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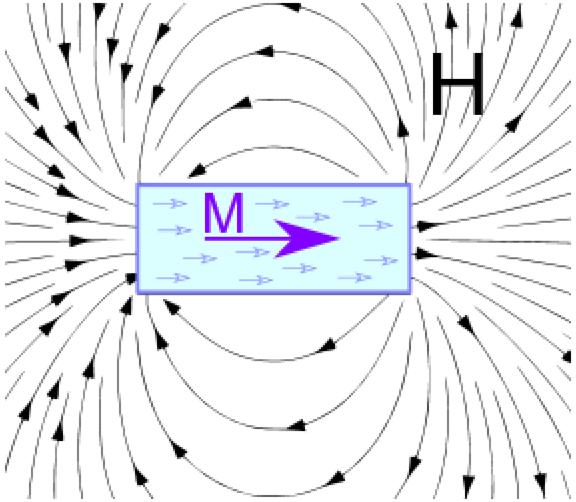
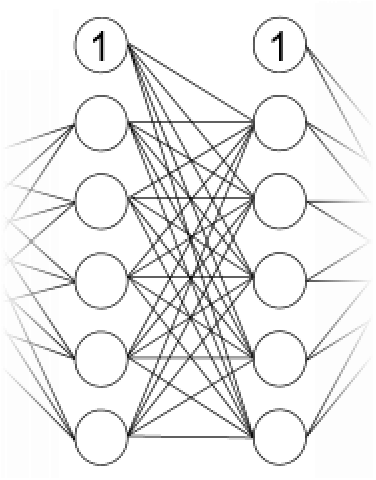
Stefan Pollok (spol@dtu.dk)
Department of Energy Conversion and Storage, Technical University of Denmark

Uncertainty estimation in magnetic field inference

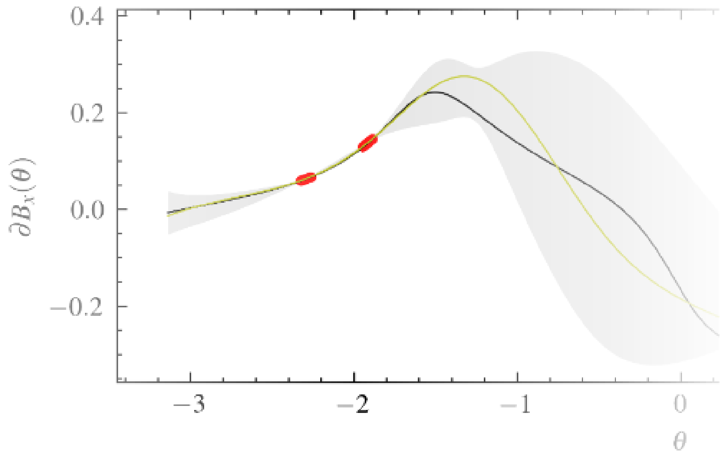
Broader perspective



Physics

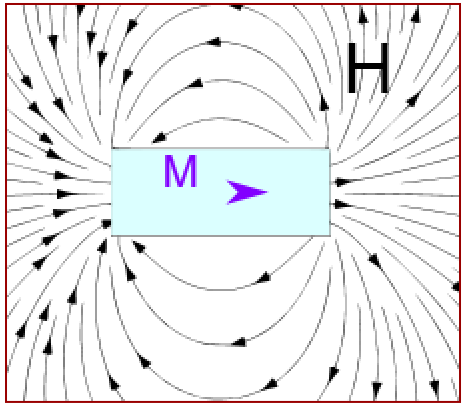


Machine Learning



Uncertainty

Physics



Magnetostatics

- Magnetic fields from steady currents / permanent magnets
- Magnetic scalar potential

$$\nabla^2 \psi_M = \nabla \cdot \mathbf{M}$$

- **Laplace's equation** (when **M**=0, i.e., outside of magnetic material)

$$\nabla^2 \psi_M = 0$$

- Solution on circular boundary in 2-D

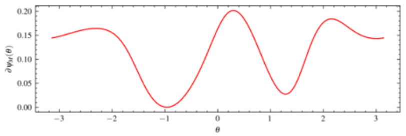
Demagnetizing field strength

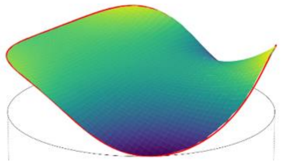
$$\mathbf{H} = -\nabla \psi_M$$

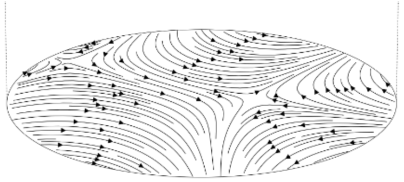
Radial coordinate r

Angular coordinate θ

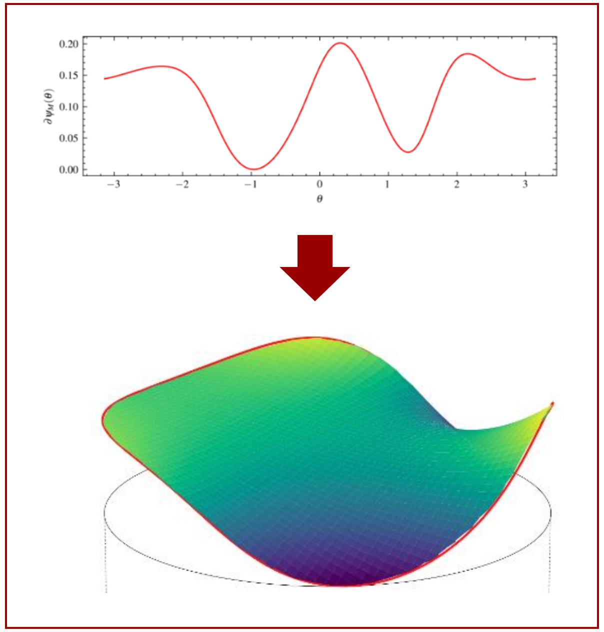
$$\psi_M(r,\theta) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta)\, r^n$$





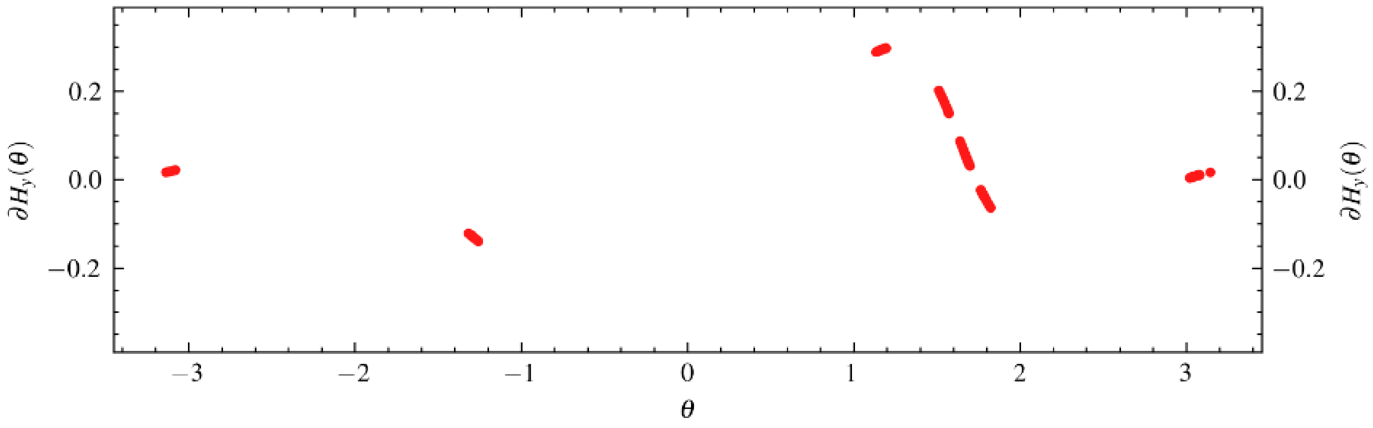


Unique solution to Laplace equation given a Dirichlet boundary condition



Research problem

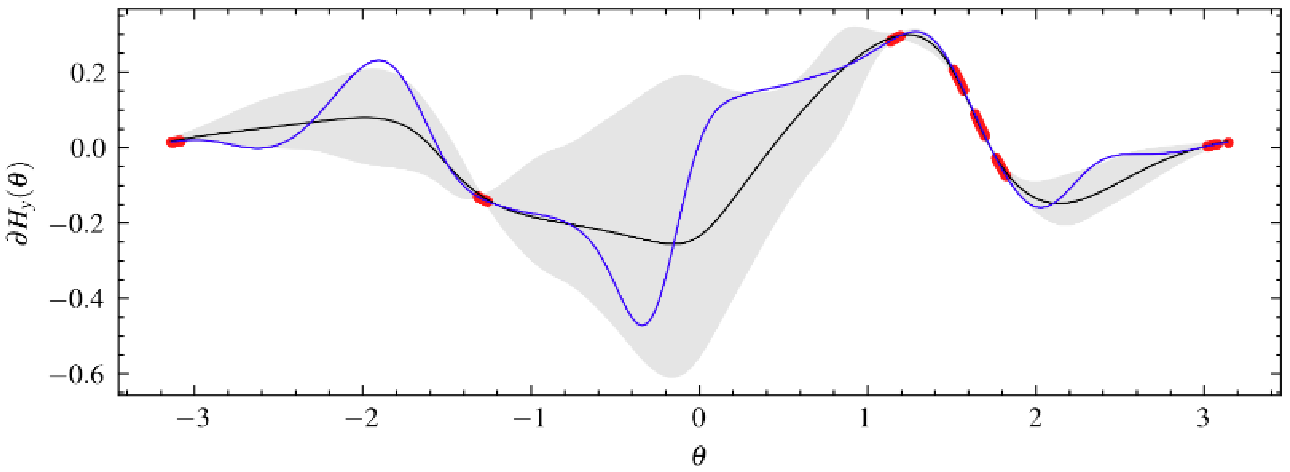
Boundary is only partially observed



μ Mean

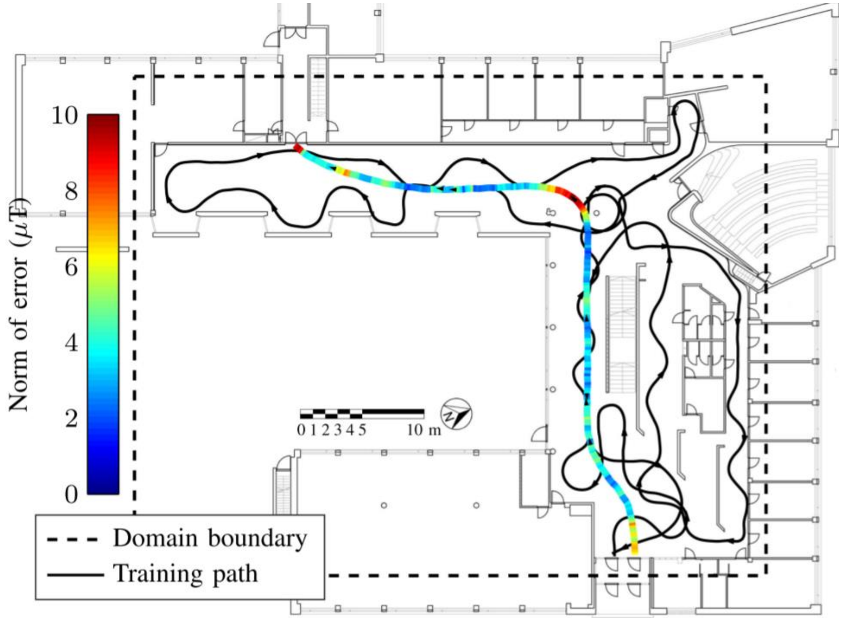
3σ – Std

Sample

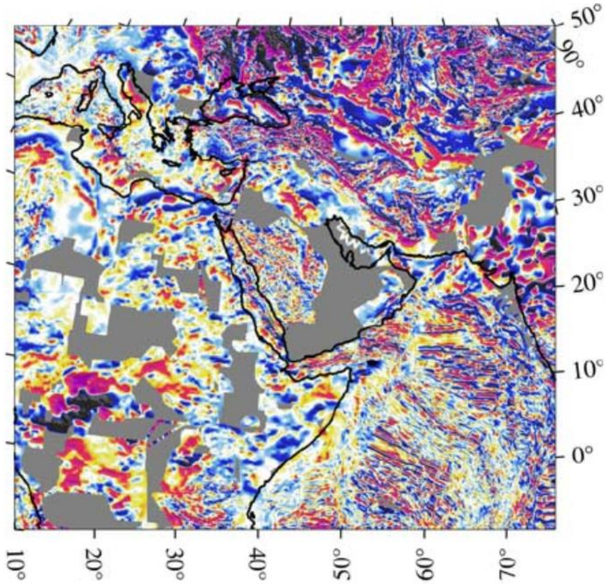


- How does the underlying $\boldsymbol{\psi}$ look like?
- How certain are we about predictions from our model in specific regions?
- How to incorporate measurements, which are obtained in form of **H**?

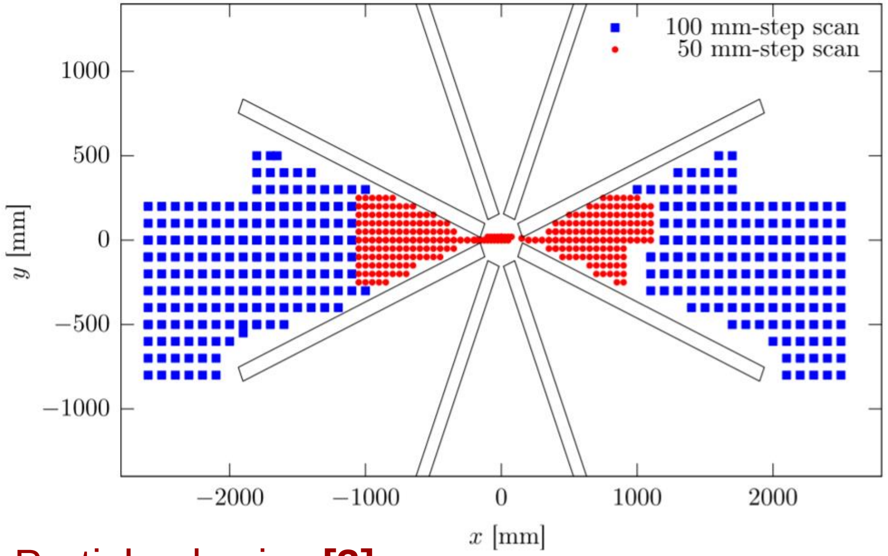
Motivation



Localization in Robotics **[1]**



Geophysics **[2]**



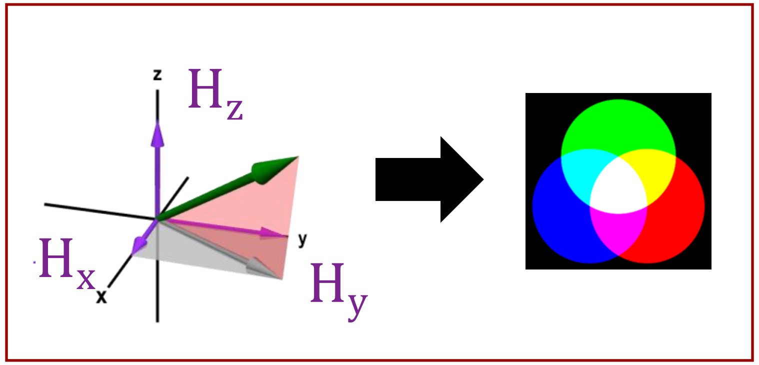
Particle physics **[3]**

[1] A. Solin et al., IEEE Trans. Robot., vol. 34, no. 4, pp. 1112-1127, Sept. 2018.

[2] S. Maus et al., Geochem. Geophys. Geosys.,vol. 10, no. 8, Aug. 2009.

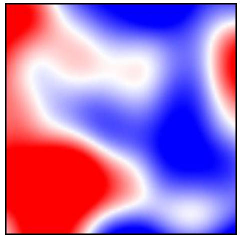
[3] J.C. Bernauer et al., Nucl. Instrum. Methods Phys. Res. A: Accel. Spectrom. Detect. Assoc. Equip., vol. 823, pp. 9-14, Jul. 2016.

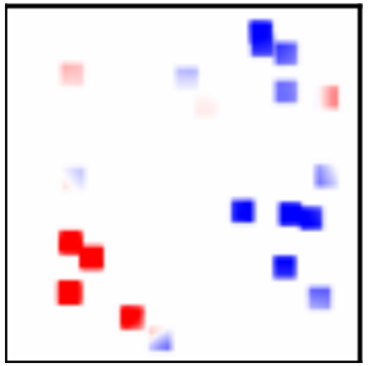
Magnetic field represented as an image



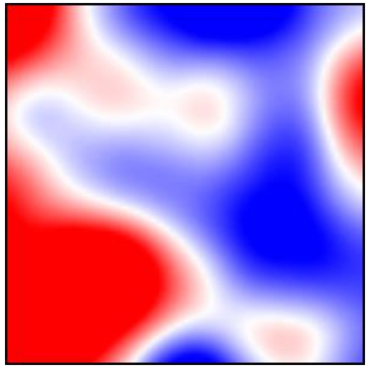
Previous work

Physics-informed Generative Adversarial Networks [4]





Available magnetic
field measurements



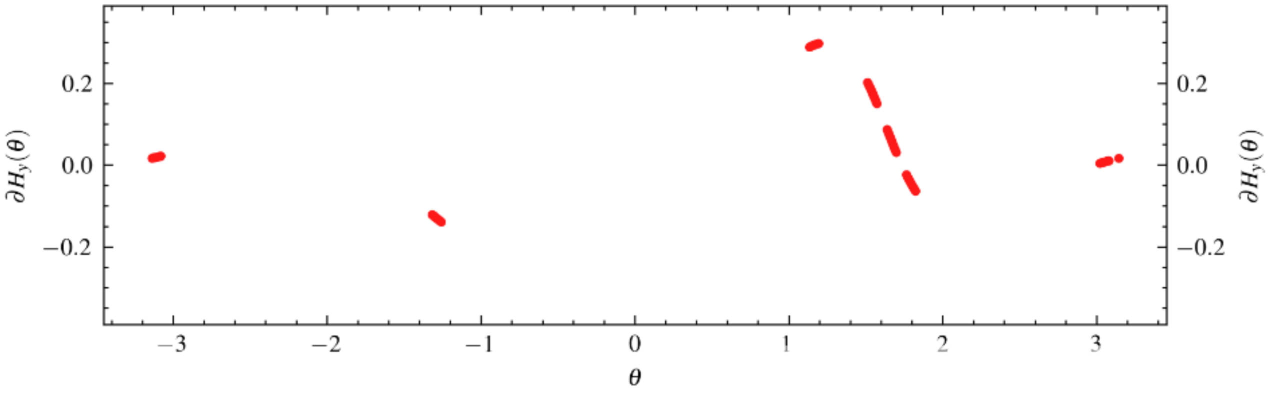
Prediction from
neural network

Limitations:

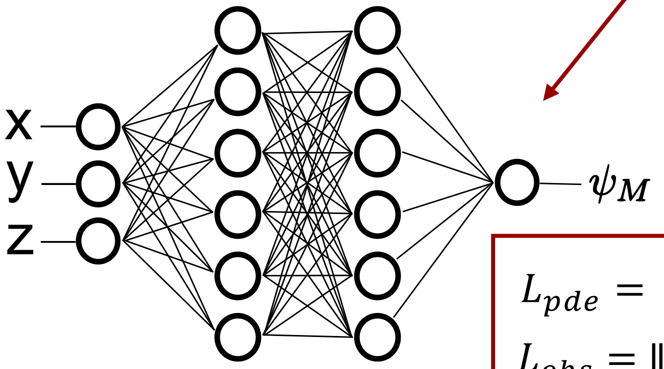
- Same input leads to identical prediction
- No built-in uncertainties
- Embedding physics only as a soft constraint (via loss function)

[4] Pollok, Stefan, et al., Journal of Magnetism and Magnetic Materials 571 (2023): 170556.

Our new approaches



Physics-informed neural networks



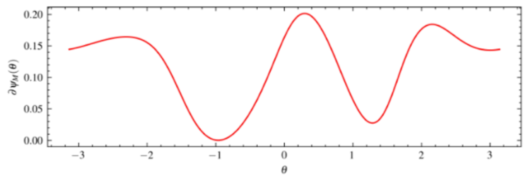
$$L_{pde} = \nabla^2 \psi_M$$
$$L_{obs} = \| -\nabla \psi_M - H_{obs} \|^2$$

Gaussian Process Regression

Exponential Sine Squared kernel

$$k(\theta, \theta') = \exp\left[-\frac{2\sin^2\left(\frac{\pi}{p}|\theta - \theta'|\right)}{\ell^2} \right]$$

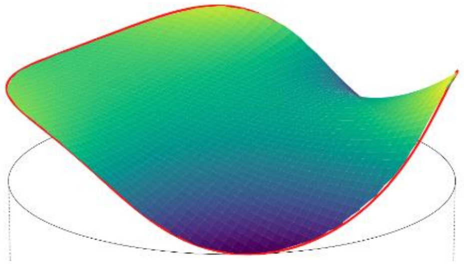
From magnetic scalar potential boundary to magnetic field



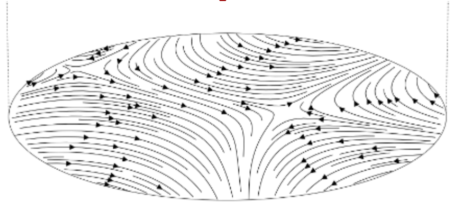
Find coefficients of Fourier series

$$\psi_M(r,\theta) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta)\, r^n$$

Evaluate solution inside circular boundary



$$\mathbf{H} = -\nabla \psi_M$$



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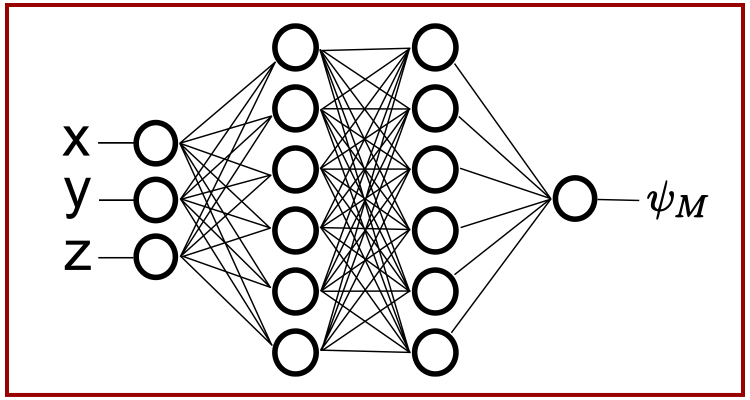
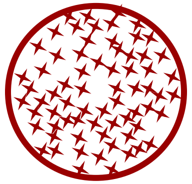
Machine Learning - PINNs



- **Architecture**
  Simple fully-connected neural network
- **Automatic differentiation**
  Losses and **H** can easily be derived
- **Collocation points**
  Randomly placed across domain as input
- **Loss functions**

$$L_{pde} = \nabla^2 \psi_M$$

$$L_{obs} = \| -\nabla \psi_M - H_{obs} \|^2$$

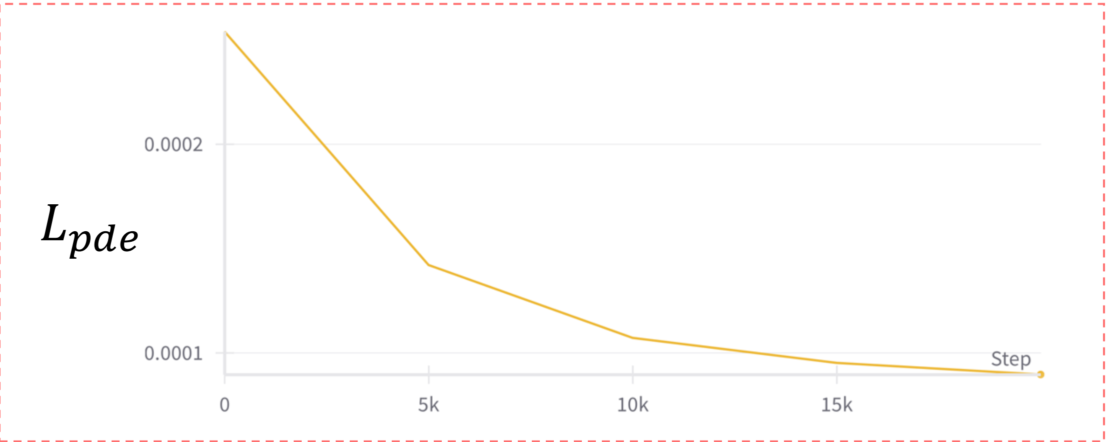


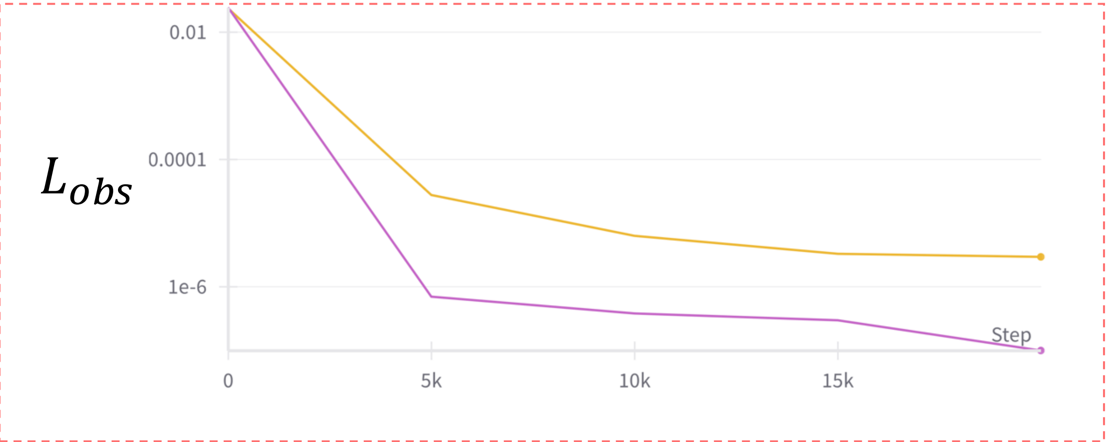
By construction

$$L_{pde,Fourier} = \nabla^2 \psi_M(r,\theta) = 0$$

Limitation to circular boundary

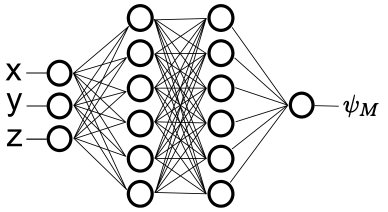
$$L_{obs,Fourier} = \| -\nabla \psi_M(r,\theta) - H_{obs} \|^2$$

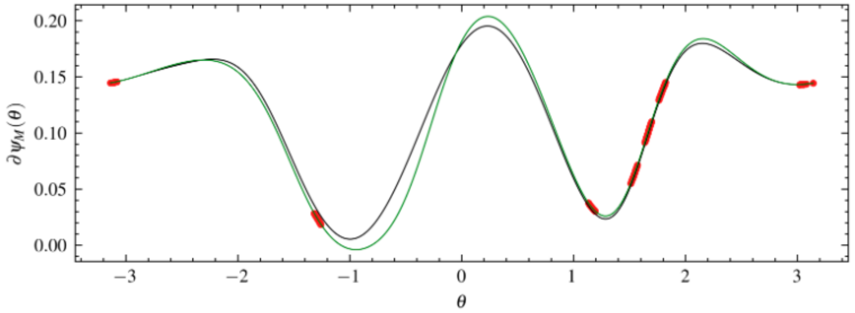




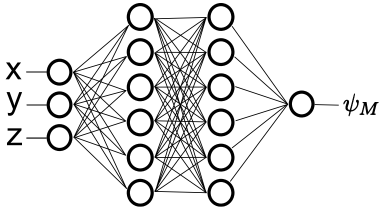
Uncertainty estimation – PINN ensemble

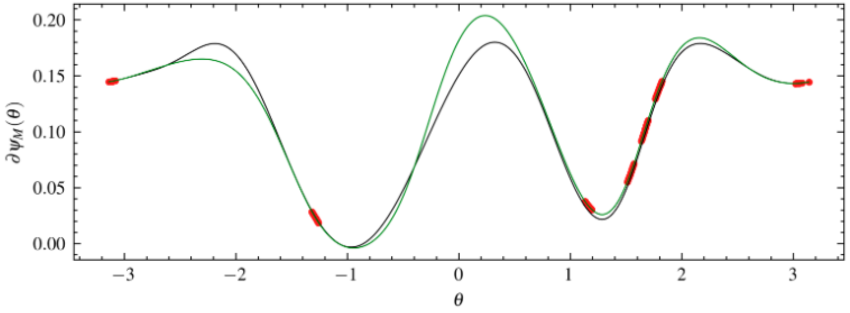
Seed 0



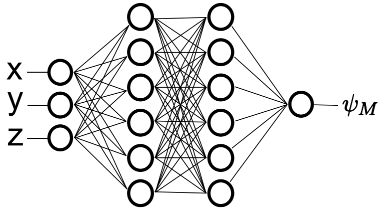


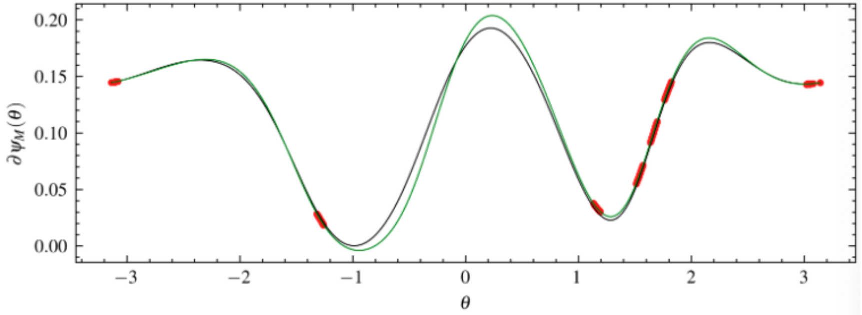
Seed 1



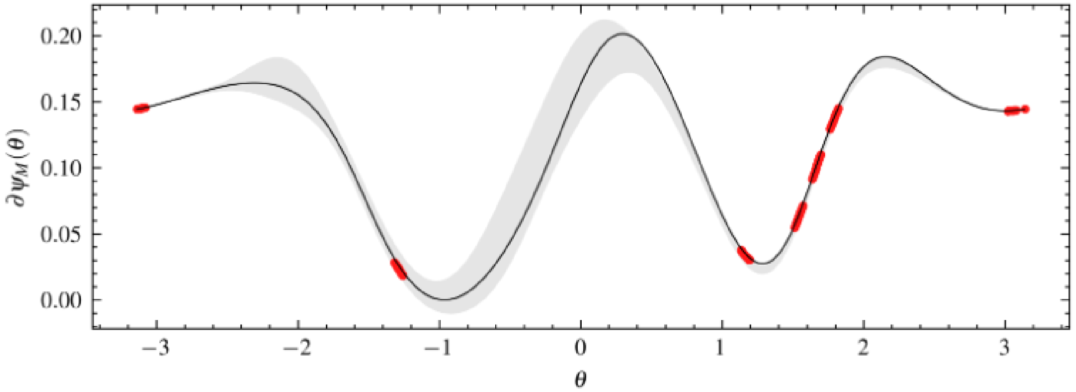


Seed 2





Mean and variance from an ensemble of 10 PINNs



Uncertainty estimation – HMC with PINNs

Specifying distribution over ϕ and the prediction

- **Bayesian neural networks**
  "Predictive distribution as an infinite ensemble of networks" [5]
  Bayesian statistics over the parameters ϕ of the PINNs based on observations $\mathcal{D}$

$$P(\phi|\mathcal{D}) = \frac{P(\mathcal{D}|\phi)P(\phi)}{P(\mathcal{D})} \cong P(\mathcal{D}|\phi)P(\phi)$$

Posterior Likelihood Prior

$$\log P(\mathcal{D}|\phi) \cong -0.5 \times 10^6 \parallel \psi_M - \psi_{M,obs} \parallel^2$$

$$\log P(\phi) = -(0.5\phi^2 + 0.5k \cdot \log 2\pi)$$

- **Monte Carlo integration**
  Usage of a finite set of random samples of ϕ to approximate the posterior
  Naive setup needs a huge number of samples due to the large dimensionality of ϕ

Alternative to random walk

- **Markov chain with Hamiltonian dynamics**
  Accept a new set ϕ^* with probability α

$$\alpha = \min[1, \exp(-H(\phi^*, p^*) + H(\phi, p))]$$

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}$$

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$$

$$H(q,p) = U(q) + K(p)$$

Negative log-probability as potential energy

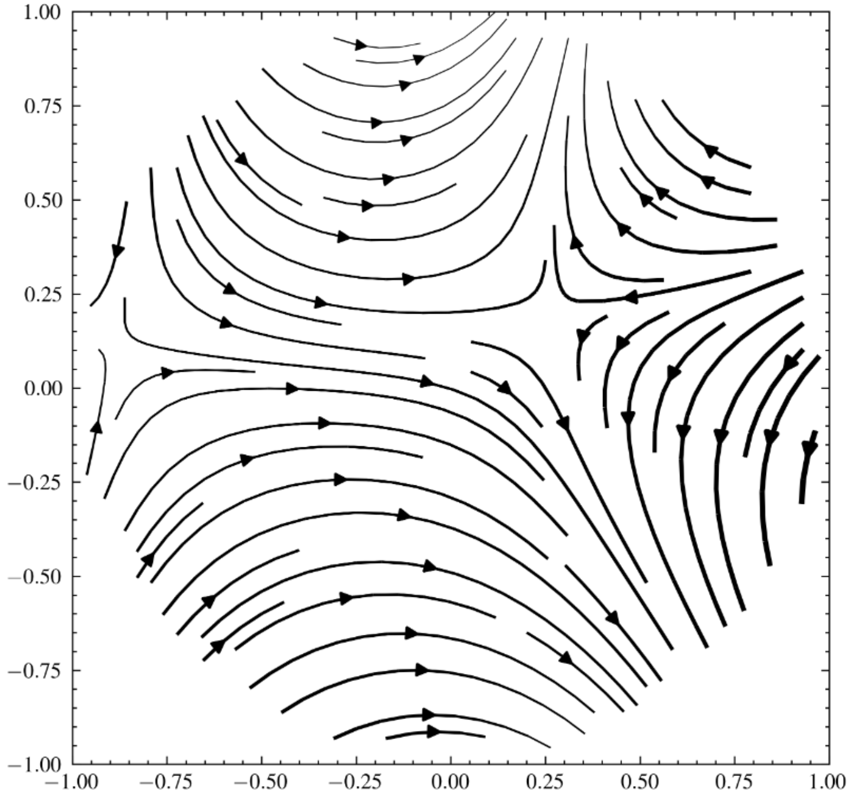
[5] Blundell, Charles, et al., International conference on machine learning. PMLR, 2015.

HMC results

$\mathbf{H} = -\nabla\psi_M$

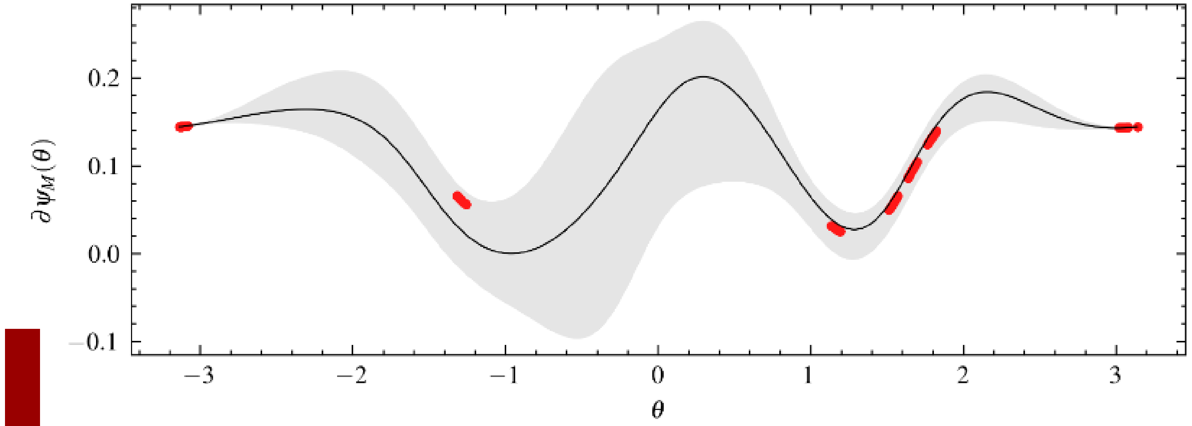
$\theta = \pi/2$

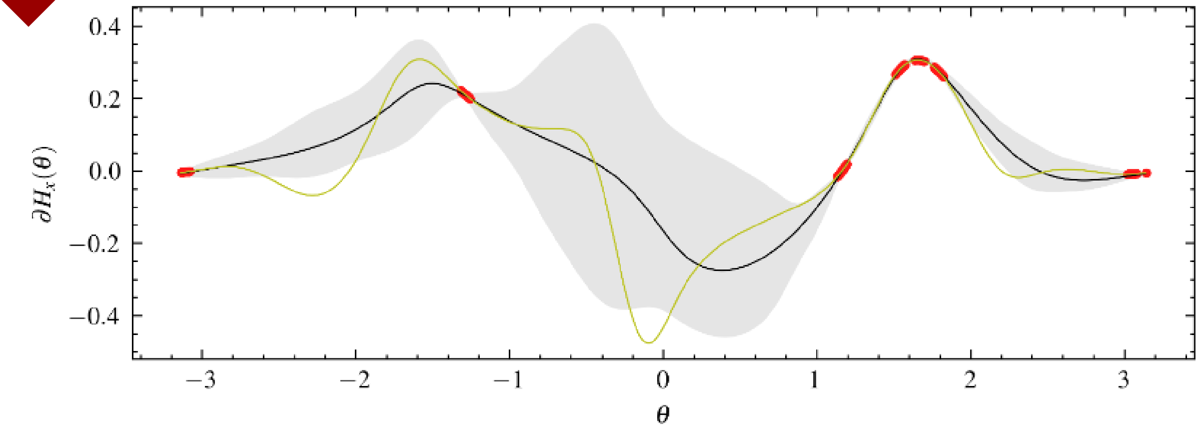
$\theta = \pi$

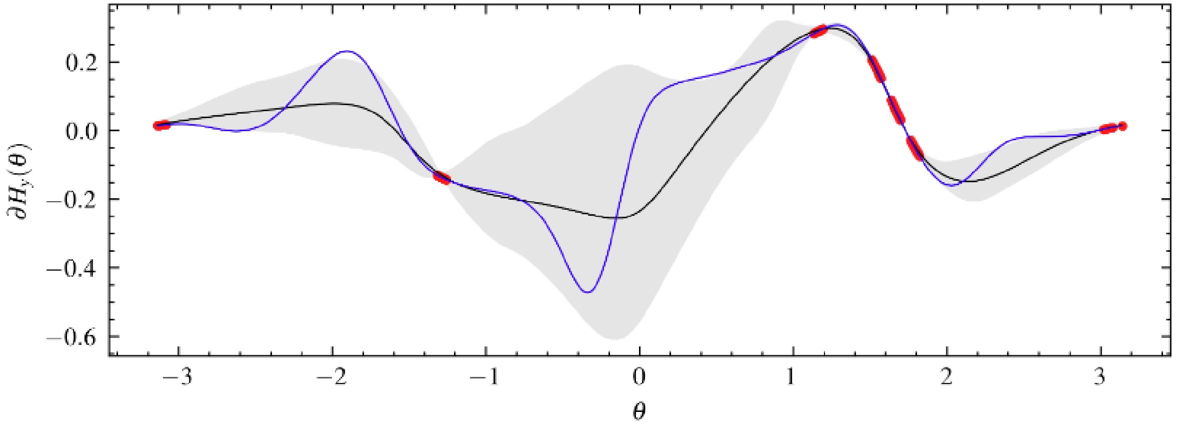


$\theta = 0$

$\theta = -\pi/2$







Future work

- Extension to 3-D with spherical harmonics (sphere as boundary)
- Arbitrary boundaries
- “physics-informed” Gaussian Processes
  ➔ kernel / covariance matrix respects Gauss’ law and Ampère’s law

Achievements

- statistical solution to Laplace’s equation from incomplete boundary
  ➔ useful for many problems in physics
- Improved decision-making
  ➔ where to measure next with limited amount of resources
  ➔ how trustworthy is the prediction

Collaborators

- Department of Energy Conversion and Storage, DTU

Berian

Rasmus

- Department of Applied Mathematics and Computer Science, DTU

Ignacio

Kristoffer

Jes

Questions / Collaborations

Contact

spol@dtu.dk

www.linkedin.com/stefanpollok

Appendix

Machine Learning – Gaussian Process Regression

- Probability distribution over possible functions

Each location is normally distributed

$$\mu(\theta_*) = \mathbf{k}_*^T(\mathbf{K} + \sigma_n^2\mathbf{I})^{-1}\mathbf{\Phi}$$
$$\text{cov}(\theta_*) = k(\theta_*, \theta_*) - \mathbf{k}_*^T(\mathbf{K} + \sigma_n^2\mathbf{I})^{-1}\mathbf{k}_*,$$

Kernel function ("pairwise influence")

$$k(\theta, \theta') = \exp\left[-\frac{2\sin^2\left(\frac{\pi}{p}|\theta - \theta'|\right)}{\ell^2}\right]$$

length as hyperparameter