# 1st August Progress

Ran PINN for 5 000 initial steps (Default: 15 000). PINN prediction of solution at that step shown in figure 1.

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| Figure 1 – Approx solution using adam, colour indicates z-axis value for all graphs. | |

Using PINN to predict solution over a dense field of random points (10 000), then evaluating absolute PDE residual at every point, figure 2 is obtained. This is the how residual-based resampling is done.

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| C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - Residual.png | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - Residual Iso.png |
| Figure 2 - PDE Residual magnitude. | |

The same approach is used for obtaining gradient and curvature graphs; but quering for the appropriate component of the Jacobian and Hessian matrix of the solution as required. The results of this are in the following page.

The ground truth gradient to compare against is obtained by using np.gradients (which uses second order finite differences) on the ground truth u solution grid, which is size 100\*256.

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| Gradient | From PINNs | From Ground Truth |
| du/dx | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - u_x.png |  |
| du/dt | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - u_t.png | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\GroundTruth2 - u_t.png |
| du/dt, isometric view | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - u_t iso.png | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\GroundTruth2 - u_t iso.png |
| Figure 3 – Gradients obtained from PINNs vs Ground Truth | | |

First, note scale in du/dt much smaller than scale in du/dx, as u changes slowly in time axis.

Qualitative agreement shows gradients obtained are what is expected; the inaccuracy could be attributed to limited number of PINN solve iterations.

I could check by obtaining gradients after running the PINN with default number of iterations and after the last resampling loop. For now, the above gradients are good enough to guide resampling of points.

Using the residual and gradient information to guide resampling, figure 4 shows how points could be redistributed. Keep in mind the information creates a probability distribution, and so re-running would produce a similar but different pattern.

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| --- |
| C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - Resampling from Gradients.png |
| Figure 4 |

The du/dx case biases points more accurately on the shock line than residual case, which positions points broadly around it. Case du/dx also biases fewer points towards the shockline, despite the magnitude of gradients being larger than the magnitude of residuals. In the du/dt case, a very slight bias is seen towards the initial area, due to the relatively smaller gradients.

The above was repeated for curvature, and how this guided point resampling is seen in figure 5. The graphs of what the curvature looked like are in the next page, in figure 6, where they are compared to curvature obtained from ground truth.

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| C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - Resampling from Curvature.png |
| Figure 5 – Whilst , the points are differently placed due to inherent randomness |

To evaluate curvature from ground truth, I used the same np.gradients function on the previous gradients obtained from ground truth. With PINNs, the different components of the Hessian matrix were analysed in turn.

These are compared to the curvature obtained from the PINN prediction below in figure 6.

|  |  |  |
| --- | --- | --- |
| Curvature | From PINNs | Ground Truth |
|  | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - u_xx.png | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\GroundTruth2 - u_xx.png |
|  | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - u_tt.png | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\GroundTruth2 - u_tt.png |
|  | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - u_xt.png | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\GroundTruth2 - u_xt.png |
|  | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\InitialTest - u_tx.png | C:\Users\mn17jilf\Uni\PhD\Projects\JPINN-Sampling\pinn-sampling\results\plots\Gradients and Curvature\GroundTruth2 - u_tx.png |
| Figure 6 - Curvature obtained from PINNs vs Ground Truth | | |

Whilst the general shapes are still broadly accurate, for the error is amplified. As the scale of curvature increases drastically, the bias towards the shock is much greater for the curvature in x only.

The results from are equal to the results from for both PINN and ground truth, which serves as an extra check.

# Next Steps

Measure the accuracy of PINN using purely gradient or curvature based resampling instead of residual-based resampling, without hyper-parameter tuning.

1. Decide which metric/s to use. Could attempt to use only , combine and information, or use curvature info too.
2. Set up code so it can be re-run multiple times on HPC without memory issues.

Re-measure and save gradients/curvature estimate after the PINN model has converged onto solution for a quantitative check.