Physics Informed Neural Networks for Parameter and Model Estimation

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Uncertainty arises from incomplete knowledge

"*...there are known knowns; ... there are known unknowns; ...there are also unknown unknowns. ...it is the latter category that tends to be the difficult one.*"

D. Rumsfeld

Physics Informed Learning Machines (PhILMs) to "Learn" Known and Unknown Unknowns

- Challenges
  - Effective (macroscale) models have partially-known physics:
    - based on conservation laws,
    - rely on empirical constitutive relationships (Darcy Law, Fourier Law, Fick's Law, Newtonian Stress),
    - no universal models for turbulence, non-Newtonian fluids, etc.
  - Multiscale models are expensive.
  - ML methods are not accurate for extrapolation and under-sampled systems, and may lack reproducibility.

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“...flawed machine learning is producing a crisis in science.” G. Allen, Rice University

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- PhILMS:*
  - Use conservation laws in addition to data to train DNN.
  - Fill gaps in data.
  - Learn parameters and unknown physics.

* “Collaboratory on Mathematics and **Ph**ysics-**I**nformed **L**earning **M**achine**s** for Multiscale and Multiphysics Problems”, ASCR, the Applied Mathematics Program

Conservation Law PDE Models with Partially-Known Physics and Partial Measurements

- Conservation Law: $\partial u/\partial t = -\nabla \cdot \mathbf{J}$.
- $\mathbf{J}$ is an unknown flux of u.
- Dirichlet boundary condition: $u(x,t) = u_D(x,t)$.
- Neumann boundary conditions: $\mathbf{J}(x,t) \cdot \mathbf{n} = q(x,t)$.
- Initial condition: $u(x,t=0) = u_0(x)$.
- Partial measurements of u, u_D, q, u_0.
- No direct measurements of $\mathbf{J}$.

Feed Forward Neural Networks

$$f(x) \approx g^L(f^{L-1}(...(g^1(x))))$$

- L - number of layers
- $g^l(x) = g(W_l x + b_l)$
- $g(x)$ - known *activation* functions of x, W_l and b_l
- W_l and b_l unknown parameters

Physics Informed DNN for PDE Models with Partially Known Physics: $\partial u/\partial t = -\nabla \cdot \mathbf{J}$

DNNs for u and $\mathbf{J}$: $\hat{u}(x,t;\theta) = \mathcal{NN}_u(x,t;\theta)$ and $\hat{\mathbf{J}}(x,t,\hat{u};\theta,\gamma) = \mathcal{NN}_u(x,t;\theta,\gamma)$.
Auxiliary DNNs to enforce conservation laws and boundary conditions:
$g_1(x,t,\theta,\gamma) = \partial\hat{u}(x,t;\theta)/\partial t + \nabla \cdot \hat{\mathbf{J}}(x,t,\hat{u};\theta,\gamma)$ and
$g_2(x,t,\theta,\gamma) = \hat{\mathbf{J}}(x,t,\hat{u};\theta,\gamma) \cdot \mathbf{n}(x)$
Jointly train all NNs:

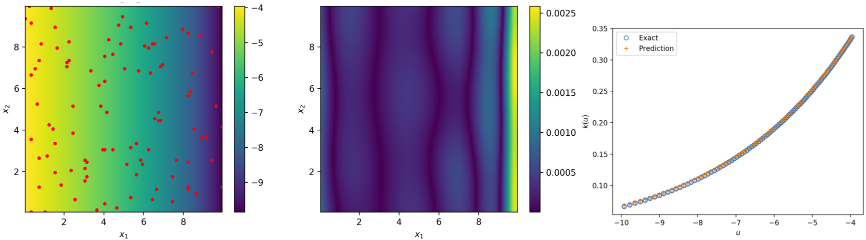
$$
\begin{aligned}
(\theta,\gamma) = \min_{\theta,\gamma} \quad [\quad & \frac{1}{N_c}\frac{1}{N_{tc}}\sum_{i=1}^{N_c}\sum_{j=1}^{N_{tc}} g_1(x_i,t_j,\theta,\gamma)^2 \\
+ \quad & \frac{1}{N_q}\frac{1}{N_{tq}}\sum_{i=1}^{N_q}\sum_{i=1}^{N_{tq}} (g_2(x_i,t_j;\theta,\gamma) - q^*(x_i,t_j))^2 \\
+ \quad & \frac{1}{N_u}\frac{1}{N_{tu}}\sum_{i=1}^{N_u}\sum_{i=1}^{N_{tu}} (\hat{u}(x_i,t_j;\theta) - u^*(x_i,t_j))^2]
\end{aligned}
$$

Tartakovsky et al, arXiv:1808.03398, 2018; *Rassi et al*, arXiv:1711.10566, 2017; arXiv:1711.10561, 2017.

Learning Relative Conductivity $k(u)$ in Unsaturated Flow Equations

$$\nabla \cdot [k(u)\nabla u(x)] = 0, \qquad \hat{u} = \mathcal{NN}_u(\mathbf{x};\theta) \text{ and } \hat{k} = \mathcal{NN}_K(\hat{u}(\mathbf{x};\theta);\gamma)$$

$$g_1(\mathbf{x};\theta,\gamma) = \nabla \cdot \left[\hat{k}\left(\hat{u}(\mathbf{x};\theta);\gamma\right)\nabla\hat{u}(\mathbf{x};\theta)\right] = \mathcal{NN}_{g_1}(\mathbf{x};\theta,\gamma)$$

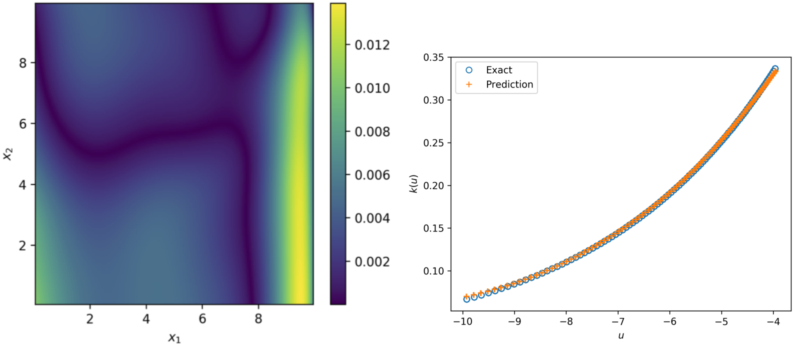


Left: Reference u field and measurements. Center: Error in the estimated u. Right: Estimated and reference $k(u)$.

Tartakovsky et al, arXiv:1808.03398, 2018

Effect of the measurement noise

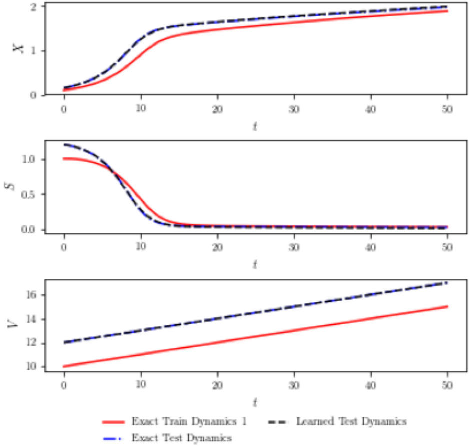
1% random noise

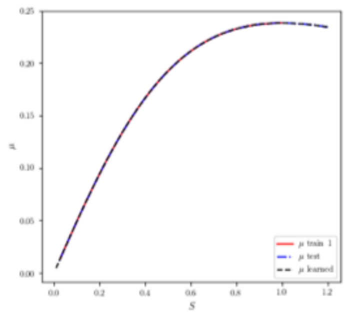


Left: Error in the estimated u. Right: Estimated and reference $k(u)$.

Bioreactor model with unknown reaction rate $\mu(S)$

$\frac{dX}{dt} = \mu(S)X(t) - \frac{F(t)X(t)}{V(t)}$, $\frac{dS}{dt} = -k\mu(S)X(t) - \frac{F(t)[S_{in} - S(t)]}{V(t)}$, $\frac{dV}{dt} = F(t)$. Only S, X and V measurements are available.

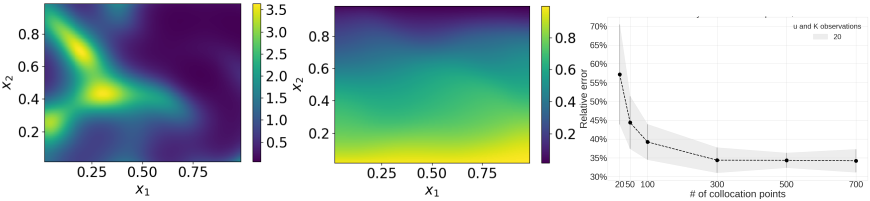




Parameter ($k(x)$) Estimation in Saturated Flow Equations

$$\nabla \cdot [k(x)\nabla u(x)] = 0, \qquad \hat{u} = \mathcal{NN}_u(\mathbf{x};\theta) \text{ and } \hat{k} = \mathcal{NN}_k(\mathbf{x};\gamma)$$

$$g_1(\mathbf{x};\theta,\gamma) = \nabla \cdot \left[\hat{k}\left(\mathbf{x};\gamma\right)\nabla\hat{u}(\mathbf{x};\theta)\right] = \mathcal{NN}_{g_1}(\mathbf{x};\theta,\gamma)$$

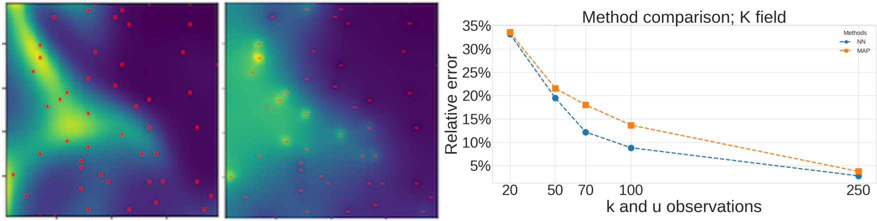


Left: Reference k field. Center: Reference u field. Right: Error in the estimated $k(u)$ versus number of collocation points.

Tartakovsky et al, arXiv:1808.03398, 2018

Comparison with the Maximum a Posteriori (MAP) Estimation Method

$$\nabla \cdot [k(x)\nabla u(x)] = 0$$



Left: PhI-DNN estimate. Center: MAP estimate. Right: MAP versus PhI-DNN.

Thank you