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ANN-MoC Approach for Solving First-Order Partial Differential Equations

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Linear first-order partial differential equations appears in the modeling of many important physical phenomena, such as heat radiative transfer [1] and neutron transport [2]. They have applications in high temperature manufacturing (e.g., class and ceramic manufactures), optical medicine, nuclear energy generation, and many others. In this work, we deal with equations of the following form

$$\Omega \cdot \nabla u + \sigma_t u = f \quad \text{in } \mathcal{D}, \tag{1}$$

where $u = u(\boldsymbol{x}) \in \mathbb{R}$, $\boldsymbol{x} = (x, y) \in \mathcal{D} = [a, b] \times [c, d]$, $\sigma_t > 0$ and a given direction $\Omega = (\mu, \eta)$ in the unitary disc centered at the origin. Incoming boundary condition is assumed as

$$u = u_{\text{in}} \quad \text{on } \Gamma^-, \tag{2}$$

where $u_{\text{in}} = u_{\text{in}}(\boldsymbol{x})$ is given on $\Gamma^- = \{\boldsymbol{x} \in \partial\mathcal{D} : \Omega \cdot \boldsymbol{n} < 0\}$, with $\boldsymbol{n}$ denoting the outward-pointing normal vector on the boundary.

The Method of Characteristics (MoC, [3]) is one of the approaches most used to solve (1)-(2). And, in this work, we discuss on an application of Artificial Neural Networks (ANNs, [4]) to assist the MoC, by providing the needed estimates of the solution on the edge of mesh cells. The idea is to explore the advantage of ANNs as universal function approximators [5] and gain advantage by a knowledge transfer strategy in the Ω direction.

The MoC approach consists in assuming the change of variables $\boldsymbol{x}(s) = \overline{\boldsymbol{x}} + s\Omega$, from where equation (1) can be rewritten as

$$\frac{du}{ds} + \sigma_t u(s) = f(s), \tag{3}$$

where $u(s) = u(\boldsymbol{x}(s))$ and $f(s) = f(\boldsymbol{x}(s))$. By applying an integrating factor, the solution of this linear first-order differential equation has the form

$$u(s) = u(0)e^{-\int_0^s \sigma_t\, ds'} + \int_0^s f(s')e^{-\int_{s'}^s \sigma_t\, ds''}\, ds'. \tag{4}$$

A common numerical strategy is to compute the solution on given mesh nodes. For simplicity, lets assume a given uniform rectangular mesh $\mathcal{M}$ build from the Cartesian product of the partitions $\mathbb{P}_{h_x} = \{x_i = a + (i-1)h_x\}_{i=1}^{n_x}$, $h_x = (b-a)/(n_x - 1)$, and $\mathbb{P}_{h_y} = \{y_j = c + h_y(j-1)\}_{j=1}^{n_y}$, $h_y = (d-c)/(n_y - 1)$, i.e. $\mathcal{M} = \mathbb{P}_{h_x} \times \mathbb{P}_{h_y}$. Without the loss of generality, lets assume Ω is in the first quarter of the unitary disc, i.e. $\mu > 0$ and $\eta > 0$. Then, from equation (4), we have

$$u(\boldsymbol{x}_{ij}) = u(\overline{\boldsymbol{x}}_{ij})e^{-\int_0^s \sigma_t\, ds'} + \int_0^s f(s')e^{-\int_{s'}^s \sigma_t\, ds''}\, ds', \tag{5}$$

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where $\boldsymbol{x}_{ij} = (x_i, y_j)$ and $\overline{\boldsymbol{x}}_{ij} = \boldsymbol{x}_{ij} - s\Omega$ is a point on one of the cell edges that has $\boldsymbol{x}_{ij}$ as a vertex. Usually, the solution is not known at the cell edges and need to be estimated from the solution previous computed on some mesh nodes. This is usually perform by interpolation techniques, which limits the accuracy of the numerical solution by the mesh size.

Alternatively, this work propose the application of ANNs of the type Multi-layer Perceptron (MLP) to estimate the solution values on cell edges. The MLP can be denoted by

$$\tilde{u}(\boldsymbol{x}) = \mathcal{N}\left(\boldsymbol{x}; \left\{\left(W^{(l)}, \boldsymbol{b}^{(l)}, f^{(l)}\right)\right\}_{l=1}^{n_l}\right), \tag{6}$$

where $\left(W^{(l)}, \boldsymbol{b}^{(l)}, f^{(l)}\right)$ denotes the triple of weights $W^{(l)}$, bias $\boldsymbol{b}^{(l)}$ and activation function $f^{(l)}$ in the l-th layer of the network, $l = 1, 2, \ldots, n_l$. By starting from the incoming boundary Γ^-, we train the neural network by solving the following minimization problem

$$\min_{\left\{\left(W^{(l)}, \boldsymbol{b}^{(l)}\right)\right\}_{l=1}^{n_l}} \frac{1}{n_s} \sum_{m=1}^{n_s} \left(\tilde{u}(\boldsymbol{x}_s) - u(\boldsymbol{x}_s)\right)^2, \tag{7}$$

where $\boldsymbol{x}_s$ are mesh nodes on Γ^-. Once trained, the ANN is applied on the computation of new mesh nodes with cell edges on Γ^-. From (5), the solution at the new mesh points is computed by

$$u(\boldsymbol{x}_{ij}) = \mathcal{N}(\overline{\boldsymbol{x}}_{ij}) e^{-\int_0^s \sigma_t \, ds'} + \int_0^s f(s') e^{-\int_{s'}^s \sigma_t \, ds''} \, ds'. \tag{8}$$

Once the solution is known on all such new nodes, the ANN is retrained with warm initialization, i.e. we use knowledge transfer from the previous training to speed up computations. By iterating, the ANN is trained and used to estimate the solution on cell edges as one moves trough all mesh nodes.

This is a work in progress that propose the use of ANN coupled to a MoC strategy to numerically solve linear first-order partial differential equations. This novel approach has the potential to provide an efficient alternative to the use of standard interpolation techniques on the solution estimates on cell edges. This can be particularly valuable in applications that requires non-uniform meshes.

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