UDC 004.032.26:532.516(045)

O.M.Glazok, c.t.s. (National Aviation University, Ukraine)

Architecture of a neural network for finding initial approximation in hydrodynamic problems

An application of neural network methods in the process of search of solution of hydrodynamic equations are offered. The architecture of a neural network for finding initial approximation in hydrodynamic problems is proposed. A model of cooperative problem solving in a computing cluster is considered.

Numerical modeling of liquids and gases motion is one of actual problems of numerical modeling. Due to lack of methods of analytical solving of the systems of equations which describe these processes, the main approach are numerical methods of solving. As estimations show, for example [1], numerical solution of hydrodynamic problems requires involving of considerable computing resources.

Machine learning is an area which develops swiftly. The growing availability of computing power, including multicore processors, distributed systems and graphic processors have become an important pre-condition to distribution of machine learning methods. For the last decade a number of programmatic instruments, which have realized important intellectual and mathematical algorithms, necessary for the construction of the systems of machine learning, have been developed, and thus considerably facilitate the construction of the systems for intellectual solution of calculation problems. Among these systems, in particular, are: MMLF, OpenAI Gym, PyBrain, RLPy, scikit-learn [2]; TensorFlow, Theano, and other. A number of applications of methods of machine learning have been offered in the solution of hydrodynamic problems [3,4]. However, on the whole these applications do not deal with the internal mechanics of hydrodynamic processes, but rather with their external descriptions. Accordingly, the solutions, offered by the researches authors, are oriented to the estimation of external side of the phenomena, but not to the methods and algorithms of solution.

The important feature of the neural networks approach is robustness of a neural model in relation to the errors in data, to the inaccuracies in determination of coefficients of equations, boundary and initial condition, errors of calculations [5]. In this work it is suggested to apply neural networks approach for charges diminishing for computation processes in the search of solution of a hydrodynamic problem. Presently, there are some works in which the neural networks approach is used for modeling of dependences and solution of differential equations in the partial derivatives. These are neural networks based on radial base functions, or radial-base neural networks, RBF-networks [6]. The important feature of radial-base neural networks is a simple algorithm of learning. With the RBF-network, forming the optimum network structure becomes the natural stage of the learning process.

The applied problems of modern hydrodynamics and aerodynamics include for itself the calculations of flows in the neighborhood of objects with complex configuration (such as an airplane, a submarine boat, a combustion engine, natural geological forms, hydrotechnical objects and others like that). The numerical approach to solution of such problems requires using calculation meshes of large dimension and complex configuration, with a variable density. A modern tendency is the use of adaptive meshes which change in the process of approximation to the solution. The issue of the day here is a considerable volume of calculations. Solutions of this problem have been offered by application of methods of machine learning, in particular neural networks methods, which will allow to prognosticate the type of approximation and pick up such form of presentation of the problem in which a process of solution will be more effective in terms of amount of calculations. It requires development of theoretical approach, finding the proper types and architectures of neural networks, development and application of the proper mathematical methods.

The modern numerical methods of solution of the systems of equations, produced by the problems of hydrodynamics, have an iterational nature. A certain initial approximation is chosen and the value of an objective function which presents the measure of accordance of the current approximate solution to the condition of optimum or to the condition of process completion is calculated. Farther, after a certain algorithm the tensor of amendments is found and the next approximation is determined, the process repeats, until the condition of completion is executed. For modern engineering problems the amount of calculation work is considerable enough and so the protracted work of calculation cluster is needed. In case of successful choice of the initial approximation, one could be able to decrease the volume of calculations considerably. In terms of the machine learning methods, this problem can be presented as a complex of problems of classification and regression (prognostication).

As an example, let us consider a problem about flat motion of liquid in a limited volume (e.g. pipe crossing). The boundary conditions near the walls of the pipe set the value of components of velocities of the media movement – v_x, v_y, and the boundary condition on the open edges of the volume determine the values of pressure on input and output cuts of model). The vector of unknown values consists of the values of the functions $f(i,j) = v_{x\ i.j}$, $g(i,j) = v_{y\ i.j}$, $h(i,j) = p_{i,j}$ in the points, where they are not determined explicitly with the boundary conditions. In all the internal points of the area the values of the functions v_x, v_y, p are unknown. In addition, there is a part of unknown values in boundary points. In most cases, ordinary mathematical algorithms of interpolation can not be applied for finding the initial approximation, as it is not enough information for this purpose and it is necessary to make additional suppositions. Using as the samples base a number of problems with the known solutions, the initial approximation can be defined through one of the following methods: choosing one instance in the samples set; forming a linear or nonlinear combination of the samples: finding such a space transformation for which one of the samples is mapped to the necessary approximation.

In the case of two-dimensional calculation, the problem of determination of such a transformation can be reduced to a problem of determination of the coordinates of a center's image and a pair of smooth functions $\beta = \beta(\alpha)$, $k = k(\alpha)$ where α and β are angles of azimuths on the prototype of point of the boundary of calculation area and its corresponding image, got as a result of application of the transform; k is an amplification coefficient, dependent on the azimuth. For the three-dimensional case it is necessary to define an analogical smooth vector function $\vec{\beta} = \vec{\beta}(\vec{\alpha})$, where the components of vectors $\vec{\alpha}$ and $\vec{\beta}$ are aggregates of angular values which determine the spatial azimuth to the point-prototype and point-image in three-dimensional space.

Modeling of the mapping transform can be performed by the combined intellectual system on the basis of neural network approach. The architecture of the system is schematically depicted in the Fig. 1.

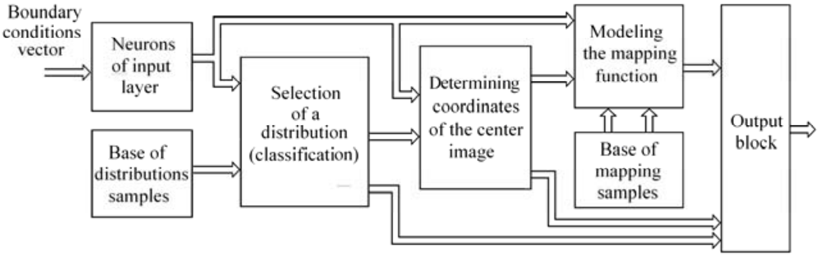

Fig..1. Architecture of an intellectual system for determination of initial numerical solution approximation of hydrodynamic problem

For modeling the transformation function, let us utilize a radial-base neural network. It is possible to describe the operation of a neuron in the i-th RBF-layer by means of the formula

$$f_i(\mathbf{X}) = \varphi\left(\left\|\mathbf{X} - \mathbf{C}_i\right\|\right) ,$$

where $\mathbf{C}_i$ is a vector of the center of activation of the radial-base function of the neuron; and . $\mathbf{X}, \mathbf{C}_i \in R^n$ The input vector and the vector of center have equal dimensions. As a radial-base function the following Gauss function can be utilized:

$$\varphi\left(\left\|\mathbf{X} - \mathbf{C}_i\right\|\right) = \exp\left(\frac{\left\|\mathbf{X} - \mathbf{C}_i\right\|^2}{2\sigma^2}\right) ,$$

where σ is a width of the activation window of the function. Thus, the i - th neuron of the hidden layer determines similarity between the input vector $\mathbf{X}$ and the standard reference vector $\mathbf{C}_i$. The activation function of the RBF-neuron gets large values in such a case . A metric can be defined as an Euclidean distance:

$$\left\|\mathbf{X} - \mathbf{C}_i\right\| = \sqrt{(x_1 - c_{i1})^2 + (x_2 - c_{i2})^2 + \ldots + (x_n - c_{in})^2} .$$

Meanwhile, the neurons of the initial layer have a linear activation function and perform the weighted addition of signals which are generated by the neurons of the working layer: $y_j = \sum_{i=1}^{n} w_{ij} f_i(\mathbf{X}),\ j = \overline{1,k}$. In this case all the factors of the radial-base layer can be taken even. The number of operating neurons is chosen in accordance with the amount of learning samples. It is necessary to find such weighing coefficients that for every input vector from the learning set $\{(\mathbf{X}_1, y_1), (\mathbf{X}_2, y_2), ..., (\mathbf{X}_n, y_n)\}$, де $\mathbf{X}_i = \{x_{i1}, x_{i2}, ..., x_{ik}\}$, the requirement $h(\mathbf{X}_i) = y_i$ would be satisfied.

The following system of correlations which must be satisfied at the successful tuning of network by means of choice of the weights:

$$\begin{vmatrix} f_i(X_1) & f_2(X_1) & \cdots & f_n(X_1) \\ f_i(X_2) & f_2(X_2) & \cdots & f_n(X_2) \\ \vdots & \vdots & \vdots & \vdots \\ f_i(X_n) & f_2(X_n) & \cdots & f_n(X_n) \end{vmatrix} \begin{vmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{vmatrix} = \begin{vmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{vmatrix}, \quad (1)$$

or, in the matrix form: $\mathbf{F}\,\mathbf{W} = \mathbf{Y}$, from where

$$\mathbf{W} = \mathbf{F}^{-1}\mathbf{Y} \quad . \quad (2)$$

One can obtain similar results at the arbitrary quantity of neurons of initial layer of the RBF-network. Let a layer contains p neurons, then the vector of output values looks like $\mathbf{Y}_i = \left[y_{i1}, y_{i2}, ..., y_{ip}\right]^T$.

The weights of neurons of the initial layer form a matrix in this case, and equation, analogical to equation (1), with the terms **W** and **Y** having the form of rectangular matrices. The sets of coefficients in the lines of the **Y** matrix describe the outputs of neurons of initial layer of a network for every input vector. The formula (2) remains true for this case.

The method of reinforcement learning is well adjusted for problems which include a compromise between a long-term and short-term reward. Exactly such situation is observed at the numerical solution of hydrodynamic problem on a multiprocessor system or a computing cluster. In such a design, each processor has its own sphere of responsibility that corresponds to a separate block of calculation mesh. A situation can be described as a Markov-type game with many players [7], the parameters of which are: the set of states S_i for each i-th player, $i = 1..N$ (the player's state includes the values of components of the sought matrices or tensors which make the current approximation in the area of responsibility for each of processors); the observation functions $O_i : S_1 \times ... \times S_N \to R^d$, which define the d-dimensional observed data for each of the players; the sets of possible actions A_i for each of the players; the reinforcement functions $r_i : S_i \times A_1 \times ... \times A_N \to R$ for each of the players. A player chooses the strategy $\pi_i : O_i \to \Delta(A_i)$.

Conclusions

An application of neural network methods in the process of search of solution of hydrodynamic equations is offered. The proposed approach will allow to prognosticate the type of approximation and chose an optimal form of problem presentation. The offered approach, in a prospect, can provide the considerable advantages in the volume of calculations, due to reducing of subproblems which arise up on the separate stages of calculations to the problems already solved before. For achievement of these results it is necessary to conduct the detailed researches in a number of directions, Among them is a problem of forming the samples base, finding a compromise between the amount of data stored in these bases and the amount of calculation work for its application; approaches to forming the mapping the reinforcement functions on condition that an exact solution is unknown, a problem of forming strategies for the participants of a distributed computing system, considered as players in co-operative games, and others. Another possible direction of research is finding approaches to effective forming of dynamic computing nets that on every stage of calculations would give an acceptable compromise between the current attained general exactness of approximation and description of the special regions.

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