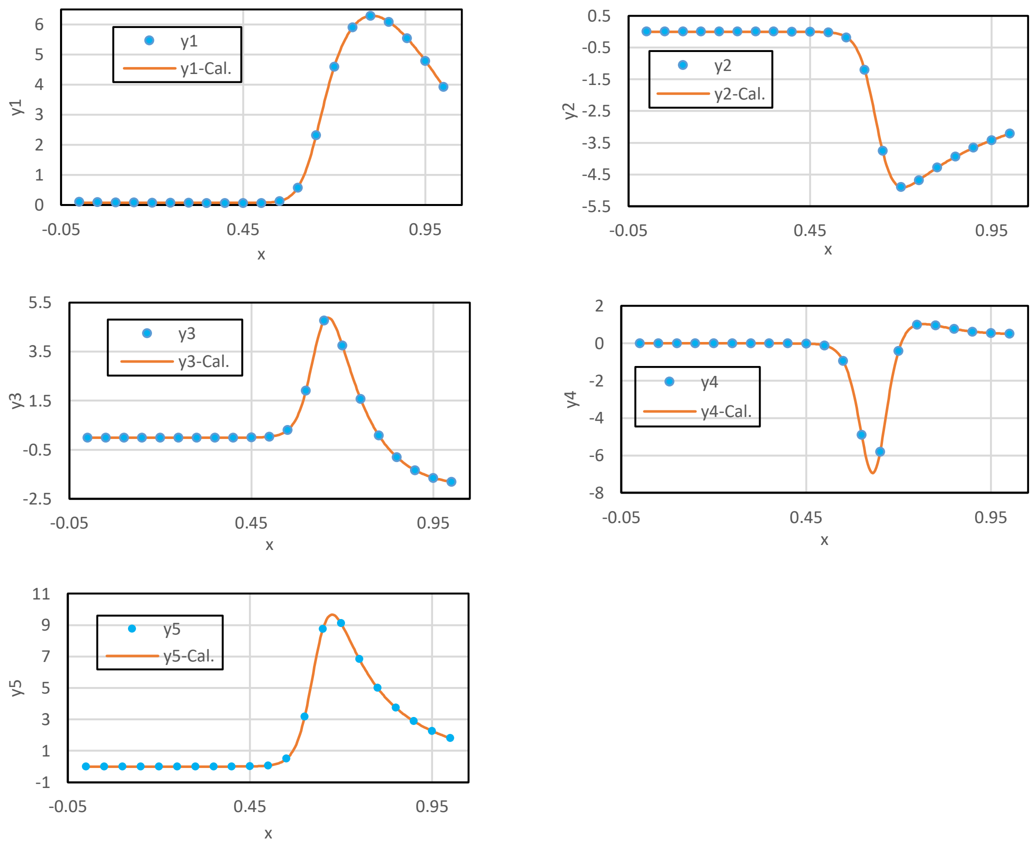


图30-19 案例4计算结果对比图

案例 5 代码

```
Algorithm = UGO1[5];
Function NNFit(NS=[2-3-3-1], TF=[1,1,7], DN=[0,0], NC=1, CT=1, Code=1, DC=[]);
Data;
x1=200,200,200,200,200,200,200,200,300,300,300,300,300,300,300,300,300,300,300,300,300,400,400,400,40
0,400,400,400,400,400,400,400,400,500,500,500,500,500,500,500,500,500,500,500,500,600,600,600,600,600,
600,600,600,600,600,600,600,700,700,700,700,700,700,700,700,700,700,700,700,800,800,800,800,800,800,80
0,800,800,800,800,800,900,900,900,900,900,900,900,900,900,900,900,900,1000,1000,1000,1000,1000,1000,1
000,1000,1000,1000,1000,1000;
x2=0.28,0.4,0.52,0.64,0.76,0.79,0.82,0.85,0.1,0.34,0.46,0.55,0.58,0.61,0.64,0.67,0.7,0.73,0.76,0.79,0.82,0.2,0.3
2,0.44,0.5,0.53,0.56,0.59,0.62,0.65,0.68,0.71,0.74,0.13,0.19,0.31,0.43,0.49,0.52,0.55,0.58,0.61,0.64,0.67,0.7,0.
15,0.27,0.39,0.42,0.45,0.48,0.51,0.54,0.57,0.6,0.63,0.66,0.13,0.19,0.25,0.31,0.37,0.4,0.43,0.46,0.49,0.52,0.55,0
.58,0.13,0.19,0.25,0.31,0.37,0.4,0.43,0.46,0.49,0.52,0.55,0.58,0.13,0.19,0.25,0.31,0.34,0.37,0.4,0.43,0.46,0.49,
0.52,0.55,0.13,0.19,0.25,0.31,0.34,0.37,0.4,0.43,0.46,0.49,0.52,0.55;
y=0.03,0.04,0.124,0.508,3.411,8.712,19.975,260.5,0.024,0.094,0.287,1,2.058,3.443,5.9,15.237,29.012,77.895,2
68.266,926.133,3226.499,0.069,0.19,0.886,1.861,2.966,5.848,12.202,32.432,91.408,161.481,705.156,2118.492
,0.065,0.104,0.315,1.929,5.122,10.026,22.473,70.457,150.428,330.854,1287.065,4971.452,0.07,0.339,1.817,3.
477,5.458,11.003,26.776,50.797,173.851,515.246,1205.304,5192.83,0.111,0.163,0.486,1.019,2.607,4.663,8.554
,17.711,37.202,109.288,266.517,801.336,0.125,0.304,0.517,1.146,4.362,8.469,19.19,42.242,100.535,269.473,7
97.309,1782.525,0.153,0.393,0.933,2.447,3.752,7.959,15.92,33.265,101.495,185.408,733.459,2062.239,0.192,
0.535,1.208,3.55,7.758,13.881,27.788,68.756,186.803,394.723,1358.639,3983.95;
```

案例 5 计算结果

Root of Mean Square Error (RMSE): 25.4670658079357
Correlation Coef. (R): 0.99960874044047
R-Square: 0.999217633964983
Adjusted R-Square: 0.999194395369884
Determination Coef. (DC): 0.999217633632817
Chi-Square: 194.474444097571
F-Statistic: 4257.10648793712

| Parameter | Best Estimate |
|---|---|
| --------- | ------------- |
| p1 | 0.000478526015697717 |
| p2 | 1.08698274898181 |
| p3 | -0.0152552253792964 |
| p4 | 1.5596594789762 |
| p5 | -1377.10979017629 |
| p6 | -8.77570525732964 |
| p7 | -1485.6250443958 |
| p8 | 3725.21290416551 |
| p9 | -10.120679925558 |
| p10 | 183.453602246203 |
| p11 | 0.117471222657448 |
| p12 | 4135096.79421982 |
| p13 | 34053.6241283155 |
| p14 | -9.81960656882674 |
| p15 | 341.401755401463 |
| p16 | 977.572358125279 |
| p17 | 137955.792304988 |
| p18 | -4688.77217456866 |
| p19 | 3.94959527258049 |
| p20 | 243.370331137084 |
| p21 | 10.3021511668467 |
| p22 | 1291.12523274526 |
| p23 | -3709.88937908792 |
| p24 | 1.3424266253167E-88 |
| p25 | 3714.11717719384 |

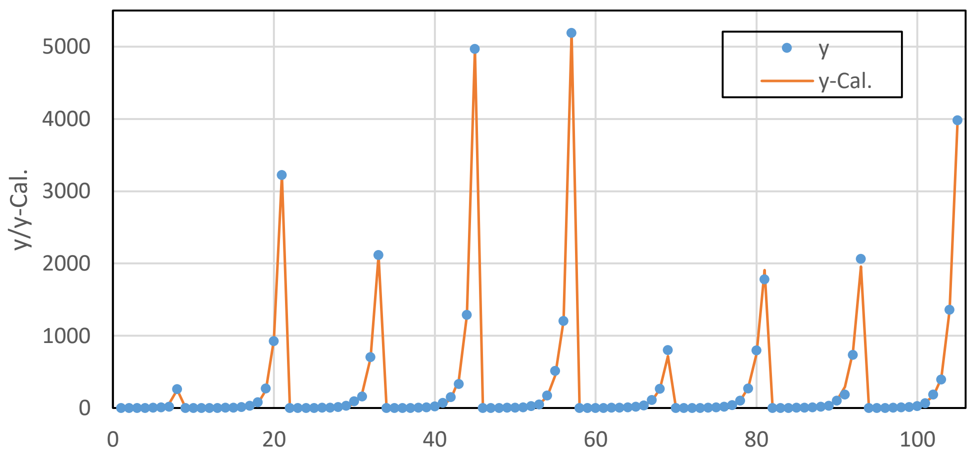


图 30-20 案例 5 计算结果对比图

五个案例计算结果都非常好，计算输出内容不仅包括各参数值以及各项拟合评价指标，还能输出完整的模型公式，如果计划将模型移植扩展，无疑是非常方便去实现的。

当求解参数较多时，如案例4有41各未知参数，案例5也有25个，未知参数数的增加也意味着求解难度加大，尤其是想求得全局最优解，需要多次计算。上述案例不排除还有更好结果。

著名的数学软件Matlab也有神经网络拟合工具箱，对大多数初次使用过该工具箱的新手用户而言，初始感觉和普遍存在的几个共同疑问是：“这完全是黑箱操作啊，具体怎么计算的？”，“有具体的模型公式吗？在哪儿？”，“如何将训练后的神经网络模型应用到其它场景？”等等，作为对比，1stOpt的神经网络拟合工具箱几乎不存在这类问题：计算步骤可视，拟合公式直接输出。

## 30.4 小结

简单而言，神经网络拟合其实与一般的数学公式拟合并无二异，只是拟合公式的产生由赋名为“神经网络”的特殊模型结构产生而已。

回到主题“神经网络是通用万能拟合器吗？”，通过5个实际案例，基本可以回答：大部分情况下是的。当模型公式未知而只有变化复杂的数据，且数据无法用常规公式去拟合得到满意的结果时，神经网络的确是一个很好的优先选择解决途径，尤其是在1stOpt中，神经网络可视化设计界面可帮助新手快速理解并掌握神经网络基本原理并产生易于理解的详细运行代码，而熟练掌握该工具箱后，用一句命令代码即可实现完整的神经网络拟合，如同处理一般的拟合问题一样，方便且强大。