https://doi.org/10.15407/dopovidi2019.12.019 UDK 517.2+519.977.58+519.8

V.I. Norkin

V.M. Glushkov Institute of Cybernetics of the NAS of Ukraine, Kyiv NTU of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" E-mail: vladimir.norkin@gmail.com

Substantiation of the backpropagation technique via the Hamilton—Pontryagin formalism for training nonconvex nonsmooth neural networks

Presented by Corresponding Member of the NAS of Ukraine P.S. Knopov

The paper observes the similarity between the stochastic optimal control over discrete dynamical systems and the learning multilayer neural networks. It focuses on contemporary deep networks with nonconvex nonsmooth loss and activation functions. The machine learning problems are treated as nonconvex nonsmooth stochastic optimization ones. As a model of nonsmooth nonconvex dependences, the so-called generalized differentiable functions are used. A method for calculating the stochastic generalized gradients of a learning quality functional for such systems is substantiated basing on the Hamilton—Pontryagin formalism. This method extends a well-known "backpropagation" machine learning technique to nonconvex nonsmooth networks. Stochastic generalized gradient learning algorithms are extended for training nonconvex nonsmooth neural networks.

Keywords: machine learning, deep learning, multilayer neural networks, nonsmooth nonconvex optimization, stochastic optimization, stochastic generalized gradient.

Introduction. The machine learning problem consists of the identification of parameters of a neural network model, e.g., neural weights, using a set of input-output observations. The training task is formulated as a task of minimizing some smooth loss functional (empirical risk), which measures the average forecast error of the neural network model.

Methods of training (identification) of large neural network models are discussed in many articles and books [1, 2]. To train deep (i.e., multilayer) neural networks, the stochastic gradient method and its modifications are mainly used [2, 3], being adopted from the theory of stochastic approximation and stochastic programming, since only they are practically applicable for training such networks. The stochastic gradient of a risk functional is a random vector whose mathematical expectation approximates the gradient of a target functional, and the stochastic gradient descent method is an iterative one for changing the desired model parameters in the direction of the stochastic (anti-) gradient.

To solve smooth neural network training problems, the BackProp method is widely used [1, 4], i.e. a special method for calculating the gradients of a target functional with respect to

various parameters. The history of the discovery, development, and application of the BackProp method was studied in [5]. Nonsmooth machine learning tasks arise, when using nonsmooth (module type) indicators of the quality of training, when applying nonsmooth regularizations, and when using nonsmooth (e. g., piecewise linear, linear rectification ReLU, etc.) activation functions in multilayer neural networks [1, 5]. Such functions give rise to essentially nonconvex nonsmooth functionals of the quality of learning, and the question arises of the convergence of the stochastic generalized gradient descent method in solving such problems. This problem has been relatively recently recognized and is already considered in the literature [6]. However, it is usually assumed using the Clarke stochastic subgradients [7] of the optimized functional, but the problem of their calculation for deep networks is not discussed.

In this paper, we extend the BackProp method to calculating the stochastic gradients of non-convex nonsmooth problems for training the multilayer neural networks and formulate the method in terms of stochastic generalized gradients of nonsmooth Hamilton—Pontryagin functions. As a model of nonsmooth nonconvex dependences, we use the so-called generalized differentiable functions [8, 9]. We also consider an important version of the BackProp method for training the so-called recurrent neural networks, i.e. networks with feedbacks and memory [1, Ch. 10].

Nonconvex nonsmooth learning problems and calculation of stochastic generalized gradients. Let us consider a standard neural network model. Let the network consist of m layers of neurons, let each layer $i \in \{1, ..., m\}$ have n_i neurons with numbers $j = 1, ..., n_i$ and let each of them have n_{i-1} inputs and one output. In the initial layer, there are n_1 neurons, each neuron of this layer has n_0 common inputs and one output. The outputs of the neurons of each layer go to the inputs of the neurons of the next layer. The output layer of the network may consist of one or more neurons.

In the theory of neural networks, the standard mathematical model of neuron (i,j) is some smooth activation function $g_i^j(x_i,w_{ij},v_{ij})$ (e.g., the logistic sigmoid, the hyperbolic tangent, etc. [1, Section 6.3.2], which expresses the dependence of the output signal $x_{(i+1)j}$ of neuron (i,j) on the input signal x_i , for example, $x_{(i+1)j} = g_i^j(x_i,w_{ij},v_{ij}) = (1+\exp\{-\langle x_i,w_{ij}\rangle-v_{ij}\})^{-1}$, where $x_i \in R^{n_{i-1}}$ is a common input of all neurons in layer i; $w_{ij} \in R^{n_{i-1}}$ and $v_{ij} \in (-\infty, +\infty)$ are the individual weight vector and the activation level of neuron $j \in \{1, ..., n_i\}$ in layer i; the expression $\langle x_i, w_{ij} \rangle$ denotes the scalar product of the vectors x_i and w_{ij} . The weights w_{ij} and thresholds v_{ij} may satisfy the constraints $w_{ij} \in W_{ij}$, $v_{ij} \in V_{ij}$. Here, the notation like R^n is used for the n-dimensional Euclidian vector space.

Note that activation functions themselves can be random, for example, neurons can accidentally fall into the so-called sleep (drop out) state, i.e. produce a zero output signal: $g_i^j(x_i, w_{ij}, v_{ij}, \omega_{ij}) = \omega_{ij} \cdot g_i^j(x_i, w_{ij}, v_{ij})$, where ω_{ij} is an additional random parameter taking values 1 or 0 with probabilities p_{ij} and $1-p_{ij}$. We assume that the random parameters $\{\omega_{ij}\}$ are independent and combined into a common vector $\omega = \{\omega_{ij}\}$ that takes values from a finite set Ω .

In what follows, we assume that the activation functions $g_i^j(x_i, w_{ij}, v_{ij}, \omega_{ij})$ of neurons $j = 1, ..., n_i$ in each layer i for any fixed value of ω_{ij} are generalized differentiable with respect of their variables (x_i, w_{ij}, v_{ij}) in the sense of the following definition, which covers all practical examples.

Definition 1 [8–10]. A function $f: \mathbb{R}^n \to \mathbb{R}^1$ is called generalized differentiable at the point $\overline{z} \in \mathbb{R}^n$, if, in some ε -neighborhood $\{z \in \mathbb{R}^n : \|z - \overline{z}\| < \varepsilon\}$ of the point \overline{z} , a multivalued mapping $\partial f(\cdot)$ upper semicontinuous at \overline{z} , with convex compact values $\partial f(z)$ is defined and is such that the following expansion holds true:

$$f(z) = f(\overline{z}) + \langle d, z - \overline{z} \rangle + o(\overline{z}, z, d)$$

where $d \in \partial f(z)$, $\langle \cdot, \cdot \rangle$ denotes a scalar product of two vectors, and the remainder term $o(\overline{z}, z, d)$ satisfies the condition: $\lim_{k \to \infty} o(\overline{z}, z^k, d^k) / \|z^k - \overline{z}\| = 0$ for all sequences $d^k \in \partial f(z^k)$, $z^k \to \overline{z}$ as $k \to \infty$. A function f is called generalized differentiable, if it is generalized differentiable at each point $\overline{z} \in \mathbb{R}^n$; the mapping $\partial f(\cdot)$ is called the generalized gradient mapping of the function f; the set $\partial f(z)$ is called a generalized gradient set of the function $f(\cdot)$ at a point z; vectors $d \in \partial f(z)$ are called generalized gradients of the function $f(\cdot)$ at a point z.

Properties of generalized differentiable functions were studied in details in [8–10]. In particular, it was shown that they are locally Lipschitzian, and their Clarke subdifferential $\partial_C f(z)$ can serve as a generalized gradient mapping $\partial f(z)$ of $f(\cdot)$, and $\partial_C f(z) \subseteq \partial f(z)$ always holds. This class of functions contains continuously differentiable, convex, and concave functions and is closed with respect to finite maximum, minimum, superposition operations, and with respect to taking the mathematical expectation.

Suppose that there is a (training) set $\{(x_1^s \in \mathbb{R}^{n_0}, y_{m+1}^s \in \mathbb{R}^{n_m}), s = 1, ..., S\}$ of observations of a network inputs-outputs. The standard training (identification) task for the network with the training quality criterion $\varphi(x_{m+1}^s, y_{m+1}^s)$ and regularization is as follows:

$$J(\{w_{ij}\}, \{v_{ij}\}) = \mathbf{E}_{\omega} \frac{1}{S} \sum_{s=1}^{S} \varphi(x_{m+1}^{s}, y_{m+1}^{s}) + \lambda \sum_{i=1}^{m} \sum_{j=1}^{n_{i}} \left(\left\| w_{ij} \right\|^{\alpha} + \left| v_{ij} \right|^{\alpha} \right) \rightarrow \min_{\{u_{ij} \in W_{ij}\}, \{v_{ij} \in V_{ij}\}, \{v_$$

where $x_{m+1}^s \in \mathbb{R}^{n_k}$ is the vector of outputs of the last network layer for a training example s; $y_{m+1}^s \in \mathbb{R}^{n_k}$ is a known, generally speaking, multidimensional vector of observations of the network outputs; $\|w_{ij}\|$ denotes the norm of the vector w_{ij} ; $\lambda > 0$, $\alpha \geqslant 1$; \mathbf{E}_{ω} is the mathematical expectation operator over ω ; the sequence of layers' outputs $\{x_i^s = (x_{i1}^s, ..., x_{in_i}^s)^T, i = 2, ..., m+1\}$ for a given first layer input $x_1^s \in \mathbb{R}^{n_0}$ is given by the relations

$$x_{(i+1)j}^{s} = g_i^{j}(x_i^{s}, w_{ij}, v_{ij}, \omega_{ij}), \quad j = 1, ..., n_i, \quad i = 1, ..., m.$$
(2)

Moreover, the training examples may contain not only the input and output of a network (e. g., features and labels of objects) $\{(x_1^s, y_{m+1}^s), s=1,...,S\}$, but also may include additional intermediate features $y_i^s \in \mathbb{R}^{n_i}$, $i \in I \subset \{2,...,m\}$, which can be used to improve the learning of the intermediate layers of the network, i.e. training examples may take the form of sequences $\{(x_1^s, \{y_i^s, i \in I\}, y_{m+1}^s), s=1,...,S\}$. That's why we consider the following general network training task:

$$J(u) = \mathbf{E}_{\theta} \sum_{i=1}^{m} f_i(x_i(\theta), u_i) + \mathbf{E}_{\theta} f_{m+1}(x_{m+1}(\theta)) \to \min_{u \in U}$$
 (3)

subject to constraints (satisfied for all values of the random parameter $\theta \in \Theta$):

$$x_{i+1}(\theta) = g_i(x_i(\theta), u_i, \theta) = \{g_i^j(x_i(\theta), u_{ij}, \theta)\}_{j=1}^{n_i}, \quad i = 1, ..., m; \quad x_1(\theta) \in \mathbb{R}^{n_0}.$$
 (4)

Here, $u = (u_1, ..., u_m) \in \mathbb{R}^l \left(l = \sum_{i=1}^m n_i \right)$ is the vector of all adjusted parameters $(u = (\{w_{ij}\}, \{v_{ij}\}))$ for problem (1), (2)); $x_i = (x_{i1}, ..., x_{in_{i-1}})^T$ is the input vector for neurons in layer i; u_{ij} is the ISSN 1025-6415. Долов. Нац. акад. наук Укр. 2019. N2 12

vector of the adjusted parameters of neuron (i,j); $u_i = \{u_{ij}\}_{j=1}^{n_i-1}$ is the vector of the adjusted parameters of all neurons in layer i; g_i^j is the activation function of neuron j in layer i; $g_i = \{g_i^j\}_{j=1}^{n_i}$ is the vector activation function of the neurons in layer i; $x_1(\theta) \in \mathbb{R}^{n_0}$ is a random vector of input signals to the network; θ is a random vector parameter that defines the distribution of input signals and influences the propagation of signals through the network $(\theta = (s, \omega))$ for problem (1), (2); and \mathbf{E}_{θ} denotes the sign of the mathematical expectation over θ .

Assumption. Suppose that, in problem (3), (4), the functions $f_i(x_i, u_i)$, $g_i^j(x_i, u_{ij}, \theta)$, and $f_{m+1}(x_{m+1})$ are generalized differentiable with respect to the totality of their arguments, respectively, (x_i, u_i) , (x_i, u_{ij}) , and x_{m+1} (for fixed θ). Here, the activation function $g_i^j(x_i, u_{ij}, \theta)$ can be of a general form, i.e. optionally, the function g_i^j may depend not on all elements of the vector x_i , and the dimension of the vector of the adjustable parameters u_{ij} may not coincide with the dimension of the vector of inputs x_i . The random parameter $\theta \in \Theta$ is a random variable defined on some probability space.

Note that, in the literature (see, e. g., [6]) for the purpose of training neural networks, it is proposed to use (stochastic) Clarke subgradients of the risk functional J(u), but these subgradients are relatively simple to be calculated only for subdifferentially regular Lipschitz functions [7, §2.3, §2.7]. For general nonconvex nonsmooth functions, their calculation is a problem.

For arbitrary generalized differentiable (over the totality of variables) vector functions $g_i(x, u) \in \mathbb{R}^{n_i}$ with arguments $x = (x^1, ..., x^n)^T \in \mathbb{R}^n$, $u = (u^1, ..., u^l)^T \in \mathbb{R}^l$, we denote the matrices:

$$g_{ix} = \begin{pmatrix} g_{ix^{1}}^{1} & \cdots & g_{ix^{n}}^{1} \\ \cdots & \cdots & \cdots \\ g_{ix^{1}}^{n_{i}} & \cdots & g_{ix^{n}}^{n_{i}} \end{pmatrix} = \begin{pmatrix} g_{ix}^{1} \\ \cdots \\ g_{ix}^{n_{i}} \end{pmatrix}, \quad g_{iu} = \begin{pmatrix} g_{iu^{1}}^{1} & \cdots & g_{iu^{l}}^{1} \\ \cdots & \cdots & \cdots \\ g_{iu^{1}}^{n_{i}} & \cdots & g_{iu^{l}}^{n_{i}} \end{pmatrix} = \begin{pmatrix} g_{iu}^{1} \\ \cdots \\ g_{iu}^{n_{i}} \end{pmatrix}.$$

For arbitrary generalized differentiable (over the totality of arguments) scalar functions $f_i(x, u)$, $x \in \mathbb{R}^n$, $u \in \mathbb{R}^l$, and $f_{m+1}(x)$, $x \in \mathbb{R}^n$, let us introduce vectors

$$(f_{ix})^T = (f_{ix^1}, ..., f_{ix^n}), (f_{iu})^T = (f_{iu^1}, ..., f_{iu^l}), (\varphi_{kx})^T = (\varphi_{kx^1}, ..., \varphi_{kx^n}),$$

where $(f_{ix}, f_{iu})^T$, $(g_{ix}^j, g_{iu}^j)^T$ are some generalized gradients of the functions $f_i(\cdot, \cdot)$, $g_i^j(\cdot, \cdot, \theta)$; $f_{(m+1)x}(\cdot)$ is some generalized gradient of the function $f_{m+1}(\cdot)$; and the expression $(\cdot)^T$ denotes the transposition of matrix (\cdot) .

The next theorem exploits the similarity between optimal control problems for discrete dynamical systems [11, 12] and multilayer neural networks and formalizes a method for calculating the stochastic generalized gradients in the problem of training a nonconvex nonsmooth neural network. It extends the well-known method of "backpropagation of the error" (BackProp) [1, 4, 5] to nonconvex nonsmooth learning problems.

Theorem 1. Under the assumptions made, the objective function J(u) of problem (3), (4) is generalized differentiable with respect to variables $u = (u_1 \in \mathbb{R}^{n_1}, ..., u_m \in \mathbb{R}^{n_m})$, and the vectors

$$h_{u}(u,\theta) = (h_{1u_{1}}(x_{1}(\theta), \psi_{1}(\theta), u_{1}), h_{2u_{2}}(x_{2}(\theta), \psi_{2}(\theta), u_{2}), ...,$$

$$..., h_{mu_{m}}(x_{mm}(\theta), \psi_{m}(\theta), u_{m}))^{T}$$
(5)

are stochastic generalized gradients of the function J(u) at a given point u, i.e., $\mathbf{E}_{\theta}h_{u}(u,\theta) \in \partial J(u)$, where $h_{i}(x_{i},\psi_{i},u_{i})=f_{i}(x_{i},u_{i})+g_{i}^{T}(x_{i},u_{i})\cdot\psi_{i}$, i=1,...,m, is a discrete (over i) Hamilton—Pontryagin function; the vector

$$h_{iu_{i}}(x_{i}(\theta), \psi_{i}(\theta), u_{i}) = (h_{iu_{i}^{1}}(x_{i}(\theta), \psi_{i}(\theta), u_{i}), \dots, h_{iu_{i}^{n_{i}}}(x_{i}(\theta), \psi_{i}(\theta), u_{i}))^{T} =$$

$$= (f_{iu_{i}^{1}}(x_{i}(\theta), u_{i}) + g_{iu_{i}^{1}}^{T}(x_{i}(\theta), u_{i}) \cdot \psi_{i}(\theta), \dots,$$

$$f_{iu_{i}^{n_{i}}}(x_{i}(\theta), u_{i}) + g_{iu_{i}^{n_{i}}}^{T}(x_{i}(\theta), u_{i}) \cdot \psi_{i}(\theta))^{T} \in \mathbb{R}^{n_{i}}$$
(6)

is the u_i -component of a generalized gradient of the function $h_i(\cdot, \psi_i, \cdot)$, i=1,...,m; $x(\theta)==(x_1(\theta),...,x_{m+1}(\theta))$ is a discrete random trajectory of process (4), corresponding to the given sequence of parameters $(u_1,...,u_m)=u$ and the random initial data $x_1(\theta)\in\mathbb{R}^{n_0}$. Here, the random sequence of auxiliary (conjugate) vector functions $(\psi_1(\theta),...,\psi_m(\theta))=\psi(\theta)$ is determined through the backpropagation equations (adopted from the Pontryagin maximum principle): $\psi_m(\theta)=f_{(m+1)x_{m+1}}(x_{m+1}(\theta))$,

$$\psi_{i-1}(\theta) = h_{ix_i}(x_i(\theta), \psi_i(\theta), u_i) = f_{ix_i}(x_i(\theta), u_i) + g_{ix_i}^T(x_i(\theta), u_i) \cdot \psi_i(\theta),
i = m, m-1, ..., 2;$$
(7)

 $(f_{ix}(x_i(\theta), u_i), f_{iu}(x_i(\theta), u_i))^T$, $(g_{ix}^j(x_i(\theta), u_i), g_{iu}^j(x_i(\theta), u_i))^T$ are some generalized gradients of the functions $f_i(\cdot, \cdot)$, $g_i^j(\cdot, \cdot, \theta)$ at the point $(x_i(\theta), u_i)$, and $f_{(m+1)x_{m+1}}(x_{m+1}(\theta))$ is some generalized gradient of the function f_{m+1} at the point $x_{m+1}(\theta)$, which are used in (6), (7).

Proof. Note that process (4) can be formally treated as a stochastic dynamic system [12, 13] in the discrete time i = 1, ..., m+1 with states x_i , control parameters u_i , a given initial state $x_1(\theta)$, and the optimality criterion (3). The stochasticity of system (4) is generated by the random input $x_1(\theta)$, a random mechanism of dropping out of neurons, and possibly other factors. Using relations (4), the vectors x_i , i = 2, ..., m+1, can be sequentially excluded from the formulation of the optimization problem (3). Then, under the sign of summation in (3), there remains some complex composite function $f(u, \theta) = \sum_{i=1}^{m} f_i(\tilde{x}_i(u_1, ..., u_{i-1}, \theta), u_i) + f_{m+1}(\tilde{x}_{m+1}(u_1, ..., u_m, \theta))$, which depends on optimization variables u, and where $\tilde{x}_i(u_1,...,u_{i-1},\theta)$, i=2,...,m+1, are complex compound functions of their arguments. Since the class of generalized differentiable functions is closed with respect to compositions, this function $f(u,\theta)$ under the made assumptions becomes generalized differentiable with respect to u for each $\theta \in \Theta$. The expectation \mathbf{E}_{θ} (in this case, summation) does not move out from the class of generalized differentiable functions. Therefore, the function $J(u) = \mathbf{E}_{\theta} f(u, \theta)$ is also generalized differentiable with respect to u. Now, similar to the proofs of Theorems 6–8 from [13], applying the rules of differentiation of the sum, the chain rule of differentiation of complex generalized differentiable functions [8, 9] (which are analogs to the rules of differentiation of smooth and convex functions), and introducing the auxiliary variables (7), after some algebraic manipulations [13], we obtain formula (6) for stochastic generalized gradients $h_u(u, \theta)$ of the function J(u).

Neural networks may have a complex heterogeneous structure. However, introducing the additional dummy neurons, such networks can be reduced to a canonical multilayer form, and, for them, one can apply the formulas of Theorem 1.

Let us consider an important special case of networks in which the adjusted parameters are the same for each layer. For example, a network can consist of identical neurons, or some identical neurons are added to each layer in an already trained network, or the network consists of duplicates of the same layer. Then, similarly to (3), (4), the training task consists in solving the following problem:

$$J(u) = \mathbf{E}_{\theta} \sum_{i=1}^{m} f_i(x_i(\theta), u) + \mathbf{E}_{\theta} f_{m+1}(x_{m+1}(\theta)) \to \min_{u=(u_1, \dots, u_l) \in U \subseteq R^l},$$
 (8)

$$x_{i+1}(\theta) = g_i(x_i(\theta), u, \theta) = \{g_i^j(x_i(\theta), u, \theta)\}_{i=1}^{n_i}, \quad i = 1, ..., m; \ x_1(\theta) \in \mathbb{R}^{n_0}.$$
(9)

Theorem 2. Under the assumptions made, the objective function J(u) of problem (8), (9) is generalized differentiable with respect to variables $u = (u_1, ..., u_l)$, and the vector

$$\left(\sum_{i=1}^{m} h_i(x_i(\theta), \psi_i(\theta), u)\right)_{u} = \left(\sum_{i=1}^{m} h_{iu_1}(x_i(\theta), \psi_i(\theta), u), \dots, \sum_{i=1}^{m} h_{iu_l}(x_i(\theta), \psi_i(\theta), u)\right)^{T}$$

is a stochastic generalized gradient of the function J(u) at the point u, i.e.

$$\mathbf{E}_{\theta} \left(\sum_{i=1}^{m} h_i(x_i(\theta), \Psi_i(\theta), u) \right)_{u} \in \partial J(u),$$

where

$$h_i(x_i, \psi_i, u) = f_i(x_i, u) + g_i^T(x_i, u) \cdot \psi_i, i = 1, ..., m,$$

is a discrete (over i) Hamilton—Pontryagin function; $x(\theta) = (x_1(\theta), ..., x_{m+1}(\theta))$ is a discrete random trajectory of process (9), corresponding to the vector parameter u and the random initial data $x_1(\theta) \in \mathbb{R}^{n_0}$. Here, the random sequence of auxiliary (conjugate) vector functions $(\psi_1(\theta), ..., \psi_m(\theta)) = \psi(\theta)$ is determined through the backpropagation equations: $\psi_m(\theta) = f_{(m+1)x_{m+1}}(x_{m+1}(\theta))$,

$$\psi_{i-1}(\theta) = h_{ix_i}(x_i(\theta), \psi_i(\theta), u) = f_{ix_i}(x_i(\theta), u) + g_{ix_i}^T(x_i(\theta), u) \cdot \psi_i(\theta), \quad i = m, m-1, ..., 2.$$

The method of stochastic generalized gradient descent and its variants. The stochastic gradient descent method [3] is the main method for training the deep neural networks, firstly, because of enormous dimensions of such networks and, secondly, due to the regularizing properties of the method. The properties of the stochastic gradient method and its modifications were studied in details in the cases of smooth and convex optimized functions [2, 3, 12]. In [9, 14, 15], this method and its modifications were substantiated for the solution of nonconvex nonsmooth stochastic programming problems (with generalized differentiable functions), and thus are applicable to nonconvex nonsmooth machine learning problems.

The work is partially supported by grant CPEA-LT-2016/10003 funded by the Norwegian Agency for International Cooperation and Quality Enhancement in Higher Education (Diku).

REFERENCES

- 1. Goodfellow, I., Bengio, Y. & Courville, A. (2016). Deep learning. Cambridge: The MIT Press. Retrieved from http://www.deeplearningbook.org
- 2. Bottou, L., Curtisy, F. E. & Nocedalz, J. (2018). Optimization methods for large-scale machine learning. SIAM Rev., 60, No. 2, pp. 223-311. https://doi.org/10.1137/16M1080173
- 3. Newton, D., Yousefian, F. & Pasupathy, R. (2018). Stochastic gradient descent: recent trends. INFORMS TutORials in Operations Research, pp. 193-220. https://doi.org/10.1287/educ.2018.0191
- 4. Rumelhart, D. E., Hinton, G. E. & Williams, R. J. (1986). Learning representations by back-propagating errors. Nature, 323, pp. 533-536. https://doi.org/10.1038/323533a0
- 5. Schmidhuber, J. (2015). Deep learning in neural networks: An overview. Neural Networks, 61, pp. 85-117. https://doi.org/10.1016/j.neunet.2014.09.003
- 6. Davis, D., Drusvyatskiy, D., Kakade, S. & Lee, J. D. (2019). Stochastic subgradient method converges on tame functions. Found. Comput. Math., pp. 1-36. https://doi.org/10.1007/s10208-018-09409-5
- 7. Clarke, F. H. (1990). Optimization and nonsmooth analysis. Classics in Applied Mathematics, Vol. 5. 2nd ed. Philadelphia, PA: SIAM.
- 8. Norkin, V.I. (1980). Generalized differentiable functions. Cybernetics, 16, No. 1, pp. 10-12. $\frac{10-12}{1007} = \frac{10-12}{1007} = \frac{10-1$
- 9. Mikhalevich, V. S., Gupal, A. M. & Norkin, V. I. (1987). Methods of nonconvex optimization. Moscow: Nauka (in Russian).
- 10. Norkin, V. I. (1986). Stochastic generalized-differentiable functions in the problem of nonconvex nonsmooth stochastic optimization. Cybernetics, 22, No. 6, pp. 804-809. https://doi.org/10.1007/BF01068698
- 11. Bryson, A. E. & Ho, Y-C. (1969). Applied optimal control: optimization, estimation, and control. Waltham: Blaisdell Publ. Co.
- 12. Ermoliev, Y. M. (1976). Methods of stochastic programming. Moscow: Nauka (in Russian).
- 13. Norkin V. I. (2019). Generalized gradients in problems of dynamic optimization, optimal control, and machine learning. Preprint. V.M. Glushkov Institute of Cybernetics of the National Academy of Sciences of Ukraine, Kyiv. Retrieved from http://www.optimization-online.org/DB HTML/2019/09/7374.html
- 14. Ermol'ev, Yu. M. & Norkin, V. I. (1998). Stochastic generalized gradient method for solving nonconvex non-smooth stochastic optimization problems. Cybern. Syst. Anal., 34, No. 2, pp. 196-215. https://doi.org/10.1007/BF02742069
- 15. Ermoliev, Y. M. & Norkin, V. I. (2003). Solution of nonconvex nonsmooth stochastic optimization problems. Cybern. Syst. Anal., 39, No. 5, pp. 701-715. https://doi.org/10.1023/B:CASA.0000012091.84864.65

Received 20.09.2019

В.І. Норкін

Інститут кібернетики ім. В.М. Глушкова НАН України, Київ НТУ України "Київський політехнічний інститут ім. Ігоря Сікорського" E-mail: vladimir.norkin@gmail.com.

ОБҐРУНТУВАННЯ ЗА ДОПОМОГОЮ ФОРМАЛІЗМУ ГАМІЛЬТОНА—ПОНТРЯГІНА МЕТОДУ ЗВОРОТНОГО ПРОСУВАННЯ ПОХИБКИ ДЛЯ НАВЧАННЯ НЕОПУКЛИХ НЕГЛАДКИХ НЕЙРОННИХ МЕРЕЖ

Простежується аналогія між задачами оптимального керування дискретними стохастичними динамічними системами та задачами навчання багатошарових нейронних мереж. Увага концентрується на вивченні сучасних глибоких мереж з негладкими цільовими функціоналами і зв'язками. Показано, що задачі машинного навчання можуть трактуватися як задачі стохастичного програмування, і для їхнього аналізу застосовано теорію неопуклого негладкого стохастичного програмування. Як модель негладких неопуклих залежностей використано так звані узагальнено диференційовані функції. Обґрунтовано метод обчислення стохастичних узагальнених градієнтів функціонала якості навчання для таких систем на основі формалізму Гамільтона—Понтрягіна. Цей метод узагальнює відомий метод "зворотного просування похибки" на

задачі навчання негладких неопуклих мереж. Узагальнені (стохастичні) градієнтні алгоритми навчання поширено на неопуклі негладкі нейронні мережі.

Ключові слова: машинне навчання, глибоке навчання, багатошарові нейронні мережі, негладка неопукла оптимізація, стохастична оптимізація, стохастичний узагальнений градієнт.

В.И. Норкин

Институт кибернетики им. В.М. Глушкова НАН Украины, Киев НТУ Украины "Киевский политехнический институт им. Игоря Сикорского" E-mail: vladimir.norkin@gmail.com.

ОБОСНОВАНИЕ ПОСРЕДСТВОМ ФОРМАЛИЗМА ГАМИЛЬТОНА—ПОНТРЯГИНА МЕТОДА ОБРАТНОГО РАСПРОСТРАНЕНИЯ ОШИБКИ ДЛЯ ОБУЧЕНИЯ НЕВЫПУКЛЫХ НЕГЛАДКИХ НЕЙРОННЫХ СЕТЕЙ

Прослеживается аналогия между задачами оптимального управления дискретными стохастическими динамическими системами и задачами обучения многослойных нейронных сетей. Внимание концентрируется на изучении современных глубоких сетей с негладкими целевыми функционалами и связями. Показано, что задачи машинного обучения могут трактоваться как задачи стохастического программирования, и для их анализа применена теория невыпуклого негладкого стохастического программирования. В качестве модели негладких невыпуклых зависимостей использованы так называемые обобщенно дифференцируемые функции. Обоснован метод вычисления стохастических обобщенных градиентов функционала качества обучения для таких систем на основе формализма Гамильтона—Понтрягина. Этот метод обобщает известный метод "обратного распространения ошибки" на задачи обучения негладких невыпуклых сетей. Обобщенные (стохастические) градиентные алгоритмы обучения распространены на невыпуклые негладкие нейронные сети.

Ключевые слова: машинное обучение, глубокое обучение, многослойные нейронные сети, негладкая невыпуклая оптимизация, стохастическая оптимизация, стохастический обобщенный градиент.