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MULTI-CLASS CLASSIFICATION METHOD BASED ON REACTIVE AGENT ENSEMBLE

Tetiana NESKORODIEVA, doctor of technical science, associate professor, head of information technology department[1],
Eugene FEDOROV, doctor of technical science, professor, professor of information technology department [2]
Olga NECHYPORENKO, PhD, (technical), associate professor, associate professor of the robotics and specialized computer systemsdepartment[3]

[1]*Vasyl' Stus Donetsk National University, 600-richcha str., 21, Vinnytsia, 21021, Ukraine, Information and applied technologies faculty, information technology department, t.neskorodieva@donnu.edu.ua*
[2]*Vasyl' Stus Donetsk National University, 600-richcha str., 21, Vinnytsia, 21021, Ukraine, Information and applied technologies faculty, information technology department, fedorovee75@ukr.net*
[3]*Cherkasy State Technological University, Cherkasy, Shevchenko blvd., 460, 18006, Ukraine, robotics and specialized computer systems department, olne@ukr.net*

Abstract

The article was created a model of the reactive agent functioning on the basis of the proposed neural network ENN-RSRO, which allows to perform a multiclass classification; efficiency criteria for this model, which allow to evaluate the proposed model, have been proposed, and a method for identifying the parameters of this model has been created, which allows to increase the accuracy of multi-class classification by model; an ensemble model of reactive agents functioning on the basis of the ENN-RSRO neural network and soft voting, which allows to perform multiclass classification of the agents team of agents, and a method of model parameters identification this is created, which allows acceleration of multiclass classification by ensemble model and increase its accuracy.

1. Introduction

Multi-agent systems are now being used to effectively manage supply chains and audit. An important example of such systems is multi-agent traffic management systems that analyses distributed information from vehicle sensors (e.g., accelerometer, gyroscope, magnetometer and audio sensor) or pictures of vehicles and classify these vehicles, which makes it possible to quickly find the required vehicle for the subject of the logistics chain and speed up the goods delivery [1]. Machine learning systems, such as neural networks, are now being used instead of expert systems in multi-agent systems [2]. Ensemble-based methods have proved to be particularly effective, and by combining basic models (such as neural networks) they provide a more accurate ensemble model. For multiagent systems, ensemble models based on bagging are suitable [3].

The aim of the work is to create a multiclass classification method based on a reactive agent's ensemble. The following objectives have been established and implemented:

- reactive agent functioning formalization;
- to propose generalized models agents functioning of reactive based on neural networks for multiclass classification;
- to create a reactive agent operating model based on the ENN-RSRO neural network for multiclass classification;
- to propose performance criteria for the reactive agent operating model based on the ENN-RSRO neural network for multi-class classification;
- to create a parameters identification method of reactive agent functioning model based on ENN-RSRO neural network for multiclass classification;
- to create an ensemble model of reactive agents functioning based on ENN-RSRO neural network and soft voting for multiclass classification;
- to create a parameters identification method of ensemble model of reactive agents functioning based on neural network ENN-RSRO and soft voting for multiclass classification.

2. Materials and Methods

Figure 1 shows the structure of the two-layer neural network ENN-RSRO. There are $N^{(x)}$ neurons in the input layer. There are $N^{(s)}$ neurons in the hidden layer. There are $N^{(y)}$ neurons in the output layer. Each *j*-th input layer neuron corresponds to the *j*-th characteristic. Each *k*-th output layer neuron corresponds to *k*-th class.

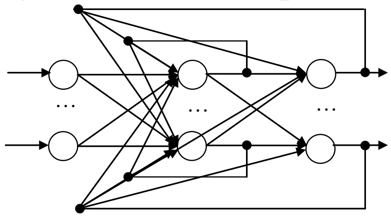

Fig. 1:ENN-RSRO two-layer neural network structure

The ENN-RSRO based reactive agent operating model for multi-class classification is presented as

$$s_j(n) = f\left(b_j^{(s)} + \sum_{i=1}^{N^{(x)}} w_{ij}^{(x-s)} x_i(n) + \sum_{i=1}^{N^{(s)}} w_{ij}^{(s-s)} s_i(n-1) + \sum_{i=1}^{N^{(y)}} w_{ij}^{(y-s)} y_i(n-1)\right),\ j \in \overline{1, N^{(s)}},$$
$$y_j(n) = g\left(b_j^{(y)} + \sum_{i=1}^{N^{(s)}} w_{ij}^{(s-y)} s_i(n) + \sum_{i=1}^{N^{(y)}} w_{ij}^{(y-y)} y_i(n-1)\right),\ j \in \overline{1, N^{(y)}},$$
$$f(z) = \max\{0, z\},\quad g(z) = \text{softmax}(z) \tag{1}$$

The criterion based on the standard error of classification is calculated as

$$\mathrm{F(w)} = \frac{1}{2N}\sum_{n=1}^{N}\sum_{j=1}^{N^{(y)}}(d_{nj} - y_j(n))^2 \to \min_{w}, \tag{2}$$

where the $\mathbf{x}_n$ is the n-th learning input vector, $\mathbf{d}_n$ is the n- th educational output vector, $N^{(x)}$ is the number of neurons of the input layer (the number of features), $N^{(y)}$ is the number of neurons of the output layer (number of classes), n is the learning implementation number, N is the power of the training set $\{(\mathbf{x}_n, \mathbf{d}_n)\}$, $\mathbf{w}$ is the weights vector. The criterion based on the accuracy of the classification is calculated as

$$F(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}[\arg\max\{d_{nj} \big| j \in \overline{1, N^{(y)}}\} = \arg\max\{y_j(n) \big| j \in \overline{1, N^{(y)}}\}] \to \max_{\mathbf{w}} ,$$
$$[a = b] = \begin{cases} 1, & a = b \\ 0, & a \neq b \end{cases} \tag{3}$$

The criterion based on the classification's computational complexity is calculated as

$$T = N \cdot (N^{(s)}(N^{(x)} + N^{(s)} + N^{(y)}) + N^{(y)}(N^{(s)} + N^{(y)})) \to \min_{N^{(s)}} \tag{4}$$

The proposed method of parameters identification of reactive agent functioning model based on ENN-RSRO for multiclass classification is based on reverse error propagation and consists in the following.

1. Training iteration number $n = 1$, initialization by uniform distribution on the interval (0,1) or [-0.5, 0.5] of offsets (thresholds) $b_j^{(s)}(n)$, $j \in \overline{1, N^{(s)}}$, $b_j^{(y)}(n)$, $j \in \overline{1, N^{(y)}}$ and weights $w_{ij}^{(x-s)}(n)$, $i \in \overline{1, N^{(x)}}, j \in \overline{1, N^{(s)}}$, $w_{ij}^{(s-s)}(n)$, $i \in \overline{1, N^{(s)}}, j \in \overline{1, N^{(s)}}$, $w_{ij}^{(y-s)}(n)$, $i \in \overline{1, N^{(y)}}, j \in \overline{1, N^{(s)}}$, $w_{ij}^{(s-y)}(n)$, $i \in \overline{1, N^{(s)}}, j \in \overline{1, N^{(y)}}$, $w_{ij}^{(y-y)}(n)$, $i \in \overline{1, N^{(y)}}, j \in \overline{1, N^{(y)}}$, where $N^{(q)}$ is the neurons number in q-th layer.

2.The learning set is set $\{(\mathbf{x}_n, \mathbf{d}_n) \,|\, \mathbf{x}_n \in R^{N^{(x)}}, \mathbf{d}_n \in R^{N^{(y)}}\}$, $n \in \overline{1, N}$, where $\mathbf{x}_n$ is the n-th learning input vector, $\mathbf{d}_n$ is the n-th learning output vector, $N^{(x)}$ is the number of the input layer's neurons, $N^{(y)}$ is the neurons number of the output layer, N is the learning set power. The current pair number from the learning set $n = 1$.

3. The output signal's initial calculation

$$x_i(n) = x_{ni},\ i \in \overline{1, N^{(x)}},\ s_i(n-1) = 0,\ i \in \overline{1, N^{(s)}}.\ y_i(n-1) = 0,\ i \in \overline{1, N^{(y)}}. \tag{5}$$

4. Calculation of the output signal for each layer (direct stroke)

$$\begin{gathered} s_j(n) = f(z1_j(n)),\ j \in \overline{1, N^{(s)}}, \\ z1_j(n) = b_j^{(s)}(n) + \sum_{i=1}^{N^{(x)}} w_{ij}^{(x-s)}(n) x_i(n) + \sum_{i=1}^{N^{(s)}} w_{ij}^{(s-s)}(n) s_i(n-1) + \sum_{i=1}^{N^{(y)}} w_{ij}^{(y-s)}(n) y_i(n-1), \\ y_j(n) = g(z2_j(n)),\ j \in \overline{1, N^{(y)}}, \\ z2_j(n) = b_j^{(y)}(n) + \sum_{i=1}^{N^{(s)}} w_{ij}^{(s-y)}(n) s_i(n) + \sum_{i=1}^{N^{(y)}} w_{ij}^{(y-y)}(n) y_i(n-1). \end{gathered} \tag{6}$$

5.Error energy calculation:

$$E(n) = \frac{1}{2}\sum_{j=1}^{N^{(y)}} e_j^2(n),\ e_j(n) = y_j(n) - d_{nj}. \tag{7}$$

6. Adjusting synaptic weights based on the generalized delta rule (reverse)

$$\begin{gathered}
b_j^{(q)}(n) = b_j^{(q)}(n) + \frac{\partial E(n)}{\partial b_j^{(q)}(n)},\quad w_{ij}^{(q-e)}(n+1) = w_{ij}^{(q-e)}(n) - \eta\frac{\partial E(n)}{\partial w_{ij}^{(q-e)}(n)},\\
\frac{\partial E(n)}{\partial b_j^{(y)}(n)} = g2_j(n),\ j \in \overline{1, N^{(y)}},\quad \frac{\partial E(n)}{\partial b_j^{(s)}(n)} = g1_j(n),\ j \in \overline{0, N^{(s)}},\\
\frac{\partial E(n)}{\partial w_{ij}^{(s-y)}(n)} = s_i(n) g2_j(n),\ i \in \overline{0, N^{(s)}},\ j \in \overline{1, N^{(y)}},\\
\frac{\partial E(n)}{\partial w_{ij}^{(y-y)}(n)} = y_i(n-1) g2_j(n),\ i \in \overline{0, N^{(y)}},\ j \in \overline{1, N^{(y)}},\\
g2_j(n) = g'(z2_j(n))(y_j(n) - d_{nj}),\quad \frac{\partial E(n)}{\partial w_{ij}^{(x-s)}(n)} = x_i(n) g1_j(n),\ i \in \overline{0, N^{(x)}},\ j \in \overline{1, N^{(s)}},\\
\frac{\partial E(n)}{\partial w_{ij}^{(s-s)}(n)} = s_i(n-1) g1_j(n),\ i \in \overline{0, N^{(s)}},\ j \in \overline{1, N^{(s)}},\\
\frac{\partial E(n)}{\partial w_{ij}^{(y-s)}(n)} = y_i(n-1) g1_j(n),\ i \in \overline{0, N^{(s)}},\ j \in \overline{1, N^{(y)}},\\
g1_j(n) = f'(z1_j(n)) \sum_{l=1}^{N^{(y)}} w_{jl}^{(s-y)}(n) g2_l(n).
\end{gathered} \tag{8}$$

7. Completion conditions validation. If $n < N$, то $n = n+1$, then go to 4.
If $n = N$ и $\frac{1}{N}\sum_{m=1}^{N} E(m) > \varepsilon$, then go to 2, otherwise stop.

Ensemble Model of Reactive Agents Functioning Based on ENN-RSRO and Soft Voting for Multiclass Classification

$$\begin{gathered}
P(k) = \frac{1}{N}\sum_{n=1}^{N}[\arg\max\{d_{nj} | j \in \overline{1, N^{(y)}}\} = k],\quad P_c(\mathbf{x} | k) = y_{ck},\quad P(\mathbf{x} | k) = \frac{1}{C}\sum_{c=1}^{C} P_c(\mathbf{x} | k),\\
k^* = \arg\max\left\{P(k | \mathbf{x}) \middle| k \in \overline{1, N^{(y)}}\right\} = \arg\max\left\{\frac{P(\mathbf{x} | k) P(k)}{\sum_{e=1}^{N^{(y)}} P(\mathbf{x} | e) P(e)} \middle| k \in \overline{1, N^{(y)}}\right\},
\end{gathered} \tag{9}$$

where C is the number of basic models,

$P(k)$ is a priori probability of occurrence of an object of k-th class,

$P_c(\mathbf{x} | k)$ is a priori probability of occurrence of an object represented by a vector $\mathbf{x}$, in the case of k-th class for c-base model, with the output values of the base model to be applied to softmax (for example, in the case of the proposed base model based on the Elman neural network with recurrent and self-recurrent output (ENN-RSRO)).

$P(k \mid \mathbf{x})$ is occurrence posterior probability of an object of *k*-th class represented by vector $\mathbf{x}$.

The proposed method of identification of parameters of the ensemble model of reactive agents functioning based on ENN-RSRO and soft voting for multiclass classification is based on bagging.

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MULTI-TASK GRAPH NEURAL NETWORK FOR PREDICTION OFADME-TOXPROPERTIES OFMOLECULES

Zakhar OSTROVSKY[1]
Volodymyr VOZNIAK[2]

[1,2]*Master of Science, Institute for Applied System Analysis, NTUU "Igor Sikorsky Kyiv Polytechnic Institute"+equal contribution*
[1]*zakharostrovsky@gmail.com*, [2]*vozniak.v.z@gmail.com*

Abstract
Prediction of ADME-Tox molecular properties is extremely important in drug discovery, as it determines the effectiveness of the drug and its success in passing the various stages of drug approval. The purpose of this work is to create a Multi-Task Graph Neural Network capable of quickly processing billion-scale databases of molecules, in order to select the most promising candidates for further experimental research.

Keywords
Graph Neural Networks, Multi-Task Learning,Drug Discovery, Molecule Property Prediction.

1. Introduction

The prediction of ADME-Tox (absorption, distribution, metabolism, excretion, and toxicity) properties of molecules is extremely important in the field of drug discovery [1, 2]. During research, scientists determine what values of these parameters the molecule must meet in order to be able to reach the causative agent of the disease, interact with it, and at the same time not be toxic to the human body and easily removed from it after treatment. That is why the effectiveness of the drug and the successful passing of the multiple stages of drug approval will depend on the accuracy of predictions of the molecules ADME-Tox properties.

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