A Hands-on Introduction to Physics-informed Machine Learning

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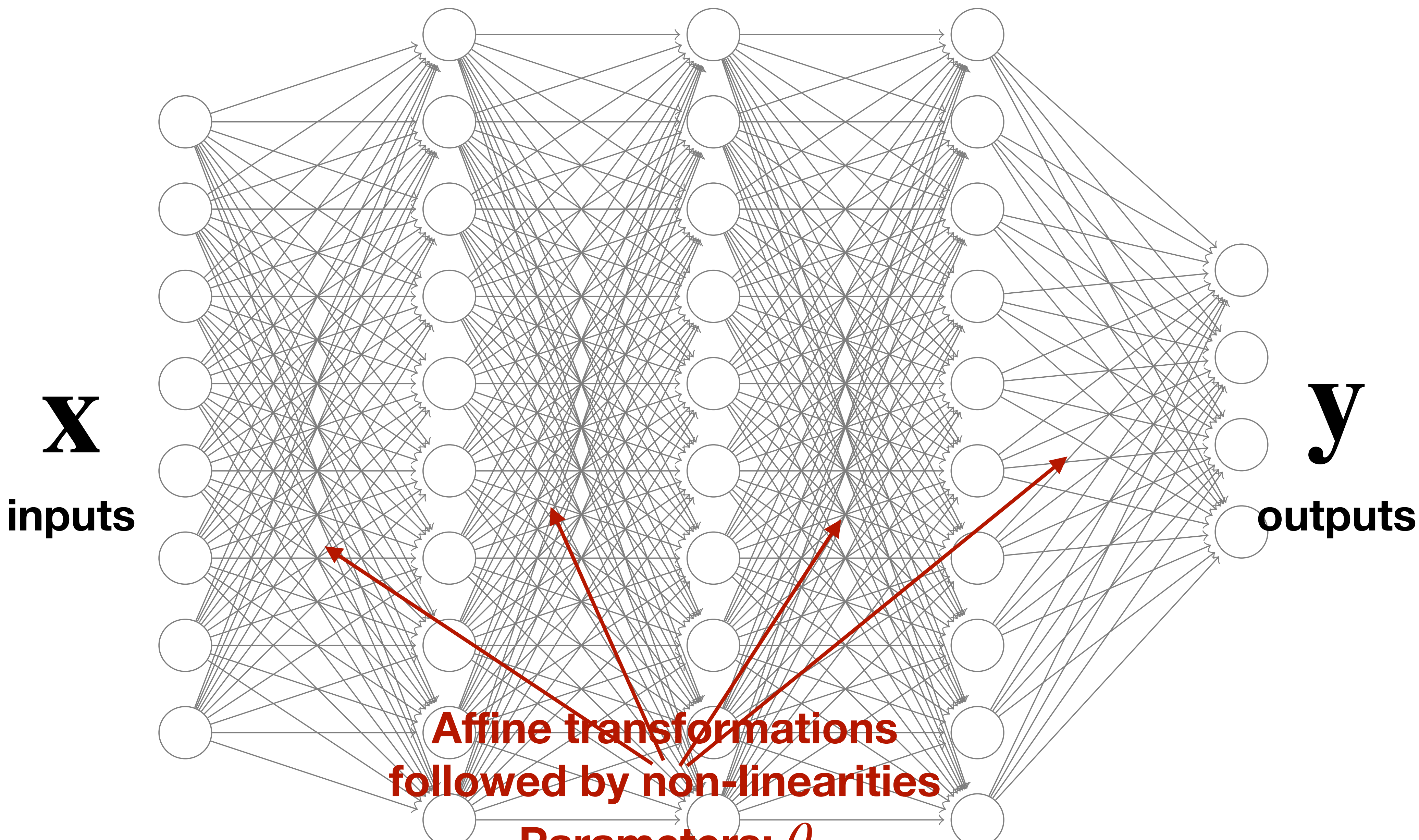
Objective

Learn how physical information in the form of differential equations can be used to regularize neural networks.

Reminder - What are neural networks?



Parameters: θ

Function: $y = N(x;\theta)$

Reminder - How do we train neural networks?

- Depends on what the task is… Focusing on **regression**.
- You have some data consisting of **inputs** $x_{1:n} = (x_1, \ldots, x_n)$ and **outputs** $y_{1:n} = (y_1, \ldots, y_n)$.
- Say you want to find a neural net $N(x;\theta)$ that goes from input to output.
- Minimize a loss function:

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left[y_i - N(x_i;\theta)\right]^2$$

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Reminder - How do we train neural networks?

Automatic differentiation for getting gradients (PyTorch, TensorFlow)

- Minimize a loss function:

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left[y_i - N(x_i;\theta)\right]^2$$

- We typically use a form of **stochastic gradient descent**

$$\theta_{t+1} = \theta_t - a_t \frac{1}{m}\sum_{j=1}^{m}\nabla_\theta\left[y_{i_j} - N(x_{i_j};\theta_t)\right]^2$$

Learning rate which has to satisfy certain constraints (Robbins-Monro, 1951)

Randomly sampled batch of inputs/outputs

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Illustrative Example 1: Solving an ODE

I. E. Lagaris, A. Likas, D. I. Fotiadis, Artificial Neural Networks for Solving Ordinary and Partial Differential Equations, 1997

From ODE to a loss function

- Consider the initial value problem:

$$\frac{d\Psi}{dx} = f(x, \Psi)$$

$$\Psi(0) = A$$

- Automatically satisfy the initial condition by parameterizing the solution as:

$$\hat{\Psi}(x;\theta) = A + xN(x;\theta)$$

- The idea is to find θ by minimizing the *integrated squared residual* of the ODE:

$$L(\theta) = \int_0^1 \left[\frac{d\hat{\Psi}(x;\theta)}{dx} - f(x, \hat{\Psi}(x;\theta))\right]^2 dx$$

Solving the problem with stochastic gradient descent

- The idea is to find θ by minimizing the *integrated squared residual* of the ODE:

$$L(\theta) = \int_0^1 \left[\frac{d\hat{\Psi}(x;\theta)}{dx} - f(x, \hat{\Psi}(x;\theta))\right]^2 dx$$

- The following algorithm converges (Robbins-Monro, 1951)

$$\theta_{t+1} = \theta_t - \frac{a_t}{n}\sum_{i=1}^{n} \nabla_\theta \left[\frac{d\hat{\Psi}(x_i;\theta_t)}{dx} - f(x_i, \hat{\Psi}(x_i;\theta_t))\right]^2$$

Spatial locations uniformly sampled in [0, 1] at each iteration.

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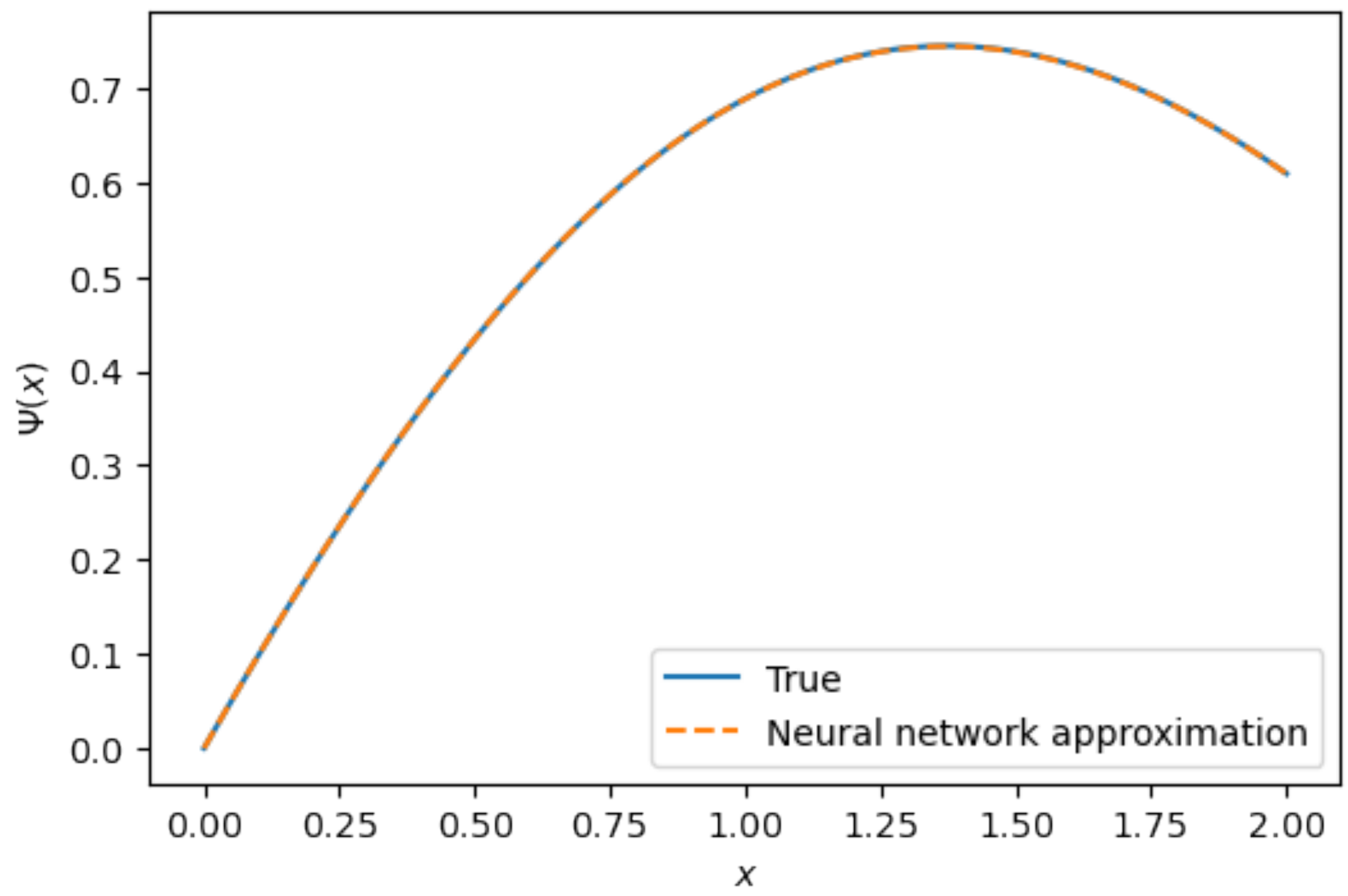
Results (Part of Hands-on activity)

$$\frac{d\Psi(x)}{dt} = \exp\left\{-\frac{x}{5}\right\}\cos x - \frac{\Psi(x)}{5}$$

$$\Psi(0) = 0$$



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Illustrative Example 2:
Solving an elliptic PDE

From PDEs to a loss function - Integrated squared approach

$$-\nabla \cdot \left[a(x)\nabla u(x)\right] + c(x)u(x) = f(x)$$

$$L(\theta) = \int \left\{ \nabla \cdot \left[a(x)\nabla \hat{u}(x;\theta)\right] + c(x)\hat{u}(x;\theta) + f(x) \right\}^2 dx$$

M. Raissi, P. Perdikaris, G. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving non-linear partial differential equations, 2019

From PDEs to a loss function - Energy approach

$$-\nabla \cdot \left[a(x)\nabla u(x)\right] + c(x)u(x) = f(x)$$

Dirichlet principle

$$L(\theta) = \int \left\{ \frac{1}{2}a(x)\nabla \hat{u}(x;\theta) + c(x)\hat{u}^2(x;\theta) - f(x)\hat{u}(x;\theta) \right\} dx - \int_{\Gamma_N} g_N \hat{u}(x;\theta) d\Gamma_N$$

S. Karumuri, R. Tripathy, I. Bilionis, Simulator-free Solution of High-dimensional Elliptic Partial Differential Equations using Deep Neural Networks, 2020

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I can already solve ODEs/ PDEs. Why is this useful?

Illustrative Example 3: Solving PDEs for all possible parameterizations

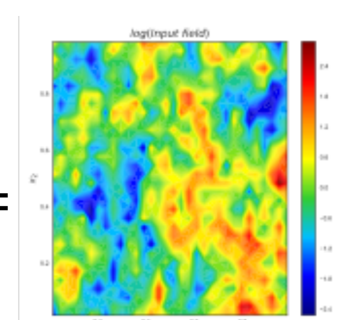
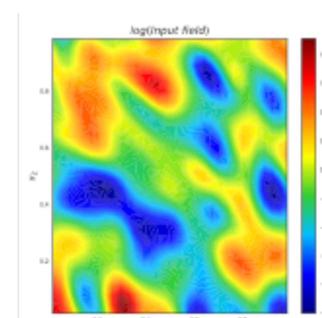
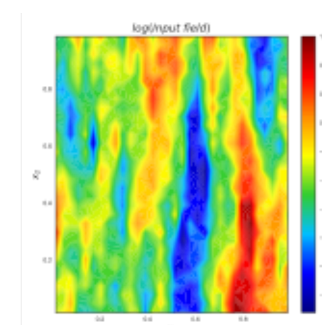
Random parameters

$$-\nabla \cdot \left[a(x;\xi)\nabla u(x;\xi)\right] + c(x)u(x;\xi) = f(x)$$

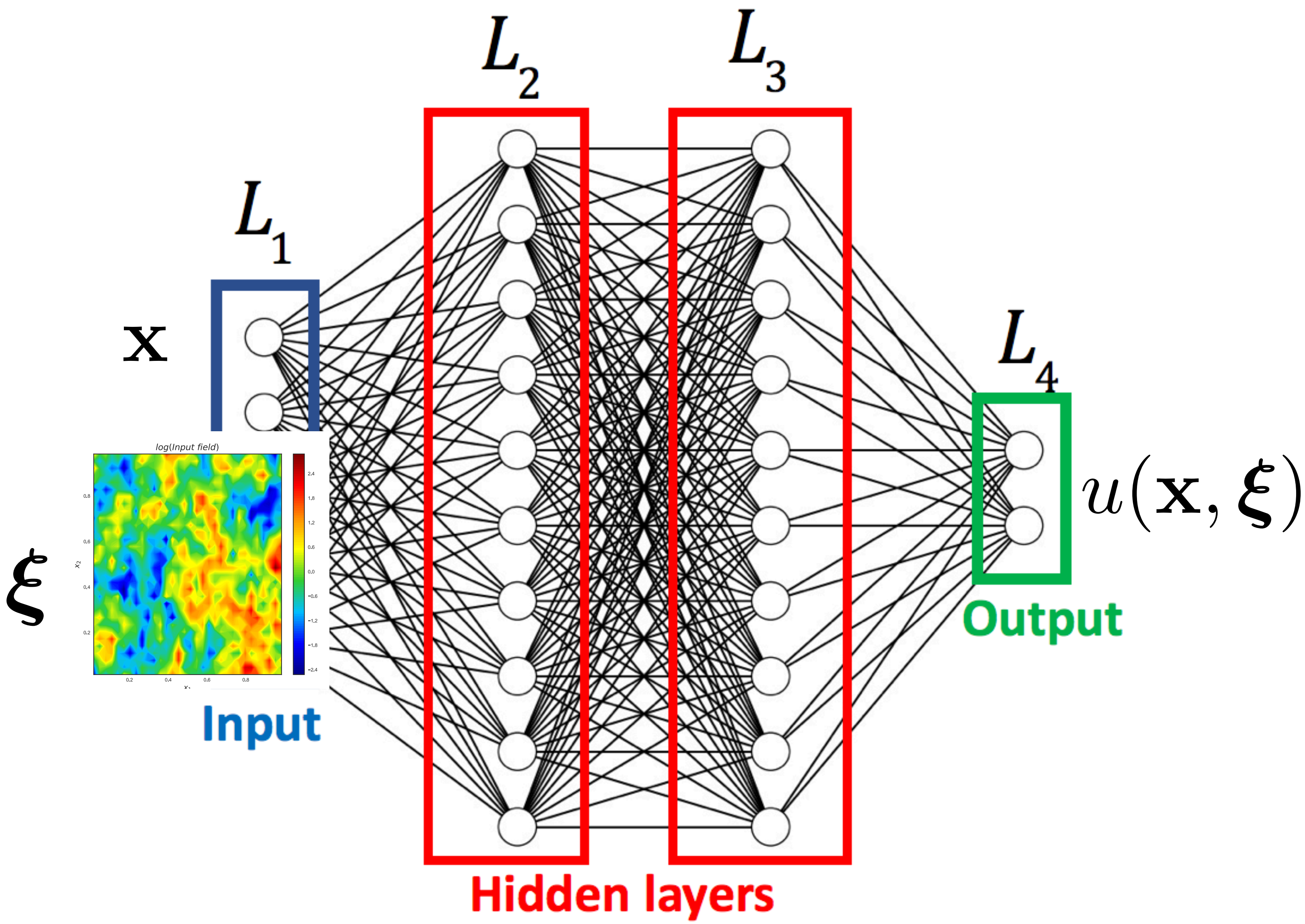
$$u = 0, \forall x_1 = 1,$$

$$u = 1, \forall x_1 = 0,$$

$$\frac{\partial u}{\partial n} = 0, \forall x_2 = 1.$$

$\log a(x,\xi) =$  or  or  ...

Representing the solution of the PDE with a DNN



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From PDEs to a loss function - Energy approach

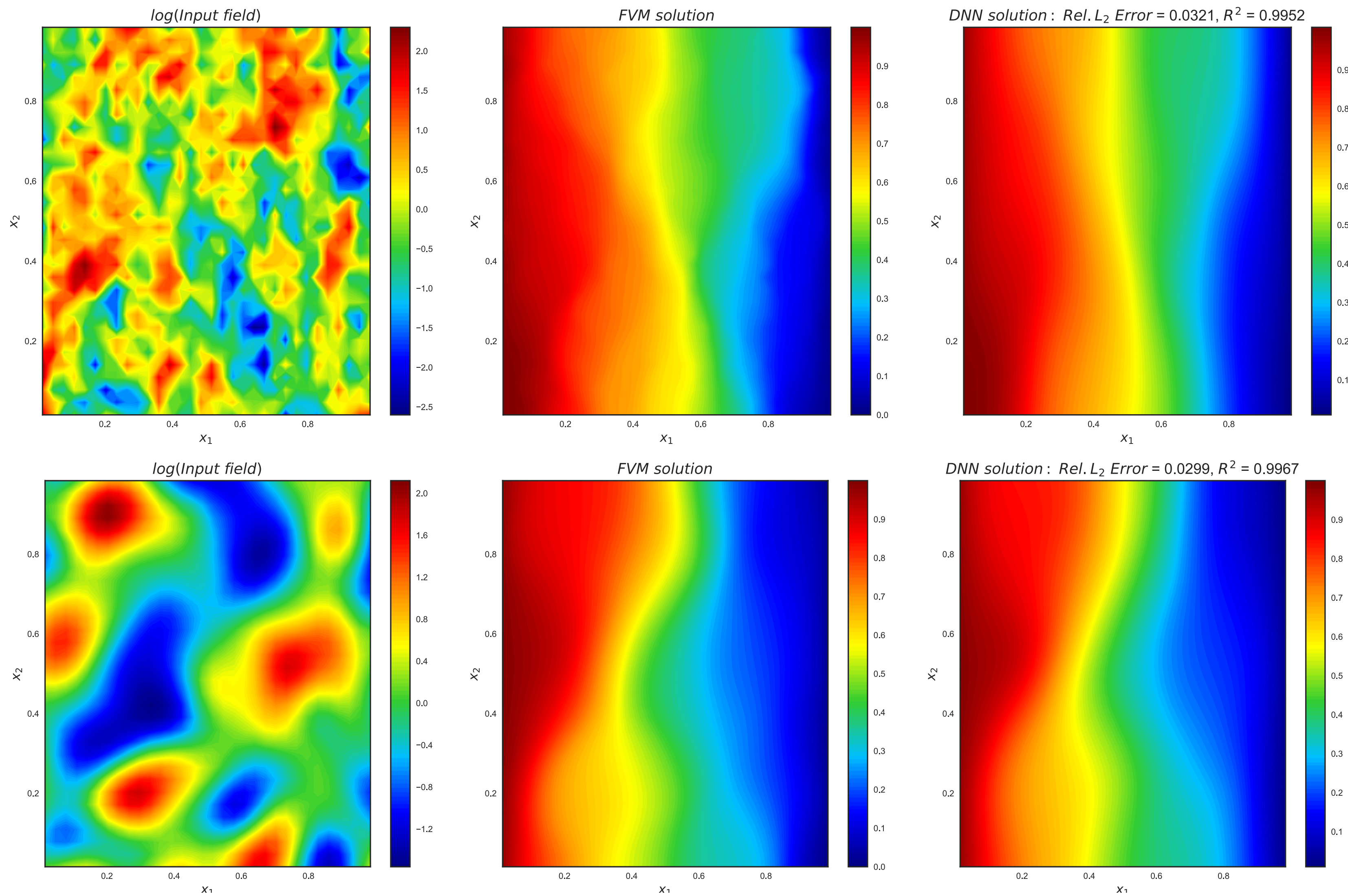
$$-\nabla \cdot \left[a(x;\xi)\,\nabla u(x;\xi)\right] + c(x)u(x;\xi) = f(x)$$

Dirichlet principle

$$L(\theta) = \mathbb{E}_{\xi}\left[\int \left\{ \frac{1}{2}a(x,\xi)\,\nabla\hat{u}(x,\xi;\theta) + c(x)\hat{u}^2(x,\xi;\theta) - f(x)\hat{u}(x,\xi;\theta) \right\} dx - \int_{\Gamma_N} g_N\hat{u}(x,\xi;\theta)d\Gamma_N]\right]$$

S. Karumuri, R. Tripathy, I. Bilionis, Simulator-free Solution of High-dimensional Elliptic Partial Differential Equations using Deep Neural Networks, 2020

One network for all kinds of random fields



Karumuri, S.; Tripathy, R.; Bilionis, I.; Panchal, J. Simulator-Free Solution of High-Dimensional Stochastic Elliptic Partial Differential Equations Using Deep Neural Networks. *Journal of Computational Physics* **2020**, *404*, 109120. https://doi.org/10.1016/j.jcp.2019.109120.

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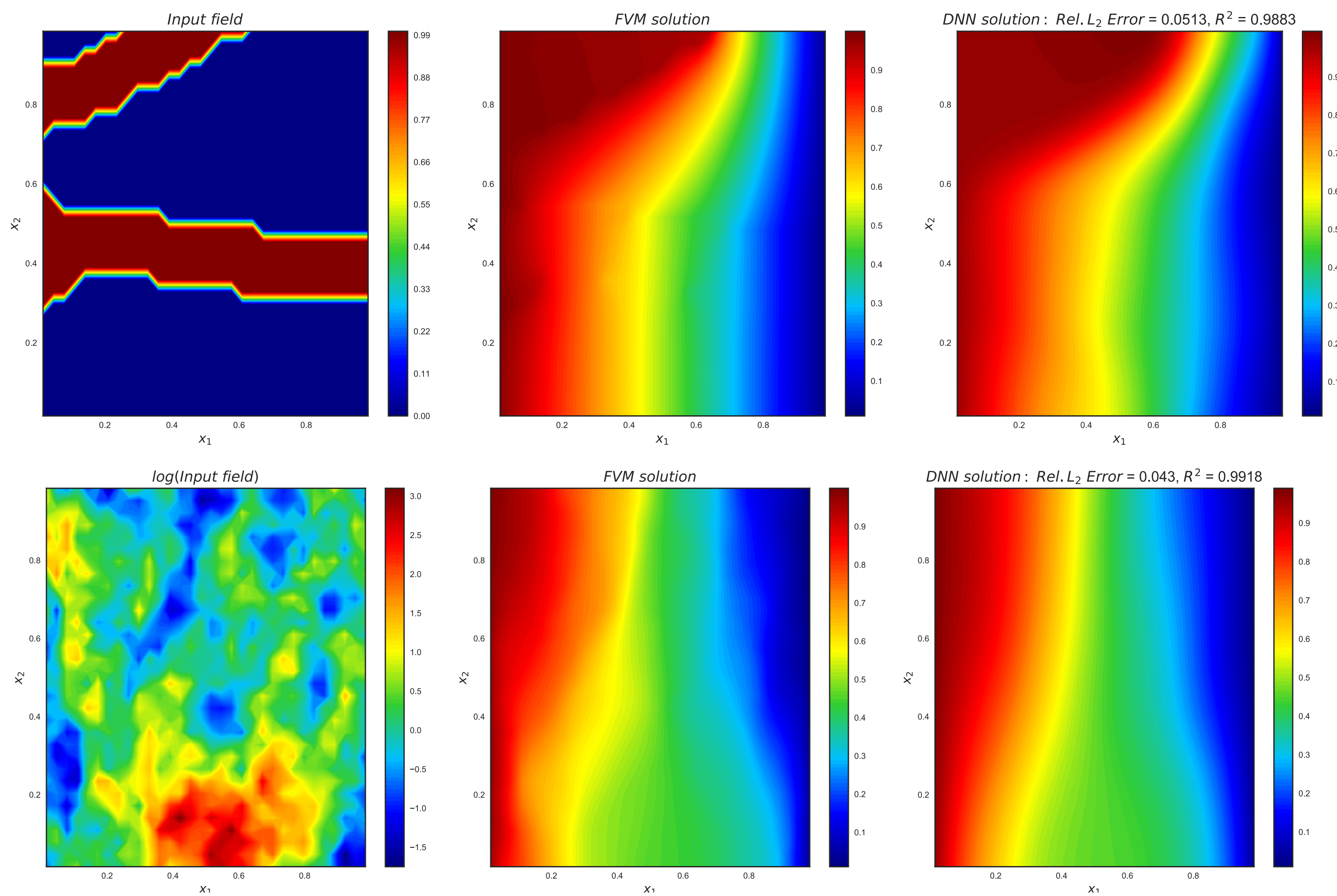

Karumuri, S.; Tripathy, R.; Bilionis, I.; Panchal, J. Simulator-Free Solution of High-Dimensional Stochastic Elliptic Partial Differential Equations Using Deep Neural Networks. *Journal of Computational Physics* **2020**, *404*, 109120. https://doi.org/10.1016/j.jcp.2019.109120.

What are the applications of this?

- High-dimensional uncertainty propagation through PDEs.
- Solving free boundary and Stefan problems (Wang, Perdikaris, 2021).
- PDE-constrained optimization (Hennigh et al., 2020).
- Inverse/model calibration problems (Raise, 2019).
- Data assimilation/filtering (no one yet).
- …

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What is the catch?

- Not as easy as it looks in practice…
- Vanishing gradients…
- Spectral bias of deep nets…
- Fine solution features…
- We address some of these in the hands-on activity by solving the physical equations for a compressible neo-Hookean material.

Hands-on activity led by Atharva Hans

https://nanohub.org/tools/handsonpinns

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