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Nonlocal Operator Learning with Uncertainty Quantification

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Table of contents

Introduction

- Nonlocal models, acting at a lengthscale δ, are widely used in engineering and scientific application[1]. The use of integro-differential equations instead of PDE leads to greater flexibility[2].
  Nonlocal Poisson's equation:

$$2\int_{d} A(\mathsf{x},\mathsf{y})\gamma(\mathsf{x},\mathsf{y})(u(\mathsf{y})-u(\mathsf{x}))d\mathsf{y} = f(\mathsf{x}), \quad \mathsf{x},\mathsf{y}\in\mathcal{R}^d.$$

  Local Poisson's equation:

$$-\nabla\cdot(a(\mathsf{x})\nabla(u(\mathsf{x}))) = f(\mathsf{x})$$

Introduction

- The nonlocal kernel defining the nonlocal operator is usually unknown. We use a data-driven learning method as in [1], used to investigate wave propagation in structural materials, to learn the functional form of nonlocal kernel in disordered materials.
- In this project we treat the presence of disordered microstructure by introducing randomness in our model, so that the material properties are treated as random fields.

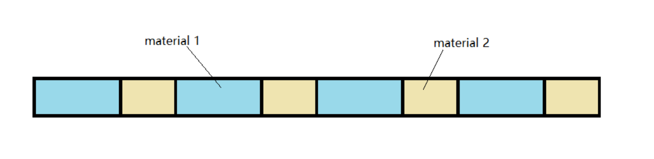


Figure 1: One-dimensional bar with periodic microstructure.

High-fidelity data

High-fidelity data

In the learning procedure, we generate the training data set by using Direct Numerical Simulations (DNS)[3] of wave propagation through a heterogeneous elastic bar.

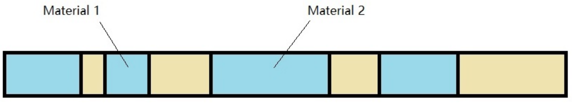


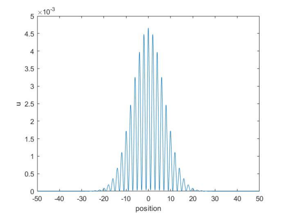
Figure 2: One-dimensional bar with disordered microstructure.

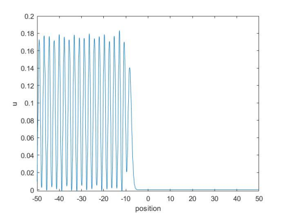
PRELIMINARY STUDY: solve the learning problem in a deterministic setting (absence of randomness).

In Figure 2, we report an example of the type of materials considered in this study. While one single microstructure is used for training, different microstructures will be considered for validation purposes.

Define a set of materials parameterized by the disorder parameter $\mathcal{D} \in [0,1]$ such that each layer in material 1 or 2 has size $w \sim \mathcal{U}((1-\mathcal{D})w_i, (1+\mathcal{D})w_i)$, where $i = 1, 2$ and $w_1 = (1-\phi)\lambda$, $w_2 = \phi\lambda$, where λ is the mean period of the microstructure. In our experiments we set $L{=}0.2$ (the bar length), $E_1{=}1$, $E_2{=}0.25$ (the Young's Modulus), $\rho{=}1$ (the density), and the symmetric domain $\Omega{=}(-b, b)$ (the spatial domain representing the bar). Two types of data are used for training:

- *1) Oscillating source.* We set $b = 50$, $v(x,0) = u(x,0) = 0$, $f(x,t) = e^{-\left(\frac{2x}{5kL}\right)^2} e^{-\left(\frac{t-t_0}{t_p}\right)^2} \cos^2\left(\frac{2\pi x}{kL}\right)$, $k = 1, 2, \ldots, 20$, $t_0 = t_p = 0.8$.
- *2) Plane wave.* For $b = 50$, $f(x,t) = 0$ and $u(x,0) = 0$, we prescribe $v(-b,t) = \sin(\omega t)$ for $\omega = 0.35, 0.7, \cdots, 3.85$.





Nonlocal Kernel Learning

- Assume that we have the following high-fidelity (HF) model which can represent the ground truth solution of the system:

$$\frac{\partial^2 u}{\partial t^2}(x,t) - \mathcal{L}_{\mathrm{HF}}[u](x,t) = f(x,t). \tag{1}$$

- We propose a nonlocal model to approximate the HF model:

$$\frac{\partial^2 u}{\partial t^2}(x,t) - \mathcal{L}_{K}[u](x,t) = f(x,t), \tag{2}$$

where

$$\mathcal{L}_K[u](x,t) = \int_{\Omega} K(|x-y|)\,(u(y,t) - u(x,t))\; dy. \tag{3}$$

Nonlocal Kernel Learning

- We represent K as a linear combination of Bernstein basis polynomials:

$$K(|x-y|) = \sum_{m=0}^{M} \frac{C_m}{\delta^{d+2}} B_{m,M}\left(\left|\frac{x-y}{\delta}\right|\right). \tag{4}$$

where the Bernstein basis functions are defined as

$$B_{m,M}(x) = \binom{M}{m} x^m (1-x)^{M-m}$$

for $0 \le x \le 1$ and where $C_m \in \mathbb{R}$.

- Learning procedure: seek for parameters C_m of the nonlocal operator whose nonlocal solution $\bar{u}$ is as close as possible to the HF data (DNS).

Numerical Result

Group Wave Velocity from Disordered DNS data

When learning material properties in the context of wave propagation, it is fundamental to recover the group wave velocity (GWV) accurately. The GWV for a disordered microsturcture will decrease to 0 rapidly when reaching a specific frequency, see Figure 3 where the GWV over 3 different samples are reported.

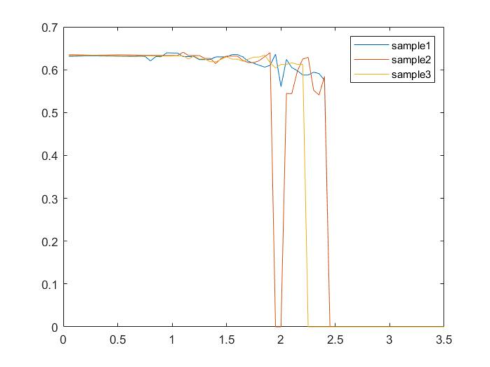


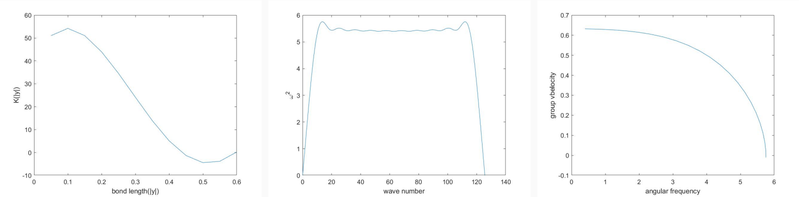
Figure 3: Group wave velocity for different samples.

Learning Results for one microstructure

Experiment settings:

- The microstructure is fixed. The random seed used to generate the microstructure is chosen to be the same as sample 1 in Figure 3.
- All the 20 samples of waves from *oscillating source* and 11 samples of waves from *plane wave* are used for training procedure.
- In the first test, we set δ=0.6 and regularization parameter ϵ=0.1. In the second one, we set δ=0.9 and regularization parameter ϵ=0.1.

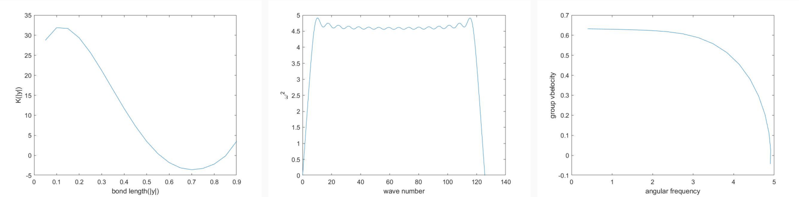
Learning Results for one microstructure



(a) Optimal kernel (b) Dispersion curve (c) Group velocity

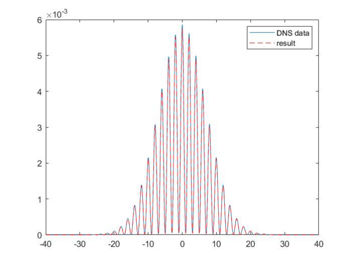
Figure 4: Disordered material, δ=0.6, ϵ=0.1

Learning Results for one microstructure

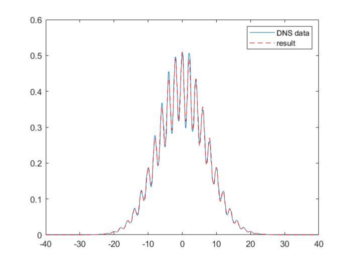


(a) Optimal kernel (b) Dispersion curve (c) Group velocity

Figure 5: Disordered material, δ=0.9, ϵ=0.1

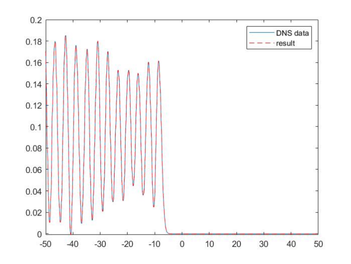


(a) t=0.2s

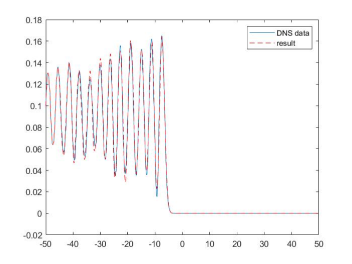


(b) t=2.0s

Figure 6: Case 10, *oscillating source* with $k = 10$.

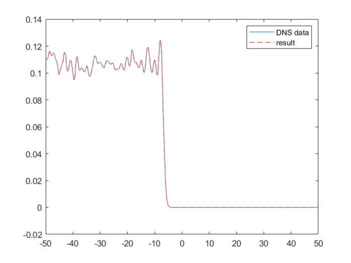


(a) t=0.2s

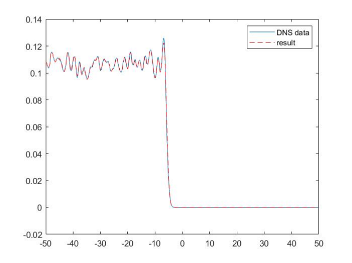


(b) t=2.0s

Figure 7: Case 23, *plane wave* with $\omega = 1.05$.



(a) t=0.2s



(b) t=2.0s

Figure 8: Case 31, *plane wave* with $\omega = 3.85$.

Conclusion

Conclusion

Process:

- We investigate the properties of wave propagation in different samples of disordered materials.
- The optimal kernel for a specific microstructure is derived, which could be used as a starting point for an uncertainty quantification algorithm (e.g. MCMC).

Future Work:

- We need to better understand the mechanism behind the mismatch of GWV, and the reason why we still do a good job even if the optimal kernel does not recover the correct GWV.
- After fully understanding the deterministic problem, we will apply an MCMC algorithm to the probability distribution of the nonlocal kernel.

[1] H. You, Y. Yu, S. Silling, and M. D'Elia, "Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws," *arXiv preprint arXiv:2012.04157*, 2020.

[2] Y. Fan, X. Tian, X. Yang, X. Li, C. Webster, and Y. Yu, "An asymptotically compatible probabilistic collocation method for randomly heterogeneous nonlocal problems," *arXiv preprint arXiv:2107.01386*, 2021.

[3] S. A. Silling, "Propagation of a stress pulse in a heterogeneous elastic bar," *Journal of Peridynamics and Nonlocal Modeling*, pp. 1–21, 2021.

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Thank you! Questions?