

A simple ODE case

A 1D dynamic system is described by

$$\frac{ds(x)}{dx} = g(s(x), u(x), x), \quad x \in [0, 1],$$

with an initial condition $s(0) = 0$. Our goal is to predict s over the whole domain $[0, 1]$ for any $u(x)$.

Linear case: $g(s(x), u(x), x) = u(x)$

Then, the operator G would be: $G : u(x) \mapsto s(x) = \int_0^x u(\tau) d\tau.$

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Learn the solution operators of parametric PDEs → We will try to approximate G (the solution of our PDE operator) by two neural networks:

$$G_{\theta}(u)(y) = \sum_{k=1}^q \underbrace{b_k(u(x_1), u(x_2), \dots, u(x_m))}_{\text{Branch}} \cdot \underbrace{t_k(y)}_{\text{Trunk}}$$

We want to obtain G , so our goal would be:

$$G_{\theta}(u)(y) \approx G(u)(y)$$

So we will enforce that condition into a loss function:

$$\mathcal{L}_{Operator}(\theta) = \frac{1}{NP} \sum_{i=1}^N \sum_{j=1}^P \left| G_{\theta}(u^{(i)})y_j^{(i)} - G(u^{(i)})y_j^{(i)} \right|^2$$
$$\mathcal{L}_{Operator}(\theta) = \frac{1}{NP} \sum_{i=1}^N \sum_{j=1}^P \left| \sum_{k=1}^q b_k(u(x_1), u(x_2), \dots, u(x_m)) \cdot t_k(y_j^{(i)}) - G(u^{(i)})y_j^{(i)} \right|^2$$

where N is the number of functions $u(x)$ in our training dataset, P is the number of points inside the domain at which we will evaluate $G(u)$.

m : Number of points at which we evaluated our input functions.

N : Number of input functions.

P : Number of points at which we evaluate the output function → output sensors.

How to generate data?

We can choose uniformly $m + 1$ points $x_j = a + j(b - a)/m$, $j = 0, 1, \dots, m$ from $[a, b]$, and define the function $u_m(x)$ as follows:

$$u_m(x) = u(x_j) + \frac{u(x_{j+1}) - u(x_j)}{x_{j+1} - x_j}(x - x_j), \quad x_j \leq x \leq x_{j+1}, \quad j = 0, 1, \dots, m - 1.$$

Regression using Gaussian:

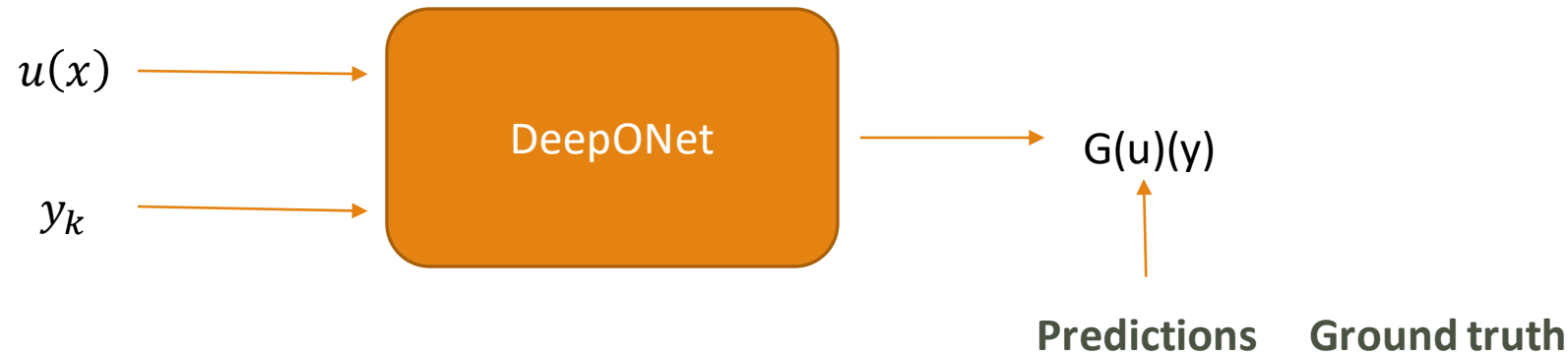
$$u \sim \mathcal{G}(0, k_l(x_1, x_2)),$$

$$\sum (x_1, x_2) = k(x_1, x_2) + I\sigma_y^2$$

$$k(x_1, x_2) = \sigma^2 e^{\frac{1}{2l^2}(x_1 - x_2)}$$

$$G : u(x) \mapsto s(x) = \int_0^x u(\tau) d\tau.$$

- We generate discrete $u_m(x)$ with discrete x values and different set of output locations $y_j, j = 1, 2, \dots, P$.
- For these output locations, we generate discrete ground truth values $\cos(y_j)$ to train our model.



Then we can define the loss function as follows:

$$L(\theta) = \frac{1}{NP} \sum_{i=1}^N \sum_{j=1}^P \left| \sum_{k=1}^q b_k(\mathbf{u}^{(i)}(\mathbf{x}_1), \dots, \mathbf{u}^{(i)}(\mathbf{x}_m)) t_k(\mathbf{y}_j^{(i)}) - s(\mathbf{y}_j^{(i)}) \right|^2,$$

- P : Total no. of output locations
- q : no. of branch nets or no. of neurons in output layer of trunk net