Generative Adversarial Nets and Application in Uncertainty Quantification

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Generative Adversarial Nets

GANs takes samples from a simple distribution $z \sim p(z)$, pass them through a Neural network $x = f_\theta(z)$ to approximate an unknown distribution $q(x)$ take their samples. The objective function is of the following form:

$$\mathbb{E}_{q(x)} \log(1 - \sigma(T_\psi(\mathbf{x}))) + \mathbb{E}_{p(z)} \log \sigma(T_\psi(G_\theta(\mathbf{z}))) \tag{1}$$

The results of the adversarial training are:

$$\begin{aligned} \hat{\psi} &= \arg\max_{\psi} \mathbb{E}_{q(x)} \log(1 - \sigma(T_\psi(\mathbf{x}))) + \mathbb{E}_{p(z)} \log \sigma(T_\psi(G_\theta(\mathbf{z}))) \\ \hat{\theta} &= \arg\min_{\theta} \mathbb{E}_{p(z)} T_\psi(G_\theta(\mathbf{z})) \end{aligned} \tag{2}$$

Here σ is the sigmoid function. ψ are the coefficients of the discriminator, θ are the coefficients for the generator.

Density ratio estimation by probabilistic classification

One may show that for fixed θ, the optimal solution for the discriminator is $T_\psi(x) = \log[\frac{p_\theta(x)}{q(x)}]$. In this case, the discriminator $T_\psi(x)$ is playing a role of estimating the log of density ratio $\frac{p_\theta(x)}{q(x)}$. Thus, the generator is playing the role that approximating of the KL divergence between $p_\theta(x)$ and $q(x)$:

$$\mathbb{KL}[p_\theta(x)||q(x)] = \mathbb{E}_{p(z)} T_\psi(G_\theta(\mathbf{z})) \tag{3}$$

$$\begin{aligned} \mathbb{KL}[p_\theta(x)||q(x)] &= \mathbb{E}_{p_\theta} \log[\frac{p_\theta(x)}{q(x)}] \\ &= -\mathbb{H}(p_\theta(x)) - \mathbb{E}_{p_\theta(x)} \log q(x) \end{aligned} \tag{4}$$

Distribution Matching and Mode Collapse in GANs

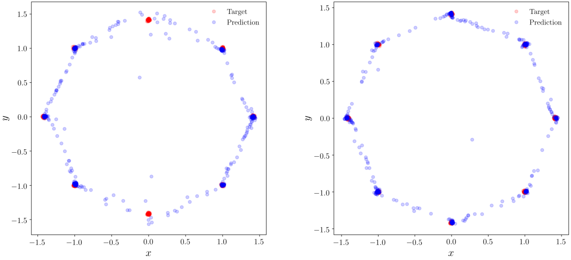


Figure: Left: Mode collapse. Right: No mode collapse.

$$
\begin{aligned}
\mathbb{KL}[p_\theta(x)||q(x)] &= \mathbb{E}_{p_\theta(x)} \log[\frac{p_\theta(x)}{q(x)}] \\
&= -\mathbb{H}(p_\theta(x)) - \mathbb{E}_{p_\theta(x)} \log q(x) \\
&= -\mathbb{H}(p_\theta(x)) - \int_{\mathcal{S}_{p_\theta} \cap \mathcal{S}_q^o} p_\theta(x) \log q(x) dx - \int_{\mathcal{S}_{p_\theta} \cap \mathcal{S}_q} p_\theta(x) \log q(x) dx
\end{aligned} \tag{5}
$$

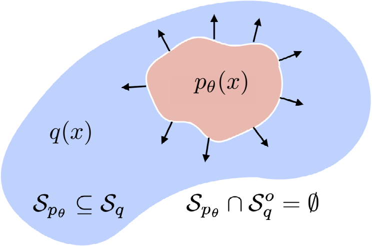
Li, C., Li, J., Wang, G., & Carin, L. (2018). Learning to Sample with Adversarially Learned Likelihood-Ratio.

Mode Collapse in GANs

Classical GANs would not suffer the risk to explore outside the support domain of the empirical distribution $q(x)$. This is so-called mode collapse issue.

Reverse KL:

$$\mathbb{KL}[p_\theta(x)||q(x)] = -\mathbb{H}[p_\theta(x)] - \mathbb{E}_{p_\theta(x)}[\log q(x)]$$
$$= -\mathbb{H}[p_\theta(x)] - \int_{\mathcal{S}_{p_\theta}\cap\mathcal{S}_q} \log q(x) p_\theta(x) dx - \int_{\mathcal{S}_{p_\theta}\cap\mathcal{S}_q^o} \log q(x) p_\theta(x) dx$$



$p_\theta(x)$: ***Generative model distribution*** $q(x)$: ***Empirical data distribution***

Use $-\lambda\mathbb{H}(p_\theta(x)) - \mathbb{E}_{p_\theta(x)} \log q(x)$ instead of $\mathbb{KL}[p_\theta(x)||q(x)]$ with $\lambda > 1$.

Mitigate Mode Collapse in GANs by Entropy Regularization

Construct a computable lower bound for the entropy $\mathbb{H}(p_\theta(\boldsymbol{x}))$.

$$\mathbb{I}(\boldsymbol{x};\boldsymbol{z}) = \mathbb{H}(\boldsymbol{x}) - \mathbb{H}(\boldsymbol{x}|\boldsymbol{z}) = \mathbb{H}(\boldsymbol{z}) - \mathbb{H}(\boldsymbol{z}|\boldsymbol{x}),$$

$$p_\theta(\boldsymbol{x},\boldsymbol{z}) = p_\theta(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z}),$$

Since in our setup, samples of $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ are generated by a deterministic function $f_\theta(\boldsymbol{z})$, it follows that $\mathbb{H}(\boldsymbol{x}|\boldsymbol{z}) = 0$. We therefore have

$$\mathbb{H}(\boldsymbol{x}) = \mathbb{H}(\boldsymbol{z}) - \mathbb{H}(\boldsymbol{z}|\boldsymbol{x}), \tag{6}$$

where $\mathbb{H}(\boldsymbol{z}) := -\int \log p(\boldsymbol{z})p(\boldsymbol{z})d\boldsymbol{z}$ does not depend on the generative model parameters θ. Now consider a general variational distribution $q_\phi(\boldsymbol{z}|\boldsymbol{x})$ parametrized by a set of parameters ϕ. Then,

$$\begin{aligned}\mathbb{H}(\boldsymbol{z}|\boldsymbol{x}) &= -\mathbb{E}_{p_\theta(\boldsymbol{x},\boldsymbol{z})}[\log(p_\theta(\boldsymbol{z}|\boldsymbol{x}))] \\ &= -\mathbb{E}_{p_\theta(\boldsymbol{x},\boldsymbol{z})}[\log(q_\phi(\boldsymbol{z}|\boldsymbol{x}))] \\ &\quad -\mathbb{E}_{p_\theta(\boldsymbol{x})}[\mathbb{KL}[p_\theta(\boldsymbol{z}|\boldsymbol{x})||q_\phi(\boldsymbol{z}|\boldsymbol{x})]] \\ &\leq -\mathbb{E}_{p_\theta(\boldsymbol{x},\boldsymbol{z})}[\log(q_\phi(\boldsymbol{z}|\boldsymbol{x}))]. \end{aligned} \tag{7}$$

Entropy Regularization

Construct a computable lower bound for the entropy $\mathbb{H}(p_\theta(\boldsymbol{x}, \boldsymbol{y}))$.

$$\mathbb{H}(p_\theta(\boldsymbol{x})) \geq \mathbb{H}(\boldsymbol{z}) + \mathbb{E}_{p_\theta(\boldsymbol{x},\boldsymbol{z})}[\log(q_\phi(\boldsymbol{z}|\boldsymbol{x}))]. \tag{8}$$

Then,

$$\begin{aligned}
& -\lambda\mathbb{H}(p_\theta(\boldsymbol{x})) - \mathbb{E}_{p_\theta(\boldsymbol{x})}\log q(\boldsymbol{x}) && (9)\\
& = -(\lambda - 1)\mathbb{H}(p_\theta(\boldsymbol{x})) - \mathbb{H}(p_\theta(\boldsymbol{x})) - \mathbb{E}_{p_\theta(\boldsymbol{x})}\log q(\boldsymbol{x}) && (10)\\
& = -(\lambda - 1)\mathbb{H}(p_\theta(\boldsymbol{x})) + \mathbb{KL}[p_\theta(\boldsymbol{x})||q(\boldsymbol{x})] && (11)\\
& \leq (1 - \lambda)\{\mathbb{H}(\boldsymbol{z}) + \mathbb{E}_{p_\theta(\boldsymbol{x},\boldsymbol{z})}[\log(q_\phi(\boldsymbol{z}|\boldsymbol{x}))]\} + \mathbb{KL}[p_\theta(\boldsymbol{x})||q(\boldsymbol{x})] && (12)
\end{aligned}$$

Matching Joint Distribution

$$\mathcal{L}_{\mathcal{D}}(\psi) = \mathbb{E}_{q(\boldsymbol{x})p(\boldsymbol{z})}[\log \sigma(T_\psi(f_\theta(\boldsymbol{z})))] + \mathbb{E}_{q(\boldsymbol{x})}[\log(1 - \sigma(T_\psi(\boldsymbol{x})))] \quad (13)$$

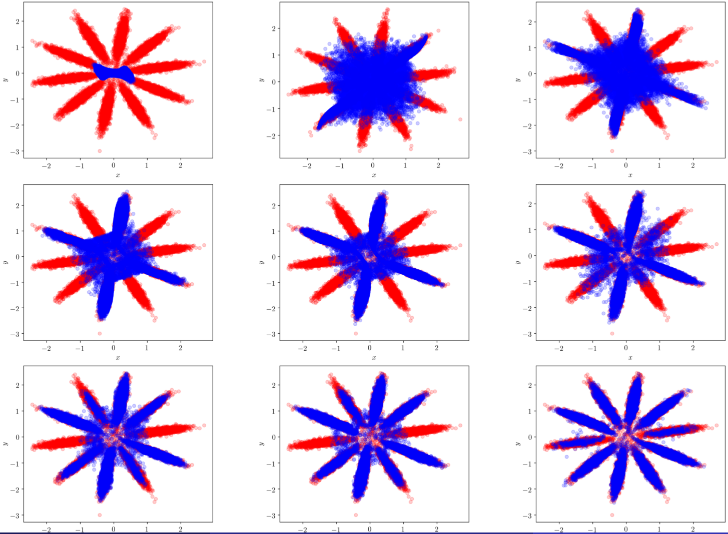
$$\mathcal{L}_{\mathcal{G}}(\theta, \phi) = \mathbb{E}_{q(\boldsymbol{x})p(\boldsymbol{z})}[T_\psi(f_\theta(\boldsymbol{z})) + (1 - \lambda)\log(q_\phi(\boldsymbol{z}|f_\theta(\boldsymbol{z})))], \quad (14)$$

the generative model can be trained by alternating between optimizing the two objectives in equations using stochastic gradient descent as

$$\max_{\psi} \ \mathcal{L}_{\mathcal{D}}(\psi) \quad (15)$$

$$\min_{\theta,\phi} \ \mathcal{L}_{\mathcal{G}}(\theta, \phi). \quad (16)$$

Distribution matching using GANs with entropy regularization



GANs for Uncertainty Quantification

We consider the uncertainty quantification for the regression task.

$$y = p_\theta(x, z), \qquad z \sim p(z) \tag{17}$$

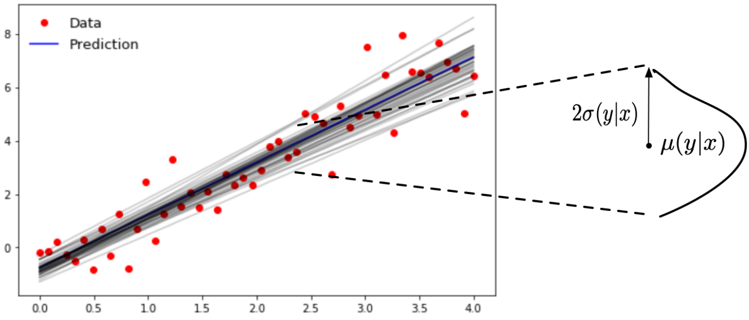


Figure: Linear Regression UQ.

Matching Joint Distribution Suffers Mode Collapse

Use simple GANs to do conditional generative model:

$$\mathcal{L}_{\mathcal{D}}(\psi) = \mathbb{E}_{q(\boldsymbol{x})p(\boldsymbol{z})}[\log \sigma(T_\psi(\boldsymbol{x}, f_\theta(\boldsymbol{x}, \boldsymbol{z})))] + \mathbb{E}_{q(\boldsymbol{x},\boldsymbol{y})}[\log(1 - \sigma(T_\psi(\boldsymbol{x}, \boldsymbol{y})))] \tag{18}$$

$$\mathcal{L}_{\mathcal{G}}(\theta, \phi) = \mathbb{E}_{q(\boldsymbol{x},\boldsymbol{y})p(\boldsymbol{z})}[T_\psi(\boldsymbol{x}, f_\theta(\boldsymbol{x}, \boldsymbol{z}))] \tag{19}$$

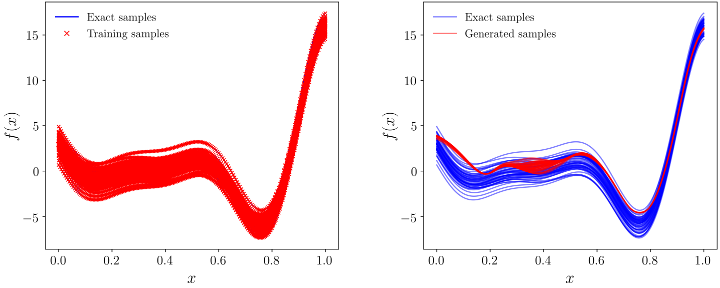
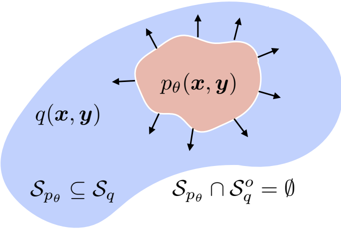


Figure: Linear Regression Mode Collapse.

Mode Collapse in GANs

Classical GANs would not suffer the risk to explore outside the support domain of the empirical distribution $q(x, y)$. This is so-called mode collapse issue.

Reverse KL: $$\begin{aligned}\mathbb{KL}\left[p_\theta(\boldsymbol{x},\boldsymbol{y})||q(\boldsymbol{x},\boldsymbol{y})\right] &= -\mathbb{H}\left[p_\theta(\boldsymbol{x},\boldsymbol{y})\right] - \mathbb{E}_{p_\theta(\boldsymbol{x},\boldsymbol{y})}\left[\log q(\boldsymbol{x},\boldsymbol{y})\right] \\ &= -\mathbb{H}\left[p_\theta(\boldsymbol{x},\boldsymbol{y})\right] \\ &\quad - \int_{\mathcal{S}_{p_\theta}\cap\mathcal{S}_q} \log q(\boldsymbol{x},\boldsymbol{y}) p_\theta(\boldsymbol{x},\boldsymbol{y}) d\boldsymbol{x}d\boldsymbol{y} \\ &\quad - \int_{\mathcal{S}_{p_\theta}\cap\mathcal{S}_q^o} \log q(\boldsymbol{x},\boldsymbol{y}) p_\theta(\boldsymbol{x},\boldsymbol{y}) d\boldsymbol{x}d\boldsymbol{y}\end{aligned}$$



$p_\theta(\boldsymbol{x},\boldsymbol{y})$: ***Generative model distribution*** $q(\boldsymbol{x},\boldsymbol{y})$: ***Empirical data distribution***

Try $-\lambda\mathbb{H}(p_\theta(x, y)) - \mathbb{E}_{p_\theta(x,y)} \log q(x, y)$ instead of $\mathbb{KL}[p_\theta(x, y)||q(x, y)]$ with $\lambda > 1$.

Matching Joint Distribution

$$\mathcal{L}_{\mathcal{D}}(\psi) = \mathbb{E}_{q(\boldsymbol{x})p(\boldsymbol{z})}[\log \sigma(T_{\psi}(\boldsymbol{x}, f_{\theta}(\boldsymbol{x}, \boldsymbol{z})))] + \mathbb{E}_{q(\boldsymbol{x},\boldsymbol{y})}[\log(1 - \sigma(T_{\psi}(\boldsymbol{x}, \boldsymbol{y})))] \tag{20}$$

$$\mathcal{L}_{\mathcal{G}}(\theta, \phi) = \mathbb{E}_{q(\boldsymbol{x},\boldsymbol{y})p(\boldsymbol{z})}[T_{\psi}(\boldsymbol{x}, f_{\theta}(\boldsymbol{x}, \boldsymbol{z})) + (1 - \lambda) \log(q_{\phi}(\boldsymbol{z}|\boldsymbol{x}, f_{\theta}(\boldsymbol{x}, \boldsymbol{z})))], \tag{21}$$

the generative model can be trained by alternating between optimizing the two objectives in equations using stochastic gradient descent as

$$\max_{\psi} \ \mathcal{L}_{\mathcal{D}}(\psi) \tag{22}$$

$$\min_{\theta,\phi} \ \mathcal{L}_{\mathcal{G}}(\theta, \phi). \tag{23}$$

Comparison with Gaussian Processes and Bayesian Neural Networks on Linear Regression

We consider 3 cases:

(i) *Gaussian homoscedastic noise:*

$$y = f(x) + \delta, \tag{24}$$

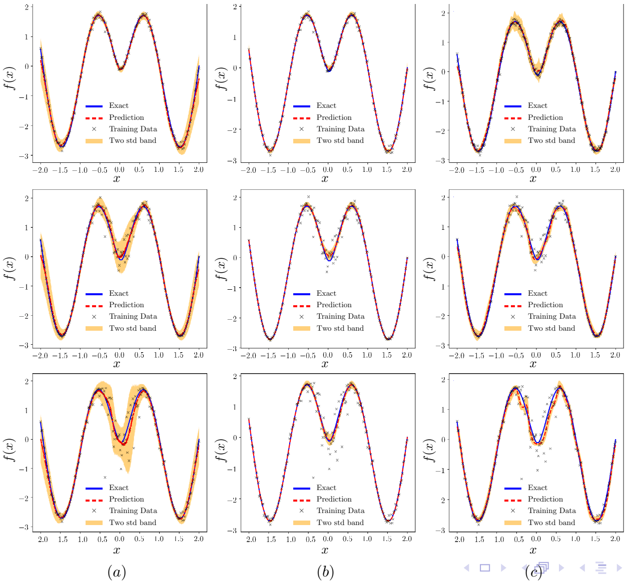
(ii) *Gaussian heteroscedastic noise:*

$$y = f(x) + \delta(x), \tag{25}$$

(iii) *Non-additive, non-Gaussian noise:*

$$y = f(x, \delta(x)) \tag{26}$$

Comparison with GP and BNN



Physics Informed Neural Networks

For a given differential equation: $u_t + \mathcal{N}[u] = 0$, one define the residual function:

$$r := u_t + \mathcal{N}[u] \tag{27}$$

The funciton used for training remains:

$$\mathrm{MSE} = \mathrm{MSE}_u + \mathrm{MSE}_r \tag{28}$$

where

$$\mathrm{MSE}_u = \frac{1}{N_u} \sum_{i=1}^{N_u} |u(t_u^i, x_u^i) - u^i|^2, \tag{29}$$

and

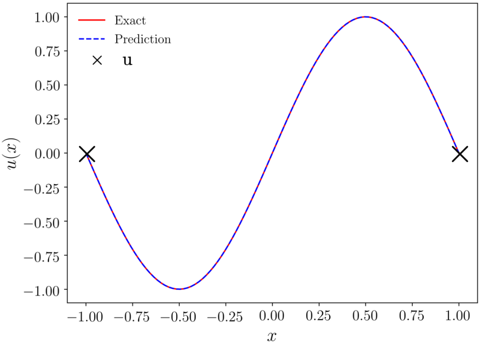
$$\mathrm{MSE}_r = \frac{1}{N_r} \sum_{i=1}^{N_r} |r(t_r^i, x_r^i)|^2, \tag{30}$$

Where, $\{t_u^i, \mathbf{x}_u^i, u^i\}_{i=1}^{N_u}$ are training data corresponding to the initial conditions and boundary conditions. $\{t_r^i, \mathbf{x}_r^i\}_{i=1}^{N_r}$ are the collocations points within the computational domain.

Physics Informed Neural Networks on Simple ODE

$$\frac{d^2u(x)}{dx^2} - u(x) = f(x), \quad x \in [-1, 1] \qquad (31)$$
$$u(-1) = 0, u(1) = 0$$

where $f(x) = -(\pi^2 + 1)\sin(\pi x)$. $N_u = 2$, $N_r = 100$.



Physics Informed Deep Generative Model

Satisfying the PDE constraint by simply minimizing the mean square loss on collocation points

$$\mathcal{L}_{PDE}(\theta) = \frac{1}{N_r}\sum_{i=1}^{N_r} \|r_\theta(\boldsymbol{x}_i, t_i)\|^2. \tag{32}$$

with

$$\begin{aligned}
\mathcal{L}_{\mathcal{D}}(\psi) = \ & \mathbb{E}_{q(\boldsymbol{x},t)p(\boldsymbol{z})}[\log \sigma(T_\psi(\boldsymbol{x}, t, f_\theta(\boldsymbol{x}, t, \boldsymbol{z})))] + \\
& \mathbb{E}_{q(\boldsymbol{x},t,\boldsymbol{u})}[\log(1 - \sigma(T_\psi(\boldsymbol{x}, t, \boldsymbol{u})))] && (33) \\
\mathcal{L}_{\mathcal{G}}(\theta, \phi) = \ & \mathbb{E}_{q(\boldsymbol{x},t)p(\boldsymbol{z})}[T_\psi(\boldsymbol{x}, t, f_\theta(\boldsymbol{x}, t, \boldsymbol{z})) && (34) \\
& + (1-\lambda)\log(q_\phi(\boldsymbol{z}|\boldsymbol{x}, t, f_\theta(\boldsymbol{x}, t, \boldsymbol{z})))], && (35)
\end{aligned}$$

Then, the resulting adversarial game for training the physics-informed model:

$$\begin{aligned}
& \max_{\psi} \ \mathcal{L}_{\mathcal{D}}(\psi) \\
& \min_{\theta,\phi} \ \mathcal{L}_{\mathcal{G}}(\theta, \phi) + \beta \mathcal{L}_{PDE}(\theta),
\end{aligned} \tag{36}$$

Physics Informed GANs on Simple ODE

Let us illustrate the basic capabilities of the proposed methods through a simple example corresponding to the following nonlinear second-order ordinary differential equation

$$
\begin{aligned}
&u_{xx} - u^2 u_x = f(x), \qquad x \in [-1, 1], \\
&f(x) = -\pi^2 \sin(\pi x) - \pi \cos(\pi x) \sin^2(\pi x),
\end{aligned}
\tag{37}
$$

subject to random boundary conditions $u(-1), u(1) \sim \mathcal{N}(\mathbf{0}, \sigma_n^2 \boldsymbol{I})$. For this simple example, the deterministic solution corresponding to $\sigma_n^2 = 0$ can be readily obtained as $u(x) = \sin(\pi x)$. Given N_u observations of $u(x)$ corresponding to different realizations of the random boundary conditions our goal is to obtain a probabilistic representation of the solution $p_\theta(u|x, \boldsymbol{z})$ by training a physics-informed generative model of the form $u = f_\theta(x, \boldsymbol{z})$, $\boldsymbol{z} \sim p(\boldsymbol{z})$ that satisfies the physics constrained.

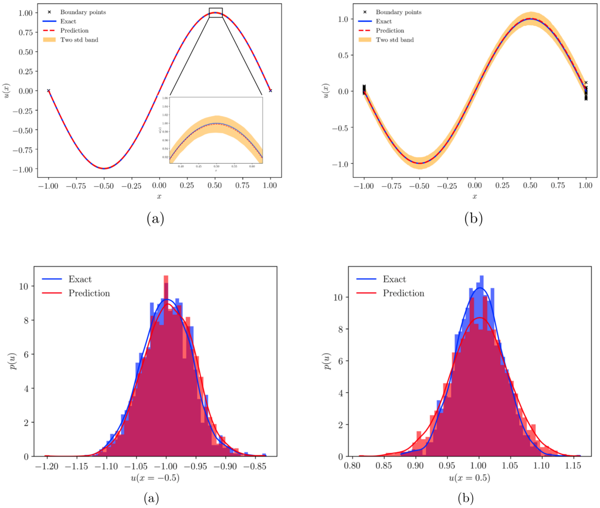


Figure: Predicted marginal densities against the reference Monte Carlo solution. (a) $p_\theta(u|x=-0.5,z)$. (b) $p_\theta(u|x=+0.5,z)$.

Shock Capturing in PDEs

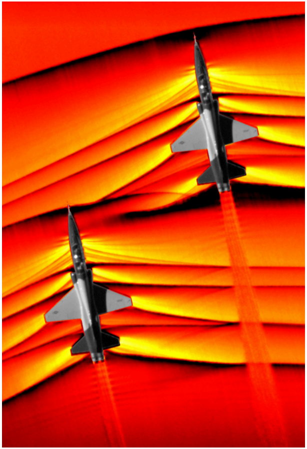


Figure: Shock wave in aerospace dynamics.

In the classical numerical methods of partial differential equations, it is hard to predict or capture the shock wave due to the nature of discretization.

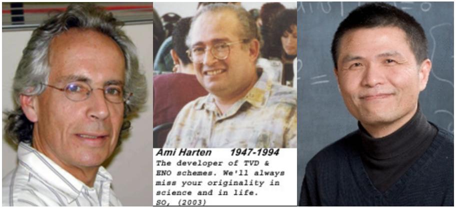


Figure: Left: Stanley Osher. Middle: Ami Harten. Right: Chi-Wang Shu.

We test a more challenging canonical problem involving the non-linear time-dependent Burgers equation in one spatial dimension:

$$\begin{aligned} &u_t + uu_x - \nu u_{xx} = 0, \qquad x \in [-1, 1], t \in [0, 1], \\ &u(0, x) = -\sin(\pi x), \\ &u(t, -1) = u(t, 1) = 0, \end{aligned} \tag{38}$$

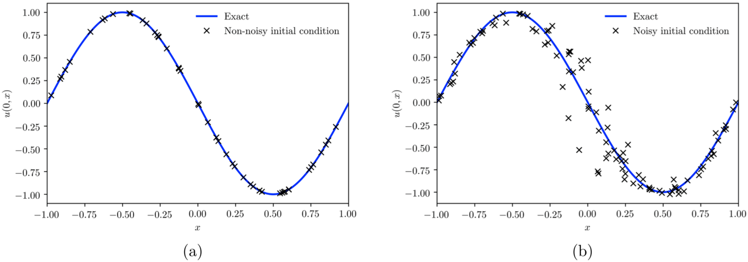


Figure: *Burgers equation:* (a) Exact initial condition and noise-free training data. (b) Training data corresponding to a single realization of the non-additive noise corruption process.

Physics Informed GANs on Burgers Equation

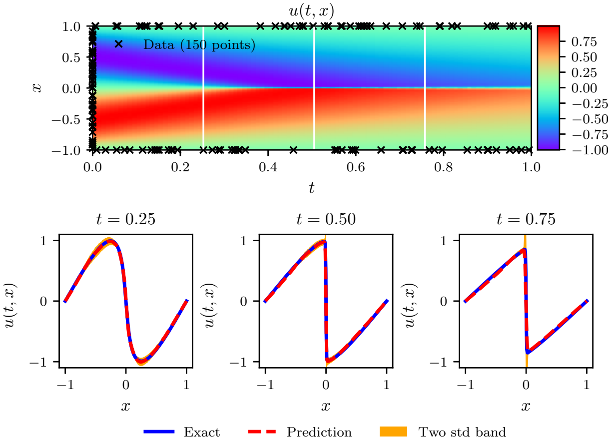


Figure: *Burgers equation with noise-free data: Top:* Mean of $p_\theta(u|x, t, z)$, along with the location of the noisy training data $\{(x_i, t_i), u_i\}$, $i = 1, \ldots, N_u$. *Middle:* Prediction and predictive uncertainty at $t = 0.25$, $t = 0.5$ and $t = 0.75$. *Bottom:* Variance of $p_\theta(u|x, t, z)$.

Physics Informed GANs on Burgers Equation

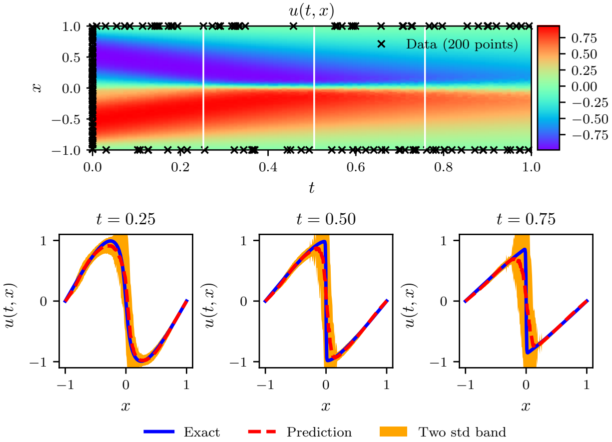


Figure: *Burgers equation with noisy data: Top:* Mean of $p_\theta(u|x,t,z)$, along with the location of the training data $\{(x_i,t_i),u_i\}$, $i = 1,\ldots,N_u$. *Middle:* Prediction and predictive uncertainty at $t = 0.25$, $t = 0.5$ and $t = 0.75$. *Bottom:* Variance of $p_\theta(u|x,t,z)$.

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