Using Machine Learning Models for Computational Fluid Dynamics

Benjamin "Trey" Brown
(join work with E. Iacob and M. Ilie)

Georgia Southern University
Department of Mathematical Sciences

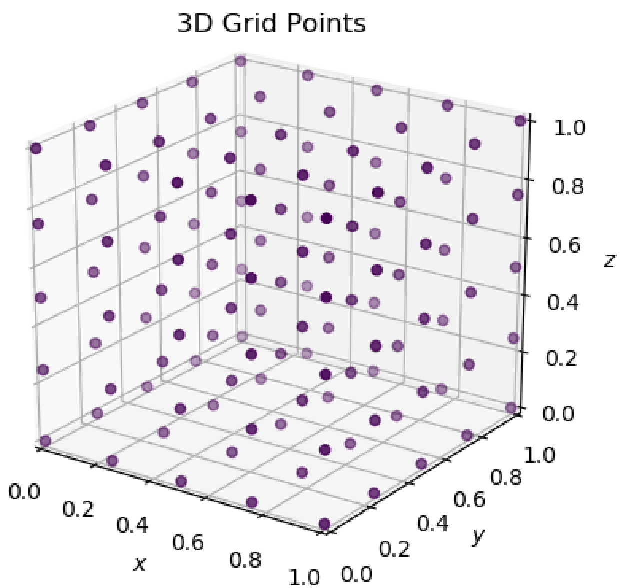
April 18, 2019

Outline

Outline

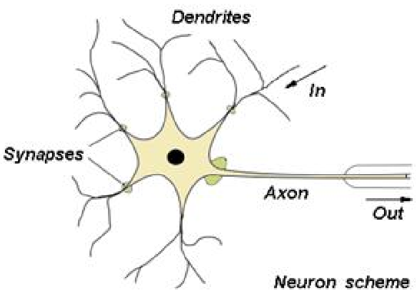
Environment That is Being Approximated

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:

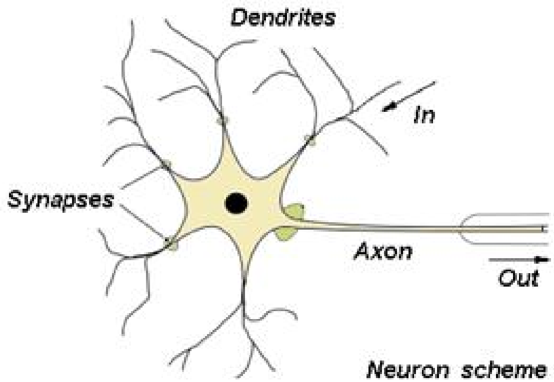


Figure 1: Human nerve cell

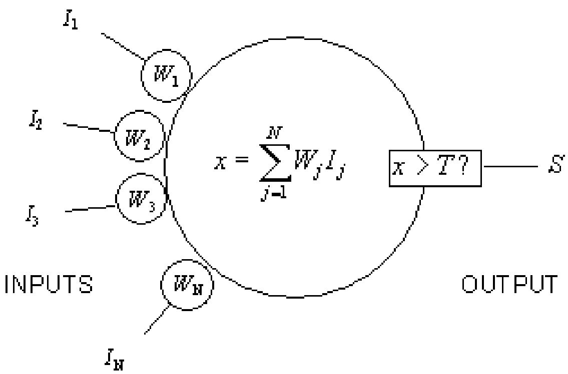
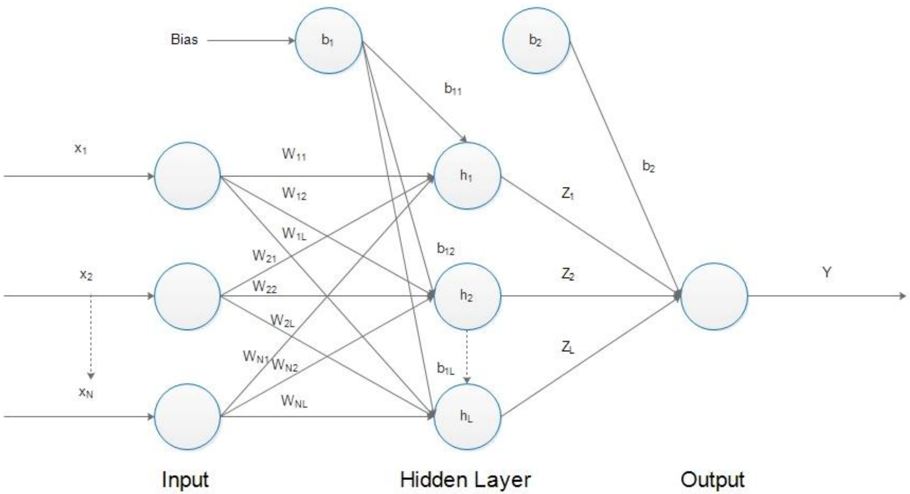


Figure 2: Neural Network

- 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

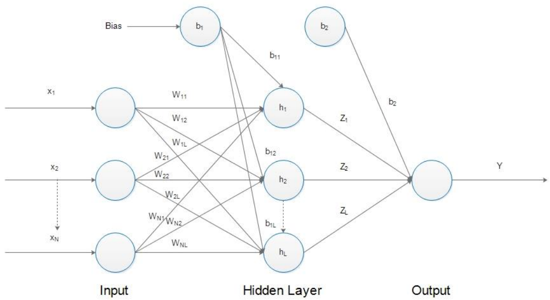


- Mathematical Model

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

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

$$\sigma\left(\sum_{j=1}^{L} z_j \sigma\left(\sum_{i=1}^{N} w_{ij} x_i + b_{1j}\right) + b_2\right)$$



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

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

Diffusion Equation

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

Our conditions:

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

- 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.

Outline

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:

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

  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

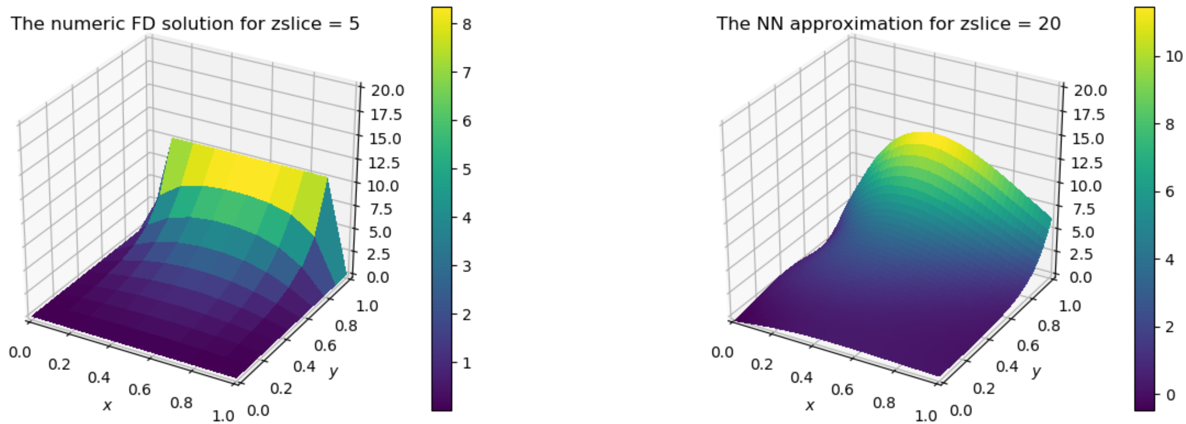


Figure 3: The FD method solution (left) and NN solution (right)

Results

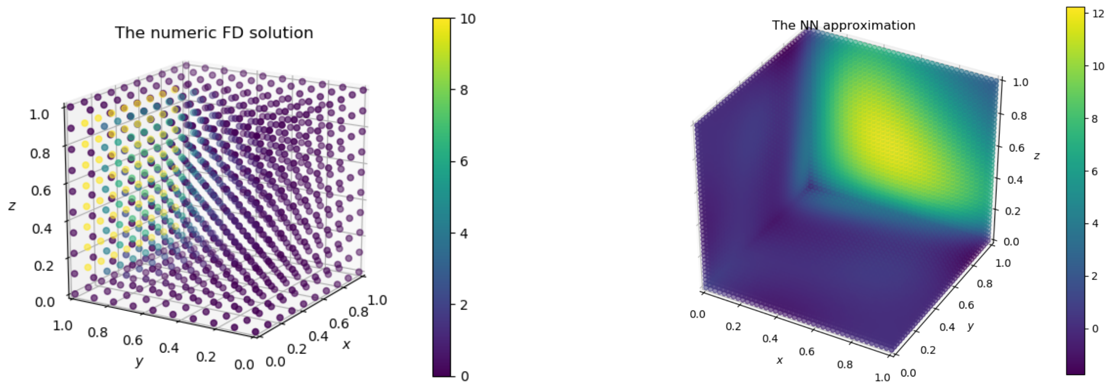


Figure 4: The FD method complete 3D solution (left) and the NN approximation on the whole domain, computed at $40 \times 40 \times 40$ grid points (right)

Outline

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

$$
\begin{aligned}
\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z} &= 0 \\
\rho\left(\frac{\partial \vec{\nu}}{\partial t} + \vec{\nu} \cdot \nabla \vec{\nu}\right) &= -\nabla p + \mu \nabla^2 \vec{\nu} + \vec{f}
\end{aligned}
$$

Outline

References

McCP W. McCulloch, W. Pitts, A logical calculus of the ideas immanent in nervous activity, Bulletin of Mathematical Biophysics, Vol. 5, 1943, 115-133.

Ros Rosenblatt, F. (1962). Principles of Neurodynamics, Spartan Books, New York.

RHW Rumelhart, D.E., Hinton, G.E., and Williams, R.J. (1986). Learning internal representations by backpropagating errors. Nature, 323:533–536.

Cyb Cybenko, G. (1989) “Approximations by superpositions of sigmoidal functions”, Mathematics of Control, Signals, and Systems, 2(4), 303–314.