SOLVING THE TRANSPORT EQUATION USING SIGMOIDAL FUNCTION APPROXIMATION

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In recent years, machine learning methods have gained popularity for solving differential equations [1]. This approach is based on the Kolmogorov-Arnold [2] and Cybenko [3] theorems on representation of function as a neural network in a sum of parameterized sigmoidal transformations of one-dimensional linear functions. This method is similar to the Galerkin method [4], where activation functions satisfying the requirements of the theorems are chosen as basis functions. These approximations allow for considering the nonlinear and even discontinuous nature of the original function's behavior.

As a test example, the solution of a mathematical physics equation in the class of infinitely smooth sigmoidal functions is considered, specifically, a one-dimensional linear transport equation with a discontinuous initial condition in the form of a step function:

$$u_t + a u_x = 0, \qquad 0 \le x \le 1, \quad 0 \le t \le 1, \qquad u(x,0) = u_0 = \begin{cases} 2, \; x \le 0.5 \\ 1, \; x > 0.5 \end{cases}, \tag{1}$$

where a is the transport speed constant. The neural network solution of the equation was verified by comparison with the exact solution: $u(x,t) = u_0(x - at)$.

To solve equation (1), an approximation using a single-layer neural network with a sigmoidal function was chosen:

$$u(x,t) \approx U(x,t) = \sum_{i=1}^{K} W_i \, \sigma\left(A_i x + B_i t + C_i\right) + D, \tag{2}$$

where W_i, A_i, B_i, C_i, D (3) are the search parameters ("weights") of the neural network, $\sigma(s) = 1/\left(1+\exp(-s)\right)$, K is the number of neurons.

Modern tensor library technologies (such as torch) enable efficient utilization of advanced mathematical algorithms in working with neural networks. For optimization problems, modifications of stochastic gradient descent are provided for an arbitrary number of parameters. The calculation of exact derivatives of functions from search parameters (3) using automatic differentiation methods is also supported. Therefore, derivatives of approximation (2) can be written for the solution of the transport equation, allowing ones to approximate the differential part:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} \approx \frac{\partial U}{\partial t} + a\frac{\partial U}{\partial x}, \tag{4}$$

$$\frac{\partial U(x,t)}{\partial x} = \sum_{i=1}^{K} W_i \, A_i \, \sigma'(A_i x + B_i t + C_i),$$

$$\frac{\partial U(x,t)}{\partial t} = \sum_{i=1}^{K} W_i \, B_i \, \sigma'(A_i x + B_i t + C_i),$$

where $\sigma'(s) = \sigma(s)\left(1 - \sigma(s)\right)$.

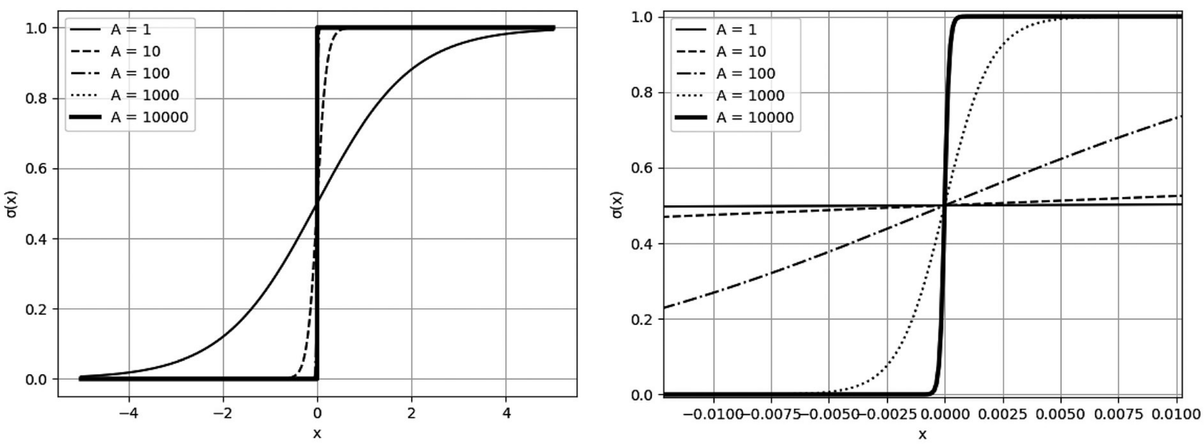
The final step involves minimizing the residual L with respect to the parameters (3) as the sum of L^2 norms of the differential equation and initial conditions using the Adam optimizer from the torch module in Python:

$$L = \left\| \frac{\partial U}{\partial x} + a\frac{\partial U}{\partial t} \right\|_{L^2} + \left\| U_0 - u_0 \right\|_{L^2} \to 0. \tag{5}$$

It was found that, due to the chosen class of infinitely smooth sigmoidal functions (2), a large value of search parameter A allows achieving the required accuracy in describing the discontinuity at x (see

Fig. 1) for the entire time interval t. This makes it possible to obtain a discontinuous solution of the transport equation with the necessary precision.

A comparison of the accuracy of the obtained neural network solution with finite-difference methods of various orders of accuracy is also performed.



a *b*

Fig. 1. Sigmoid function converging to the Heaviside step function as a function of the parameter at *x*:
a – domain from –5 to 5; *b* – 800× magnification

References

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