relationship between the average persistence and the same ML-based metrics. Together, these results provide additional insight into how changing the architecture of a neural network like ResNet-20 can result in a "smoother" (and thereby easier to optimize) loss landscape.

3.2 Physics-Informed Neural Networks

In our second experiment, we look at a set of physics-informed neural network (PINN) models trained to solve increasingly difficult convection problems. Specifically, we consider the one-dimensional convection problem, a hyperbolic partial differential equation that is commonly used to model transport phenomena:

$$\frac{\partial u}{\partial t} + \beta \frac{\partial u}{\partial x} = 0, \quad x \in \Omega, \quad t \in [0, T] \tag{1}$$

$$u(x,0) = h(x), \quad x \in \Omega, \tag{2}$$

where β is the convection coefficient and $h(x)$ is the initial condition. The general loss function for this problem is

$$L(\theta) = \frac{1}{N_u} \sum_{i=1}^{N_u} (\hat{u} - u_0^i)^2 + \frac{1}{N_f} \sum_{i=1}^{N_f} \lambda_i (\frac{\partial \hat{u}}{\partial t} + \beta \frac{\partial \hat{u}}{\partial x})^2 + L_B, \tag{3}$$

where $\hat{u} = NN(\theta, x, t)$ is the output of the NN, and L_B is the boundary loss. The goal of this case study is to investigate the PINN's soft regularization and how it helps (or fails to help) the optimizer find optimal solutions to seemingly simple convection problems. As shown in Krishnapriyan et al. [2021], increasing the wave speed parameter, β, can make it harder for the PINN to find a reasonable solution. This difficulty has been linked to changes in the loss landscape, which becomes increasingly complicated, such that optimizing the model becomes increasingly difficult.

In Fig. 2, we show that increasing the wave speed indeed results in a more complicated loss landscape. In the bottom row, we show the spatiotemporal patterns predicted by the PINN models. Note, increasing β makes the problem harder to solve, and here we can see that our PINN models fail to

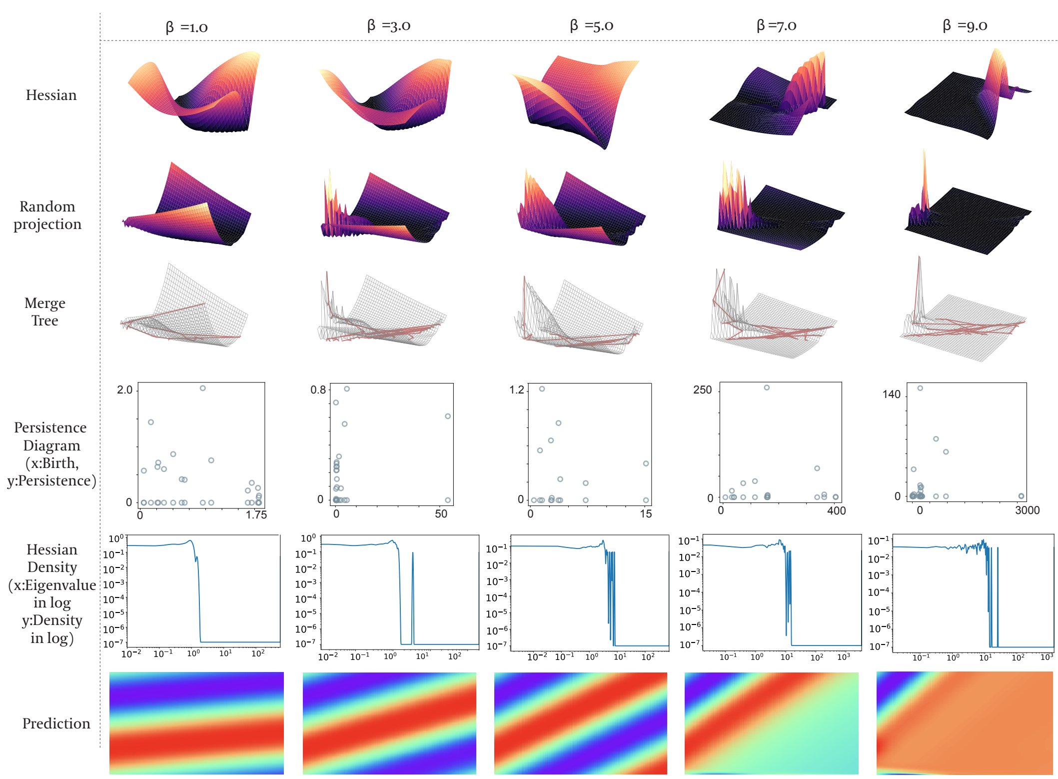

Figure 2: Visualizing the failure modes of PINNs. Compare with Krishnapriyan et al. [2021].

accurately predict the pattern around $\beta = 7.0$. Looking at the first three rows, we observe increasingly complex loss landscapes as β increases, in both versions of the loss landscape and further revealed by the more complicated and branched structure of the merge tree (i.e., with many more minima and saddle points). The change in complexity of the landscape is further supported by higher persistence values in the persistence diagrams. We also relate our observations to the Hessian Density, which suggests that the volume and complexity of the loss landscape increases with β. Together, these different views give us a more holistic understanding of how the loss landscape changes as β increases. Interestingly, these observations agree with previous findings that increasing β results in a more complicated loss landscape, corresponding to a harder optimization problem [Krishnapriyan et al., 2021]. We further verify these observations numerically in Fig. 6 (in the appendix). These plots provide additional insights beyond the qualitative changes in the loss landscapes we observed, confirming that the number of saddle points in the merge tree (left column) increases, along with the average persistence (right column), as the value of β increases. We observe similar trends in the Absolute Error, Top-1 Hessian Eigenvalue, and Hessian Trace as β increases. Together, these results reaffirm previous findings and provide new insights into the failure modes of PINNs, revealing that the topology of the loss landscape becomes significantly complex as PINNs start to fail.

4 Conclusion and Future Work

In this work, we study neural network loss landscapes through the lens of TDA. Specifically, we capture the underlying shape of loss landscapes using merge trees and persistence diagrams. By quantifying these topological constructs, we reveal new insights about the landscapes. Furthermore, we explore the relationship between our TDA-based metrics and relevant traditional ML metrics. For ResNet models, we find that the number of saddle points is inversely related to the average persistence and to the other ML-based metrics. For PINN models, we find that the number of saddle points and average persistence increase together along with the other ML-based metrics. These relationships reflect the curvature and sharpness of the landscape, which in turn strongly impacts the model's performance and generalization abilities. Note, in this work we only show the 0-dimensional persistence diagram, which is exactly what the branches in the merge tree encode. Since here our original focus was on extracting merge trees, we decided to limit our analysis to these lower-dimensional features. We leave the analysis of higher-dimensional holes for future work.

Moreover, since the merge tree and persistence diagram can be computed for arbitrary-dimensional spaces, our generalized and scalable approach opens up the door to studying loss landscapes in higher dimensions. In the future, we hope to extend our approach to characterize higher-dimensional loss landscapes, under the hypothesis that more information (hidden in these additional dimensions) could perhaps provide new insights into the loss function and properties relating neural network architecture to learning dynamics. One simple way to do this would be to sample along more directions. So, for example, we could construct a subspace based on the top 3 to 10 Hessian eigenvectors. While this would still be far from the potentially billions of dimensions in the true high-dimensional loss landscapes of modern ML models (with potentially billions of parameters), we expect that there exists a much lower-dimensional manifold upon which the interesting variation can be observed.

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