Neural networks catching up with finite differences in solving partial differential equations in higher dimensions

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Abstract—Fully connected multilayer perceptrons are used for obtaining numerical solutions of partial differential equations in various dimensions. Independent variables are fed into the input layer, and the output is considered as solution’s value. To train such a network one can use square of equation’s residual as a cost function and minimize it with respect to weights by gradient descent. Following previously developed method, derivatives of the equation’s residual along random directions in space of independent variables are also added to cost function. Similar procedure is known to produce nearly machine precision results using less than 8 grid points per dimension for 2D case. The same effect is observed here for higher dimensions: solutions are obtained on low density grids, but maintain their precision in the entire region. Boundary value problems for linear and nonlinear Poisson equations are solved inside 2, 3, 4, and 5 dimensional balls. Grids for linear cases have 40, 159, 512 and 1536 points and for nonlinear 64, 350, 1536 and 6528 points respectively. In all cases maximum error is less than $8.8 \cdot 10^{-6}$, and for nonlinear 64, 350, 1536 and 6528 points respectively. The same effect is observed here for higher dimensions: solutions are obtained on low density grids, but maintain their precision in the entire region. Boundary value problems for linear and nonlinear Poisson equations are solved inside 2, 3, 4, and 5 dimensional balls. Grids for linear cases have 40, 159, 512 and 1536 points and for nonlinear 64, 350, 1536 and 6528 points respectively. In all cases maximum error is less than $8.8 \cdot 10^{-6}$, and for nonlinear 64, 350, 1536 and 6528 points respectively.

This particular expression represents a real valued function $u$ of one argument $x$. Here $\sigma$ is a special kind of nonlinear scalar mapping that is applied to each component of its input independently. For example, $x$ is first multiplied by a vector (matrix of a single column) $W^0$ and then each component goes through $\sigma$. The result is then multiplied by matrix $W^1$ and again nonlinear $\sigma$ is applied. Process is repeated as many times as there are layers in a network. This one has four of them. Numbers of neurons in hidden layers set ranges for $i$, $j$ and $k$. Numerical parameters are represented by weights matrices:

$$W^0, W^1, W^2, W^3$$

and they can be tuned by methods like gradient descent. Functions of this class are able to represent arbitrary mappings in various dimensions, as well as their derivatives, as their derivatives.

II. Background

Feedforward neural networks are able to solve partial differential equations by weights minimization technique that uses the equation itself as a cost function, so, if it reaches small enough values, one can conclude that the equation holds within some error margin. The input of such network is considered as a vector of independent variables and the output as value of solution. All necessary derivatives of output with respect to input and of cost function with respect to weights can be calculated by the extended backpropagation procedure. Including boundary conditions into cost function itself usually does not produce very accurate results, so a process of function substitution is required. For brevity, 2D case will be described, however, generalization is straightforward. Consider a boundary value problem for partial differential equation written for function $u(x, y)$:

$$U(x, y, u, u_x, u_y, ...) = 0$$

in a region $\Gamma$ with boundary $\partial \Gamma$ and condition:

$$u_{|\partial \Gamma} = f$$

A new function $v$ is introduced by relation:

$$u(x, y) = v(x, y) \cdot \phi(x, y) + f$$

where $\phi(x, y) = 1$ in $\Gamma$. This equation is then solved by neural network. The function $v$ satisfies the following equation:

$$v(x, y) = \phi(x, y) \cdot \left(U(x, y, v, v_x, v_y, ...) = 0\right)$$

This equation can be solved by neural network as well.

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where $\phi$ is known and carefully chosen to be smooth, vanish on $\partial \Gamma$:

$$\phi|_{\partial \Gamma} = 0$$

to have reasonable normal derivative on the boundary:

$$\frac{\partial \phi}{\partial n}|_{\partial \Gamma} \sim 1$$

and to behave on $\Gamma$ “as simply as possible”. The complete set of requirements for such functions has not yet been formulated. After writing the equation for $v(x, y)$, one can notice that boundary condition turns into:

$$v|_{\partial \Gamma} < \infty$$

It seems that it’s not necessary to account for that during the weights minimization since neural networks do not converge to infinite valued functions if there is a finite solution nearby. In applications $\phi$ is usually chosen as the simplest analytical expression that vanishes on boundary and has maximum value equal to 1, which is reached at a single point inside region $\Gamma$. Condition $\frac{\partial \phi}{\partial n} \sim 1$ is imposed to exclude situations when said derivative is too small. Otherwise, $v$ near the boundary would have to be too large in order to produce correct $\frac{\partial u}{\partial n}$, which is expected to be of the order of 1. In trivial cases, like boundary problem inside a sphere of radius 1, one can choose:

$$\phi = 1 - r^2$$

After substitution, the equation for $v(x, y)$ can be written as

$$V(x, y, v, v_x, v_y, \ldots) = 0$$

Minimization will use cost function $e = V^2$. A set of grid points $(x_i, y_i)$, $i \in 1...N$ inside the region $\Gamma$ is generated as a matrix $X$ with two rows and $N$ columns. All derivatives that are encountered in $V$ for $v$ like $\frac{\partial}{\partial x}$, $\frac{\partial}{\partial y}$ and so on have to be calculated for $X$. For example, $\frac{\partial}{\partial x} X$ is a matrix with the first row elements equal to 1 and the second row ones equal to 0, vice versa for $\frac{\partial}{\partial y} X$. All higher derivatives of $X$ are zero. Said set of matrices:

$$X, \frac{\partial}{\partial x} X, \frac{\partial}{\partial y} X, \ldots$$

is propagated forward from one layer to another, and when the final layer is reached, an output set is obtained:

$$v_1, \frac{\partial}{\partial x} v_1 \equiv v_1^x, \frac{\partial}{\partial y} v_1 \equiv v_1^y, \ldots$$

All of its members are matrices of size $1 \times N$. Cost function is discretized as:

$$E = \mu \sum_{x,y \in \Gamma} \frac{1}{N} \sum_{i=1}^{N} V^2(x_i, y_i, v_i, v_x^i, v_y^i, \ldots)$$

Extended backward pass requires calculating derivatives of $E$ with respect to each element of the output matrices:

$$\frac{\partial E}{\partial v_i}, \frac{\partial E}{\partial v_x^i}, \frac{\partial E}{\partial v_y^i}, \ldots$$

and these derivatives are gathered in matrices of the same size $1 \times N$. They are propagated backward in order to obtain gradient of $E$ with respect to the weights of each layer. The whole procedure is described in [2]. One can mention a few features of the neural network approach:

- Derivatives are calculated analytically, so numerical effects can only be brought by rounding errors and/or incorrect discretization of the cost function’s measure $\mu$, that can happen when grids have large spacing.
- The solution is obtained as a neural network, which is a smooth closed-form expression. It exists naturally in the entire region rather than on finite set of points. This allows to modify the grid during the training as much as necessary without algorithm forgetting solution’s values in points that were removed.
- Parallelization is trivial: dense grids can be split into parts and processed by different computational nodes, which would only have to synchronize few megabytes of weights data during each step regardless of the grid size.
- Training is based on matrix multiplications and its careful implementation allows to achieve very high hardware efficiency on modern GPUs [2].

### III. Method’s Extension

Previously described approach is more or less standard for direct solving of partial differential equations with neural networks, although no papers prior to [2] formulated it in a form that was suitable for networks of arbitrary topology. In the same study the method was enhanced by adding extra terms to cost function. Namely, for equation:

$$V(x, y, v, v_x, \ldots) = 0$$

one can write a trivial consequence:

$$\frac{\partial}{\partial x} V = 0$$

and include it into cost $e = V^2 + V_x^2$. Applying operators

$$\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial y^2}$$

to $V$ and adding the corresponding terms to $e$ for 2D case allowed to increase precision and avoid overfitting to such a degree that solving boundary value problem on a grid of 59 points inside a unit circle produced $2 \cdot 10^{-5}$ accurate result for the entire region, whereas training with no extra terms could only achieve accuracy of $2 \cdot 10^{-3}$ [1]. In this paper additional derivatives up to the fourth order are calculated along two directions $\xi$ and $\zeta$, which are random orthonormal vectors in space of independent variables. Since the cost function now includes terms like $V_{\xi}^2$ and $V_{\zeta}^2$, which depend on $v_\xi$ and $v_\zeta$ and so on, it is necessary to initialize matrices like $\frac{\partial}{\partial \xi} X$ and $\frac{\partial}{\partial \zeta} X$ at the input layer of the network. Using coordinates in $(x, y)$ basis:

$$\xi = (a_1, a_2), \zeta = (b_1, b_2)$$

one can write:

$$\frac{\partial}{\partial \xi} = a_1 \frac{\partial}{\partial x} + a_2 \frac{\partial}{\partial y}$$

and similarly for $\frac{\partial}{\partial \zeta}$. Therefore, $\frac{\partial}{\partial \xi} X$ is a linear combination of $\frac{\partial}{\partial x} X$ and $\frac{\partial}{\partial y} X$ with coefficients $a_1$ and $a_2$, and so is $\frac{\partial}{\partial \zeta} X$.
but with $b_1$ and $b_2$. Higher order terms like $\frac{\partial^2}{\partial x^2} X$ are all zeros. Those extra matrices are used by forward pass to calculate derivatives $v_\xi$, $v_\zeta$, $v_{\xi \zeta}$ and others on the output layer of the perceptron.

Forward propagation works independently for every grid point $(x_i, y_i)$, and each point with index $i$ is represented by $i^{th}$ columns of all matrices initialized at the input layer. Noting that columns of $\frac{\partial}{\partial x} X$ and $\frac{\partial}{\partial y} X$ are coordinates of vectors $\xi$ and $\zeta$ in $x, y$ basis, one can conclude that different points can have different and, more importantly, random directions $\xi_i$ and $\zeta_i$. To implement that, one can generate $2N$ uniformly distributed unit vectors, split them into pairs, run Gram-Schmidt process on each pair, and then write one vector to $\frac{\partial}{\partial x} X$ and another to $\frac{\partial}{\partial y} X$. For 2D case $\xi_i$ and $\zeta_i$ form a basis in the input space that is randomly rotated from point to point. For higher dimensions it is possible to include more directional derivatives that will not be a linear combination of $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$, but since $\xi$ and $\zeta$ are different in each point, all directions of the input space are somewhat covered. Using one direction instead of two was found to produce less accurate results, and using three directions did not bring much improvement in higher dimensions.

In all cases training is split into three phases that use extra derivatives up to fourth order. Cost functions are built using the following terms:

$$V_0 = V$$
$$V_1 = V^2 + V_\zeta^2$$
$$V_2 = V_{\xi \zeta}^2 + V_{\zeta \zeta}^2$$
$$V_3 = V_{\xi \xi \zeta}^2 + V_{\xi \zeta \zeta}^2 + V_{\zeta \zeta \zeta}^2$$
$$V_4 = V_{\xi \xi \xi \xi \zeta}^2 + V_{\xi \xi \zeta \xi \zeta} + V_{\xi \zeta \zeta \xi \zeta}$$

The first phase uses terms from 0 to 4. The second one uses terms from 0 to 3 and the last one from 0 to 2. Cost functions can be written as:

$$e_s = \sum_{j=0}^{s} V_j$$

for $s = 4, 3$ and 2. They spawn a considerable amount of matrices that one should propagate. For example, 5D Poisson equation itself requires 2 derivatives for each dimension, 10 in total:

$$\frac{\partial}{\partial x_i}, \frac{\partial^2}{\partial x_i^2}, j \in \{1...5\}$$

(1)

Then 8 additional operators are casted:

$$\frac{\partial}{\partial \xi^2}, \frac{\partial^2}{\partial \xi^2 \xi^2}, \frac{\partial^3}{\partial \xi^3 \xi^3}, \frac{\partial^4}{\partial \xi^4 \xi^4}$$

(2)

$$\frac{\partial}{\partial \zeta^2}, \frac{\partial^2}{\partial \zeta^2 \zeta^2}, \frac{\partial^3}{\partial \zeta^3 \zeta^3}, \frac{\partial^4}{\partial \zeta^4 \zeta^4}$$

(3)

Results of (2), (3), their combinations with (1) and function values themselves constitute to a total number of 99 different matrices. For $s = 3$ it’s 77 and for $s = 2$ it’s 55.

A. Renormalization

For certain functions derivatives of various orders have vastly different magnitude. For example, $\sin 10x$ has values of the order of 1 and its $n^{th}$ derivative with respect to $x$ is of the order of $10^n$. If solution of a partial differential equation demonstrates similar properties, backpropagation will mostly minimize high order terms without proper attention to low order ones. Such cases require normalization. For each grid point the largest derivative along additional direction is spotted:

$$M_\xi = \max(v_\xi, v_{\xi x}, v_{\xi \xi x}, v_{\xi \xi \xi x}, v_{\xi \xi \xi \xi x}, ...)$$

If $M_\xi > 4$, vector $\xi$ is divided by $\sqrt[M_\xi]{M_\xi}$, where $k$ is the order of the largest derivative with respect to $\xi$. Similar procedure is done for $\zeta$. Renormalization requires one forward pass and is usually done once after each portion of epochs $r_{int}$. Note that even if solution does not produce derivatives of various magnitude, neural network can still exhibit this behavior somewhere along the training.

IV. RESULTS

To have non trivial analytical solutions, against which one could verify numerical results, formulas $u_a$ for those solutions were first picked and then substituted into linear:

$$\Delta u = g$$

and nonlinear Poisson equation:

$$\Delta u + u^2 = h$$

to find the corresponding source terms $g$ and $h$ that would produce them. In all cases equations are solved inside $n$-dimensional ball of radius 1 with vanishing boundary condition:

$$\Gamma : r < 1$$

$$u|_{\partial \Gamma} = 0$$

which is then simplified by function substitution:

$$u = v \cdot (1 - r^2)$$

After numerical solutions are obtained for $v$, functions $u$ are calculated using them and compared against analytical expressions $u_a$ on dense enough sets of random points distributed uniformly inside $\Gamma$. Maximum and median values of absolute error $\varepsilon = |u - u_a|$ are calculated.

Grids are comprised of two parts. Surface part contains equidistant points from $\partial \Gamma$ with angular distance $\theta$. Internal part is a regular grid, which is generated in three steps. At first, a Cartesian grid with spacing $\lambda$ inside $[-1, 1]^n$ is created. Two random vectors in $\mathbb{R}^n$ are then chosen, and the grid is rotated from one to another. Finally, it is shifted along each direction by random value from interval $[-\frac{\lambda}{3}, \frac{\lambda}{3}]$ and after that all points with $r > 1$ are excluded.

Training is based on RProp [22] procedure with parameters $\eta_+ = 1.2$, $\eta_- = 0.5$. Weights are forced to stay in $[-20, 20]$ interval, no min/max bonds for steps are imposed. Initial steps $\Delta_0$ are set to $2 \cdot 10^{-4}$, unless otherwise stated. Weights for neurons are initialized [9], [11] with random values from range
$\pm 2/\sqrt{3}$, where $s$ is the number of senders. Thresholds are initialized in range $\pm 0.1$. All layers, but input and output, are nonlinear with activation function:

$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

The procedure is implemented according to [2] with no intermediate load/saves and run on Google Cloud instance with Nvidia Tesla P100 using 32 bit precision. All training points are processed in one batch. During the training original equation’s residual $V_0 = V_0$ is monitored, and its root mean squared is calculated for grid points. Training phases are thoroughly described for 2D case and applied without changes to higher dimensions. After figuring out grid requirements and network topologies all solutions were obtained from the first try.

### A. Two dimensions

Analytical solution is written as:

$$u(x_1, x_2) = \frac{10}{17} (1 - r^2)(x_1 + \sin x_2 + x_1^2 + x_2 \cos x_1)$$

$$r^2 = x_1^2 + x_2^2$$

Ratio $\frac{u^2}{u^3}$ is introduced, so that $u_{\text{max}} - u_{\text{min}} \approx 1$. Source term for linear equation is:

$$g = -\frac{10}{17} (-x_1^2 - x_2^2 + 1) \sin x_2 -$$

$$-\frac{10}{17} x_1 (2x_1 - x_2 \sin x_1 + 1) +$$

$$+ \frac{10}{17} (-x_1^2 - x_2^2 + 1) (2 - 2x_2 \cos x_1) -$$

$$-\frac{40}{17} x_2 (\cos x_1 + \cos x_2) -$$

$$-\frac{40}{17} (x_1^2 + x_1 + \sin x_2 + x_2 \cos x_1)$$

and for nonlinear equation is:

$$h = -\frac{10}{17} (-x_1^2 - x_2^2 + 1) \sin x_2 -$$

$$-\frac{10}{17} x_1 (2x_1 - x_2 \sin x_1 + 1) +$$

$$+ \frac{10}{17} (-x_1^2 - x_2^2 + 1) (2 - 2x_2 \cos x_1) -$$

$$-\frac{40}{17} x_2 (\cos x_1 + \cos x_2) -$$

$$-\frac{40}{17} (x_1^2 + x_1 + \sin x_2 + x_2 \cos x_1) +$$

$$+ \frac{100}{289} (-x_1^2 - x_2^2 + 1)^2 (x_1^2 + x_1 + \sin x_2 +$$

$$+ x_2 \cos x_1)$$

In both cases new function $v$ is introduced:

$$u(x_1, x_2) = v(x_1, x_2) \cdot (1 - x_1^2 - x_2^2)$$

Linear equation turns into:

$$(1 - x_1^2 - x_2^2) \Delta v - 4x_1 \frac{\partial v}{\partial x_1} - 4x_2 \frac{\partial v}{\partial x_2} - 4v = g \quad (4)$$

and nonlinear into:

$$(1 - x_1^2 - x_2^2) \Delta v - 4x_1 \frac{\partial v}{\partial x_1} - 4x_2 \frac{\partial v}{\partial x_2}$$

$$- (1 - x_1^2 - x_2^2)^2 v^2 - 4v = h \quad (5)$$

Boundary conditions are now trivial:

$$v|_{\partial \Gamma} < \infty$$

Neural network is a fully connected perceptron with the following layer structure:

$$2, 96, 96, 96, 96, 96, 96, 1$$

1) Linear 2D equation: Surface grid contains 13 points of a circle with $\theta = \frac{\pi}{6}$. Internal grid has spacing $\lambda = \frac{1}{3}$ and contains 27 points, the total number is 40 (see Fig. 1).

The first training phase uses $e_4$ and lasts for 2000 epochs with $r_{\text{int}} = 200$. After the first 1000 epochs, steps $\Delta$ are reset back to $2 \cdot 10^{-4}$. RMS of equation’s residual at the end: $V_0 = 4 \cdot 10^{-4}$.

The second phase uses $e_3$, $\Delta_0 = 2 \cdot 10^{-5}$ and lasts for 2000 epochs with $r_{\text{int}} = 200$. At the end of it $V_0 = 1.3 \cdot 10^{-4}$.

The third phase uses $e_2$, $\Delta_0 = 2 \cdot 10^{-5}$ and lasts for 2000 epochs with $r_{\text{int}} = 200$. The final RMS of the residual:

$V_0 = 4 \cdot 10^{-5}$.

$u(x_1, x_2)$ is obtained in 114 seconds on grid of 40 points and tested on 4000 points against the analytical solution with the following results:

$$\epsilon_{\text{max}} = 3.5 \cdot 10^{-6}, \epsilon_{\text{median}} = 6.8 \cdot 10^{-7}$$

2) Nonlinear 2D equation: Surface grid contains 17 points of a circle with $\theta = \frac{\pi}{6}$. Internal grid has spacing $\lambda = \frac{1}{3}$ and contains 47 points, the total number is 64.

The first training phase uses $e_4$, lasts for 3000 epochs and is split into 5 intervals. The first one contains 160 epochs, $r_{\text{int}} = 15$. The second has 340 epochs and $r_{\text{int}} = 50$. The third is 500 epochs and $r_{\text{int}} = 50$. The fourth is 1000, $r_{\text{int}} = 50$ and the final one is another 1000 epochs with $r_{\text{int}} = 100$. Steps $\Delta$ are reset back to $2 \cdot 10^{-4}$ at the end of each interval but the last one. At the end of this phase $V_0 = 4 \cdot 10^{-2}$.

The second phase uses $e_3$, $\Delta_0 = 2 \cdot 10^{-5}$ and lasts for 2000 epochs with $r_{\text{int}} = 200$. At the end of it $V_0 = 1 \cdot 10^{-5}$.

The third phase uses $e_2$, $\Delta_0 = 2 \cdot 10^{-5}$ and lasts 2000 epochs with $r_{\text{int}} = 200$. The final RMS of the residual $V_0 = 1 \cdot 10^{-4}$.

$u(x_1, x_2)$ is obtained in 180 seconds on grid of 64 points and tested on 4000 points against the analytical solution with the following results:

$$\epsilon_{\text{max}} = 8 \cdot 10^{-6}, \epsilon_{\text{median}} = 2.4 \cdot 10^{-6}$$

B. Three dimensions

Analytical solutions is written as:

$$u(x_1, x_2, x_3) = \frac{3}{5} (1 - r^2)(x_1 + \sin x_2 + x_3^2 + x_2 \cos x_1)$$

$$r^2 = x_1^2 + x_2^2 + x_3^2$$

Substitution of function is implemented in a similar manner:

$$u(x_1, x_2, x_3) = v(x_1, x_2, x_3) \cdot (1 - r^2)$$
Equations and corresponding sources \( g \) and \( h \) are obtained by exactly the same procedure as in two-dimensional case. Results are similar and for brevity they are omitted. Neural network is a fully connected perceptron with the following layer structure:

\[
3, 96, 96, 96, 96, 96, 1
\]

1) **Linear 3D equation**: Surface grid contains 51 points of a sphere with \( \theta = \frac{\pi}{6} \). Internal grid has spacing \( \lambda = \frac{1}{3} \) and contains 108 points, the total number is 159.

The first phase is the same as phase 1 of 2D Linear case. At the end of it \( V_0 = 1.5 \cdot 10^{-3} \).

The second phase is the same as phase 2 of 2D Linear case and it ends with \( V_0 = 3 \cdot 10^{-4} \).

The third phase is the same as phase 3 of 2D Linear case and the final \( V_0 = 1.3 \cdot 10^{-4} \).

\( u(x_1, x_2, x_3) \) is obtained in 226 seconds on grid of 159 points and tested on 35000 points against the analytical solution with the following results:

\[
\varepsilon_{\text{max}} = 6.5 \cdot 10^{-6}, \varepsilon_{\text{median}} = 1.4 \cdot 10^{-6}
\]

2) **Nonlinear 3D equation**: Surface grid contains 87 points of a sphere with \( \theta = \frac{\pi}{6} \). Internal grid has spacing \( \lambda = \frac{1}{4} \) and contains 265 points, the total number is 343.

The first phase is the same as phase 1 of 2D Nonlinear case and it leaves \( V_0 = 3.2 \cdot 10^{-2} \).

The second phase is the same as phase 2 of 2D Nonlinear case and it ends with \( V_0 = 6 \cdot 10^{-4} \).

The third phase is the same as phase 3 of 2D Nonlinear case and the final \( V_0 = 1.8 \cdot 10^{-4} \).

\( u(x_1, x_2, x_3) \) is obtained in 380 seconds on grid of 343 points and tested on 35000 points against the analytical solution with the following results:

\[
\varepsilon_{\text{max}} = 8.2 \cdot 10^{-6}, \varepsilon_{\text{median}} = 1.9 \cdot 10^{-6}
\]

C. **Four dimensions**

Analytical solutions is written as:

\[
u(x_1, x_2, x_3, x_4) = \frac{7}{9}(1 - r^2)(x_1 + \sin x_2 + x_3^2 + x_4 \cos x_4)\]

\[
r^2 = x_1^2 + x_2^2 + x_3^2 + x_4^2
\]

Substitution is similar:

\[
u(x_1, x_2, x_3, x_4) = v(x_1, x_2, x_3, x_4) \cdot (1 - r^2)
\]

Neural network is a fully connected perceptron with the following layer structure:

\[
4, 148, 148, 148, 148, 148, 1
\]

1) **Linear 4D equation**: Surface grid contains 154 points of a 3-sphere with \( \theta = \frac{\pi}{6} \). Internal grid has spacing \( \lambda = \frac{1}{3} \) and contains 358 points, the total number is 512.

Phase 1 (see phase 1 of 2D Linear): \( V_0 = 1.5 \cdot 10^{-3} \).

Phase 2 (see phase 2 of 2D Linear): \( V_0 = 3.3 \cdot 10^{-4} \).

Phase 3 (see phase 3 of 2D Linear): \( V_0 = 1.7 \cdot 10^{-4} \).

\( u(x_1, x_2, x_3, x_4) \) is obtained in 560 seconds on grid of 512 points and tested on 500,000 points against the analytical solution with the following results:

\[
\varepsilon_{\text{max}} = 6.5 \cdot 10^{-6}, \varepsilon_{\text{median}} = 9.7 \cdot 10^{-7}
\]

2) **Nonlinear 4D equation**: Surface grid contains 357 points of a 3-sphere with \( \theta = \frac{\pi}{6} \). Internal grid has spacing \( \lambda = \frac{1}{4} \) and contains 1179 points, the total number is 1536.

Phase 1 (see phase 1 of 2D Nonlinear): \( V_0 = 5 \cdot 10^{-2} \).

Phase 2 (see phase 2 of 2D Nonlinear): \( V_0 = 1.2 \cdot 10^{-3} \).

Phase 3 (see phase 3 of 2D Nonlinear): \( V_0 = 2.5 \cdot 10^{-4} \).

\( u(x_1, x_2, x_3, x_4) \) is obtained in 1160 seconds on grid of 1536 points and tested on 500,000 points against the analytical solution with the following results:

\[
\varepsilon_{\text{max}} = 8.6 \cdot 10^{-6}, \varepsilon_{\text{median}} = 1.2 \cdot 10^{-6}
\]

D. **Five dimensions**

Analytical solutions is written as:

\[
u(x_1, x_2, x_3, x_4, x_5) = \frac{7}{9}(1 - r^2)(x_1 + \sin x_2 + x_3^2 + x_4 \cos x_5)\]

\[
r^2 = x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2
\]

Substitution is as usual:

\[
u(x_1, x_2, x_3, x_4, x_5) = v(x_1, x_2, x_3, x_4, x_5) \cdot (1 - r^2)
\]

Neural network is a fully connected perceptron with the following layer structure:

\[
5, 160, 160, 160, 160, 160, 1
\]

1) **Linear 5D equation**: Surface grid contains 399 points of a 4-sphere with \( \theta = \frac{\pi}{6} \). Internal grid has spacing \( \lambda = \frac{1}{3} \) and contains 1137 points, the total number is 1536.

Phase 1 (see phase 1 of 2D Linear): \( V_0 = 1.5 \cdot 10^{-3} \).

Phase 2 (see phase 2 of 2D Linear): \( V_0 = 3.2 \cdot 10^{-4} \).

Phase 3 (see phase 3 of 2D Linear): \( V_0 = 2.1 \cdot 10^{-4} \).

\( u(x_1, x_2, x_3, x_4, x_5) \) is obtained in 1280 seconds on grid of 1536 points and tested on 5,000,000 points against the analytical solution with the following results:

\[
\varepsilon_{\text{max}} = 8.7 \cdot 10^{-6}, \varepsilon_{\text{median}} = 1.2 \cdot 10^{-6}
\]
2) Nonlinear 5D equation: Surface grid contains 1217 points of a 4-sphere with $\theta = \frac{\pi}{5}$. Internal grid has spacing $\lambda = \frac{1}{4}$ and contains 5311 points, the total number is 6528. Phase 1 (see phase 1 of 2D Nonlinear): $V_0 = 3.2 \cdot 10^{-2}$, Phase 2 (see phase 2 of 2D Nonlinear): $V_0 = 2 \cdot 10^{-3}$, Phase 3 (see phase 3 of 2D Nonlinear): $V_0 = 3.3 \cdot 10^{-4}$.

$u(x_1, x_2, x_3, x_4, x_5)$ is obtained in 5000 seconds on grid of 6528 points and tested on 5,000,000 points against the analytical solution with the following results:

$$\varepsilon_{\text{max}} = 8.8 \cdot 10^{-6}, \varepsilon_{\text{median}} = 1.5 \cdot 10^{-6}$$

V. CATCHING UP WITH FINITE DIFFERENCES

Linear Poisson equations will be considered in this section. For estimation of time required to solve those with classical methods, a simple 2n+1 point stencil in n dimensions is considered. For example, in 2D case it states:

$$\Delta u = \frac{1}{h^2} u(x_1 + h, x_2) + u(x_1 - h, x_2) - 2u(x_1, x_2) + u(x_1, x_2 + h) + u(x_1, x_2 - h) - 2u(x_1, x_2) + h^2 \left( \frac{\partial^4 u}{\partial x_1^4} + \frac{\partial^4 u}{\partial x_2^4} \right) + O(h^4)$$

In 5D it gives the following discretization error:

$$\epsilon = \frac{h^2}{12} \left( \frac{\partial^4 u}{\partial x_1^4} + \frac{\partial^4 u}{\partial x_2^4} + \frac{\partial^4 u}{\partial x_3^4} + \frac{\partial^4 u}{\partial x_4^4} + \frac{\partial^4 u}{\partial x_5^4} \right) + O(h^4)$$

For analytical solution $u_a(x_1, x_2, x_3, x_4, x_5)$ it turns into:

$$\epsilon = \frac{7}{108} h^2 \left( -24 - 8x_4 x_5 \sin x_5 + 8x_2 \cos x_2 - \left( x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2 - 13 \right) \cdot (\sin x_2 + x_4 \cos x_4) \right) + O(h^4)$$

For estimation this whole expression can be reduced to the first term:

$$\epsilon \approx \frac{7 \cdot 24 h^2}{108} \approx 1.6 \cdot h^2$$

Now instead of original equation:

$$\Delta u = h$$

discretization results in solving:

$$\Delta \bar{u} = h - \epsilon$$

The difference $\Psi$ between analytical and discrete solutions can be obtained using the following equation:

$$\Delta (u - \bar{u}) = \Delta \Psi = \epsilon$$

(7)

with vanishing boundary condition:

$$\Psi|_{\partial \Gamma} = 0$$

For constant $\epsilon$ it can be readily solved:

$$\Psi = -\frac{\epsilon}{10} \left( 1 - x_1^2 - x_2^2 - x_3^2 - x_4^2 - x_5^2 \right)$$

which gives:

$$\max |u - \bar{u}| \approx \frac{|\epsilon|}{10}$$

(8)

Note that for other dimensions instead of 10 one should put $2n$. This result is confirmed for low dimensions by solving numerically with no terms of $\epsilon$ omitted.

One can argue that since neural network is solving another equation - the one that is written for $v$, its discretization error $\epsilon_v$ is different. Closer look reveals that terms of $\epsilon_v$ related to Laplacian indeed become $\sim 18$ times smaller, however the most part of the error now comes from the first order derivatives (see (4), (5)):

$$4x_i \frac{\partial v}{\partial x_i}$$

Leading terms of $\epsilon_v$ for those:

$$\frac{4h^2}{6} \frac{\partial^3 v}{\partial x_i^3} \sim 0.5h^2$$

The later equivalence is due to the third derivatives of the analytical solution:

$$v_a = \frac{7}{9} (x_1 + \sin x_2 + x_3^2 + x_4 \cos x_4)$$

being of the order of $7/9$. To make sure that the ratio of 3 between $\epsilon_v$ and $\epsilon$ is not a significant advantage for a neural network, the term $x_3^2$ in $v_a$ was replaced with $x_3^2/2$. This increases discretization error for $v$ by three times. After neural network solution was recalculated, the effect of that on precision turned out to be subtle and was fully compensated by setting $r_{int} = 20$ for the first 1000 epochs of phase 1 and extending said phase for another 500 epochs. This increased total running time by 10%. However, all those changes also produced even better final result:

$$\varepsilon_{\text{max}} = 6.5 \cdot 10^{-6}, \varepsilon_{\text{median}} = 1.13 \cdot 10^{-6}$$

Using established estimations for $\epsilon$ and setting maximum allowed error to $\delta = 10^{-5}$, the grid spacing for the second order finite difference scheme can be written as:

$$\sqrt{\frac{10\delta}{1.5}} \approx 0.008$$

It results in $125^5 \approx 3 \cdot 10^{10}$ points for each unit of 5D volume. Solution is obtained in the region $\Gamma$, which is a ball of radius 1. Its volume is:

$$\frac{8\pi^2}{15} \approx 5.26$$

Therefore, to cover internal part of $\Gamma 1.6 \cdot 10^{11}$ points are needed. The lower bond for the size of the external part can be calculated using similar considerations: 4D surface of 5D sphere has a measure of:

$$\frac{8\pi^2}{3} \approx 26.3$$

And it should at least be uniformly covered by points with the same spacing, which gives:

$$125^4 \cdot 26.3 \approx 6.4 \cdot 10^9$$

This value is about 5% of the internal one and is going to be omitted.

After discretization a linear system is to be solved. Its number of variables is equal to that of the grid points. Matrix
for such system is \(2n + 1 = 11\) diagonal. Solving time will be extrapolated using the data from H. Liu et al. [20]. They investigated performance of parallel AMG solvers run on Nvidia Tesla C2070 for various matrices and different implementations. Apart from relatively fast solution times [14], [19], [21] they use similar hardware, which eases the task of extrapolation. Tesla C2070 achieves 515 GFLOPS as it was used in double precision mode. In this paper Tesla P100 is operating with single precision for which it delivers 9340 GFLOPS. To make some room for estimation error one can consider that AMG solvers can run on single precision just as well. Therefore, the total ratio between theoretical computational powers is 18. The most similar matrix is \(P3D7P_{100}\). It was created by similar 7 point stencil for 3D Poisson equation on \(100^3\) grid. The least processing time mentioned for this matrix is 0.34 seconds. Using linear extrapolation, one can write an approximate running time for solving 5D linear Poisson equation:

\[
t_{5D} = 0.34\sec \cdot \frac{1.6 \cdot 10^{11}}{18 \cdot 100^3} \approx 3000\sec
\]

Estimation does not account for a fact that \(P3D7P_{100}\) is 7 diagonal, and the matrix to be solved is 11 diagonal. Similarly, for lower dimensions one can find:

\[
t_{4D} \approx 23\sec
\]
\[
t_{3D} \approx 0.15\sec
\]
\[
t_{2D} \approx 0.001\sec
\]

Plots of solving time against the number of dimensions can be seen on Fig. 2.

VI. CONCLUSION

Neural network method was applied to boundary value problems for linear and nonlinear Poisson equations inside 2, 3, 4 and 5 dimensional unit balls. It’s based on direct approximation of functions by multilayer perceptrons: independent variables are fed into input layer, and solution’s values are obtained at the output. Procedure was improved by considering, in addition to equation itself, it’s trivial consequences, obtained by differentiation. Prior to enhancements the method was mostly fringe and used as a proof of concept. With the additional cost terms and hardware efficient implementation it was able to compete with a second order finite difference scheme in solving 5D boundary value problem. For 4D cases and lower, classical method was far more effective. In higher dimensions neural networks managed to get ahead due to their ability to operate on grids with spacing as low as \(1/3\) provided solution’s derivatives up to 6th were of the order of 1. Even though it was compared against the simplest second order scheme, one can imagine some hard times trying to apply high order stencils to a grid that has no more than 6 points in each direction. Therefore, regardless of the order, the minimal number of points per dimension will probably always stay lower for neural networks so there is always a high dimensional task, for which finite differences are slower. One can also mention a decrease in memory complexity: if obtained on a grid, 5D solution would utilize at least 640GB of memory whereas neural network required about 2GB during the training and 640KB to store the result. This gap is mostly due to ineffective usage of resources by classical methods. For example, values of \(125^5\) grid can easily describe 125 completely different solutions of 4D equations, whereas training a 5D neural network to represent such a mess would probably not end very well. On the other hand for functions that do not change too fast almost any grid representation is a waste of memory since a set of independent values has too many degrees of freedom. From this point of view neural networks can provide much more efficient representation, which matters for higher dimensions.

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REFERENCES

[1] V.I. Avrutskiy. Avoiding overfitting of multilayer perceptrons by training derivatives. arXiv preprint, available 1 Jan 2018.
[2] V.I. Avrutskiy. Enhancing approximation abilities of neural networks by training derivatives. arXiv preprint [arXiv:1712.04473] 2017.
[3] Francesco Bassi and Stefano Rebay. A high-order accurate discontinuous finite element method for the numerical solution of the compressible navier-stokes equations. Journal of computational physics, 131(2):267–279, 1997.
[4] Arthur Earl Bryson. Applied optimal control: optimization, estimation and control. CRC Press, 1975.
[5] Pierre Cardaliaguet and Gaëlle Euvrard. Approximation of a function and its derivative with a neural network. Neural Networks, 5(2):207–220, 1992.
[6] Alexandre Joel Chorin. Numerical solution of the navier-stokes equations. Mathematics of computation, 22(104):745–762, 1968.
[7] George Cybenko. Approximation by superpositions of a sigmoidal function. Mathematics of Control, Signals, and Systems (MCSS), 2(4):303–314, 1989.
[8] Robert Eymard, Michael Gutnic, and Danielle Hilhorst. The finite volume method for Richards equation. Computational Geosciences, 3(3):259–294, 1999.
[9] Xavier Glorot and Yoshua Bengio. Understanding the difficulty of training deep feedforward neural networks. In Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, pages 249–256, 2010.
[10] Ernst Hairer, Christian Lubich, and Gerhard Wanner. Geometric numerical integration: structure-preserving algorithms for ordinary differential equations, volume 31. Springer Science & Business Media, 2006.

[11] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Delving deep into rectifiers: Surpassing human-level performance on imagenet classification. In Proceedings of the IEEE international conference on computer vision, pages 1026–1034, 2015.

[12] Kurt Hornik. Approximation capabilities of multilayer feedforward networks. Neural networks, 4(2):251–257, 1991.

[13] Kurt Hornik, Maxwell Stinchcombe, and Halbert White. Multilayer feedforward networks are universal approximators. Neural networks, 2(5):359–366, 1989.

[14] Marcin Krotkiewski and Marcin Dabrowski. Efficient 3d stencil computations using cuda. Parallel Computing, 39(10):533–548, 2013.

[15] Manoj Kumar and Neha Yadav. Multilayer perceptrons and radial basis function neural network methods for the solution of differential equations: a survey. Computers & Mathematics with Applications, 62(10):3796–3811, 2011.

[16] Vera Kurkova. Kolmogorov’s theorem and multilayer neural networks. Neural networks, 5(3):501–506, 1992.

[17] IE Lagaris, A Likas, and DI Fotiadis. Artificial neural network methods in quantum mechanics. Computer Physics Communications, 104(1-3):1–14, 1997.

[18] Isaac E Lagaris, Aristidis Likas, and Dimitrios I Fotiadis. Artificial neural networks for solving ordinary and partial differential equations. IEEE Transactions on Neural Networks, 9(5):987–1000, 1998.

[19] Hui Liu, Zhangxin Chen, and Bo Yang. Accelerating preconditioned iterative linear solvers on gpu. International Journal of Numerical Analysis and Modelling: Series B, 5(1-2):136–146, 2014.

[20] Hui Liu, Bo Yang, and Zhangxin Chen. Accelerating algebraic multigrid solvers on nvidia gpus. Computers & Mathematics with Applications, 70(5):1162–1181, 2015.

[21] Stoyan Markov, Peicho Petkov, Damyan Grancharov, and Georgi Georgiev. High performance poisson equation solver for hybrid cpu/gpu systems. 2013.

[22] Martin Riedmiller and Heinrich Braun. A direct adaptive method for faster backpropagation learning: The rprop algorithm. In Neural Networks, 1993., IEEE International Conference on, pages 586–591. IEEE, 1993.

[23] David E Rumelhart, Geoffrey E Hinton, Ronald J Williams, et al. Learning representations by back-propagating errors. Cognitive modeling, 5(3):1, 1988.

[24] Yazdan Shirvany, Mohsen Hayati, and Rostam Moradian. Multilayer perceptron neural networks with novel unsupervised training method for numerical solution of the partial differential equations. Applied Soft Computing, 9(1):20–29, 2009.

[25] Gordon D Smith. Numerical solution of partial differential equations: finite difference methods. Oxford university press, 1985.

[26] Allen Tallove and Susan C Hagness. Computational electrodynamics: the finite-difference time-domain method. Artech house, 2005.