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Physics-informed neural network with unknown measurement noise

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Outline

Introduction to physics-informed neural networks

Limitations and extensions

Physics-informed neural networks with unknown measurement noise

Introduction to physics-informed neural networks

Physics-informed machine learning

There are two main strategies to derive and deduce models

- **theory-based** first principles or
- **data-driven** approaches.

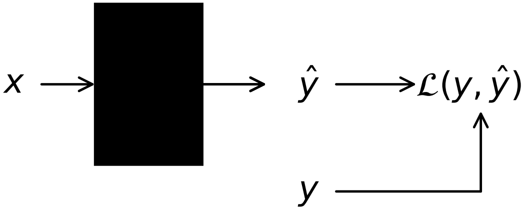
My overall research aim is to create new tools for using these two modeling strategies in conjunction.

Why do we want to do this?

- **Leverage performance** of data-driven ML models
- Make ML models more **interpretable**

Integrating prior knowledge into machine learning models

The combination of **machine learning** with **prior knowledge** from physics results in the field of **physics-informed machine learning**.



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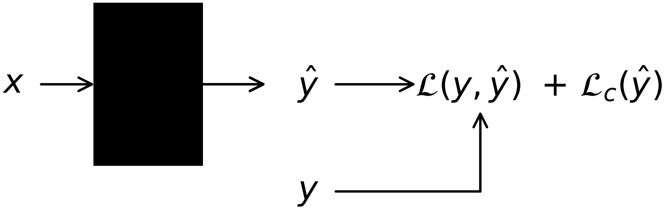
- additional term in the **loss function**



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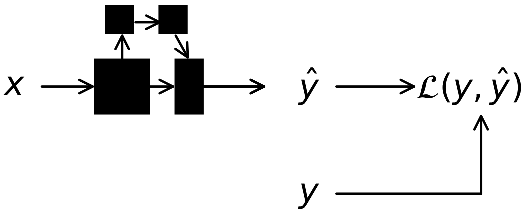

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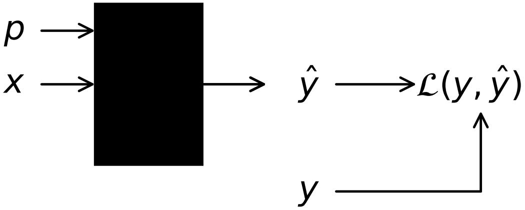
- additional **inputs** to the ML model



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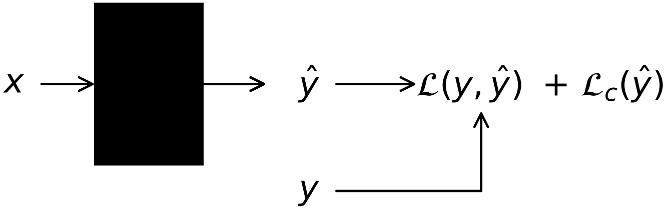
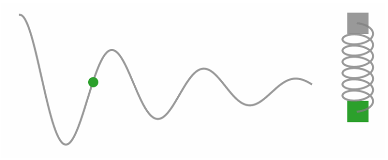
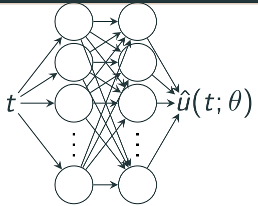


Solving PDEs with machine learning

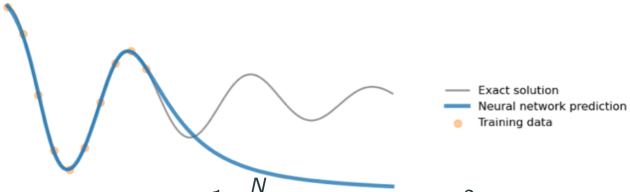


Damped harmonic oscillator

$$m\frac{d^2}{dt^2}u + \mu\frac{d}{dt}u + k = 0$$



Naive approach: Supervised learning

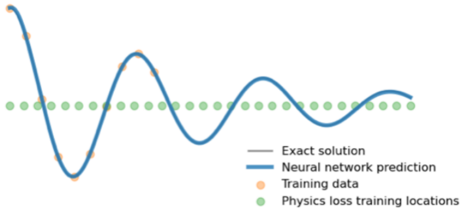


$$\min_\theta \frac{1}{N}\sum_{i=1}^{N}\left(\hat{u}(t_i;\theta) - u_i\right)^2$$

Main problems:

- No guarantee that the model obeys the conservation laws
- May require a lot of training data, not always feasible

Physics-informed neural network



$$L(\theta) = \overbrace{\frac{1}{N}\sum_{i=1}^{N}\left(\hat{u}(t_i,\theta) - u_i\right)^2}^{\text{supervised loss}} + \underbrace{\frac{1}{N_c}\sum_{j=1}^{N_c}\left(\left[m\frac{d^2}{dt^2} + \mu\frac{d}{dt} + k\right]\hat{u}(t_j,\theta)\right)^2}_{\text{physics loss}}$$

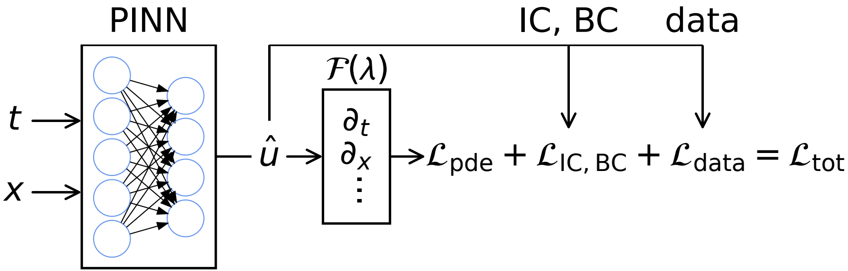
From a ML perspective:

- Physics loss is an unsupervised regularizer, which adds prior knowledge

From a mathematical perspective:

- PINNs provide a way to solve PDEs
  - Neural network is a mesh-free functional approximation of PDE solution
  - Physics loss is used to assess if the solution is consistent with PDE
  - Supervised loss is used to include boundary/initial conditions and potential observations

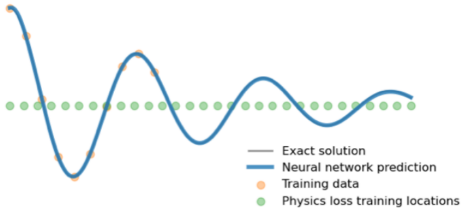
PINNs constitute an **alternative** to **classical solvers** of PDEs.



$$\mathcal{L}_{\mathrm{PDE}} = \frac{1}{N_c} \sum_{j=1}^{N_c} (\mathcal{F} \hat{u}(x_j, t_j; \theta))^2 \qquad \mathcal{L}_{\mathrm{BC}} = \frac{1}{N_{\mathrm{BC}}} \sum_{i=1}^{N_{\mathrm{BC}}} (\hat{u}(x_i, t_i; \theta) - f(x_i, t_i))^2$$

$$\mathcal{L}_{\mathrm{data}} = \frac{1}{N_d} \sum_{k=1}^{N_d} (\hat{u}(x_k, t_k; \theta) - u_k)^2$$

PINN training loop



$$L(\theta) = \overbrace{\frac{1}{N}\sum_{i=1}^{N}\left(\hat{u}(t_i,\theta) - u_i\right)^2}^{\text{supervised loss}}$$
$$\underbrace{+\frac{1}{N_c}\sum_{j=1}^{N_c}\left(\left[m\frac{d^2}{dt^2} + \mu\frac{d}{dt} + k\right]\hat{u}(t_j,\theta)\right)^2}_{\text{physics loss}}$$

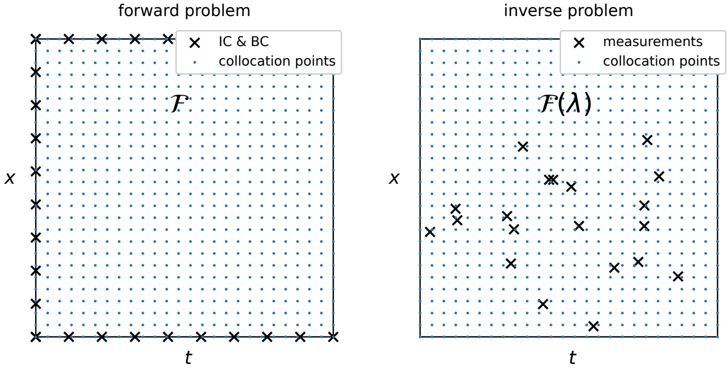
Training loop

1. Sample boundary/collocation points $\{t_i\}_{i=1}^{N}$ and $\{t_j\}_{j=1}^{N_c}$
2. Compute network outputs
3. Compute **gradients** of network with respect to **network input** $\frac{d}{dt}\hat{u}$, $\frac{d^2}{dt^2}\hat{u}$
4. Compute loss
5. Compute **gradient** of loss function with respect to **network parameters** $\frac{d}{d\theta}L$
6. Take gradient descent step

We can apply **autodifferentiation** to compute both $\frac{d}{dt}\hat{u}$ and $\frac{d}{d\theta}L$

Forward problem vs inverse problem

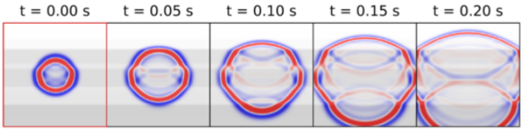
PINNs are **flexible** in their use.

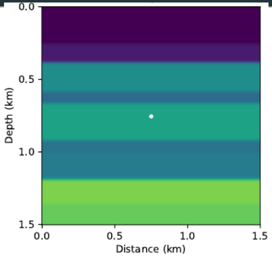


$$\mathcal{L}_{\text{tot}} = \mathcal{L}_{\text{BC}} + \mathcal{L}_{\text{PDE}} \qquad \mathcal{L}_{\text{tot}} = \mathcal{L}_{\text{data}} + \mathcal{L}_{\text{PDE}}$$

PINNs for forward simulation

Ground truth FD

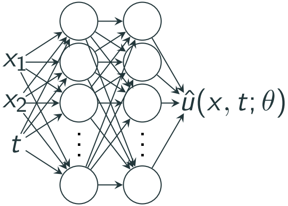




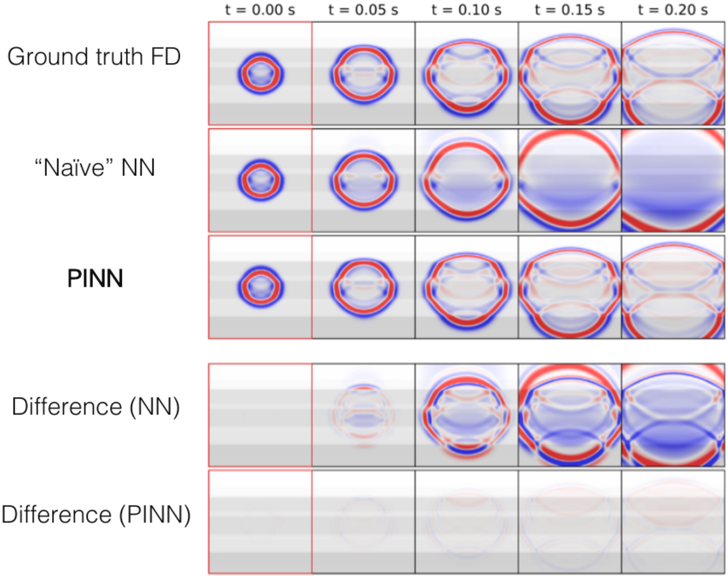
Solving the wave equation with physics-informed deep learning – Moseley et al, ArXiv (2020)

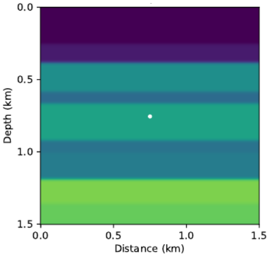
$$\mathcal{L}_{\mathrm{PDE}} = \frac{1}{N_c}\sum_{j=1}^{N_c}\left(\left[\nabla^2 - \frac{1}{c(x_j)^2}\frac{\partial^2}{\partial t^2}\right]\hat{u}(x_j, t_j)\right)^2$$

$$\mathcal{L}_{\mathrm{IC}} = \frac{1}{N_{\mathrm{IC}}}\sum_{i=1}^{N_{\mathrm{IC}}}(\hat{u}(x_i, t_i) - u_{\mathrm{FD}}(x_i, t_i))^2$$



PINNs for forward simulation





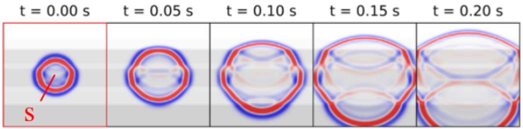
Solving the wave equation with physics-informed deep learning – Moseley et al, ArXiv (2020)

- Mini-batch size $N_c = N_{IC} = 500$
- Fully connected NN, 10 layers, 1024 hidden units
- Softplus activation
- Adam optimizer

Training time: 1 hour

PINNs for forward simulation

Ground truth FD



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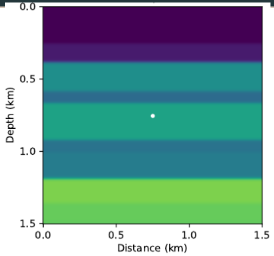
$$\mathcal{L}_{\mathrm{IC}} = \frac{1}{N} \sum_{i=1}^{N} (\hat{u}(x_i, t_i, s_i) - u_{\mathrm{FD}}(x_i, t_i, s_i))^2$$

Conditioned PINNs

Idea: Add IC/BCs as additional network input parameters.

Network **does not** need to be retrained for each simulation

$\Rightarrow$ much faster!



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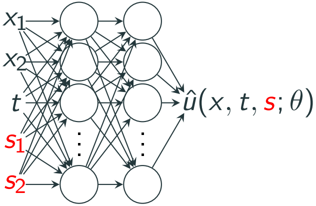
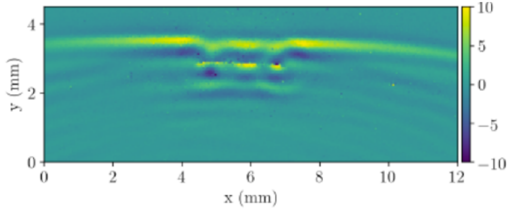
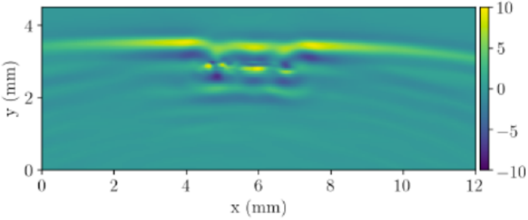




(a) Actual data at $t = 12.38\ \mu s$.

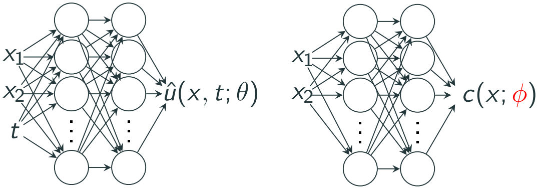


(b) Data recovered from PINN simulation at $t = 12.38\ \mu s$.

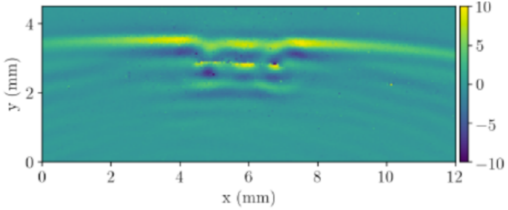
$$\mathcal{L}_{\mathrm{PDE}}(\theta, \phi) = \frac{1}{N_c}\sum_{j=1}^{N_c}\left(\left[\nabla^2 - \frac{1}{c(x_j;\phi)^2}\frac{\partial^2}{\partial t^2}\right]\hat{u}(x_j, t_j;\theta)\right)^2$$

$$\mathcal{L}_{\mathrm{data}} = \frac{1}{N_{\mathrm{d}}}\sum_{i=1}^{N_{\mathrm{d}}}(\hat{u}(x_i, t_i;\theta) - f(x_i, t_i))^2$$

Treat velocity as another neural network and simultaneously learn it



Shukla K et al, **Physics-Informed Neural Network for Ultrasound Nondestructive Quantification of Surface Breaking Cracks**, Journal of Nondestructive Evaluation (2020)



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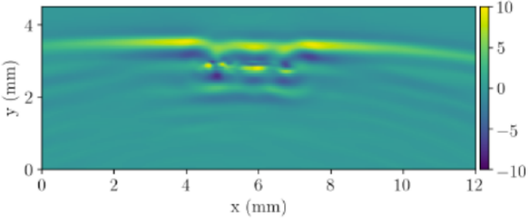

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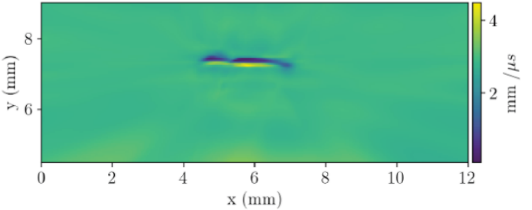

(d) Speed $v(x, y)$ recovered from PINN simulation.

Treat velocity as another neural network and simultaneously learn it

Shukla K et al, **Physics-Informed Neural Network for Ultrasound Nondestructive Quantification of Surface Breaking Cracks**, Journal of Nondestructive Evaluation (2020)

Limitations and extensions

Advantages and limitations of PINNs

Advantages

- **Mesh-free**
- Can perform well for **high-dimensional PDEs**
- Can be extended to **inverse problems**
- Perform best on **messy/mixed problems**
    - Noisy data
    - Physics not perfectly known
- Analytical gradients (e.g. sensitivity analysis)

Disadvantages

- **Computational cost** is high
- No guarantee to converge, **convergence properties** less well understood
- Challenging to scale to more **complex problems** (larger domains, multi-scale, multi-physics)

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Problem: How to pick the weight(s)?

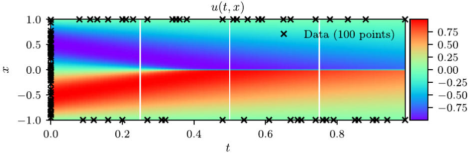
$\mathcal{L}_{\text{tot}} = \mathcal{L}_{\text{BC}} + \omega \mathcal{L}_{\text{PDE}}$

ω too small $\Rightarrow$ only learns boundary conditions ω too large $\Rightarrow$ no unique solution

Example: Burgers' equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - v\frac{\partial^2 u}{\partial x^2} = 0 \qquad u(x,0) = -\sin(\pi x)$$

$$u(-1,t) = u(1,t) = 0$$



Let the solution be approximated by

$$\hat{u}(x,t;\theta) = (x-1)(x+1)(t-0)\text{NN}(x,t;\theta) - \sin(\pi x)$$

Only one loss term to optimize

$$\mathcal{L}_{\text{PDE}}(\theta) = \frac{1}{N_c}\sum_{j=1}^{N_c}\left(\left[\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - v\frac{\partial^2 u}{\partial x^2}\right]\hat{u}(x_j,t_j;\theta)\right)^2$$

Can be challenging to use this approach for complex boundary conditions.

There also exist adaptive schemes for updating the weights.

Adaptive collocation points

Idea Place additional collocation points where the PDE residuals are large.

Algorithm 1 Residual-based adaptive refinement (RAR)

Sample the initial collocation points $\mathcal{T}$;
Train the PINN for a certain number of iterations;
while Training **do**
  Sample a set of points S_0;
  Compute the PDE residuals for the points in S_0;
  S $\leftarrow$ m points with largest residuals in S_0;
  $\mathcal{T} \leftarrow \mathcal{T} \cup S$;
  Train the PINN for a certain number of iterations;
end while

Many variations exist, e.g. use PDE residuals to construct a distribution from which new collocation points can be sampled.

Wu et al. **A comprehensive study of non-adaptive and residual-based adaptive sampling for physics-informed neural networks**. Computer

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Physics-informed neural networks with unknown measurement noise

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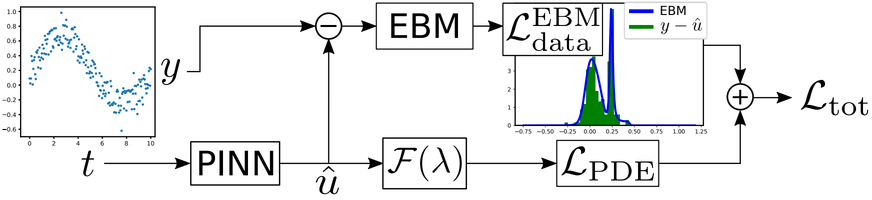
We aim to **train PINNs** in case of **unknown measurement noise**.

- **Energy-based model** (EBM) to model unknown noise distribution
- $\mathcal{L}_{\text{data}}^{\text{EBM}}$ ... NLL of **measurement-residuals** given the learned PDF

$$\mathcal{L}_{\text{tot}} = \mathcal{L}_{\text{data}}^{\text{EBM}}(\{y_d - \hat{u}(t_i)\}_{i=1}^{N_d}) + \omega \mathcal{L}_{\text{PDE}}(\mathcal{F}, \hat{u}, \{t_j\}_{j=1}^{N_c})$$

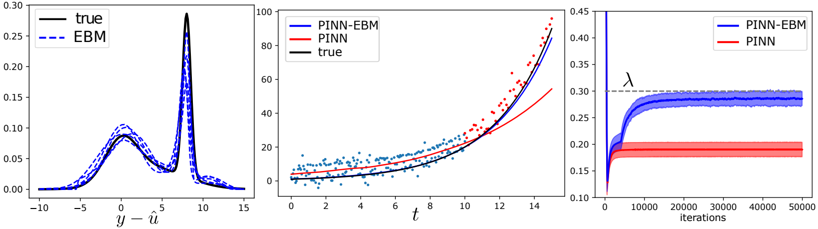


Pilar and Wahlström, Physics-informed neural networks with unknown measurement noise, L4DC (2024)

Example – exponential differential equation

- The solution u is **governed** by an **ODE** with unknown λ.
- The measurements y are contaminated by **homogeneous measurement noise** ϵ of unknown form.

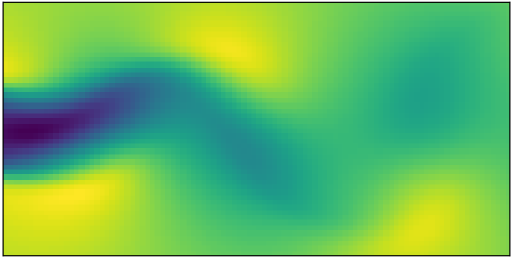
$$\dot{u}(t) = \lambda u(t)$$
$$y(t) = u(t) + \epsilon$$



Pilar and Wahlström, **Physics-informed neural networks with unknown measurement noise**, L4DC (2024)

The **PINN-EBM** also improved the results when considering the **Navier-Stokes equations** in the presence of **non-Gaussian noise**.

$$f = u_{\mathrm{t}} + \lambda_1(uu_{\mathrm{x}} + vu_{\mathrm{y}}) + p_{\mathrm{x}} - \lambda_2(u_{\mathrm{xx}} + u_{\mathrm{yy}}) \stackrel{!}{=} 0,$$
$$g = v_{\mathrm{t}} + \lambda_1(uv_{\mathrm{x}} + vv_{\mathrm{y}}) + p_{\mathrm{y}} - \lambda_2(v_{\mathrm{xx}} + v_{\mathrm{yy}}) \stackrel{!}{=} 0,$$



noise		PINN-EBM	PINN-off	PINN
3G	$100\lvert\Delta\lambda_1\rvert$	**1.19**±0.67	2.92±0.47	23.10±0.11
	$100\lvert\Delta\lambda_2\rvert$	**0.04**±0.03	0.09±0.05	0.08±0.06
	RMSE	**0.06**±0.01	0.11±0.01	0.20±0.02
	NLL	**-0.03**±0.08	0.15±0.07	0.40±0.30
	$100f^2$	**0.04**±0.00	0.10±0.01	0.18±0.01

Pilar and Wahlström, **Physics-informed neural networks with unknown measurement noise**, L4DC (2024)

Summary

PINNs constitute an **alternative** to **classical solvers** of PDEs.

- Flexible method, both forwards and inverse problems.
- Particularly useful on **messy/mixed problems**
- Unknown **measurement noise** can be taken into account in **PINNs**.

Some pointers if you want to learn more:

- **An expert's guide to training physics-informed neural networks**, Wang et al., arXiv (2023)
- **Scientific Machine Learning Through Physics–Informed Neural Networks: Where we are and What's Next**, Journal of Scientific Computing (2022)
- Course: **ETH Zürich Deep Learning in Scientific Computing** (2023) Lectures available on Youtube (some slides heavily inspired from that sources)

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Random Fourier features

Problem: PINNs are biased towards learning low-frequency solutions $\rightarrow$ **spectral bias**

Idea: transform inputs to higher-frequency functions $\rightarrow$ **Random Fourier features**

$$\gamma(\mathbf{x}) = \begin{bmatrix} \cos(\mathbf{B}\mathbf{x}) \\ \sin(\mathbf{B}\mathbf{x}) \end{bmatrix}$$

where $\mathbf{B} \in \mathbb{R}^{mxd}$ with $\mathbf{B}_{ij} \sim \mathcal{N}(0, \sigma^2)$ and σ is a hyperparameter.

- The coordinate embedding $\gamma(\mathbf{x})$ serves as input to the PINN.
- Enables more effective learning of high frequencies.
- The value of the parameter σ is an important design choice.
- In practice, often $\sigma \in [1, 10]$.

Tancik et al. **Fourier features let networks learn high frequency functions in low dimensional domains**, NeurIPS (2020)