Is it time to swish? Comparing activation functions in solving the Helmholtz equation using physics-informed neural networks

Introduction

Forward modeling lies at the heart of most inversion algorithms. Solving the wave equation numerically constitutes the majority of the computational cost for applications like seismic imaging and full waveform inversion (FWI). Frequency-domain solutions of the wave equation allow a reduction in dimensionality as they provide solutions of the Helmholtz equation per frequency. This approach to model wavefields gained popularity with the rise of waveform inversion (Pratt, 1999); however, such solutions require inverting a stiffness matrix that can become computationally intractable for large 3D models or for modeling high frequencies. Moreover, conventional algorithms do not have a mechanism to transfer information gained from solving one problem to the next. For example, the same amount of computational effort is needed to model wavefields corresponding to a small perturbation in the velocity model. This results in a computational bottleneck when repeated modeling is needed for updated velocity models, as in the case of FWI.

Recently, Alkhalifah et al. (2020) demonstrated the use of physics-informed neural networks (PINNs) to address some of the challenges associated with the conventional Helmholtz solvers, including the flexibility of modeling additional physics. By considering a homogeneous background model, for which the wavefield solution is obtained analytically, Alkhalifah et al. (2020) trained a neural network to solve for the scattered wavefield. Contrary to conventional deep learning approaches, instead of a labeled set, the training of the neural network is done through a loss function, which embeds the residual of the underlying Helmholtz equation. For an input given by a location in the computational domain, the neural network learns to map it to the scattered wavefield solution at the input location, thanks to the universal approximation theorem. The key enabler of PINNs is automatic differentiation that allows for fast and accurate derivative computation of the neural network’s output w.r.t. the inputs, which is needed to evaluate the loss function. By using machine learning techniques like transfer learning and surrogate modeling, the method can be used to speed up repeated wavefield computations, as suggested by Waheed et al. (2020) for the eikonal equation. The PINN-based Helmholtz solver has recently been extended for the vertically transversely isotropic (VTI) case (Song et al., 2021).

However, several challenges remain to be addressed in making the PINN-based Helmholtz solver fully practicable. Chief among them is the slow convergence of the neural network in the presence of sharp heterogeneities in the velocity model. Although fully-connected neural networks can approximate arbitrary functions, they have been shown to prioritize learning low frequency features of the underlying function, and hence exhibit a bias towards smooth functions. This poses difficulty in training them to approximate, for example, solutions corresponding to high frequencies or solutions for sharply varying velocity models that generate high-frequency features in the wavefield solution. These observations have been confirmed both in theory and practice (Rahaman et al., 2019; Cao et al., 2019).

Therefore, in this study, we explore the role of activation functions in improving convergence speed for the PINN-based Helmholtz solver. We do a comparative study of different activation functions that are routinely used in the PINN literature, namely hyperbolic tangent (tanh), inverse tangent (atan), and exponential linear unit (elu). In addition, we consider another variant of the ReLU activation function, named ‘swish’, which has shown superior performance over other activation functions on a number of challenging image classification and machine translation problems (Ramachandran et al., 2017). Through tests on a synthetic model, we find that the swish activation function shows markedly improved convergence rate and accuracy in solving the Helmholtz equation.

Theory

The Helmholtz equation in an acoustic, isotropic medium with constant density is given as:

\[
\left(\nabla^2 + \frac{\omega^2}{v^2}\right) u(x) = f(x),
\]
where $v$ is the wave velocity, $\omega$ is the angular frequency. The goal is to solve equation (1) for the complex valued wavefield $u(x) = \{u_r, u_i\}$ as a function of the angular frequency $\omega$. Then the time domain solution can be found using inverse Fourier transform of the superposition of the mono-frequency solutions. To avoid the problem of sampling near the source location, Alkhalifah et al. (2020) suggests solving the Lippmann-Schwinger form of the Helmholtz equation:

$$\left(\nabla^2 + \frac{\omega^2}{v^2}\right) \delta u = -\omega^2 \delta m u_0,$$

(2)

for the scattered wavefield $\delta u = u - u_0$, where $u_0$ is the background wavefield satisfying equation (1) for the background velocity $v_0$, and $\delta m = \frac{1}{v^2} \frac{\partial v}{\partial x} \frac{1}{v_0}$ is the velocity model perturbation. By using a background model with a constant velocity in which we can calculate the background wavefield $u_0$ analytically, we use equation (2) to calculate the scattered wavefield $\delta u$ per frequency, from which we find the solution to the Helmholtz equation (1) as:

$$u_r = \delta u_r + u_{0r}, \quad u_i = \delta u_i + u_{0i}.$$

To solve equation (2) using a deep neural network (DNN), we consider a network with two neurons in the input layer for the spatial coordinates $(x,z)$, two output neurons for the real and imaginary parts of the scattered wavefield, and a number of hidden layers. The second derivatives of the outputs $(\delta u_r, \delta u_i)$ w.r.t. the inputs $(x,z)$ can be computed using automatic differentiation. We seek to minimize the following loss function:

$$\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} \left[ |\omega^2 m^{(i)} \delta u_r^{(i)} + \nabla^2 \delta u_r^{(i)} + \omega^2 \delta m u_0^{(i)}|_2^2 + |\omega^2 m^{(i)} \delta u_i^{(i)} + \nabla^2 \delta u_i^{(i)} + \omega^2 \delta m u_0^{(i)}|_2^2 \right],$$

(3)

for the real and imaginary parts of the scattered wavefield $(\delta u_r, \delta u_i)$. Here $N$ is the number of training samples, which consists of a randomly selected collocation points from the computational domain, and $i$ is the sample index. The role of this loss function is to impose the validity of the Helmholtz equation on a given number of training points. The set of network parameters $\theta^*$ that minimize the loss function given in equation (3) on this set of training samples can be found by solving the following optimization problem:

$$\theta^* = \arg\min_{\theta} \mathcal{L}(x^*, z^*; \theta).$$

(4)

Once the DNN is trained, we evaluate it on a regular grid to obtain the predicted scattered wavefields, which are then added to the background wavefields to obtain the final wavefield solution.

**Activation functions**

The choice of activation function in DNNs has a significant impact on the training dynamics and convergence of the network. Activation functions are sources of nonlinearity as they transform the neural network function to a superposition of nonlinear basis functions. Choosing the right basis function can make a significant impact in efficiently representing a function. Therefore, in this study, we consider activation functions that are routinely used in the PINN literature (atan, tanh, and elu) in addition to the swish activation function, which is given as $f(x) = x \cdot \text{sigmoid}(x)$. Swish is a smooth, non-monotonic function that has consistently matched or outperformed ReLU on DNNs applied to a variety of challenging problems, including image classification and machine translation. It is believed that the reason for this improvement is that swish is able to better alleviate the problem of vanishing gradients during backpropagation.

**Results**

In this section, we present a comparative study of different activation functions to solve equation (2) for a two-scatter velocity model, shown in Figure 1. We keep all the hyper-parameters fixed to ensure fairness of the comparison. We use a DNN architecture with 8 hidden layers and 20 neurons in each layer, as used by Alkhalifah et al. (2020) for the considered velocity model. We randomly select 5000 locations from
Figure 1 A two-scatter velocity model taken from Alkhalifah et al. (2020) for the tests. The background has a homogeneous velocity of 2 km/s.

Figure 2 Loss history for training of the PINN model using different activation functions in the hidden layer.

the computational domain and train the PINN model using the Adam optimizer for 15,000 epochs with mini-batch optimization having a batch size of 256. The PINN model is implemented using the SciANN package (Haghighat and Juanes, 2021) – a high-level Tensorflow wrapper for scientific computations.

Figure 2 shows the loss history for training the PINN model using different activation functions considered. We observe that elu performs the worst with tanh and atan yielding similar performances, while swish has a markedly improved convergence compared to all the considered activation functions. For all activation functions, the convergence plateaus after an initial reduction of the loss value; however, swish recovers faster than the other activation functions. This can be observed by comparing the loss curves for the first 2000 epochs. We also tabulate the $L_2$ and $L_{\infty}$ errors for both the real and imaginary components of the wavefield solution using these activation functions (see Table 1). We clearly observe improved accuracy for the swish activation function compared to the rest.

In Figure 3, we show the scattered wavefield solution obtained from the PINN model trained using the swish activation function. We also plot the wavefield errors on the same color scale. The overall errors are considerably smaller than for the solutions computed using other activation functions as confirmed by Table 1.

Conclusions

We studied the routinely used activation functions from the PINN literature in solving the Helmholtz equation. In addition, we also considered the swish activation function, which is a variant of ReLU. Swish had shown improved performance compared to other activation functions in training DNNs for a variety of data science problems, thanks to its robustness against the problem of vanishing gradients. We also observed superior convergence using the swish activation function in solving the Helmholtz equation. Although these results are preliminary, they demonstrate the potential of selecting better
activation functions to improve the convergence of PINN solvers. To focus on the activation functions in this study, we only used the Adam optimizer for all cases. However, to converge faster, typically the optimization process begins with a first-order optimizer like Adam and then switches to a second-order optimizer like L-BFGS after a suitably low value of the loss function. Seeing the loss curves, it can be noted that swish allows early switching to a second-order optimizer compared to other studied activation functions, which would compound its efficacy.

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References


<table>
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<th>Activation functions</th>
<th>( L_2 )</th>
<th>( L_{\infty} )</th>
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<td>Imag.</td>
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<td>tanh</td>
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<td>swish</td>
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<td>( 4.7 \times 10^{-5} )</td>
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Table 1: \( L_2 \) and \( L_{\infty} \) errors for the real and imaginary parts of the PINN Helmholtz solution obtained using different activation functions.