Predicting time dependent shock propagation using Machine Learning

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Overview

We study the ability of both shallow learning methods and deep learning methods to predict shock behavior, with the goal of producing a model that can infer the underlying physics of shock propagation.

Background

Shocks are propagating discontinuities in flow parameters

- Hydrodynamic equations allow for discontinuous solutions
- Shocks appear in high energy situations such as explosions and fusion events

The Viscous Burgers' Equation models shock behavior

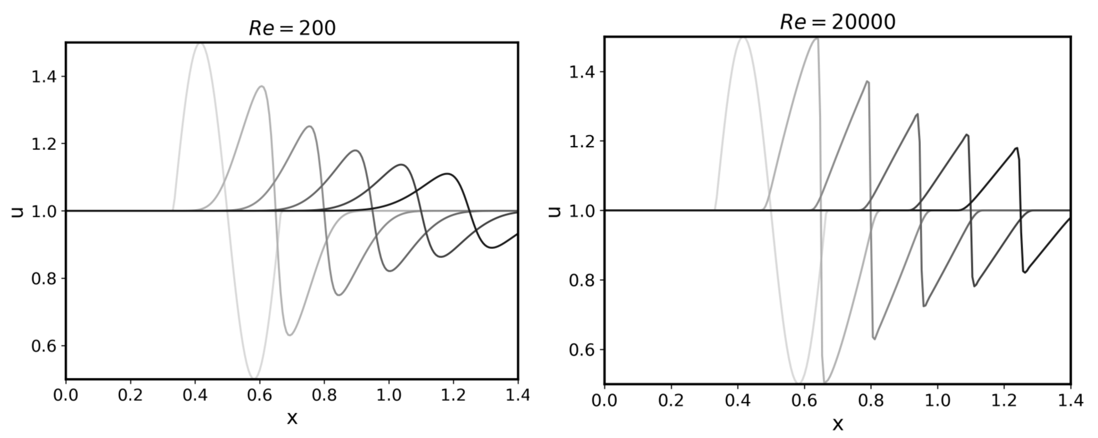
- Fundamental PDE describes fluid flow, gas dynamics and acoustics in one dimension
- Derived from the Navier-Stokes Equation by neglecting pressure and body-force terms, and assuming incompressibility

$$\overbrace{\underbrace{\frac{\partial \mathbf{u}}{\partial t}}_{\text{Variation}} + \underbrace{(\mathbf{u}\cdot\nabla)\mathbf{u}}_{\text{Convection}}}^{\text{Inertia (per volume)}} \overbrace{- \underbrace{\nu\nabla^2\mathbf{u}}_{\text{Diffusion}} = \underbrace{\cancel{-\nabla w}}_{\substack{\text{Internal}\\ \text{source}}}}^{\text{Divergence of stress}} + \underbrace{\cancel{\mathbf{g}}}_{\substack{\text{External}\\ \text{source}}} . \longrightarrow \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$$

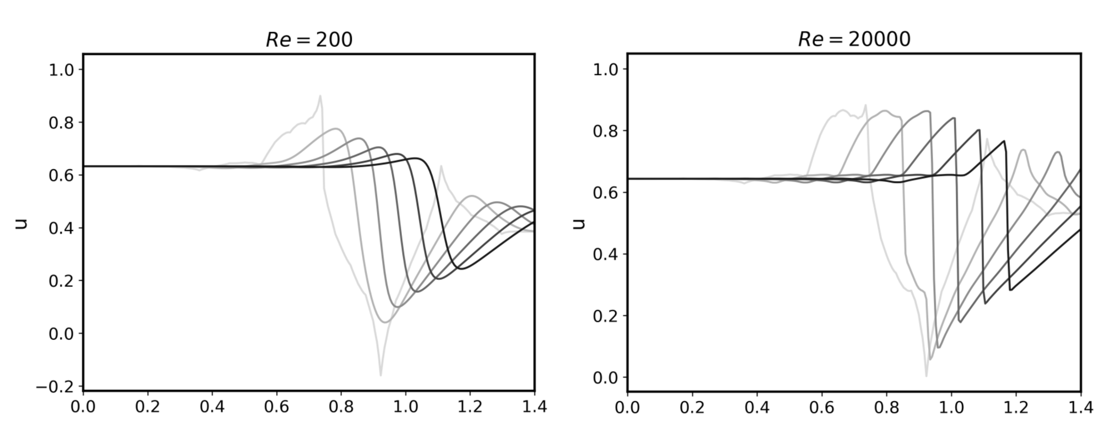
Navier-Stokes Equation *Burgers' Equation*

Data Generation

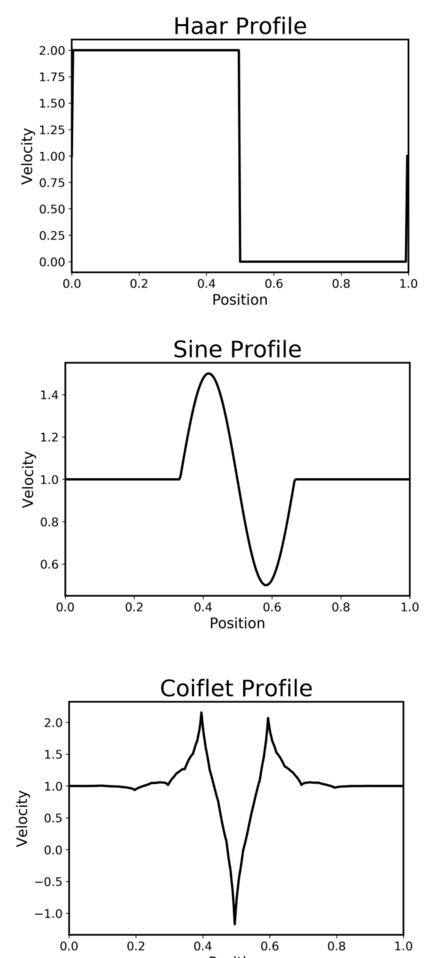
- Eulerian method solves the Burgers equation by implementing **second-order advective and diffusive updates**, after an **initial velocity profile is specified**
- Four datasets were created to explore the performance of the model in isolated situations -
  - Single and multiple shock systems, each with both sinusoidal and "complex" velocity initial profiles
  - Complex velocity profiles generated by randomly weighting linear combinations of sine, coiflet and haar wavelet profiles
  - Reynolds number varied from 10 – 20 000



Shocks with sinusoidal initial profiles propagating through space



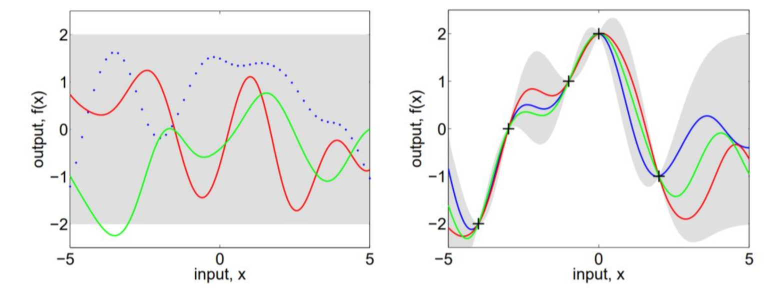
Shocks with complex initial profiles propagating through space



Methodology

- The input to the prediction algorithm contains the velocity initialization, time elapsed from the initial state, and the Reynolds number.

Gaussian Process Regression

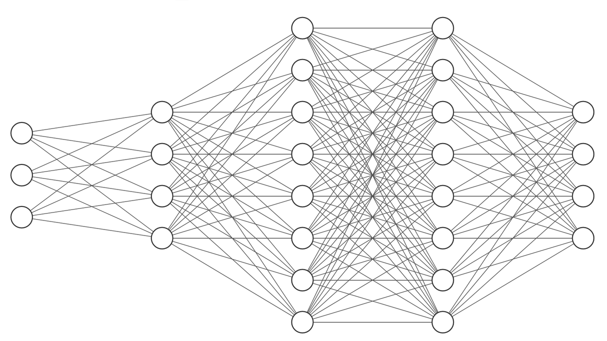


- Prior distribution of functions specified by a covariance kernel
- Posterior distribution based on observed data

Matérn covariance kernel with ν = 0.5 captures discontinuity present in shocks

$$C_\nu(d) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\frac{d}{\rho}\right)^\nu K_\nu\left(\sqrt{2\nu}\frac{d}{\rho}\right)$$

Deep Neural Network

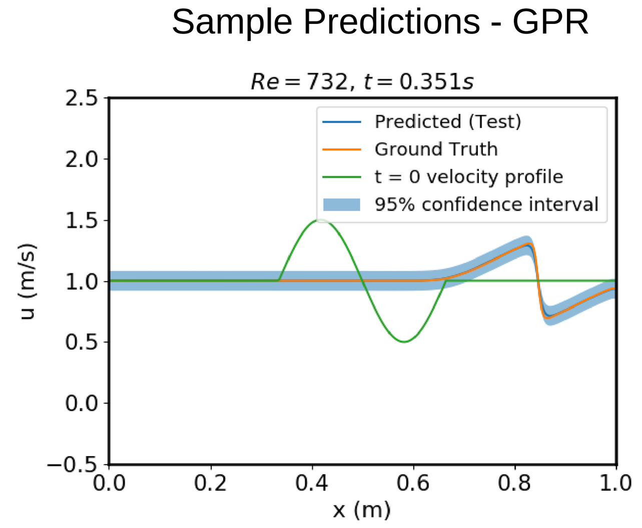


- **Five fully connected layers**
  - ReLU activation functions
  - 512 neurons per hidden layer
- Final linear layer predicts shock profiles
- Trained with *Adam* stochastic gradient descent

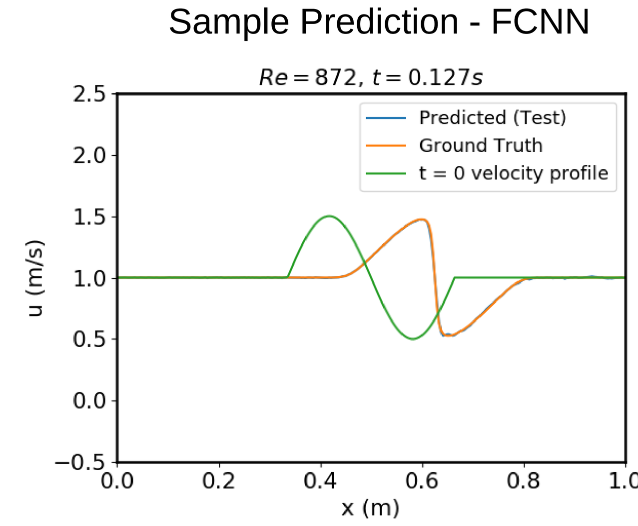
Results – Single Shock

The GPR model and the FCNN can both predict the shock physics accurately when initial velocity profiles are sinusoidal and relatively similar across the dataset, the GPR's ability to interpolate between datapoints results in a smoother prediction.

Sample Predictions - GPR



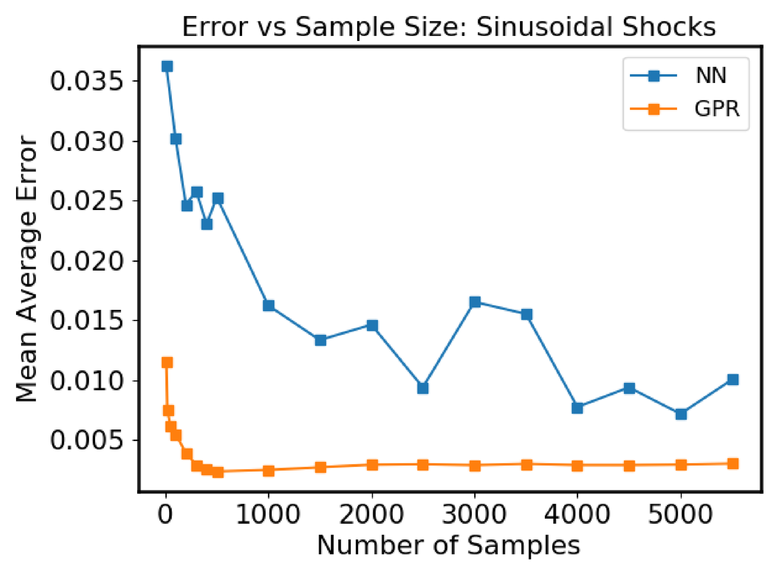
Sample Prediction - FCNN



$$\text{MAE} = \frac{1}{n}\sum_{j=1}^{n} |y_j - \hat{y_j}| \times 100\%$$

Velocity Profile	Algorithm	Cross Validated MAE (5-Fold)
Sinusoidal	**GPR**	**0.296%**
	FCNN	0.700%
Complex	GPR	4.71%
	FCNN	**1.36%**

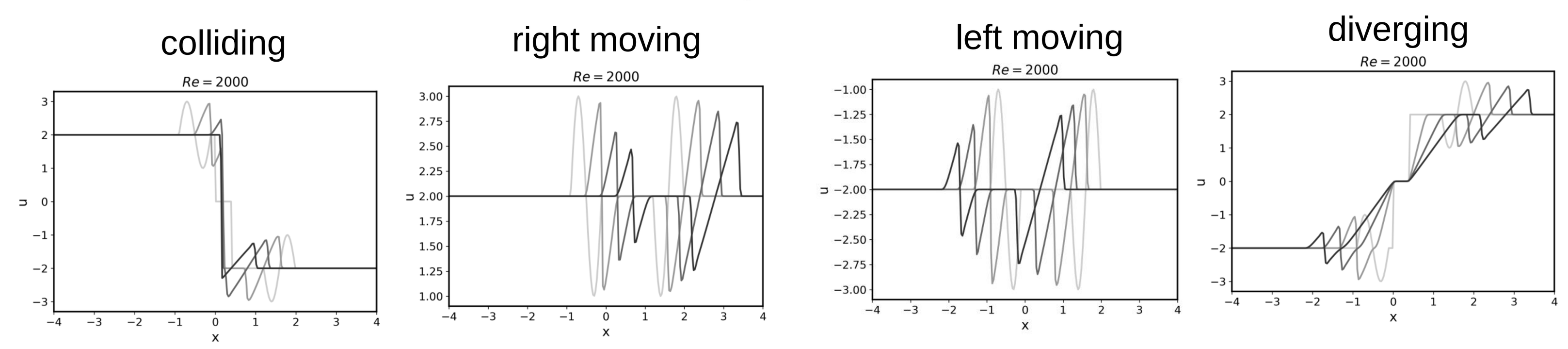
The FCNN has better generalization ability across different complex velocity initializations that require more data for inference, while GPR struggles to perform inference on large and high-dimensional datasets.



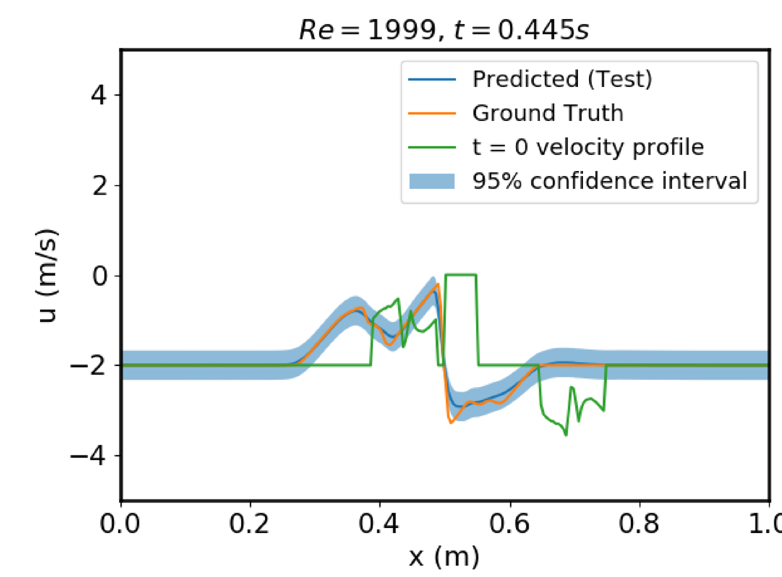
Results – Multiple Shocks

Systems with multiple interacting shocks (four different orientations shown below) introduce more difficulty to the inference problem.

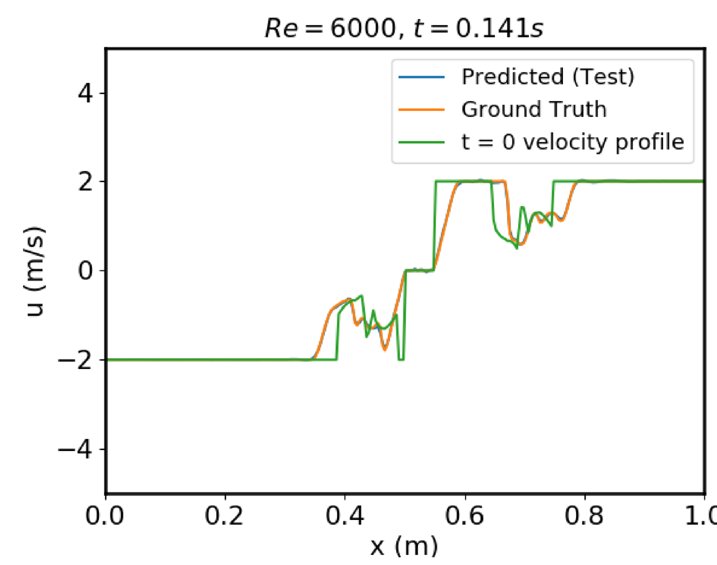
Both the GPR and FCNN model can generate accurate predictions in these cases, with similar trends in accuracy.



Sample Prediction - GPR



Sample Prediction - FCNN



Velocity Profile	Algorithm	Cross Validated MAE (5-Fold)
Sinusoidal	**GPR**	**0.92%**
	FCNN	1.02 %
Complex	GPR	5.82%
	FCNN	**2.38%**

Conclusion

- A Gaussian Process Regression model and a Deep Neural Network are presented for predicting shock propagation in different flow properties and velocity initializations.
- While **GPR performs better with small datasets**, the **FCNN is more efficient** in complex cases that require **larger datasets** for inference

Limitations and Future Work

- Both models fail to extrapolate accurate predictions when the training dataset does not resemble the conditions seen in the test dataset.
- **Convolution operations** are necessary for an understanding of the physics that can extrapolate and generalize to situations with a **previously unseen number of shocks.**
- **Sequential wavelet transforms** can act as an **explainable analogue** to a traditional Convolutional Neural Network.

References

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Acknowledgements

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