



Application of Physics-Informed Neural Networks to Neutron Star Magnetospheres

International Conference on Machine Learning for Astrophysics

Petros Stefanou

Co-authors:
Jorge Urbán
Jose Pons

July 2024

1/20



Universitat
d'Alacant



BLADES



GENERALITAT
VALENCIANA

Conselleria de Educació,
Universitats y Empleo



**MACHINE LEARNING
FOR ASTROPHYSICS**
2ND EDITION
CATANIA, 8-12 JULY, 2024



Table of Contents

- ▶ Introduction
- ▶ Motivation
- ▶ Optimisation method
- ▶ Application to neutron star magnetospheres
- ▶ Summary



Table of Contents

1 Introduction

- ▶ Introduction
- ▶ Motivation
- ▶ Optimisation method
- ▶ Application to neutron star magnetospheres
- ▶ Summary



Physics-informed neural networks

1 Introduction



Physics-informed neural networks

1 Introduction

Basics

- Solve PDEs using neural networks
- Input: coordinates in some domain
- Output: an approximate solution
- Loss: the residuals of the PDE describing the system
- Training set: Large number of random points
- Boundary conditions imposed through hard-enforcement

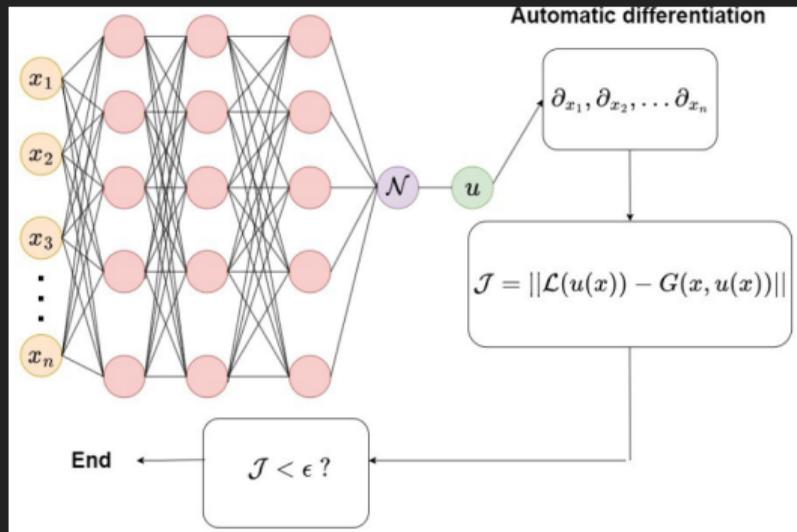


Figure 1: A physics-informed neural network



Optimisation process

1 Introduction



Optimisation process

1 Introduction

Correction step

$$\Theta_{k+1} = \Theta_k + \alpha_k \mathbf{p}_k$$

$$\mathbf{p}_k = -H_k \nabla \mathcal{J}(\Theta_k)$$

Line search methods

- Trainable parameters Θ
- Loss function \mathcal{J}
- Θ are adjusted so that $\mathcal{J}(\Theta) \rightarrow 0$
- α_k determines the step size
- \mathbf{p}_k determines the direction



Table of Contents

2 Motivation

- ▶ Introduction
- ▶ **Motivation**
- ▶ Optimisation method
- ▶ Application to neutron star magnetospheres
- ▶ Summary



Improve convergence

2 Motivation



Improve convergence

2 Motivation

PINNs vs. classical methods

- Precision
- Efficiency



Improve convergence

2 Motivation

PINNs vs. classical methods

- Precision
- Efficiency

Ill-conditioning

- Loss function in PINNs is poorly-scaled
- Broad eigenvalue spectrum of $\text{hess}(\mathcal{J})$ close to minimum
- Condition number $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}} \gg 1$
- Some directions are flat
- Gradient-based methods **fail miserably**



Improve convergence

2 Motivation

PINNs vs. classical methods

- Precision
- Efficiency

Ill-conditioning

- Loss function in PINNs is poorly-scaled
- Broad eigenvalue spectrum of $\text{hess}(\mathcal{J})$ close to minimum
- Condition number $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}} \gg 1$
- Some directions are flat
- Gradient-based methods **fail miserably**

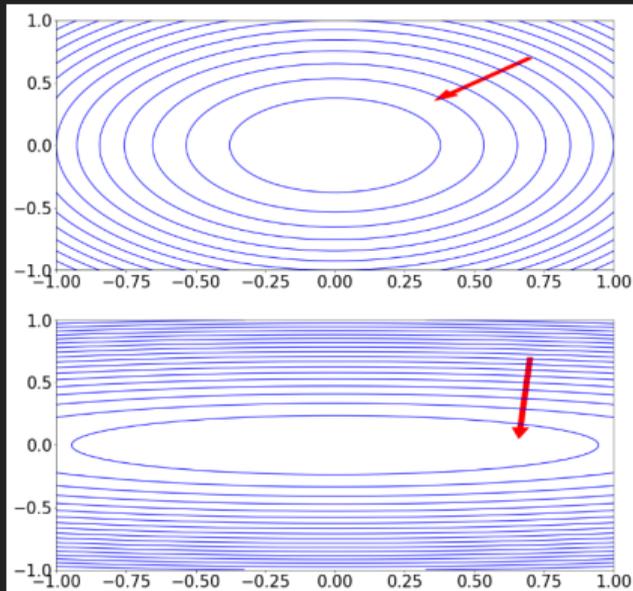


Figure 2: Contours of a loss function



Table of Contents

3 Optimisation method

- ▶ Introduction
- ▶ Motivation
- ▶ **Optimisation method**
- ▶ Application to neutron star magnetospheres
- ▶ Summary



Quasi-Newton methods

3 Optimisation method



Quasi-Newton methods

3 Optimisation method

Broyden class

$$H_{k+1} = \frac{1}{\tau_k} \left[H_k - \frac{H_k \mathbf{y}_k \otimes H_k \mathbf{y}_k}{\mathbf{y}_k \cdot H_k \mathbf{y}_k} + \phi_k \mathbf{v}_k \otimes \mathbf{v}_k \right] + \frac{\mathbf{s}_k \otimes \mathbf{s}_k}{\mathbf{y}_k \cdot \mathbf{s}_k}$$

- H_k approximates the inverse Hessian of the loss
- Depends on Θ_k and $\nabla \mathcal{J}(\Theta_k)$
- $\tau_k = 1, \phi_k = 1$ define the BFGS optimizer
- Different τ_k, ϕ_k define different methods



The role of H_k

3 Optimisation method



The role of H_k

3 Optimisation method

Curvature information

- H_k is associated with curvature
- Step direction points towards minimum
- Less iterations to converge



The role of H_k

3 Optimisation method

Curvature information

- H_k is associated with curvature
- Step direction points towards minimum
- Less iterations to converge

Preconditioning

- Define new variables $\mathbf{z} = H_k^{-1/2} \Theta$
- Update rule becomes

$$\mathbf{z}_{k+1} = \mathbf{z}_k - \alpha_k \nabla \mathcal{J}(\mathbf{z}_k)$$

- Hessian matrix in \mathbf{z} -space

$$\text{hess}(\mathcal{J}(\mathbf{z})) = H_k^{1/2} \text{hess}(\mathcal{J}(\Theta)) H_k^{1/2}$$

- Spectrum concentrated around ~ 1



Optimisation algorithm choices

3 Optimisation method



Optimisation algorithm choices

3 Optimisation method

Self-scaled BFGS

$$\tau_k^{(1)} = \min \left\{ 1, \frac{\mathbf{y}_k \cdot \mathbf{s}_k}{\mathbf{s}_k \cdot H_k^{-1} \mathbf{s}_k} \right\}$$

$$\phi_k^{(1)} = 1$$

Self-scaled Broyden

$$\tau_k^{(2)} = \begin{cases} \tau_k^{(1)} \min \left(\sigma_k^{-1/(n-1)}, \frac{1}{\theta_k^{(1)}} \right) & \text{if } \theta_k > 0 \\ \min \left(\tau_k^{(1)} \sigma_k^{-1/(n-1)}, \sigma_k \right) & \text{if } \theta_k \leq 0 \end{cases}$$

$$\phi_k^{(2)} = \frac{1 - \theta_k}{1 + a_k \theta_k}$$



Table of Contents

4 Application to neutron star magnetospheres

- ▶ Introduction
- ▶ Motivation
- ▶ Optimisation method
- ▶ **Application to neutron star magnetospheres**
- ▶ Summary



Neutron star magnetospheres

4 Application to neutron star magnetospheres



Neutron star magnetospheres

4 Application to neutron star magnetospheres

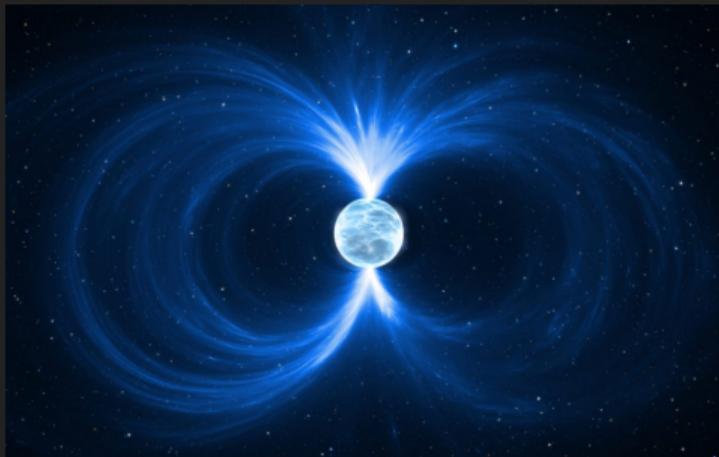


Figure 3: An artist's conception of a NS

Features

- Plasma flowing along the star's magnetic field
- Large scale field is dipolar
- Toroidal fields
- Force-free regime
- Non-rotating limit
- Axisymmetry

$$q^2 \frac{\partial}{\partial q} \left(q^2 \frac{\partial \mathcal{P}}{\partial q} \right) + (1 - \mu^2) q^2 \frac{\partial^2 \mathcal{P}}{\partial \mu^2} + \mathcal{T} \frac{d\mathcal{T}}{d\mathcal{P}} = 0$$



Results

4 Application to neutron star magnetospheres



Results

4 Application to neutron star magnetospheres

Current-free case

- $\mathcal{T}_{\mathcal{P}}^{\mathcal{T}} = 0$
- Simple problem to check our method
- Analytical solution for comparison



Results

4 Application to neutron star magnetospheres

Current-free case

- $\mathcal{T} \frac{\mathcal{T}}{\mathcal{P}} = 0$
- Simple problem to check our method
- Analytical solution for comparison

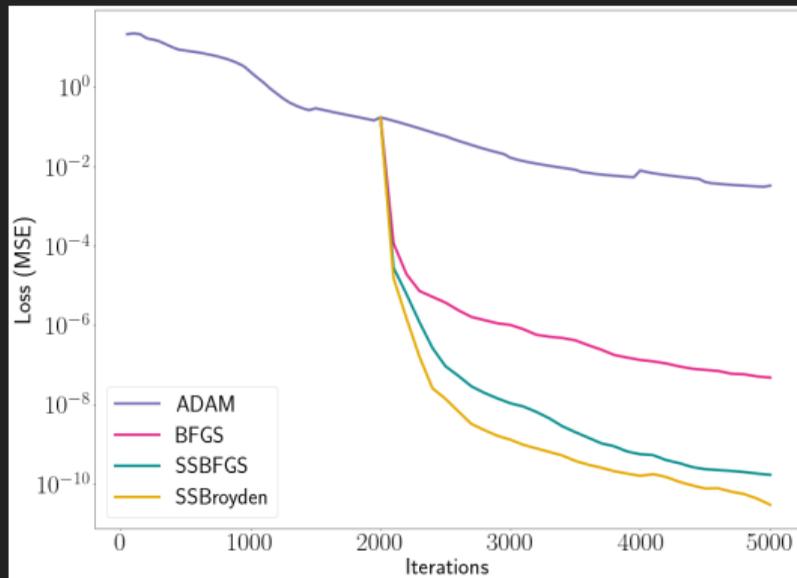


Figure 4: Loss function vs iterations



Results

4 Application to neutron star magnetospheres

Current-free case

- $\mathcal{T} \frac{\mathcal{T}}{\mathcal{P}} = 0$
- Simple problem to check our method
- Analytical solution for comparison

Main points

- Quasi-Newton methods are vastly superior to gradient-based methods
- New algorithms further improve convergence compared to BFGS
- Relative error wrt analytical $\sim 10^{-7}$

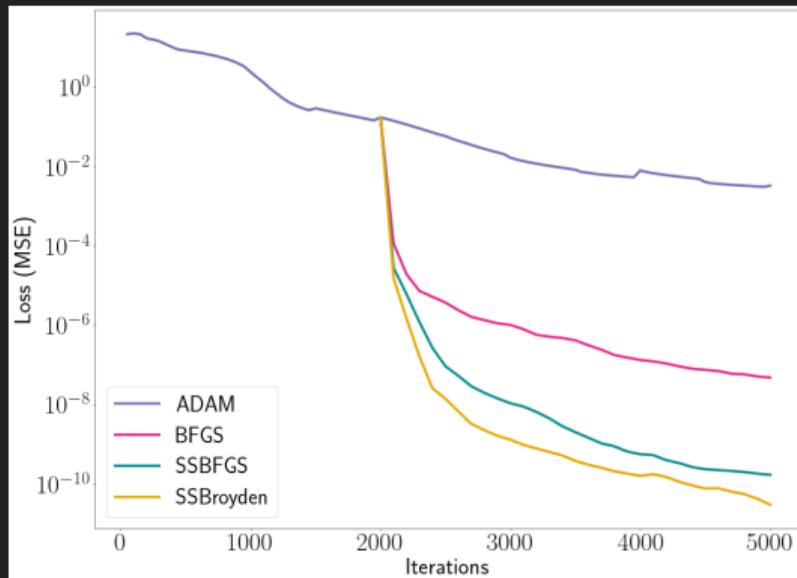
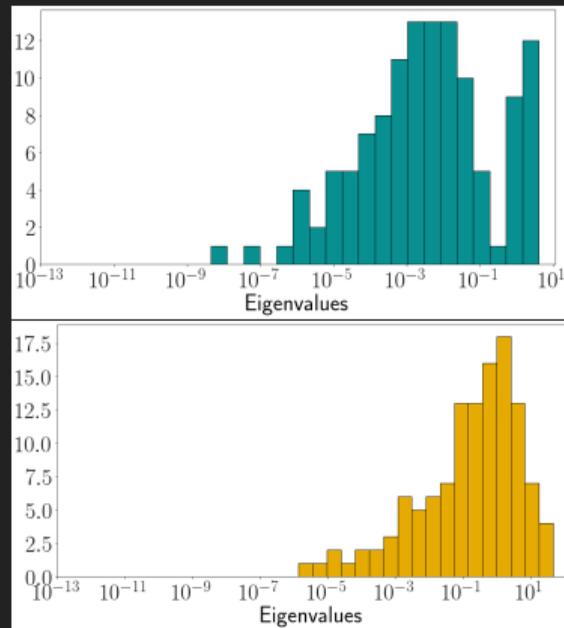
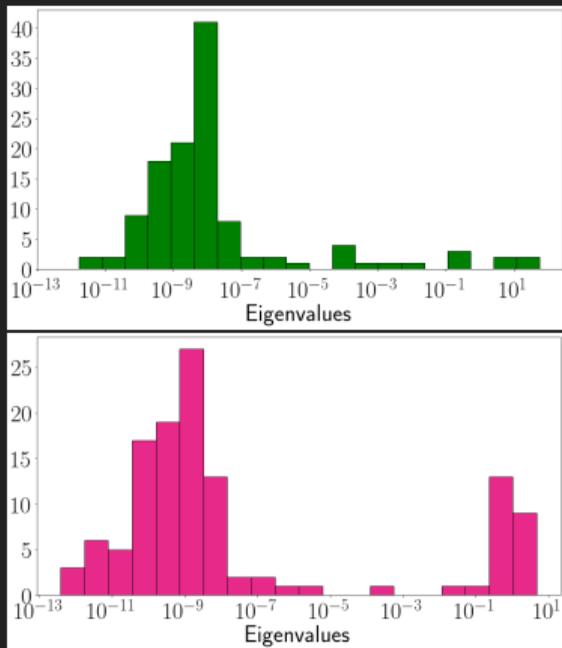


Figure 4: Loss function vs iterations



Results

4 Application to neutron star magnetospheres



15/20 **Figure 5:** Upper:Adam. Lower:BFGS

Figure 6: Upper: SSBFGS. Lower:SSBroyden



Results

4 Application to neutron star magnetospheres

Force-free case

- Multipolar content
- Non-linear source term

$$\mathcal{T}(\mathcal{P}) = \begin{cases} s(|\mathcal{P}| - \mathcal{P}_c)^\sigma & \text{if } |\mathcal{P}| > \mathcal{P}_c \\ 0 & \text{if } |\mathcal{P}| < \mathcal{P}_c, \end{cases}$$

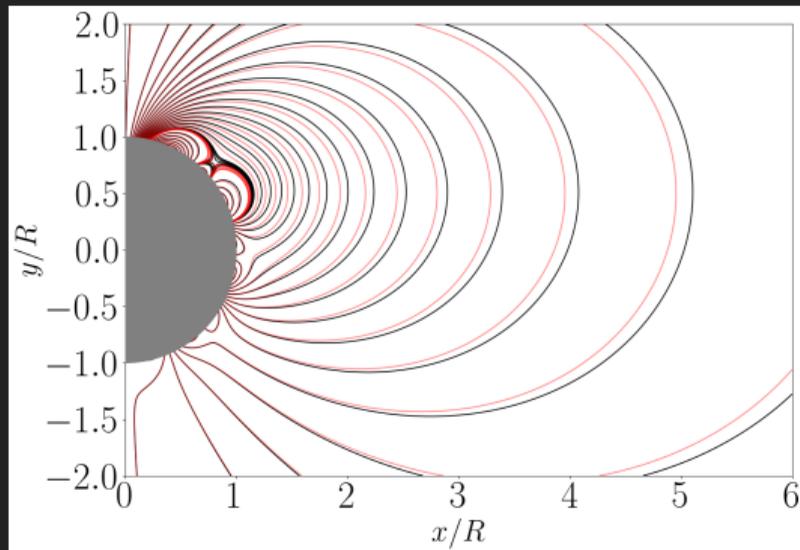
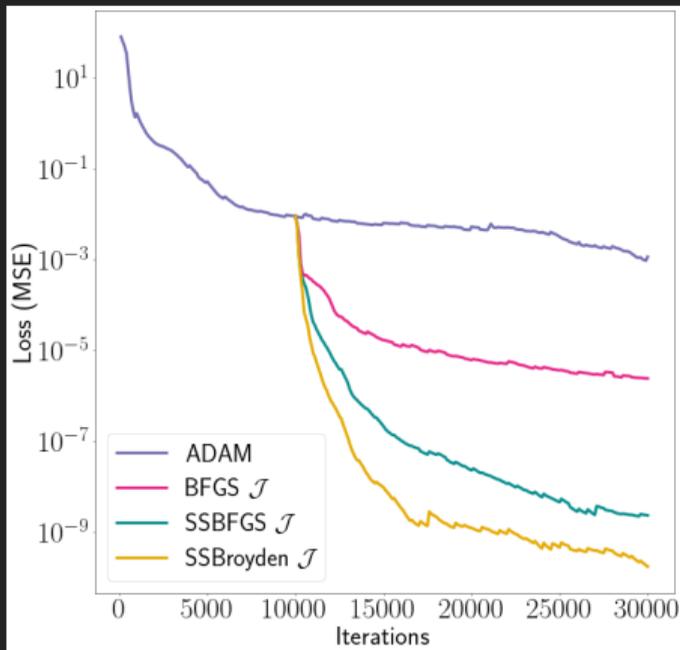


Figure 7: A force-free solution



Results

4 Application to neutron star magnetospheres



17/20 Figure 8: Loss function vs iterations

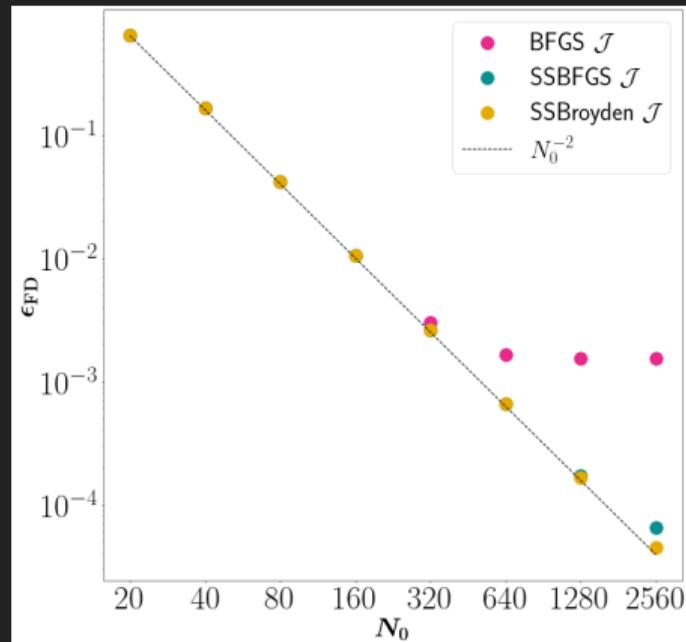


Figure 9: PINN error estimation



Table of Contents

5 Summary

- ▶ Introduction
- ▶ Motivation
- ▶ Optimisation method
- ▶ Application to neutron star magnetospheres
- ▶ **Summary**



Key points

6 Summary

- Optimisation process plays a crucial role
- Suitable choice of optimisation algorithm leads to state-of-the-art precision
- Smaller networks can be employed leading to improved efficiency
- Results extend to other problems
- Preprint for more details:



Urbán, Jorge F., Petros Stefanou, and José A. Pons (May 2024).

“Unveiling the optimization process of Physics Informed Neural Networks: How accurate and competitive can PINNs be?” In: *arXiv e-prints*. DOI: [10.48550/arXiv.2405.04230](https://doi.org/10.48550/arXiv.2405.04230).





Application of Physics-Informed Neural Networks to Neutron Star Magnetospheres

Thank you