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用神经网络预测饱和液体密度
Using Neural Network to Predict the Density of Saturated Liquid

韦藤幼 黄瑞华
Wei Tengyou Huang Ruihua

(广西大学工业测试实验中心 南宁市西乡塘路 530004)
(The Industrial Testing Experiment Centre, Guangxi University, Xixiangtanglu, Nanning, Guangxi, 530004, China)

摘要 使用前向神经网络,采用带阻尼的牛顿二阶学习方法,学习纯物质的饱和液体密度与温度的关系,在熔点到临界点的温度范围内,预测平均误差小于0.03%。适宜的网络工作区间 $[a_{min}, a_{max}]$ 为 [0.5, 0.7]
关键词 神经网络 液体密度 预测 牛顿二阶学习方法
中图法分类号 O 645.1

Abstract The feed-forword neural network is used to study the relationship between the density of the pure saturated liquid matters and the temperature. The weighs of the neural network are updated by using the damped Newton second order method. The estimated average errors are less than 0.03% between the melting point and the critical point. The suitable working range $[a_{min}, a_{max}]$ is [0.5, 0.7] for the network.
Key words neural network, density of liquid, estimation, Newton second order method

饱和液体密度是物质的一个重要性质,为此人们进行了大量精确实验及理论研究,给出了比较权威的密度数据及估算方法[1,2],这些估算方法平均误差为1%~3%。文献[3, 4]使用神经网络预测液体的基本物性,但没有预测密度与温度的关系。本文采用三层前向神经网络,对不同温度下的液体密度进行预测,当中间层为三个单元时,平均误差小于0.03%,最大误差为0.2%。本文给出的使用神经网络进行高精度预测的方法具有广泛的应用前景。

1 神经网络模型及学习过程

1.1 前向神经网络

已有的研究表明,在很宽的条件下,三层前向网络能以任意精度逼近任意连续函数及其各阶导数[5]。具有1个输入和1个输出的三层前向神经网络见图1

其中,第 j 中间层的输入为:

$$s_j = \theta_j + w_j t_i, \quad (j = 1,\cdots,p) \tag{1}$$

其输出采用 S 函数,为:

$$b_j = 1/(1+\exp(-s_j)), \quad (j = 1,\cdots,p) \tag{2}$$

输出层的输入为:

$$l = r + \sum_{i=1}^{p} v_j b_j, \quad (j = 1,\cdots,p) \tag{3}$$

最后输出为:

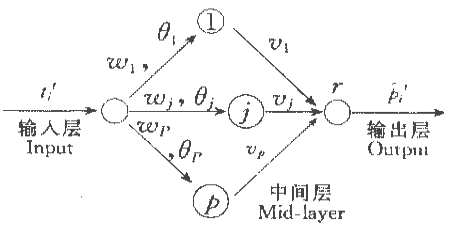

图1 三层前向神经网络模型

Fig. 1 Three layer feed-forward neural neural model

$$\hat{d}_i' = 1/(1+\exp(-l)). \tag{4}$$

1.2 学习过程

网络训练时使用相对误差型平方和目标函数:

$$E = \sum_{i=1}^{n} \left[\frac{d_i' - \hat{d}_i'}{d_i'}\right]^2, \tag{5}$$

网络中的权值 w_i, v_j 及阀值 θ_j, r 通过学习训练确定。最著名的学习方法是误差反向传播(EBP)算法,它是一个一阶学习方法,开始网络收敛很快,但后来很慢,有时不能达到期望解。

牛顿的二阶学习方法如下:

$$w^{i+1} = w^i - H^{-1}(w_i)G(w_i), \tag{6}$$

上式中,w_i 为网络权值及阀值失量,而 H 为 Hessian 矩阵,G 为梯度。对图1的网络,G 及 H 均可通过解析式求出。

式(6)的学习过程往往容易发散,改进的方法是增加步长因子或阻尼因子。本文采用后者,其方法是式(6)使用带阻尼的 Hessian 矩阵 H', H' 是在 H

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矩阵的对角线元素加上一阻尼因子 μ,当网络不收敛时,μ增加 1倍,否则 μ减少 1倍。学习过程见图 2

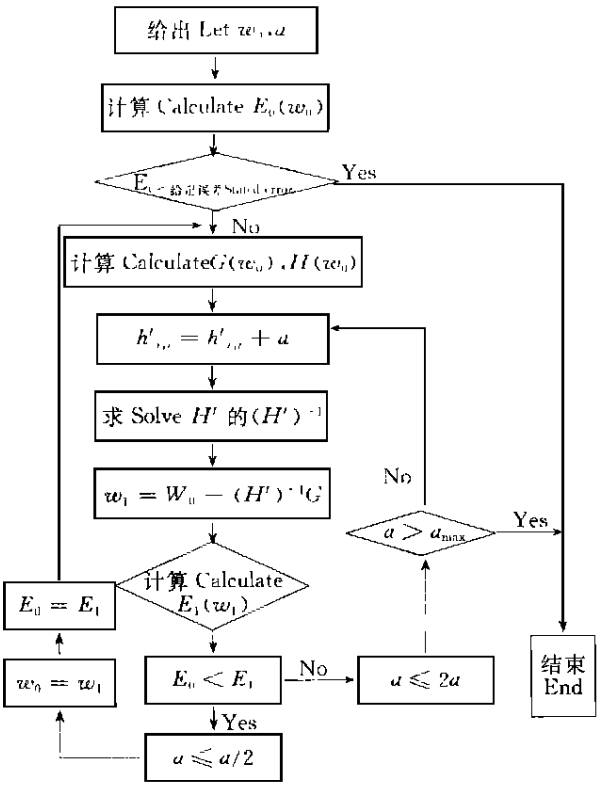

图 2 阻尼牛顿法学习过程

Fig. 2 The Learning process of the damped Newton method

表 1为水体系网络学习过程收敛情况,可见收敛很快。

表 1 水体系学习过程

Table 1 The learning process of water system

学习次数 Learning times	误差 E Error	学习次数 Learning times	误差 E Error
0	2.18	1 000	6.42E-6
100	1.04E-4	2 000	3.97E-6
200	3.08E-5	3 000	3.06E-6
300	1.77E-5	5 000	1.68E-6

2 数据的准备及组织

对每一个体系的密度 d与温度 t 的训练数据,本文选用文献 [1]。但用于学习之前,还必须把文献的 t, d数据变换为图 1所用的 t', d',使 t'及 d'的取值范围是从 0到 1 变换公式如下:

$$t' = \frac{a_{max} - a_{min}}{t_{max} - t_{min}} t + a_{min}, \quad (7)$$

$$d' = \frac{a_{max} - a_{min}}{d_{max} - d_{min}} d + a_{min}, \quad (8)$$

上式中,t_{max}, t_{min} 为训练数据的最高及最低温度,d_{max}及 d_{min}为训练数据的最大及最小密度,而 a_{max}及 a_{min}是 t'及 d'的工作区间范围。

表 2表明,a_{max}, a_{min} 取值对学习精度是有影响的。对绝大多数体系的计算表明,a_{max}取 0.7, a_{min}取 0.5效果都满意。

表 2 水体系学习过程 a_{min}的影响 (a_{max}= 0.7)

Table 2 a_{min} Influence of learning process of water system (a_{max}= 0.7)

a_{min}	平均误差 Average error (%)	a_{min}	平均误差 Average error (%)
0.3	0.020	0.6	0.018
0.4	0.019	0.65	0.04
0.5	0.018		

3 结果

3.1 中间单元数的影响

表 3是 6个体系不同中间单元的学习结果。可见,随着中间单元数的增加,学习误差减少,采用 2个中间单元能满足一般要求,使用 4个中间单元时,误差下降不多,但学习过程及预测都较复杂。因此,选择 3个中间单元是比较合适的。

表 3 中间单元数的影响

Table 3 Influence of numbers of middle units

体系 System	平均误差 Average error (%)			
	1单元 Unit 1	2单元 Unit 2	3单元 Unit 3	4单元 Unit 4
水 Water	0.356	0.088	0.0187	0.0150
氨 Ammonia	1.45	0.143	0.0074	0.004
丙烷 Propane	1.034	0.108	0.009	0.003
乙醇 Ethanol	1.503	0.210	0.0193	0.003
甲酸 Formic acid	0.952	0.200	0.0452	0.021
乙酸 Ethanoic acid	0.492	0.130	0.0297	0.0152

3.2 不同种类体系的学习结果

表 4给出了采用 3个中间单元的 6类体系学习结果。从中可知,对各种类型体系,平均误差都很小,

表 4 不同种类体系的学习结果

Table 4 The study result of different systems

体系类型 Type of system	体系数 System number	总数据点 Total data point	平均误差 Average error (%)	最大误差 Max error (%)
烷烃 Alkane	23	676	0.026	0.20
烯烃、炔烃 Alkene, alkyne	11	297	0.020	0.20
卤代烃 Halohydrocarbon	8	219	0.030	0.15
醇 Alcohol	11	410	0.022	0.12
有机酸 Organic acid	8	256	0.028	0.18
无机气体及水 Inorganic gas, water	5	108	0.016	0.07

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levels were significant lowering before oral given in diabetic rats induced by STZ. Comparing with model group, insulin levels in high and low dose groups of AP picked up significantly after oral administration for 30 days. The results showed that AP had positive influrence on the protection of β cells of pancreas island injured by STZ.

Table 4 Effect of AP on the insulin levels in serum of diabeticrats induced by STZ ($\bar{x} \pm s$)

Group	Doses (g/kg)	n	Serum insulin (MIU/L)	
			Before p.o	After p.o
Control		10	20.13± 6.08	21.2± 7.71
Model		10	6.38± 2.14	4.41± 2.24
XKW	2.5	10	6.48± 2.51	9.40± 2.40*
AP	0.25	10	5.99± 2.42	9.01± 2.31*
AP	0.125	10	6.38± 2.61	7.70± 3.42

Compared with model group* $P < 0.05$.

2.5 Histologic examination

As can be seen in Histologic examination, the pancreas is sublobe shape, and pancreatic island is round rope, dividing line clear, no inflammatory cell and fiber. There were 17 pancreatic islands and 36.2 island cells on average in each case in rats of control group. In the model group, number of pancreatic island decreased significantly, only 8 pancreatic islands on average in each case. Either its volume or its cell number decreased, showing little inflammatory cells and fiber tissue. The numbers of pancreatic island and its cells were significant increasing, and there were 15.7 pancreatic islands and 14.9 pancreatic island cells on average in each case, and no fibrosis in pancreatic island and only little cells were atrophy, but no inflammatory cells infiltration was found in AP groups. The results showed that AP had definite anti-oxidation, decreasing injuring of STZ on pancreatic island cells.

3 Discussion

The tender stem and leaves of Teng Cha have been used to treat with common cold and pyretic fever, pain-swelling of pharynx and larynx as well as jaundice hepatitis[4]. AP extracted from Teng Cha could resist constrictive action on rabbit thoracic aorta induced by epinephrine and high concetration K^+, thus expecting AP might be effective in treating with hypertension[5]. According to the previous studies, the flavonoid exhibits wide pharmacological activity on physiological systems of cardiovascular, respiratory and endocrine etc[6]. Thus, the results in our study showed that AP could lowered blood sugar levels in diabetic rats induced by STZ, increasing SOD activity and decreasing MDA content, levels of improving lipids, rising insulin levels in serum, and lightening the injuring of pancreatic island cells. Those suggests that AP has the effect of hypoglycemia, anti-oxidation, lipid-lowering, and protecting pancreatic island cells.

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而且最大误差都不超过0.2%，对有机酸及卤代烃等极性较强体系，误差稍大于其它类型体系。

4 结论

(1) 带阻尼的牛顿二阶学习方法，收敛快、精度高；(2) 本网络的工作区间 $[a_{min}, a_{max}]$ 为 [0.5, 0.7]，比较合适；(3) 本网络的学习平均误差很小，能满足绝大多数液体密度应用领域的要求。

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