Using Machine Learning Models for Computational Fluid Dynamics

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- Background
 - Motivation
 - Neural Networks
 - Mathematical Model
 - Fluid Diffusion Equation
 - Contributions
- 2 Our work
 - Neural Networks: universal approximators
 - Finite Differences
 - Results
- Conclusions and future work
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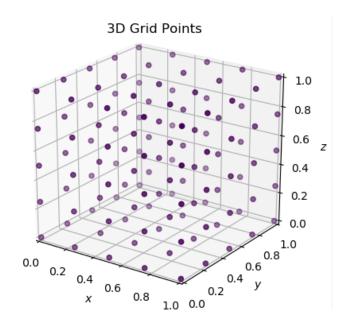


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Environment That is Being Approximated



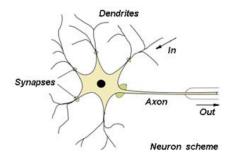
These grid points are set up in a perfect sequence. We chose how many points to have along each axis.



Neural Networks



- How does brain work?
- Dendrites Collect information.
- Cell body processes the information.
- The processed information passed through synapses.
- Axons receive the information and conveys to the dendrites of the next nerve cell.



Neural networks



• Early implementation of the idea:

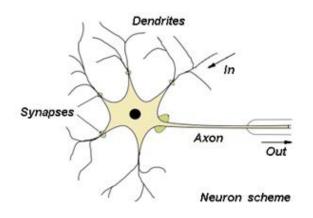


Figure 1: Human nerve cell

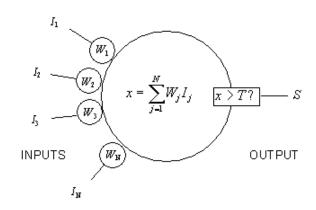
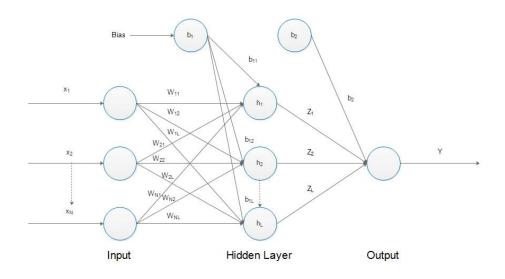


Figure 2: Neural Network

- Dendrites can be compared to input units, cell body to nodes, synapses to activation function and axons to the output units.
- In 1943, neurophysiologist Warren McCulloch and mathematician Walter Pitts wrote a paper on how neurons might work.

Generic ANN, one hidden layer





Generic ANN, one hidden layer

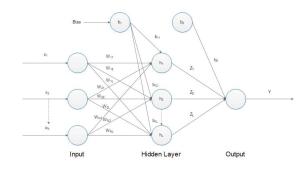


• Mathematical Model

$$y: \mathbb{R}^{N} \to (0,1)$$

$$y(\mathbf{x}; \mathbf{w}, \mathbf{b}) =$$

$$\sigma \left(\sum_{j=1}^{L} z_{j} \sigma \left(\sum_{i=1}^{N} w_{ij} x_{i} + b_{1j} \right) + b_{2} \right)$$



where $\sigma()$ is the sigmoid function:

$$\sigma: \mathbb{R} \to \mathbb{R}, \quad \sigma(x) = \frac{1}{1 + e^{-x}}$$

Diffusion Equation



$$\dot{E}_{in} + \dot{E}_g - \dot{E}_{out} = \dot{E}_s$$

Our conditions:

$$\begin{cases} \dot{E}_g = \dot{q} dx dy dz = 0 \\ \dot{E}_s = \rho C_p \frac{\partial T}{\partial t} dx dy dz = 0 \end{cases}$$

• At equilibrium, when diffusion stops (temperature does not change over time), the distribution of temperature in a space $D \subset \mathbb{R}^3$ is given by $u: D \longrightarrow \mathbb{R}$, the solution of the Laplace equation:

$$\Delta u(x, y, z) = 0 \tag{1}$$

• The Laplace equation (1) with boundary conditions may have an analytical solution, but, in practice, numerical solutions can be always computed.



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Neural Networks: universal approximators



Theorem (Cybenko, 1989)

Let σ be the sigmoid function. The finite sums of the form:

$$G(\boldsymbol{x}) = \sum_{i=1}^{N} \alpha_i \sigma \left(\boldsymbol{y}_i^T \boldsymbol{x} + b_i \right)$$

are dense in $C([0,1]^n)$. That is, for any $f \in C([0,1]^n)$ and $\varepsilon > 0$, there is a sum $G(\boldsymbol{x})$ of the above form such that:

$$|G(\boldsymbol{x}) - f(\boldsymbol{x})| < \varepsilon \qquad \forall \boldsymbol{x} \in [0, 1]^n$$

Finite Differences solution



• A popular choice is the Finite Differences (FD) method, which produces a numerical solution by iteratively solving a linear system of equations. For instance, the FD method using second order approximations produces a numerical solution by solving the system:

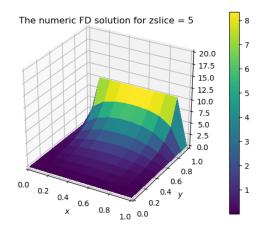
$$u_{i,j,k}^{k+1} = (u_{i-1,j,k}^k + u_{i+1,j,k}^k + u_{i,j-1,k}^k + u_{i,j+1,k}^k + u_{i,j,k-1}^k + u_{i,j,k+1}^k)/6$$
(2)

on the domain D typically divided in an equally spaced grid of points (x_i, y_j, z_k) .

• The numerical solution produced by the FD method is stable and quite efficient.

Results





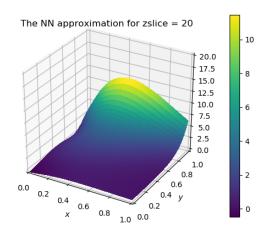


Figure 3: The FD method solution (left) and NN solution (right)

Results



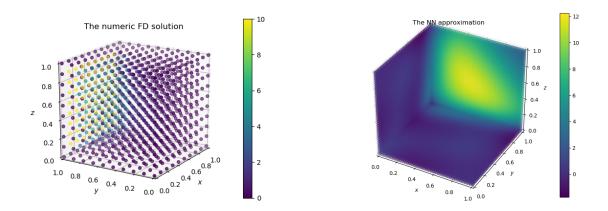


Figure 4: The FD method complete 3D solution (left) and the NN approximation on the whole domain, computed at $40 \times 40 \times 40$ grid points (right)



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Conclusions and future work



- We interpolate the numerical solutions from Finite Differences method and produce analytical solutions using an Artificial Neural Network approximation model.
- Next: Navier-Stokes Equation

$$\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z} = 0$$

$$\rho \left(\frac{\partial \vec{\nu}}{\partial t} + \vec{\nu} \cdot \nabla \vec{\nu} \right) = -\nabla p + \mu \nabla^2 \vec{\nu} + \vec{f}$$



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References



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