Using Physics-Informed Regularization to Improve Extrapolation Capabilities of Neural Networks

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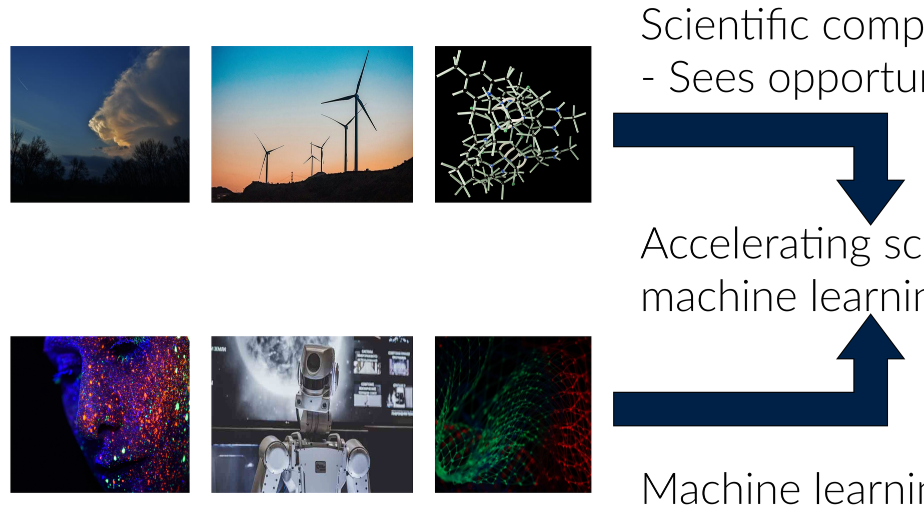
Scientific Computing meets Machine Learning



Scientific computing community
- Sees opportunity for improvement

Accelerating scientific applications with machine learning ("AI for Science")

Machine learning community
- Building on prior success, wants to expand

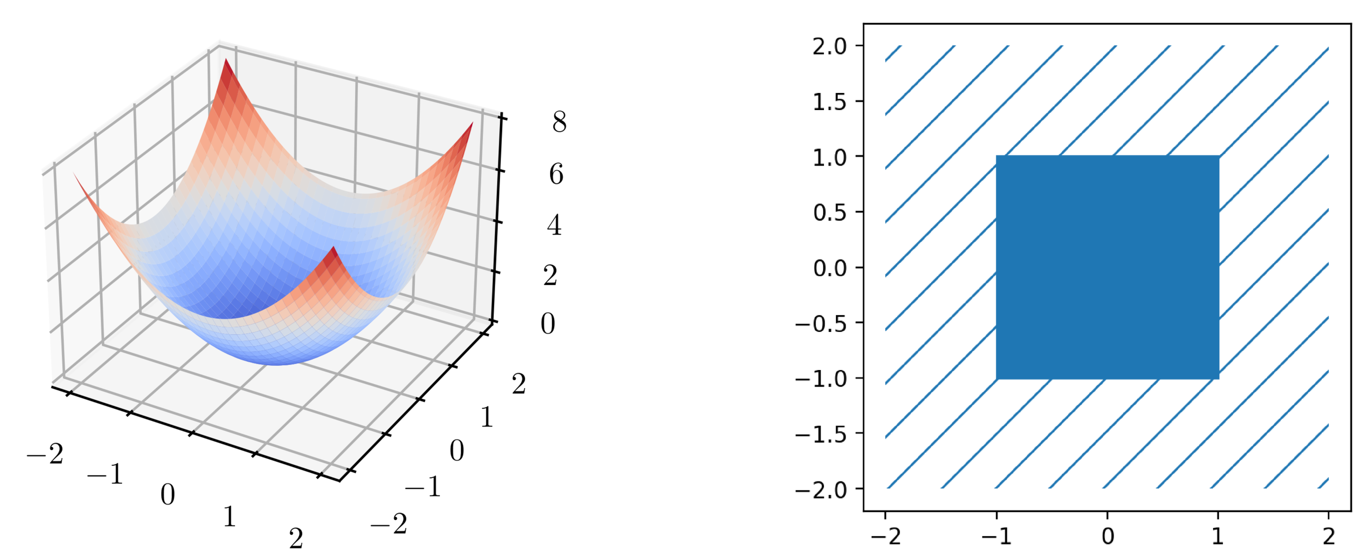
However, neural network based physics emulators suffer from a lack of extrapolation capabilities. We explore physics-based regularization to address this challenge.

Improving Extrapolation Capabilities via Regularization: Developing a Strategy Based on a Two-Dimensional Function

Model

$$f(x, y) = x^2 + y^2$$

using a neural network over the domain $[-2, 2] \times [-2, 2]$.



(a) Function to model over the domain $[-2, 2] \times [-2, 2]$

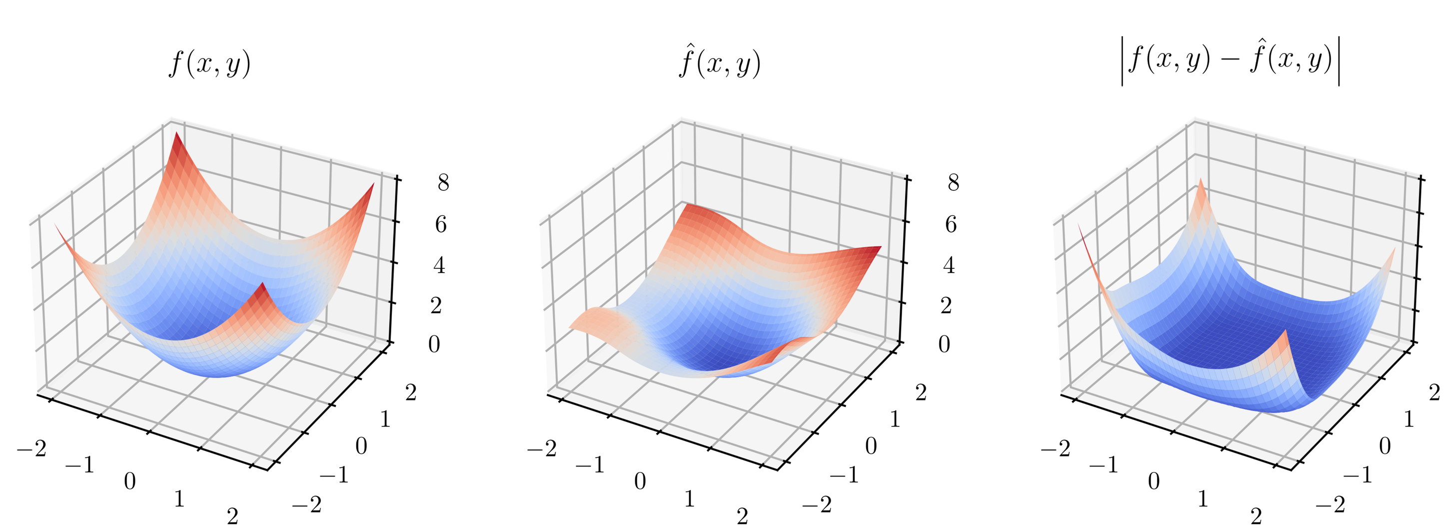
(b) Interpolation region is the square from $[-1, 1] \times [-1, 1]$ (shown in blue). Extrapolation region is the rest of the domain (shown in hatched lines)

Main goal: Improve the accuracy of a neural network in the extrapolation region while only using labeled data in the interpolation region

Paraboloid: Baseline Model

Loss Function is just MSE on labeled points in the interpolation region $[-1, 1]\times[-1, 1]$

$$\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N} \left| f\left(\mathbf{x}^{\{i\}}\right) - \hat{f}\left(\mathbf{x}^{\{i\}}\right)\right|^2$$



(a) Target Function (b) Model Prediction (c) Absolute Error

Paraboloid: Physics-Informed Regularizers

Seek to regularize the neural network based on information embedded into the function we are trying to predict, but without using additional data. For example,

All second derivatives are constant

$$E_2\left(\hat{f}, \mathbf{x}\right) = \mathrm{Var}\left(\hat{f}_{xx}(\mathbf{x})\right) + \mathrm{Var}\left(\hat{f}_{yy}(\mathbf{x})\right) + \mathrm{Var}\left(\hat{f}_{xy}(\mathbf{x})\right) + \mathrm{Var}\left(\hat{f}_{yx}(\mathbf{x})\right) \approx 0$$

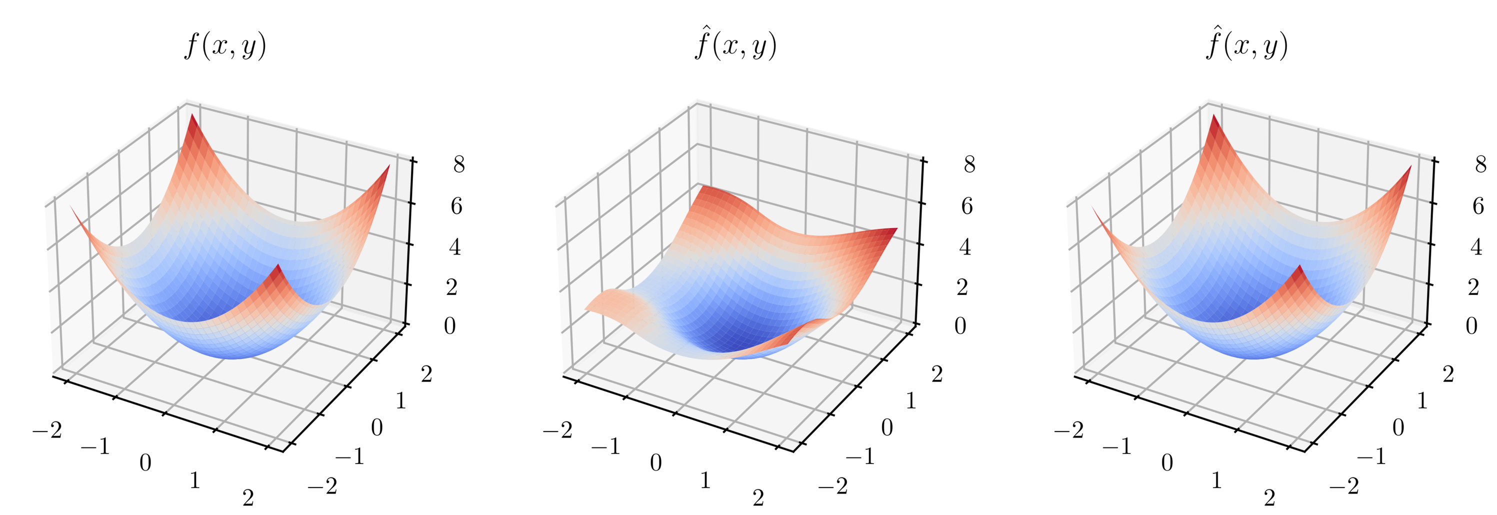
All third derivatives are zero

$$E_3\left(\hat{f}, \mathbf{x}^{\{i\}}\right) = \left|\hat{f}_{xxx}\left(\mathbf{x}^{\{i\}}\right)\right| + \left|\hat{f}_{xxy}\left(\mathbf{x}^{\{i\}}\right)\right| \ldots + \left|\hat{f}_{yyx}\left(\mathbf{x}^{\{i\}}\right)\right| + \left|\hat{f}_{yyy}\left(\mathbf{x}^{\{i\}}\right)\right| \approx 0$$

Using E_3, the loss function can now become

$$\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N} L\left(\hat{f}, \mathbf{x}^{\{i\}}\right) \text{ where}$$

$$L\left(\hat{f}, \mathbf{x}^{\{i\}}\right) = \begin{cases} \left|f\left(\mathbf{x}^{\{i\}}\right) - \hat{f}\left(\mathbf{x}^{\{i\}}\right)\right|^2 + \lambda E_3\left(\hat{f}, \mathbf{x}^{\{i\}}\right) & \text{if } \mathbf{x}^{\{i\}} \in \Omega_{\text{int}} \\ \lambda E_3\left(\hat{f}, \mathbf{x}^{\{i\}}\right) & \text{if } \mathbf{x}^{\{i\}} \in \Omega_{\text{ext}} \end{cases}$$



(a) Target Function (b) Baseline Model. Ext. Error: 8.46×10^{-1} (c) Third Order Regularizer. Ext. Error: 1.90×10^{-2}

Improving Extrapolation Capabilities via Regularization: Two-Dimensional Acoustic Wave Equation

$$\frac{\partial p}{\partial t} + \kappa \nabla \cdot \mathbf{v} = 0$$
$$\frac{\partial \mathbf{v}}{\partial t} + \frac{1}{\rho}\nabla p = 0$$

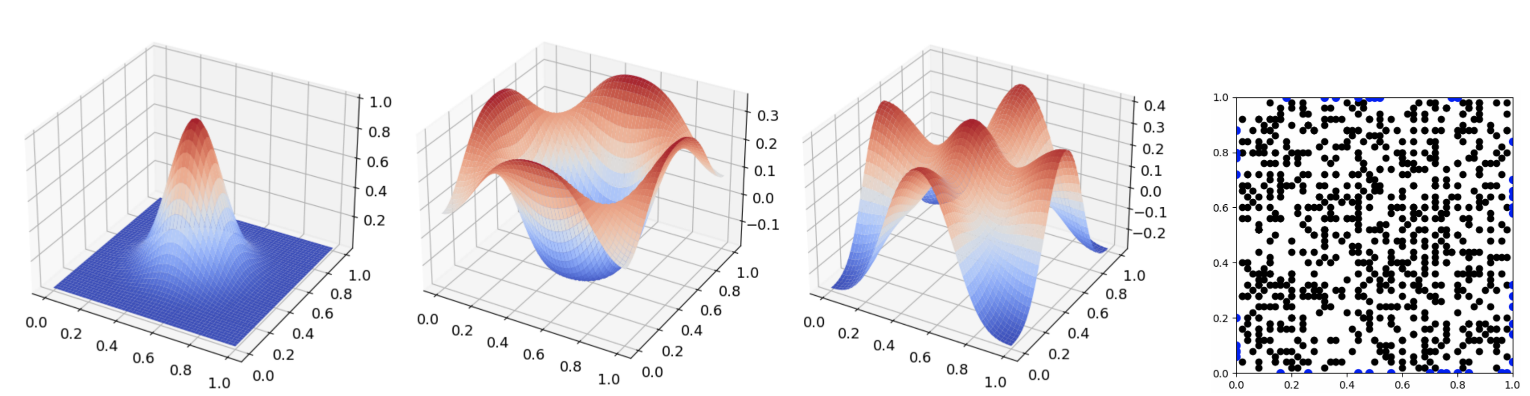
(a) First Order System

$$\frac{\partial^2 p}{\partial t^2} = c^2\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2}\right)$$

(b) Second Order Equation

Main Goal: Improve accuracy of neural network in extrapolation region ($t > 1$) while only using labeled data in the interpolation region ($t \leq 1$)

- Reflecting boundary conditions ($\mathbf{v}_n = 0$)
- Labeled data: data sampled in space every 10^{th} time step for $t \leq 1$. Spatial samples based on on random selection of 1% of discretization points
- 10% of boundary points are also selected, where a boundary-condition regularizer can be applied



(a) Simulation ($t = 0.0$) (b) Simulation ($t = 0.4$) (c) Simulation ($t = 1.0$) (d) Data collection at $t = 0.25$

Augment the loss function with physics-based regularization that does not require labeled data

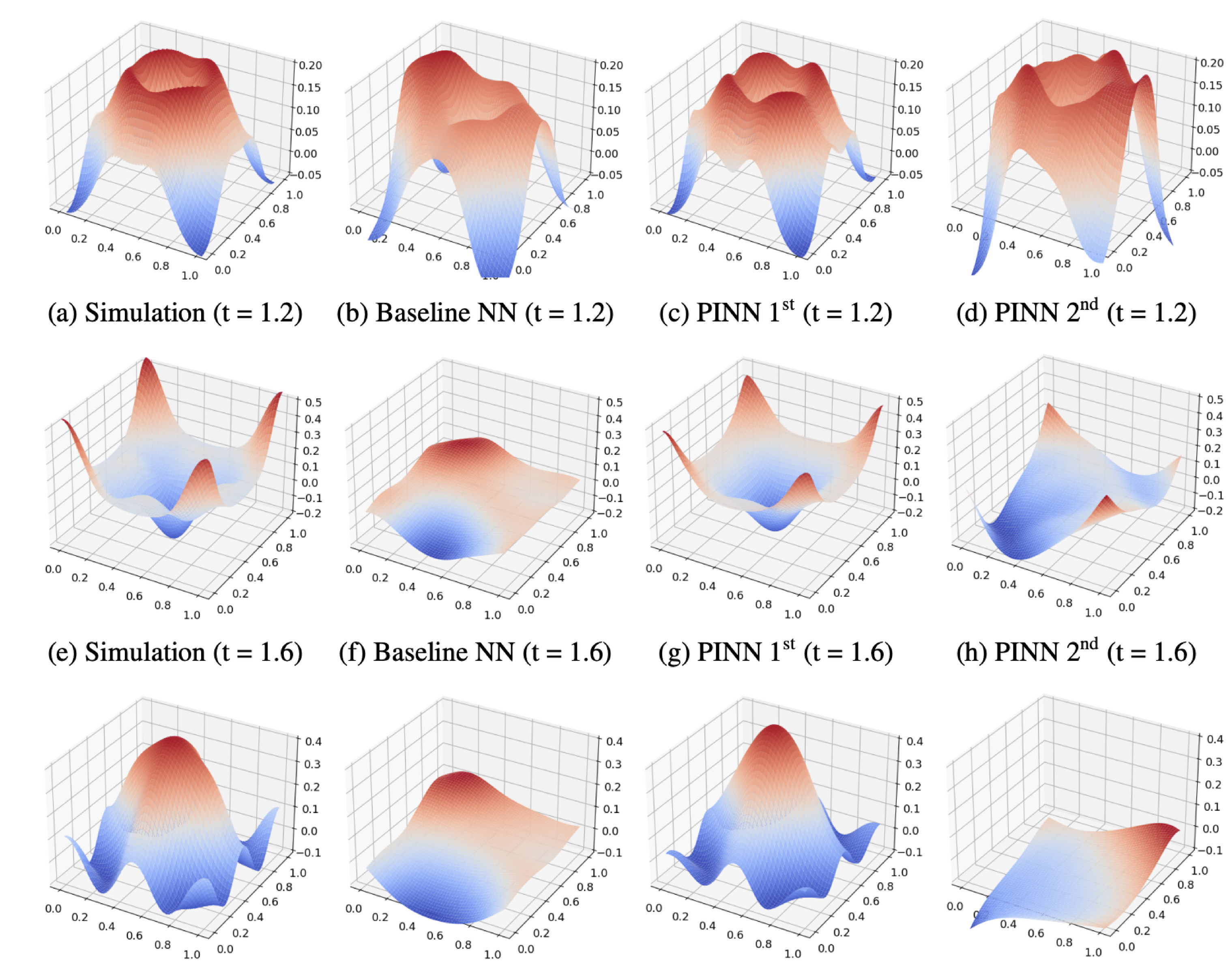
$$\mathcal{L} = \mathrm{MSE} + \lambda_r E_r + \lambda_b E_b$$

where E_r is a PDE-based regularizer that does not require labeled data and E_b is a boundary condition regularizer that does not require labeled data.

Two Dimensional Acoustic Wave Results

Name	E_r	E_b	Interp Error	Extrap Error
Baseline	N/A	N/A	1.8×10^{-3} (43%)	1.8×10^{-1} (16%)
PINN 1st	$\lvert\hat{p}_t - \nabla \cdot \hat{\mathbf{v}}\rvert + \lVert\hat{\mathbf{v}}_t + \nabla\hat{p}\rVert$	$\lVert\hat{\mathbf{v}}_n\rVert$	7.3×10^{-3} (9%)	3.1×10^{-2} (35%)
PINN 2nd	$\lvert\hat{p}_{tt} - \nabla^2\hat{p}\rvert$	N/A	1.8×10^{-2} (7%)	1.9×10^{-1} (25%)

Table 1. Performance of various physics-based regularization strategies (average of five runs with standard deviation shown in parentheses)



(a) Simulation (t = 1.2) (b) Baseline NN (t = 1.2) (c) PINN 1st (t = 1.2) (d) PINN 2nd (t = 1.2)

(e) Simulation (t = 1.6) (f) Baseline NN (t = 1.6) (g) PINN 1st (t = 1.6) (h) PINN 2nd (t = 1.6)

(i) Simulation (t = 2.0) (j) Baseline NN (t = 2.0) (k) PINN 1st (t = 2.0) (l) PINN 2nd (t = 2.0)

Figure 6. Comparison of extrapolation performance between simulation (left column) and predictions from neural networks trained with different regularization strategies

Future Work

Develop an a posteriori error estimate and devise more efficient sampling strategies based on a measure of neuron saturation.

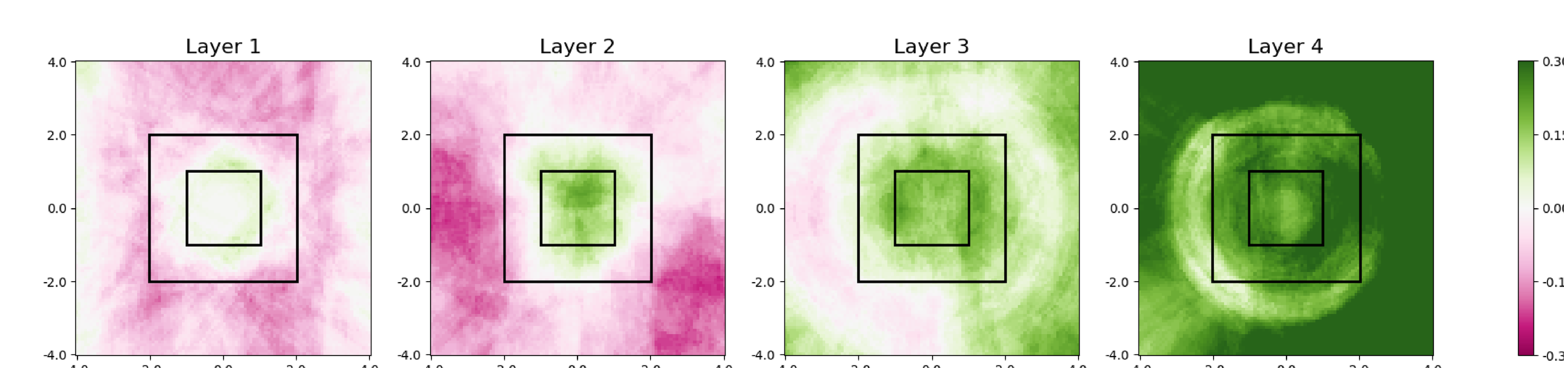


Figure 7. Difference in layer-wise saturation between a PINN with a 2^{nd} order regularizer and a baseline NN for the paraboloid target function. Negative (pink) values indicate the PINN is less saturated in the region while positive (green) values indicate the PINN is more saturated in that region compared to the baseline NN.

* These five authors contributed equally. Work performed while first five authors attended UCLA/IPAM's Research in Industrial Projects for Students summer program (Ha and White were academic and industrial mentors, respectively).