

Physics-Informed Neural Networks for Structural Concrete Engineering

Master's Thesis FS 2021

Rafael Bischof

Supervisors

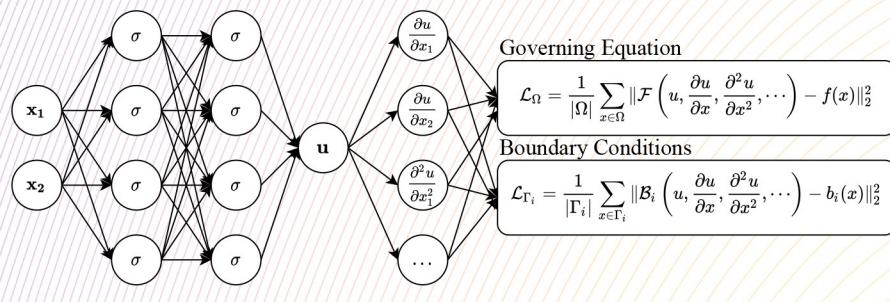
Dr. Michael Kraus

Prof. Dr. Olga Sorkine-Hornung

Prof. Dr. Walter Kaufmann

Introduction

Physics-Informed Neural Networks (PINN) present a way of parameterising partial differential equation (PDE) by including the governing equation and boundary conditions into their loss function.



Structure of a Physics-Informed Neural Network

Their continuity, flexibility and the perspective of solving arbitrary instances of a given PDE in a single forward pass, might turn PINNs into a valuable alternative to established, mesh-based numerical techniques like the Finite Element Method.

Adaptive Loss Balancing

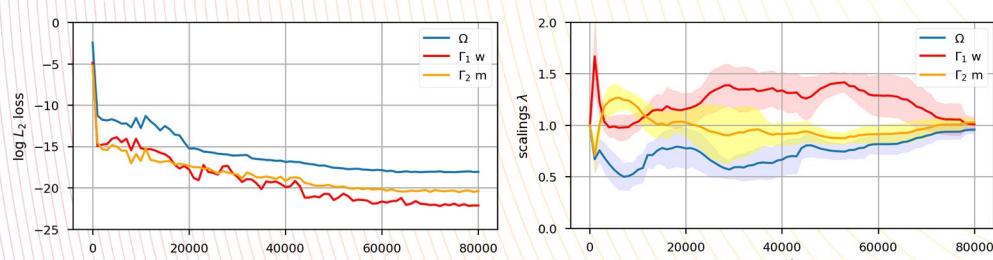
In a first step, we address the issue of gradient pathologies arising because of terms with different units of measurements and thus of varying magnitudes in the loss function.

$$\mathcal{L} = \lambda_0 \mathcal{L}_\Omega + \sum_{i=1}^M \lambda_i \mathcal{L}_{\Gamma_i}$$

Linear scalarisation of the loss terms

Adaptive loss balancing techniques are automated heuristics for selecting the scaling factors, therefore eliminating the need for extensive grid-search. We implemented and compared several techniques proposed in the context of PINNs (Learning Rate Annealing) as well as Computer Vision (GradNorm, Softadapt). Finally, we propose a new approach by combining the best attributes of the aforementioned solutions.

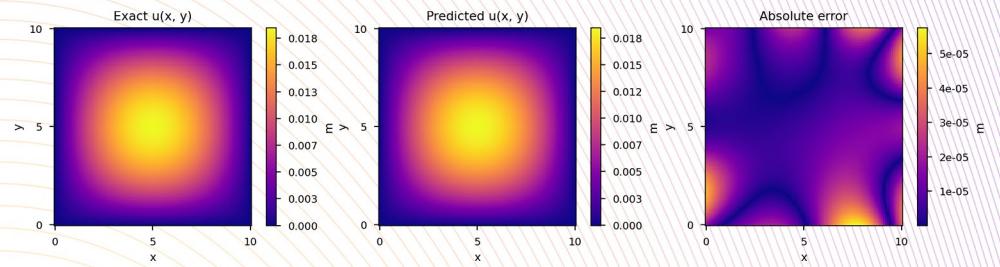
We employ SoftAdapt's balancing method using the rate of change between consecutive training steps and normalizing them through a softmax function. Similar to Learning Rate Annealing, we update the scalings using an exponential decay in order to utilise loss statistics from more than just one training step in the past. In addition, we introduce a random lookback into the exponential decay, where a Bernoulli random variable decides whether to use the previous steps' loss statistics to calculate the scalings, or whether to look all the way back until the start of training.



Our approach proved to perform considerably better than existing methods on the Kirchhoff plate bending problem, while also being about six times more computationally efficient. Furthermore, we showed that the adaptively chosen scalings λ can be inspected to learn about the training process and identify weak points. This allows to make informed decisions in order to improve the framework.

Parameter Study on Kirchhoff Plate Bending Problem

In a second step, we focus on applying PINNs to the Kirchhoff plate bending problem and study the effects of a wide selection of state-of-the-art techniques proposed in the context of PINNs. More specifically, we test several network architectures by varying the depth, width and adding residual connections, the activation functions *tanh*, *sigmoid* and *sine*, as well as sampling the collocation points randomly, dynamically at every iteration or adversarially. In addition, we also re-implement the adaptive loss balancing techniques introduced in the previous section.

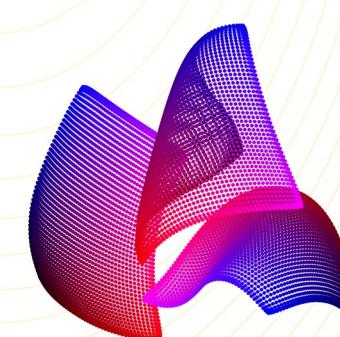


We analysed the results in perspective with important properties from structural engineering, highlighted hyperparameters and extensions which improve the model's performance compared to the original PINN, and identified a number of trade-offs that need to be addressed on a per-task basis. The best performing models achieved accuracies exceeding minimum requirements for practical applications, thus showing the PINN's potential at parameterising Kirchhoff's PDE.

fully connected (tanh)	4.7e-08 6.2e-07	1.7e-09 4.7e-10	1.9e-09 5.4e-09	1.8e-08 1.3e-08	2.9e-09 2.7e-09	8.3e-10 1.9e-10	4.6e-09 1.1e-09	1.6e-09 4.4e-09	1.7e-09 7.3e-10
fully connected (sigmoid)	9.2e-08 3.8e-05	7.1e-08 2.3e-08	3.1e-09 2.3e-09	3.9e-08 4.4e-06	1.6e-08 7.0e-09	6.9e-09 4.7e-09	1.2e-08 1.1e-07	5.4e-09 5.9e-10	2.5e-09 5.1e-10
fully connected (sine)	1.7e-08 1.3e-09	2.4e-10 2.7e-11	1.3e-10 1.2e-10	3.0e-09 3.3e-09	2.7e-10 2.2e-10	1.0e-10 2.8e-11	3.0e-08 3.0e-08	1.1e-09 1.5e-09	1.0e-09 3.0e-09
multiplicative residual	4.0e-08 2.1e-07	7.8e-10 4.4e-09	1.9e-09 1.4e-09	2.5e-08 4.8e-08	1.8e-09 1.6e-09	1.9e-09 9.1e-10	1.5e-08 8.6e-06	7.5e-10 5.2e-10	5.5e-10 4.8e-10

2 layer, 32 nodes 2 layer, 128 nodes 2 layer, 256 nodes 3 layer, 32 nodes 3 layer, 128 nodes 3 layer, 256 nodes 5 layer, 32 nodes 5 layer, 128 nodes 5 layer, 256 nodes

The results (median values and standard deviations over five runs) indicate that wider networks tend to perform better, whereas shallow networks of only two or three layers are enough to approximate the latent function very accurately. Not only do additional layers not bring any gains in prediction accuracy, the computation time required to train them also increases exponentially. Therefore, we see no benefit in exploring deeper networks. This is contrary to the general trend in Deep Learning, where it is widely understood that depth in networks incites learning features at various levels of abstraction and increases their ability to extrapolate. To understand better the inner workings of PINNs, we inspected the latent representations within the network using t-SNE visualisations.



Finding the mathematical explanation for this phenomenon might open up a vast number of new possibilities for improving the performance of PINNs, e.g. allowing to build specialised architectures that favour this kind of internal representations. Furthermore, the clear shapes in the hidden representations could give hints as to how PINNs make their predictions and potentially reveal weak-points, which would be a great boost to their interpretability and thus also to their adequacy for use in practice.

Hypernetworks

Finally, we successfully implemented hypernetworks to generate task-specialised PINNs and learn priors over the space of functions that define them. A hypernetwork converts input embeddings to weights and biases of another, main network (e.g. a PINN), therefore eliminating the need for a backward pass at inference time and thus greatly reducing computation time compared to other techniques like transfer learning or meta learning. While not yet as accurate and reliable as other, established techniques, PINNs generated by hypernetworks could become a valuable tool for fast prototyping by providing engineers with instant predictions in a single forward pass.