Adversarial Uncertainty Quantification in Physics-Informed Neural Networks

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The model: UQPINN

$$\text{UQPINN} = \text{GAN} + \text{PINN}$$

1. **UQPINN** : Uncertainty Quantification Physics-Informed Neural Network
2. **GAN** : Generative Adversarial Network
3. **PINN** : Physics-Informed Neural Network

Novalty

”we will develop a flexible variational inference framework that will allow us to train such models directly from noisy input/output data, and predict outcomes of non-linear dynamical systems that are partially observed with quantified uncertainty”

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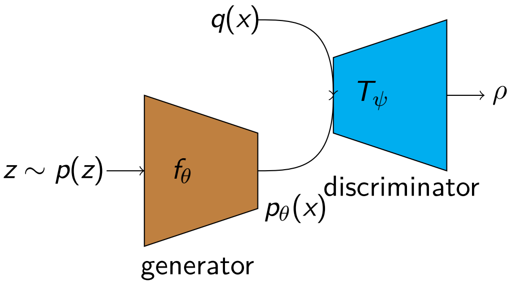
Using adversarial approach to handle randomness in observations.

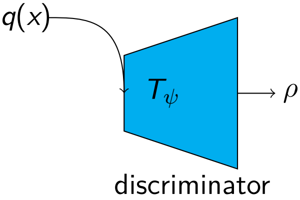
GAN



$$\max_{\psi} \mathcal{L}_{\mathcal{D}}(\psi)$$

$$\min_{\theta,\phi} \mathcal{L}_{\mathcal{G}}(\theta, \phi) + \beta\ \mathcal{L}_{PDE}(\theta)$$

GAN

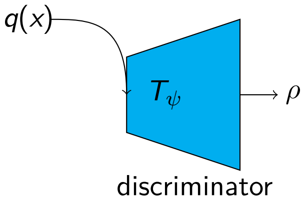


$$\underset{\psi}{argmin} \frac{\rho(y = +1|x, t, u)}{\rho(y = -1|x, t, u)}$$

$$p_\theta(x, t, u) = \rho(x, t, u|y = +1)$$

$$q(x, t, u) = \rho(x, t, u|y = -1)$$

GAN



$$\underset{\psi}{argmin} \frac{\rho(y=+1|x,t,u)}{\rho(y=-1|x,t,u)}$$

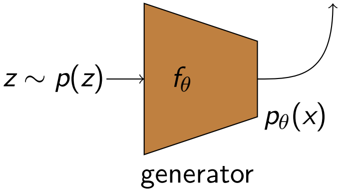
$$p_\theta(x,t,u) = \rho(x,t,u|y=+1)$$

$$q(x,t,u) = \rho(x,t,u|y=-1)$$

$$T_\psi \approx \rho(y=+1|x,t,u)$$

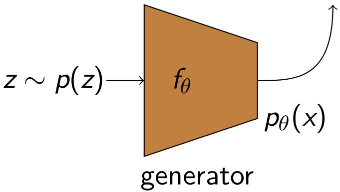
$$\mathcal{L}_D(\psi) = \mathbb{E}_{q(x,t)p(z)}[log\, \sigma(T_\psi(x,t,f_\theta))] + \mathbb{E}_{q(x,t,u)}[log(1-\sigma(T_\psi))]$$

GAN



$$\underset{\theta}{\mathrm{argmax}}\ \mathbb{KL}\left[p_\theta(x, t, u) \| q(x, t, u)\right]$$

GAN



$$\underset{\theta}{argmax}\ \mathbb{KL}\left[p_\theta(x, t, u) \| q(x, t, u)\right]$$

$$\begin{aligned}\mathcal{L}_G(\theta, \psi) = \mathbb{E}_{q(x,t)p(z)}[&T_\psi(x, t, f_\theta(x, t, z)) \\ &+ (1-\lambda) log(q_\phi(z|x, t, f_\theta(x, t, z)))]\end{aligned}$$

Experiment Setup

Author's Experiment Setup

GPU	NVIDIA Tesla P100(16GB)
DL framework	Tensorflow v1.10
Formula	1. pedagogical ODE 2. Burgers' equation 3. Darcy flow
Model	UQPINN

Experiment Setup

	Author's Experiment Setup	My Experiment Setup
GPU	NVIDIA Tesla P100(16GB)	MX450(2GB)
DL framework	Tensorflow v1.10	Pytorch v1.9.0
Formula	1. pedagogical ODE 2. Burgers' equation 3. Darcy flow	1. pedagogical ODE 2. Burgers' equation 3. Darcy flow
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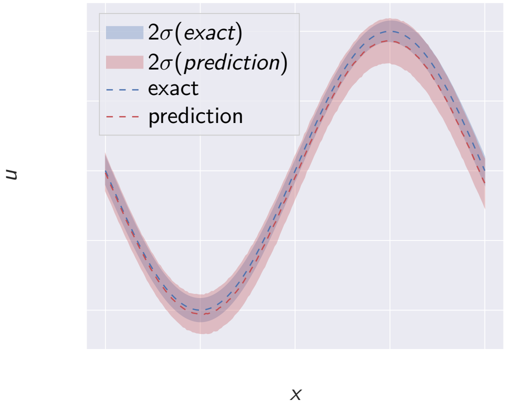
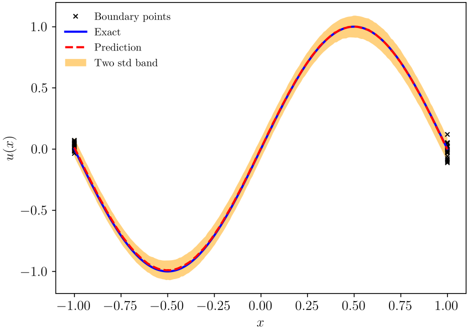
parameters are set to be the same as the author's

pedagogical ODE

$$
\begin{aligned}
&\frac{\partial^2 u}{\partial x^2} - u^2 \frac{\partial u}{\partial x} f(x) && x \in [-1, 1] \\
&f(x) = -\pi^2 sin(\pi x) - \pi cos(\pi x) sin(\pi x)^2 \\
&u(x) \sim \mathcal{N}(sin(\pi), noise) && x = \{-1, 1\}
\end{aligned}
$$



$2\sigma(exact)$
$2\sigma(prediction)$
exact
prediction
u
x



Boundary points
Exact
Prediction
Two std band
1.0
0.5
0.0
−0.5
−1.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
$u(x)$
x

Burgers Equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0 \qquad x \in [-1, 1], t \in [0, 1]$$

$$u(0, x) = -sin(\pi x)$$

$$u(t, x) = 0 \qquad x = \{-1, 1\}$$

$$\nu = \frac{0.01}{\pi}$$

Darcy

$$
\begin{aligned}
\nabla_{\vec{x}}(K(u)\nabla_{\vec{x}}u(\vec{x})) &= 0 & \vec{x} &\in [0, L_1] \times [0, L_2] \\
u(\vec{x}) &= 0 & x_1 &= L_1 \\
-K(u)\frac{\partial u(\vec{x})}{\partial x_1} &= q & x_1 &= 0 \\
K(u) &= K_s\sqrt{s(u)}\left(1 - (1 - s(u)^{\frac{1}{m}})^m\right)^2 & x_2 &= \{0, L_2\} \\
s(u) &= \left(1 + (\alpha(u_g - u))^{\frac{1}{1-m}}\right)^{-m}
\end{aligned}
$$