Physics-informed Machine Learning: A very gentle introduction

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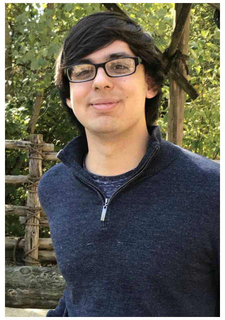
Alex Alberts


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Physics-informed Machine Learning Subgroup

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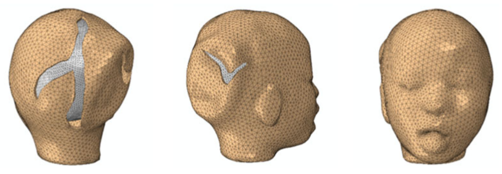
Three basic problems that we would like to be able to solve.

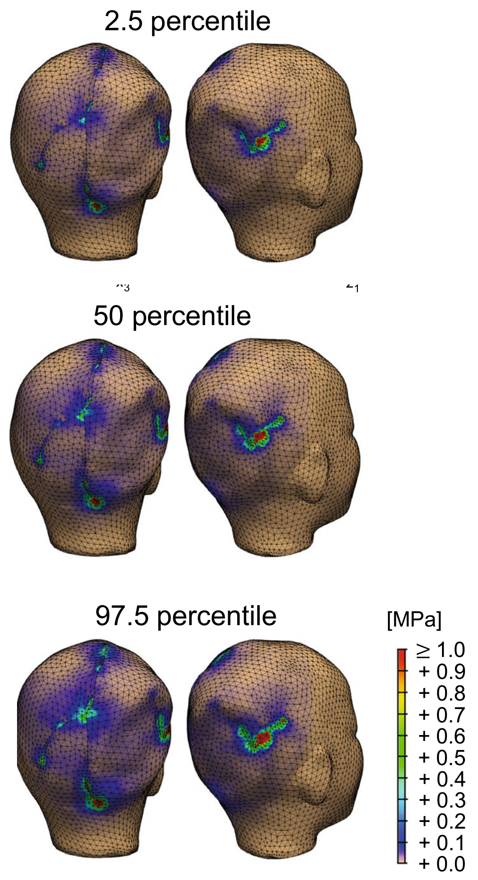
The Uncertainty Propagation Problem (reconstructive surgery)

Table 1 Range of HGO parameters based on Annaidh et al. (2012) and Tonge et al. (2013)

Parameter	Range	Mean
μ (MPa)	[0.004774, 0.2014]	0.04498
k_1 (MPa)	[0.000380, 24.530]	4.9092
k_2 (–)	[0.133, 161.862]	76.64134



Non-linear Elasticity



Stress statistics

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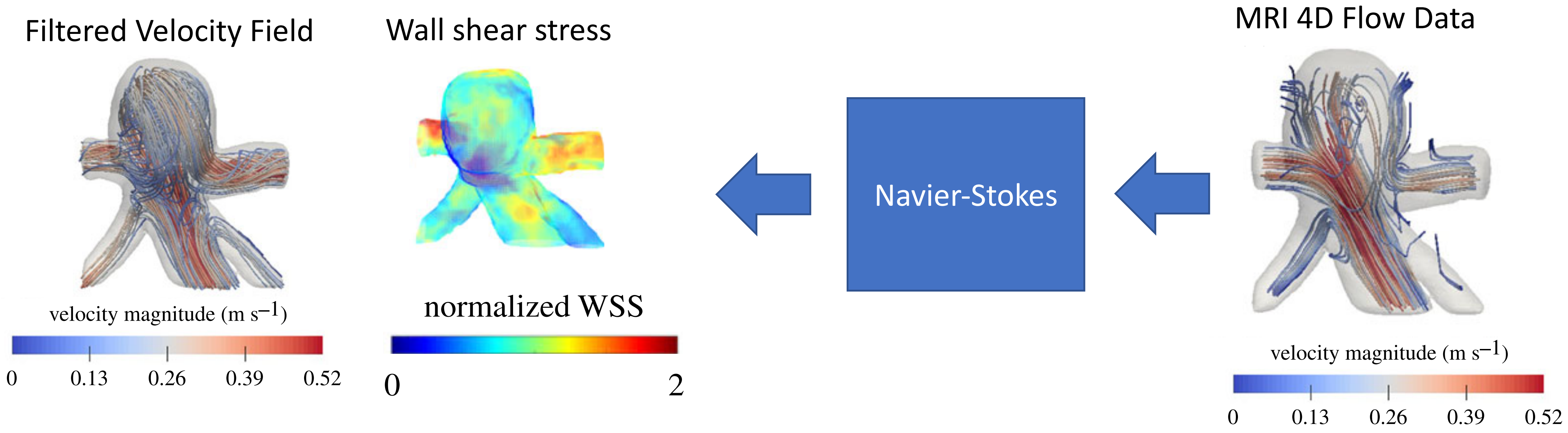
Lee, T., Turin, S.Y., Gosain, A.K. et al. Biomech Model Mechanobiol (2018) 17: 1857. https://doi-org.ezproxy.lib.purdue.edu/10.1007/s10237-018-1061-

Inverse Problem Example (Cerebral aneurysm)



Melissa C. Brindise, Sean Rothenberger, Benjamin Dickerhoff, Susanne Schnell, Michael Markl, David Saloner, Vitaliy L. Rayz, Pavlos P. Vlachos, Multi-modality cerebral aneurysm haemodynamic analysis: *in vivo* 4D flow MRI, *in vitro* volumetric particle velocimetry and *in silico* computational fluid dynamics **16** *J. R. Soc. Interface* http://doi.org/10.1098/rsif.2019.0465

Example of a Design Problem (reconstructive surgery)

Table 1 Range of HGO parameters based on Annaidh et al. (2012) and Tonge et al. (2013)

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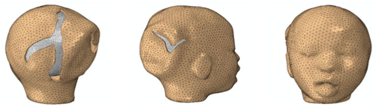
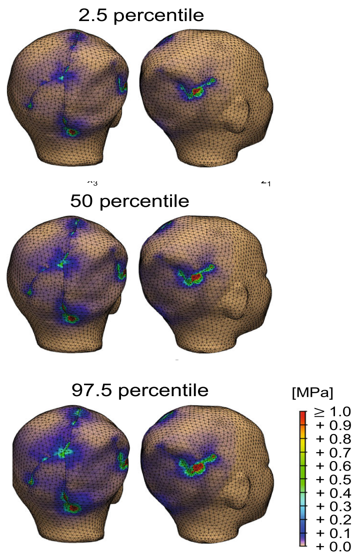
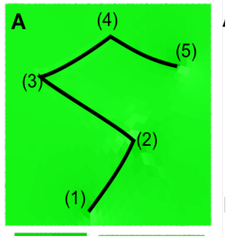


Non-linear Elasticity



Stress statistics



Optimal flap design

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Figures courtesy of Buganza's group.

We know how to pose these problems mathematically!

We just can’t solve them…

Common Solution Approaches and Their Computational Intractability

- All problems can, in principle, be solved by Monte Carlo sampling.
- Infeasible to do directly with physical simulator.
- Idea -> Replace the simulator with a surrogate model.
- Problem -> ***Curse of dimensionality***.

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IDEA 1: Use Deep Neural Networks (DNN) to Represent the Response Surface

- Universal function approximators.
- Layered representation of information.
- Tremendous success in high-dimensional applications such as *image classification*, *autonomous driving*.
- Availability of libraries such as *tensorflow*, *keras*, *theano*, *PyTorch*, *caffe* etc.

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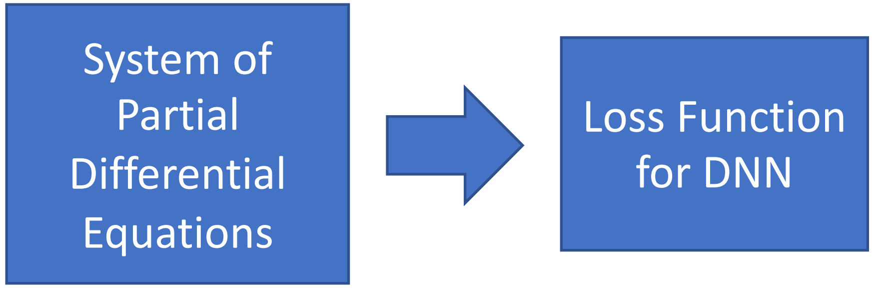
Tripathy, R. K.; Bilionis, I. Deep UQ: Learning Deep Neural Network Surrogate Models for High Dimensional Uncertainty Quantification. Journal of Computational Physics 2018, 375, 565–588. https://doi.org/10.1016/j.jcp.2018.08.036.

IDEA 2: Get rid of PDE Solver



- Lagaris et al., 1991
- Raisi, Predikaris, Karniadakis, 2019.
- {Raisi, Perdikaris, Karniadakis, Zabaras}* {2018, 2019}.
- Karumuri, Tripathy, Bilionis, Panchal, 2019.
- …

Illustrative Uncertainty Propagation Example With Physics-Informed DNN

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 2019 (under review). https://arxiv.org/abs/1902.05200.

Stochastic Elliptic Partial Differential Equation

PDE:

$$\nabla(a(\mathbf{x})\nabla u(\mathbf{x})) = 0,$$

$$\mathbf{x} = (x_1, x_2) \in \Omega = [0,1]^2,$$

Boundary conditions:

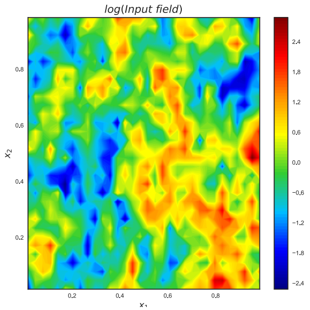
$$u = 0, \forall x_1 = 1,$$

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

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

Uncertain conductivity:

$\log a(x) =$



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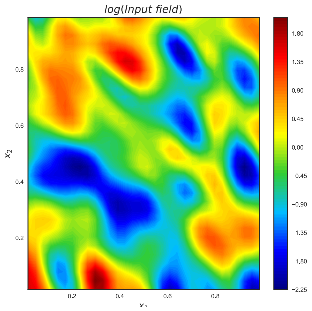
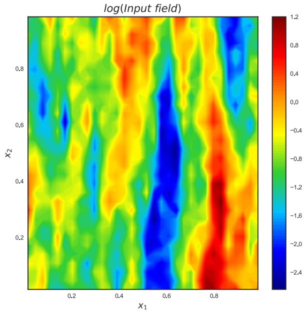


or



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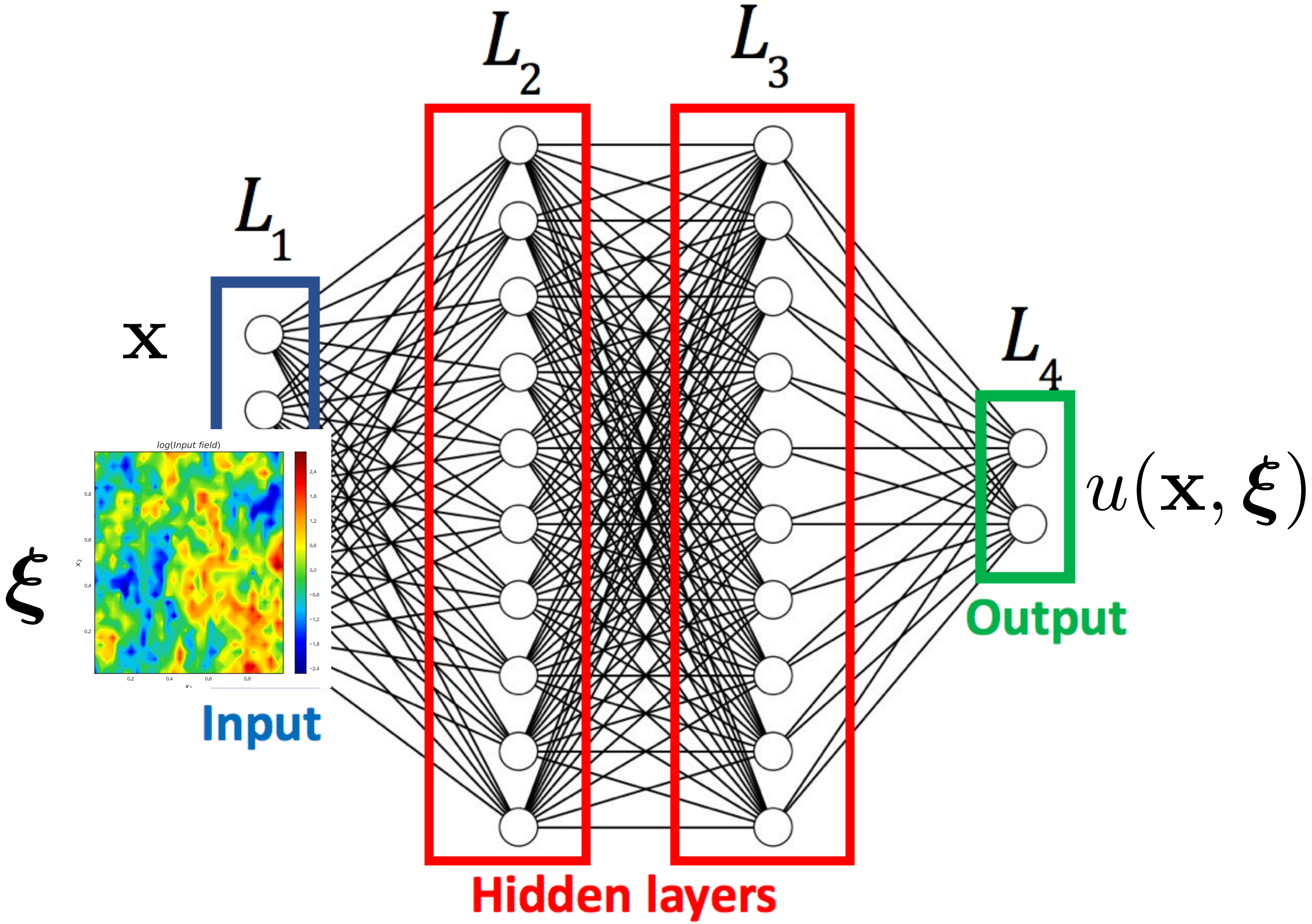
Representing the Solution of the Stochastic PDE as a DNN



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How to turn the PDE into a loss function? Integrated Squared Residual

- Move all PDE terms to the left hand side.
- Square and integrate over space/time.
- Take expectation over random parameters.
- Minimize what you get over the space of DNNs subject to any boundary conditions.

$$J[u] = \mathbb{E}_{\xi}\left[\int_{[0,1]^2} \left(\nabla \cdot (a(x,\xi)\nabla \mathrm{u})\right)^2 dx\right].$$

Works, but may have lots of local minima…

Can we do better?

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How to turn the PDE into a loss function? Energy-based Residual

- Write down energy functional for system.
- Take expectation over random parameters.
- Minimize what you get over the space of DNNs subject to any boundary conditions.

$$J[u] = \mathbb{E}_{\xi}\left[\int_{[0,1]}^{2} a(x,\xi) \parallel \nabla u \parallel_2^2 \, dx\right].$$

Energy-based loss is better because you can often prove uniqueness of solution!

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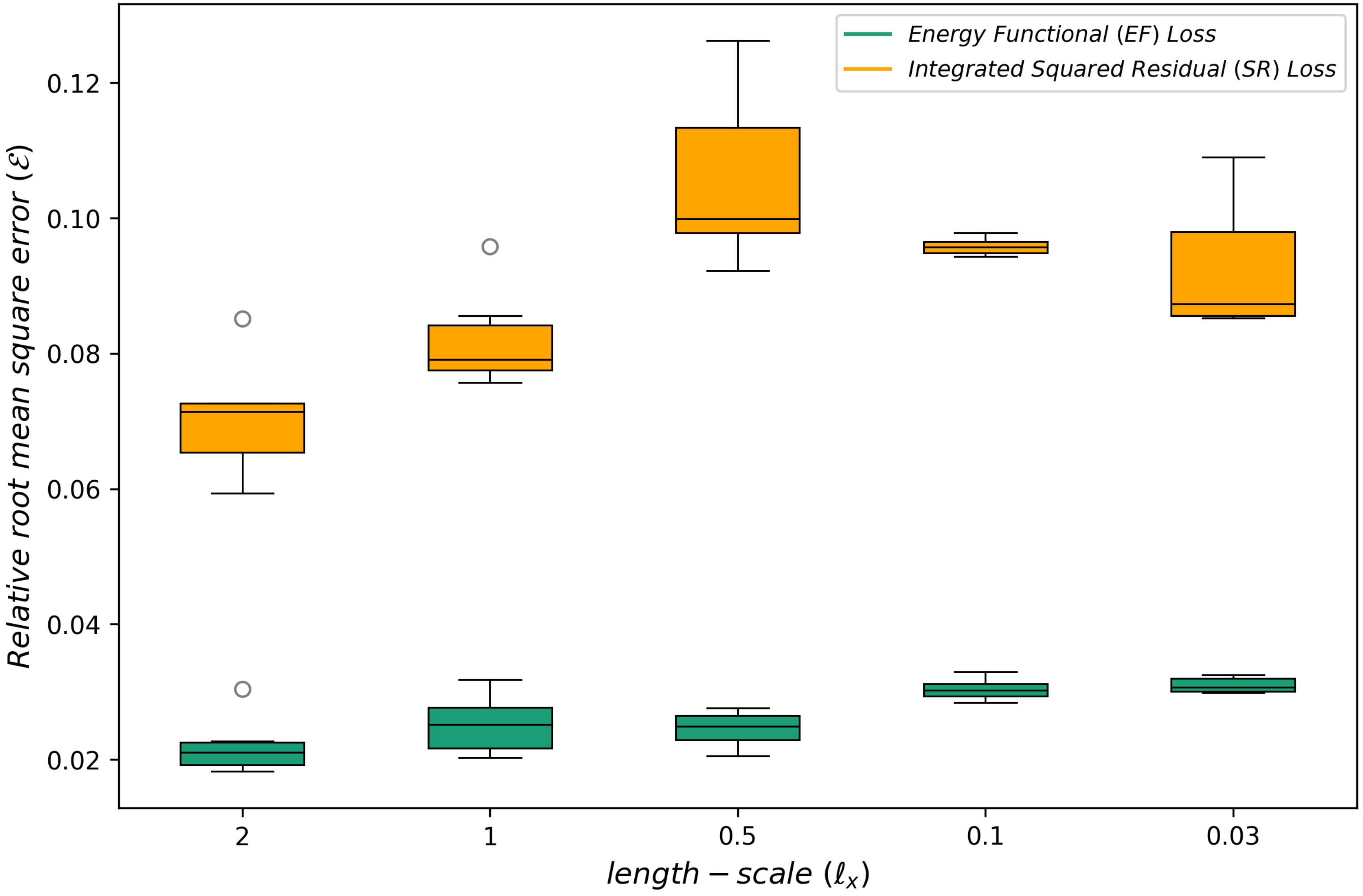
Integrated Square Residual vs Energy Loss



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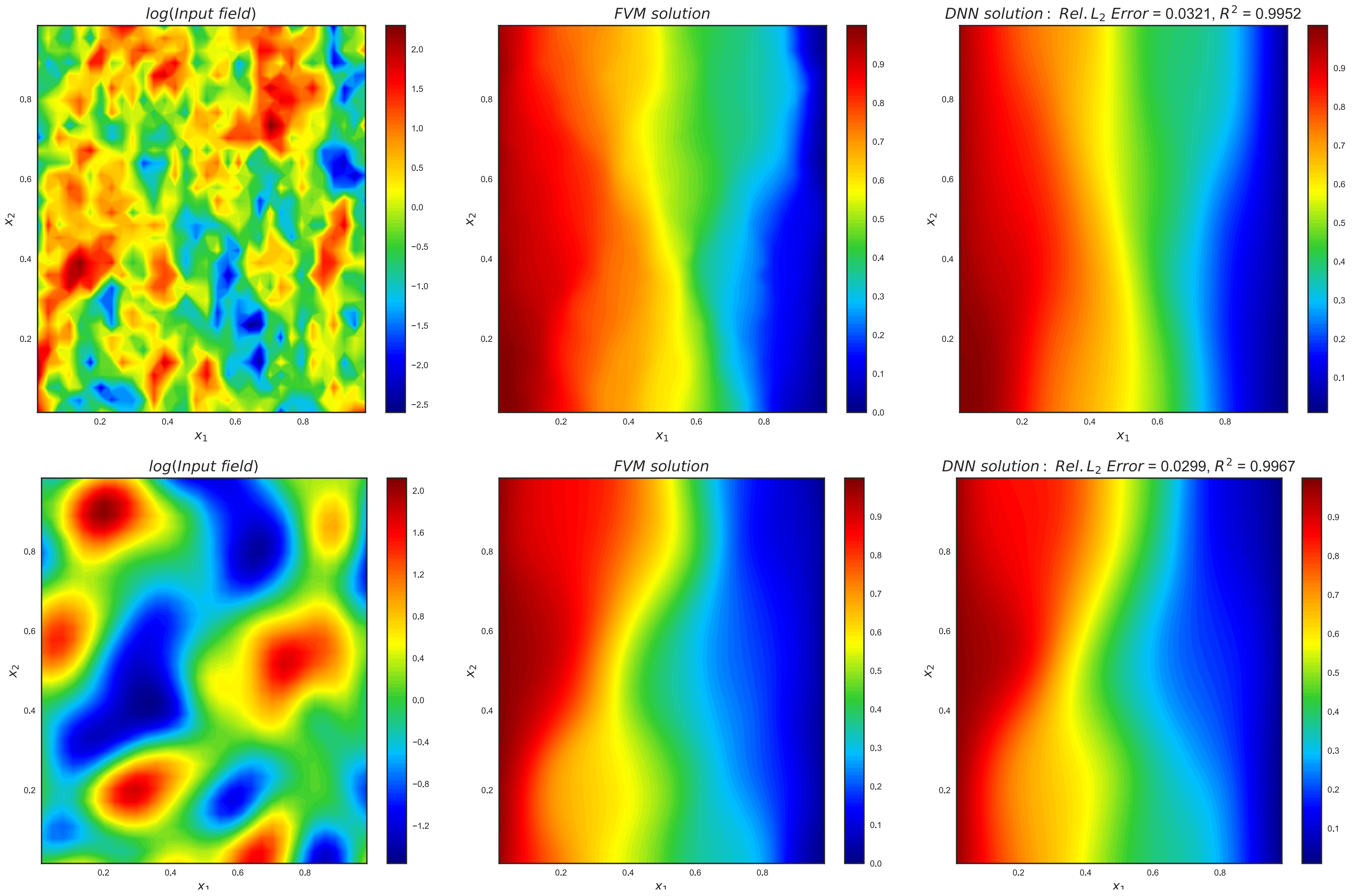
Numerical Examples: Point-wise Predictions



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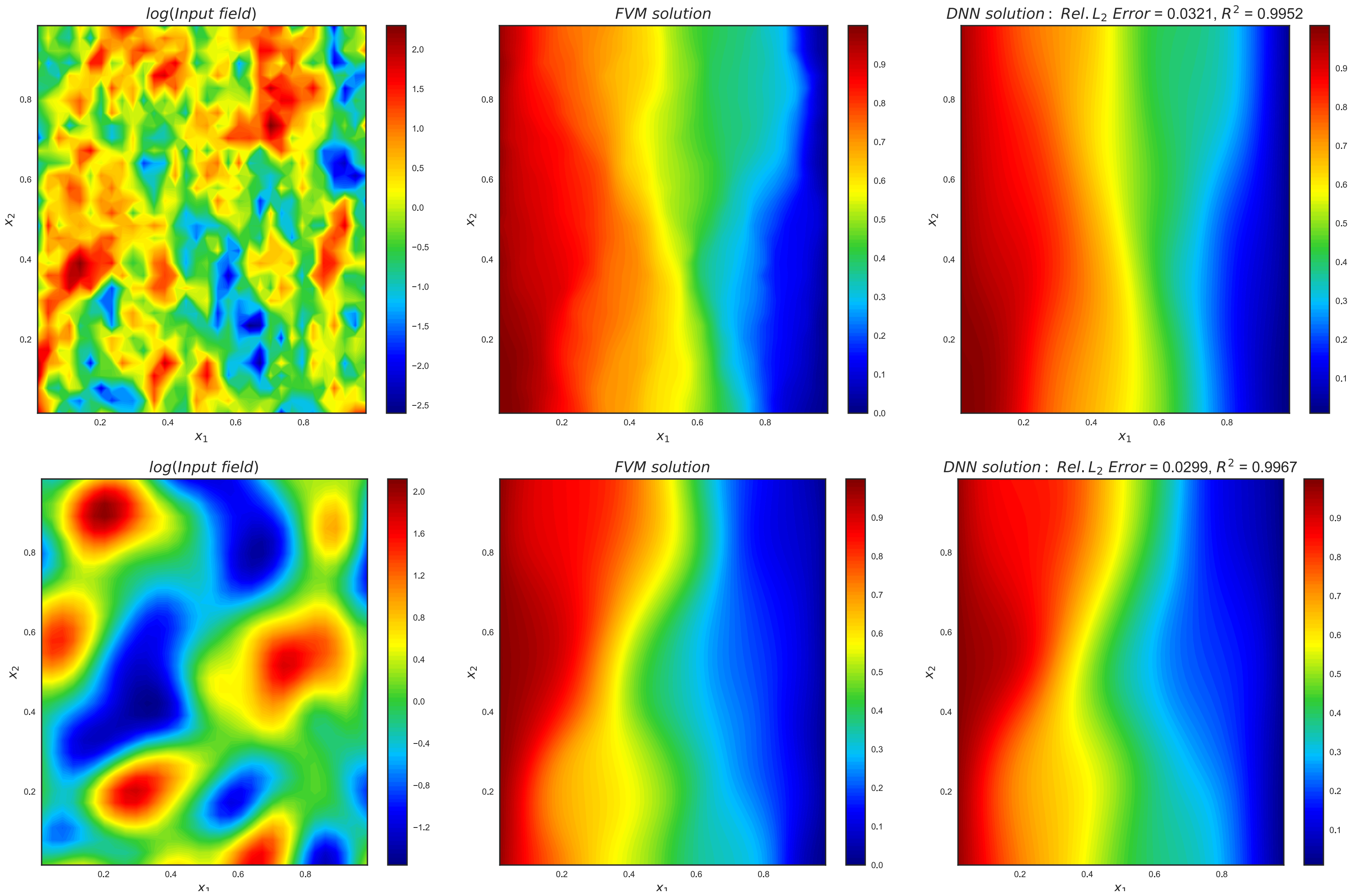
Numerical Examples: Point-wise Predictions



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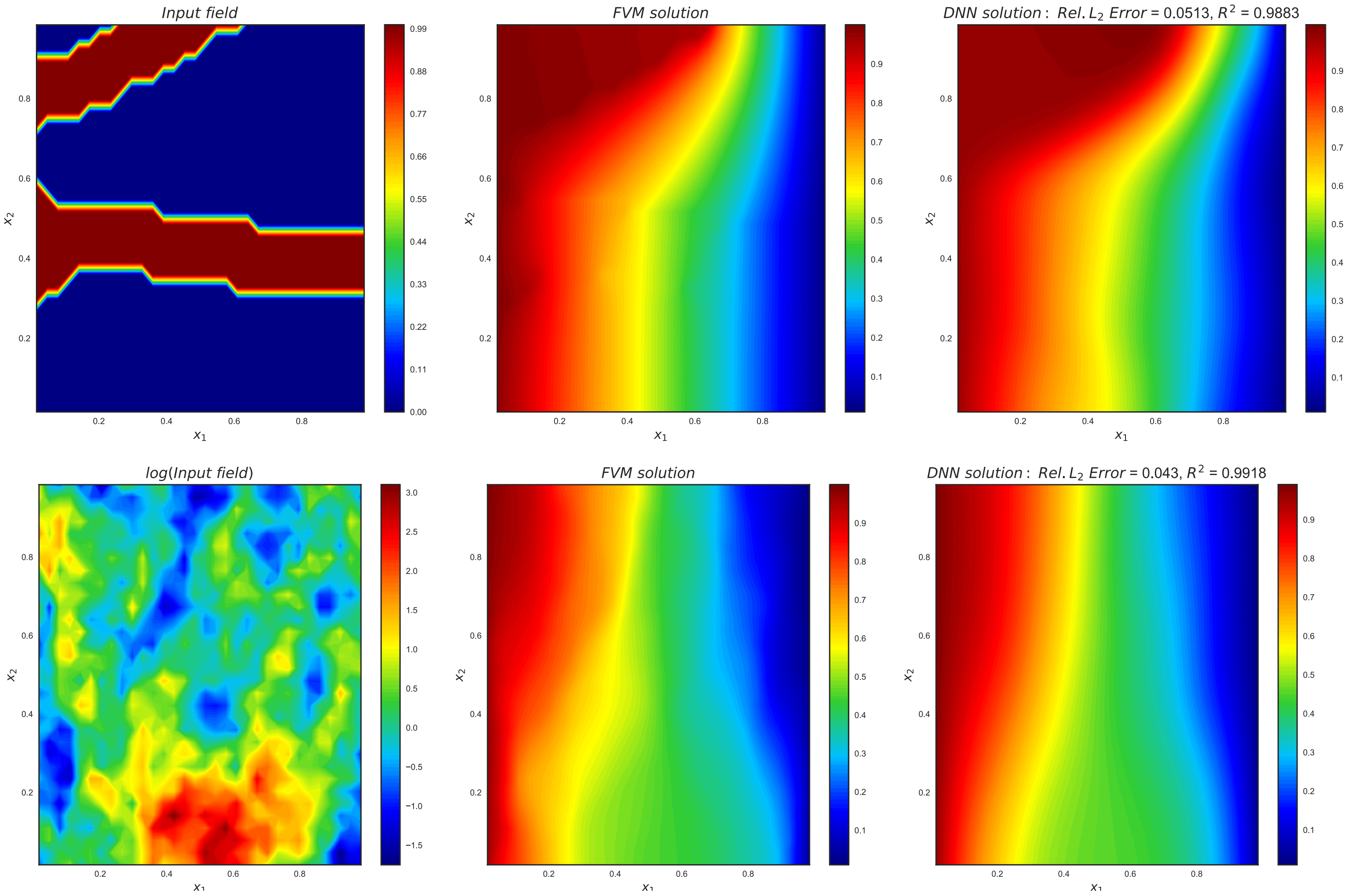
Numerical Examples: Point-wise Predictions



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Ending Remarks

- Lot's of nuances that did not talk about (see paper).
- Can we ditch traditional solvers completely?
- How to pose inverse problems?
- How to pose design problems?
- Best DNN structures?
- Best optimization algorithms?
- Bayesian formulation?

Thank you
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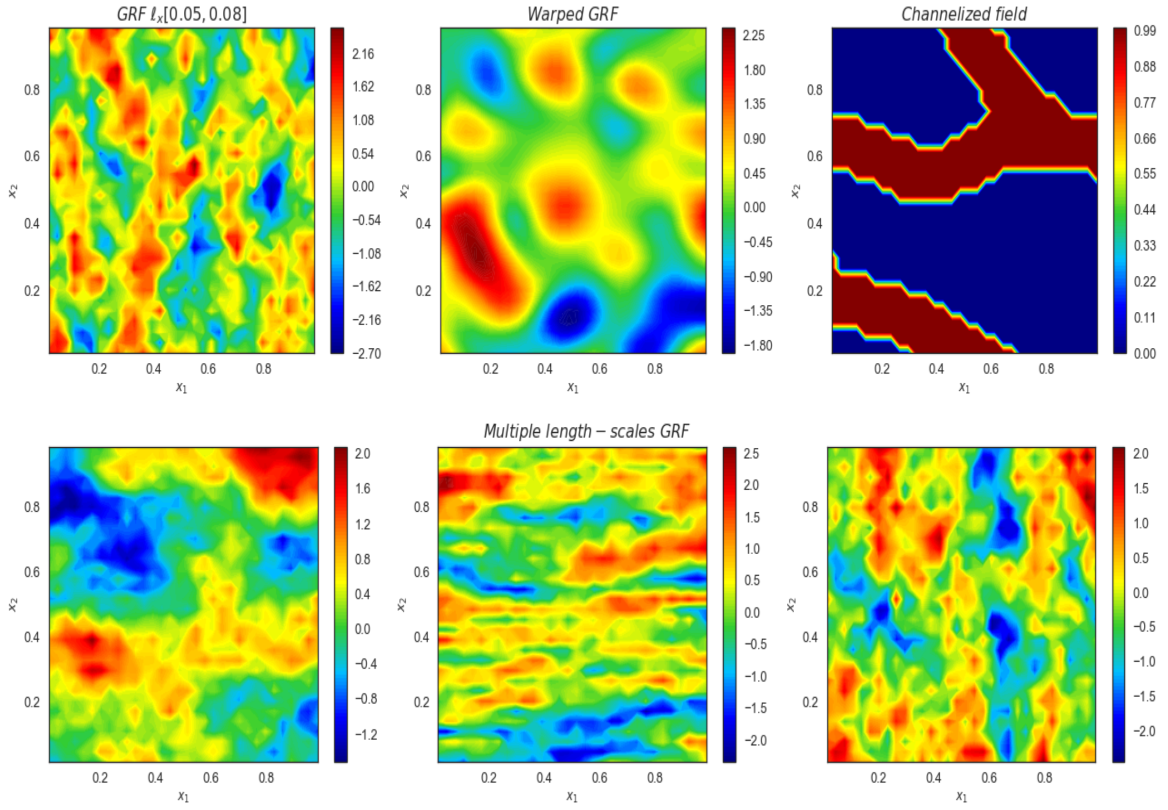
But how do I do the integrals?

- You don't have to do the integrals.
- All you need is the ability to sample:
  - uniformly in spatial domain
  - random parameters
- This is sufficient to construct stochastic algorithms that provably converge to a local minimum of the loss (Robbins-Monro, 1956).

Numerical Examples: Results Summary



Datasets	K	L	n	Number of test samples	$\mathcal{E}$	Number of trainable parameters θ
GRF ℓ_x $[0.05, 0.08]$	3	2	350	2,000	4.45%	1,096,901
Warped GRF	5	2	300	1,000	4.68%	1,211,401
Channelized field	3	2	300	512	5.30%	850,201
Multiple length-scales GRF	3	2	500	9,000	3.86%	2,017,001

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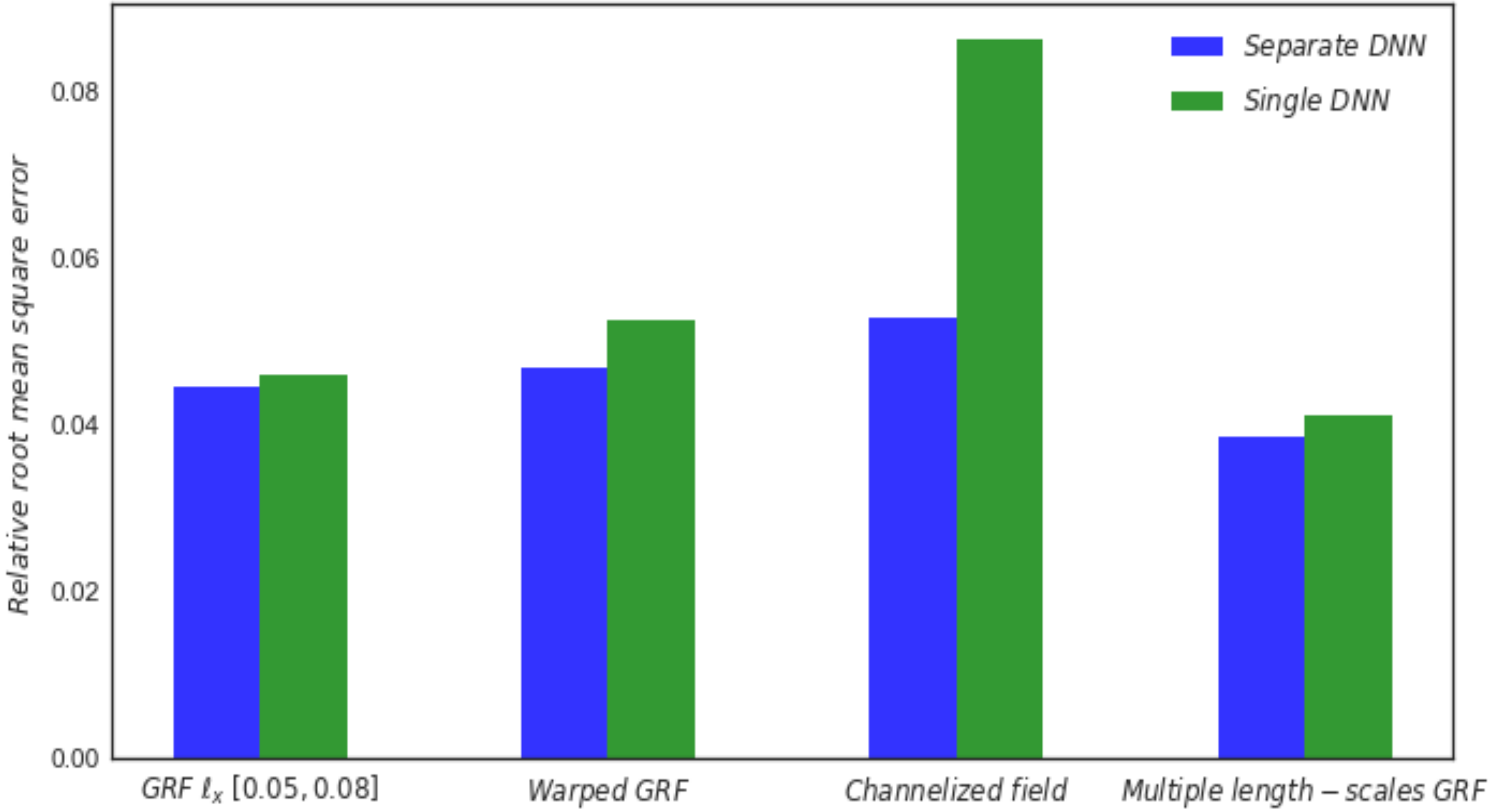
Numerical Examples: One DNN for all fields?



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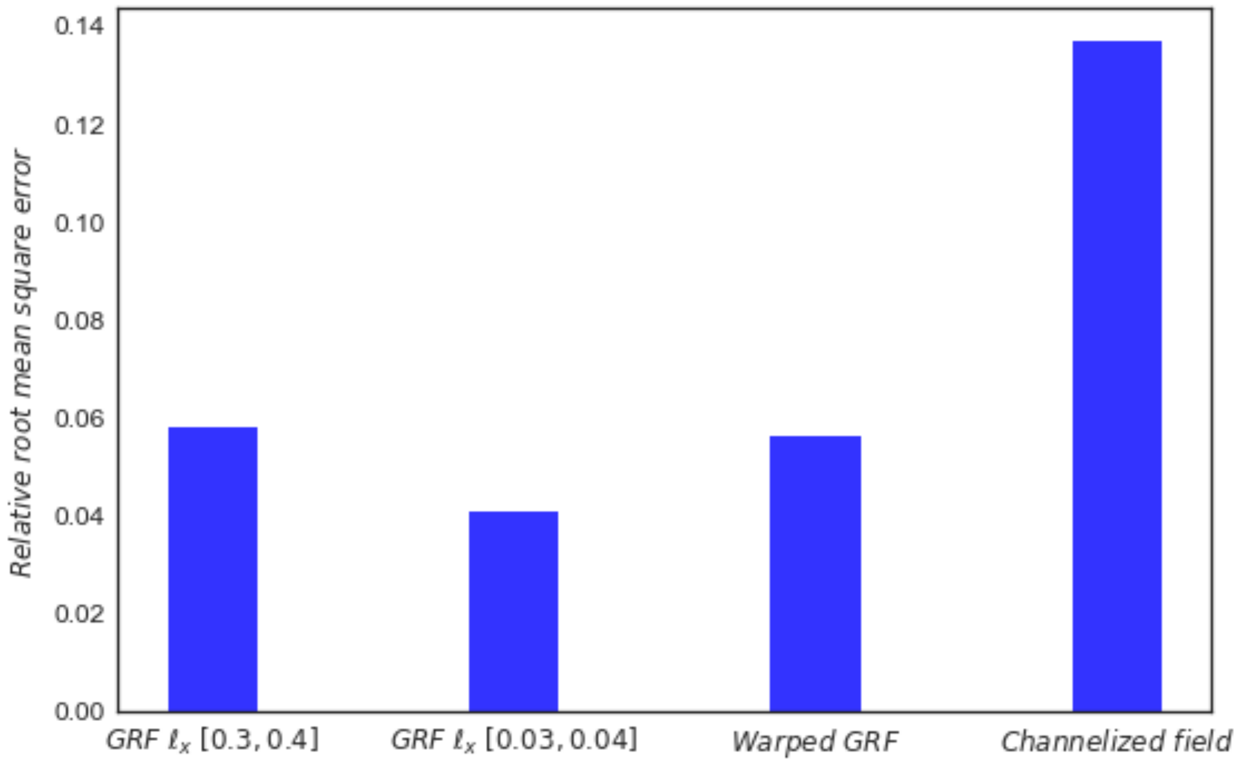
Numerical Results: Transfer Learning

- Trained on GRF with multiple length scales predicting on other:



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