Course project: Reaction-diffusion system in porous media

Contributed by Dr. Xuhui Meng
Huazhong University of Science and Technology

Project statement

Here we consider a diffusion-reaction system in porous media, e.g., the transport of contaminant in soil, which can be expressed as follows [1]:

$$\begin{aligned}
\partial_t u &= D\partial_x^2 u - \lambda u^3 + f(x),\ x \in [-1, 1], \\
u(t, -1) = u(t, 1) &= 0.5,\ u(0, x) = 0.5\cos^2(\pi x), \\
\lambda(x) &= 0.2 + \exp(x)\cos^2(2x), \\
f(x) &= \exp\left(-\frac{(x - 0.25)^2}{2l^2}\right)\sin^2(3x),\ l = 0.4,
\end{aligned} \tag{1}$$

where t and x are the time and space coordinates, respectively, $u(t, x)$ represents the concentration, $\lambda(x)$ and $f(x)$ are the space-dependent reaction rate and source term, respectively, and $D = 0.01$ is the diffusion coefficient.

Generally, the reaction rate is determined by the pore structure, which is difficult to measure directly. We would like to infer the reaction rate based on partial measurements on u, f as well as λ. Specifically, all measurements are noisy, and we would like to quantify the uncertainties in predictions.

Dataset

- We employ the Matlab PDE Toolbox to solve Eqs. (1) and (2) to generate the training data.
- Details on the training data, e.g., the number of training data, locations of measurements, etc., can be found in Sec. 6.2 of [1].

Tasks

- Comparison between B-PINNs [2] and PINNs. Given noisy data, PINN is likely to give overfitting results.
- Study the effect of noise scale (e.g., 5%, 10%, 15%, etc.) on the predicted accuracy.
- A more complicated case: steep boundary layer. Specifically, we consider the following diffusion-reaction system:

$$\begin{aligned}
\partial_t u &= D\partial_x^2 u - \lambda u^3 + f(x),\ x \in [-1, 1], \\
u(t, -1) = u(t, 1) &= 1,\ u(0, x) = \cos^2(\pi x), \\
\lambda(x) &= 0.2 + \exp(x^2)\cos^2(3x),\ D = 0.01, \\
f(x) &= \exp\left(-\frac{(x - 0.25)^2}{2l^2}\right)\sin^2(3x),\ l = 0.4,
\end{aligned} \tag{2}$$

Programming Options

You may use TensorFlow, PyTorch, or DeepXDE for completing the tasks.

References

[1] A. F. Psaros, X. Meng, Z. Zou, L. Guo, and G. E. Karniadakis. Uncertainty quantification in scientific machine learning: Methods, Metrics, and Comparisons. *arXiv preprint arXiv:2201.07766*, 2022.

[2] L. Yang, X. Meng, and G. E. Karniadakis. B-PINNs: Bayesian physics-informed neural networks for forward and inverse PDE problems with noisy data. *Journal of Computational Physics*, 425:109913, 2021.