Two Approaches using Deep Learning to solve Partial Differential Equation

PDE solver and operator learning

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  - Physics Informed Neural Network (PINN)
  - My interests on PDE solver

- **Operator learning**
  - CNN encoder-decoder
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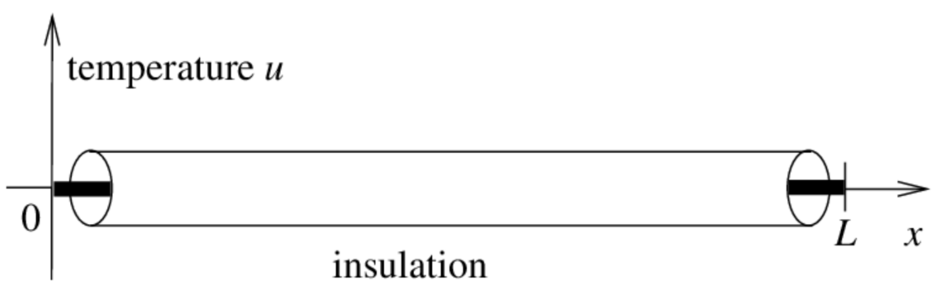
Partial differential equation (PDE)

- **In mathematics, a differential equation is an equation that relates one or more functions and their derivatives.**
  - The functions generally represent **physical quantities.**
  - The derivatives represent **their rates of change.**
  - The differential equation defines a **relationship between the above two**.

(e.g.)

Let $u(t,x)$ denote the temperature at point x at time t.



Governing equation (heat equation) :

$$\frac{\partial u(t,x)}{\partial t} = k\frac{\partial^2 u(t,x)}{\partial x^2}.$$

Initial condition (IC) :

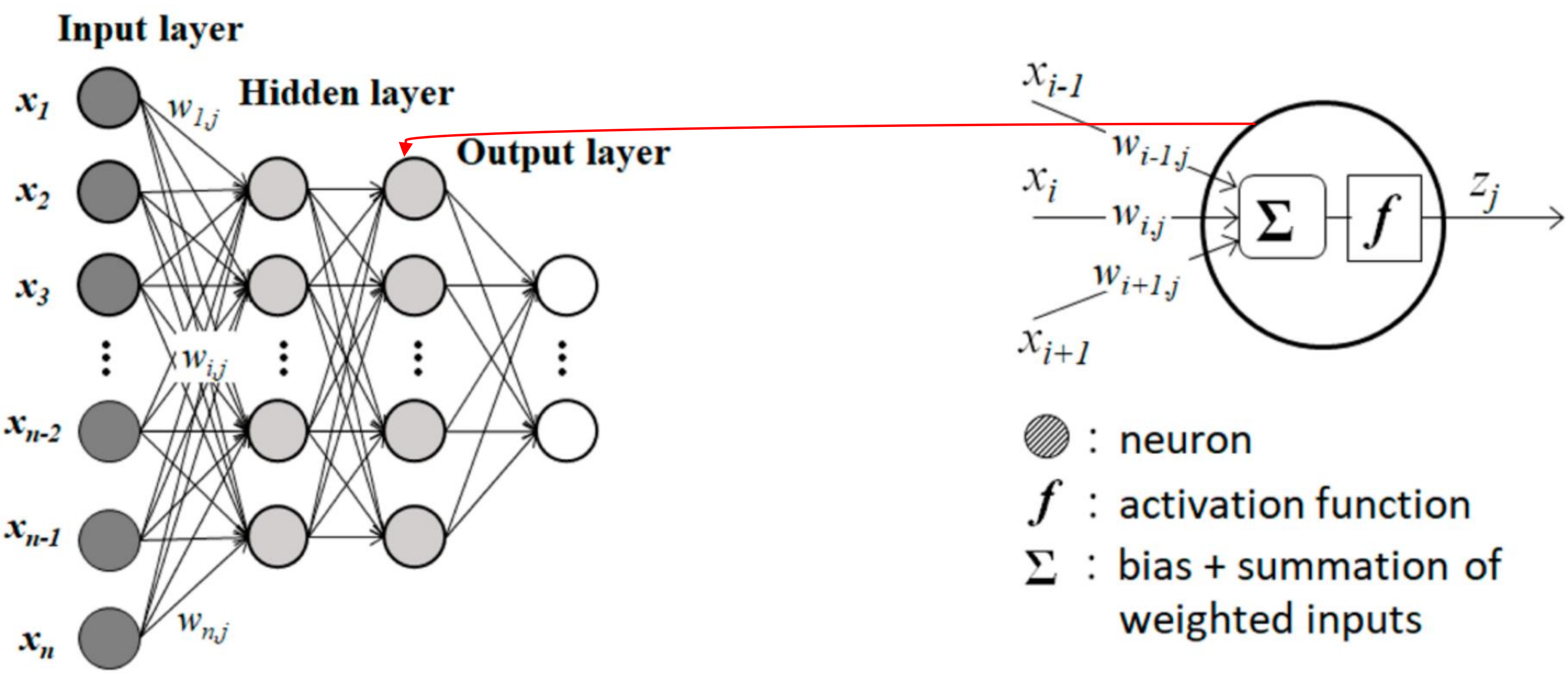
$$u(t=0,x) = f(x).$$

Boundary condition (BC) :

$$u(t,x=0) = h(x), \qquad u(t,x=L) = g(x).$$

https://math.libretexts.org/Bookshelves/Differential_Equations/Book%3A_Differential_Equations_for_Engineers_(Lebl)/4%3A_Fourier_series_and_PDEs/4.06%3A_PDEs_separation_of_variables_and_the_heat_equation

Deep Neural Network and Deep Learning



(**a**) Deep neural network (**b**) Inner structure of the neuron

https://www.researchgate.net/publication/338190342_Convolutional_Neural_Network_Coupled_with_a_Transfer-Learning_Approach_for_Time-Series_Flood_Predictions/figures?lo=1

Two mainstream on deep learning approach to PDEs

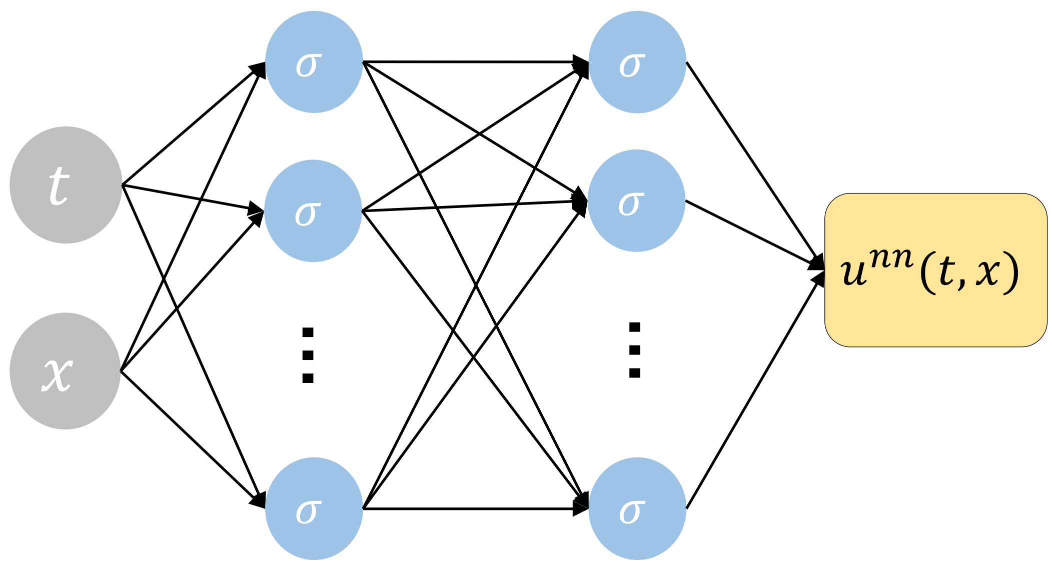
- **PDE solver**
  - Using neural networks directly to parametrize the solution to PDEs.
  - Solve one instance of PDE at a time.
  - Models
    - Deep Ritz Method (DRM)
    - Physics Informed Neural Network (PINN)

Find $\boldsymbol{u(t,x)}$ satisfying

$$\mathcal{L}_{PDE} = f(u, u_t, u_x, u_{xx}, \ldots) = 0$$

$$\mathcal{L}_{IC} = u(0,x) - g(x) = 0$$

$$\mathcal{L}_{BC} = u|_{\partial\Omega} - h(t,x)|_{\partial\Omega} = 0$$



Two mainstream on deep learning approach to PDEs

- **Operator learning**
  - Learning a mapping from the parameters (e.g. external force, initial, and boundary conditions) of the PDEs to the corresponding solution.
  - Learning a family of PDEs from data.
  - Models
    - Deep Operator Network (DeepONet)
    - Fourier Neural Operator (FNO)

Find a map $\boldsymbol{\mathcal{G}}: \boldsymbol{g(x)} \mapsto \boldsymbol{u(t,x)}$ satisfying

$$\mathcal{L}_{PDE} = f(u, u_t, u_x, u_{xx}, \dots) = 0$$

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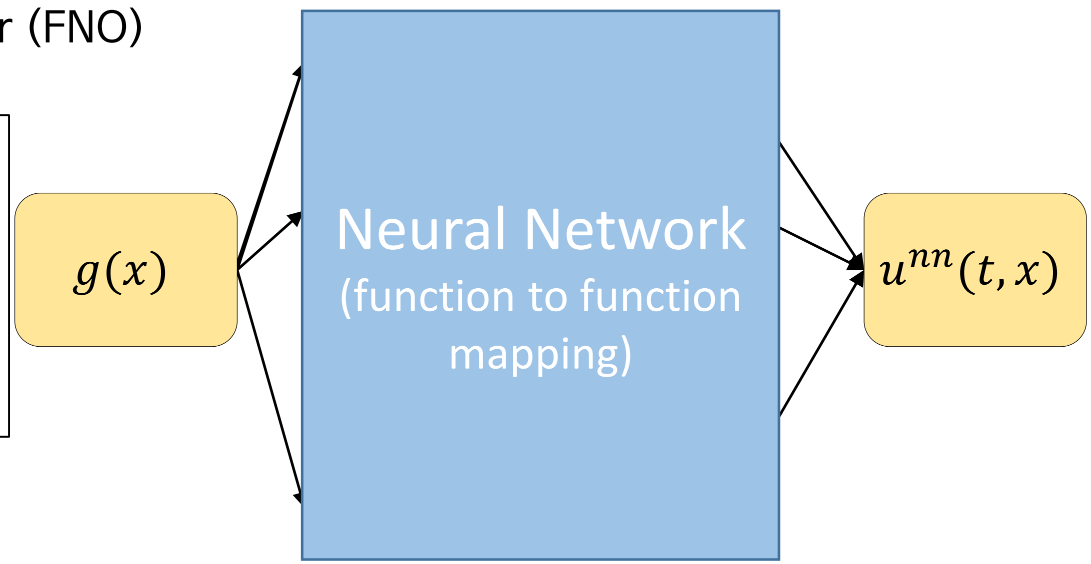


Part 1. PDE solver

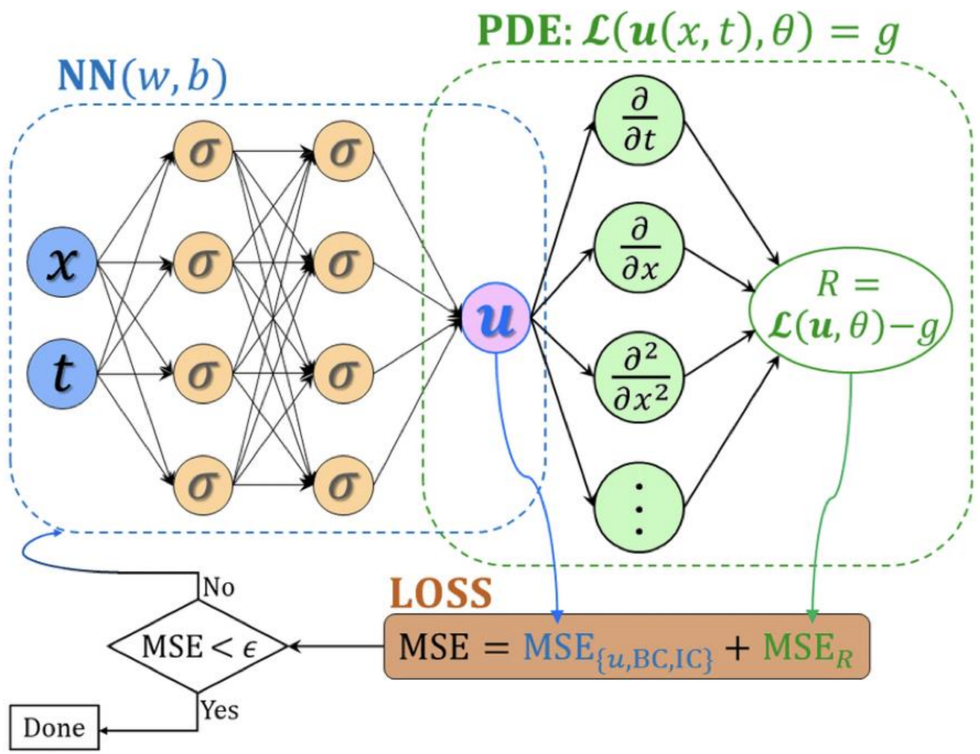
Physics-informed neural network (PINN)

Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computation al physics*, *378*, 686-707.

Automatic differentiation and the back-propagation algorithm

“Here we revisit them using modern computational tools, and apply them to more challenging dynamic problems described by time-dependent nonlinear partial differential equations.”

[Schematic of a PINN]



Lu, L., Meng, X., Mao, Z., & Karniadakis, G. E. (2021). DeepXDE: A deep learning library for solving differential equations. *SIAM Review*, *63*(1), 208-228

Physics-informed neural network (PINN) - Forward problem

(e.g.) Burgers' equation

Eq : $u_t + uu_x - (0.01/\pi)u_{xx} = 0$

IC : $u(0, x) = -\sin(\pi x)$ $\qquad x \in [-1,1], t \in [0,1]$

BC : $u(t, -1) = u(t, 1) = 0$

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Loss function

$$\boldsymbol{L}(\boldsymbol{\theta}) = \frac{1}{N_{Eq}} \sum_{i=1}^{N_{Eq}} \left| u_t(t^i, x^i) + u(t^i, x^i) u_x(t^i, x^i) - (0.01/\pi) u_{xx}(t^i, x^i) \right|^2 + \frac{1}{N_{IC}} \sum_{j=1}^{N_{IC}} \left| u(t^j, x^j) + \sin(\pi x^j) \right|^2 + \frac{1}{N_{BC}} \sum_{k=1}^{N_{BC}} \left| u(t^k, x^k) \right|^2$$

Data:

$(t_i, x_i) \in [0,1] \times [-1,1]$

$(t_j, x_j) \in \{0\} \times [-1,1]$

$(t_k, x_k) \in [0,1] \times \{-1,1\}$

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Physics-informed neural network (PINN) - Forward problem

(e.g.) Burgers' equation

$$\text{Eq}: u_t + uu_x - (0.01/\pi)u_{xx} = 0$$
$$\text{IC}: u(0,x) = -\sin(\pi x) \qquad x \in [-1,1], t \in [0,1]$$
$$\text{BC}: u(t,-1) = u(t,1) = 0$$

Loss function

$$\boldsymbol{L(\theta)} = \frac{1}{N_{Eq}} \sum_{i=1}^{N_{Eq}} \left| u_t(t^i,x^i) + u(t^i,x^i)u_x(t^i,x^i) - (0.01/\pi)u_{xx}(t^i,x^i) \right|^2 + \frac{1}{N_{IC}} \sum_{j=1}^{N_{IC}} \left| u(t^j,x^j) + \sin(\pi x^j) \right|^2 + \frac{1}{N_{BC}} \sum_{k=1}^{N_{BC}} \left| u(t^k,x^k) \right|^2$$

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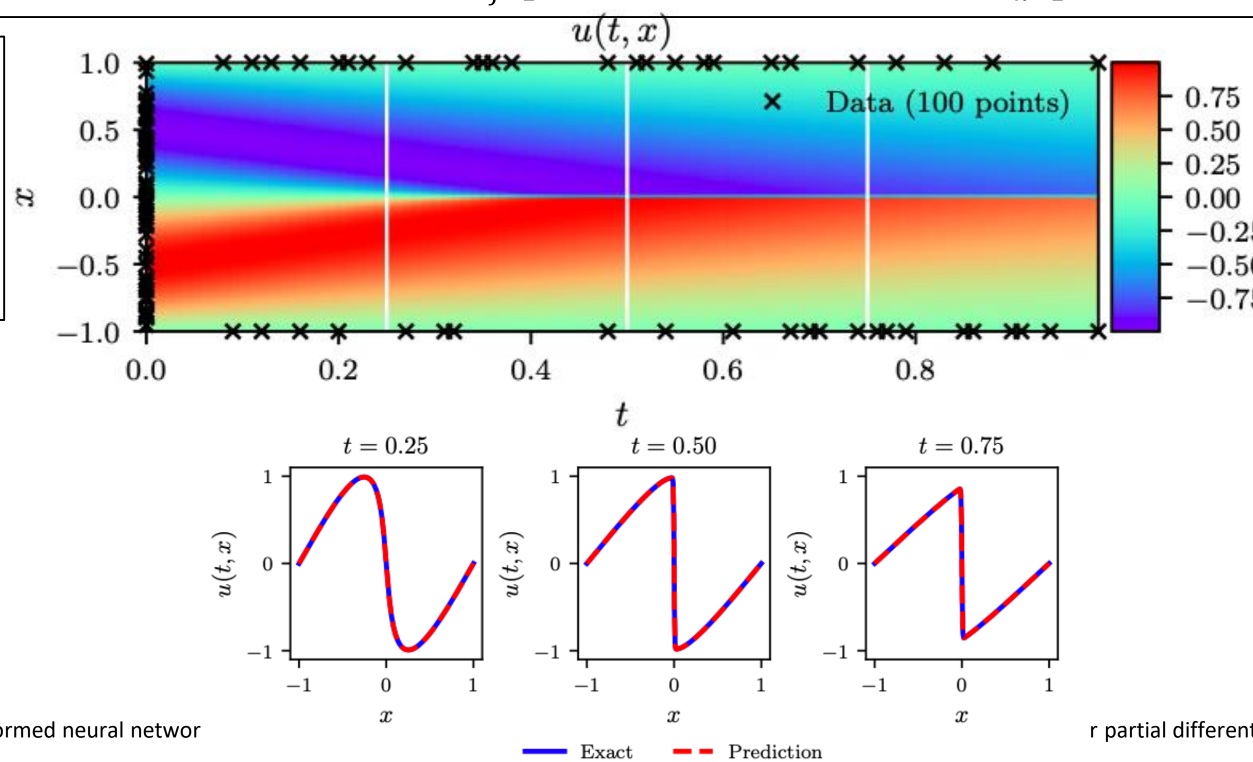

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My interest [1]

Hwang, H. J., Jang, J. W., Jo, H., & **Lee, J. Y.** (2020). Trend to equilibrium for the kinetic Fokker-Planck equation via the neural network a pproach. *Journal of Computational Physics*, *419*, 109665.

- **Using PINN to the kinetic Fokker-Planck equation.**

The kinetic Fokker−Planck equation in a bounded interval $\Omega = [-1,1]$ is written as

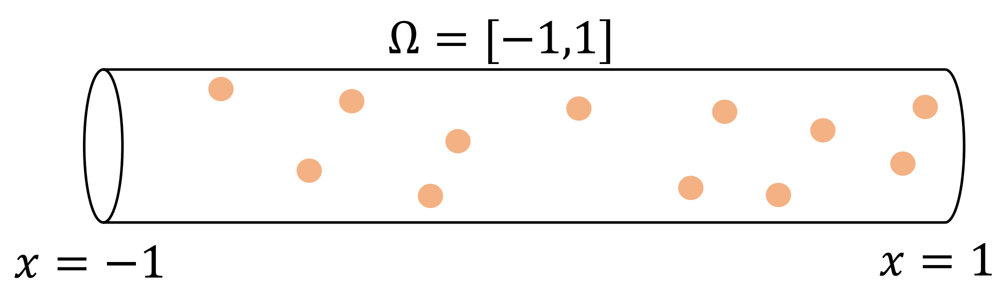
$$\partial_t f(t,x,v) + v \cdot \nabla_x f = \partial_v(\sigma \partial_v f + \beta v f),$$

subject to the initial condition

$$f(0,x,v) = f_0(x,v)$$

- $t \in [0,T]$ where T=5 or 10.
- $x \in [-1,1]$: unit ball in $\mathbb{R}^1$.
- $v \in [-10,10]$.

where σ is the diffusion coefficient, β is the friction coefficient, and the $f(t,x,v)$ is the pro babilistic density distribution of particles.



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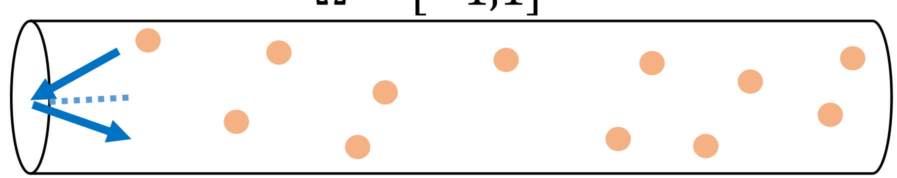
* Boundary conditions

– **Ex) Specular reflection** boundary condition

- $f(t,x,v) = f(t,x,-v)$, for $x=-1$ and $x=1$

$\Omega = [-1,1]$



$x=-1$ $x=1$

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* Boundary conditions

- **Absorbing** boundary condition: $f(t,x,v)|_{\gamma_-} = 0$, for x=−1 and 1.
- **Inflow** boundary condition: $f(t,x,v)|_{\gamma_-} = g(t,x,v)$, for x=−1 and 1 with a given function $g(t,x,v)$.
- **Specular reflection** boundary condition: $f(t,x,v) = f(t,x,-v)$, for x=−1 and 1.
- **Periodic** boundary condition: $f(t,x,v) = f(t,-x,v)$, for x=−1 and 1.
- **Diffusive** reflection boundary condition: $f(t,x,v) = C\mu(v)\int_{w\cdot n_x>0} f(t,x,w)|w\cdot n_x|dw,$ for x=−1 and 1, where $C = \left(\int_{v\cdot n<0}\mu(v)|v\cdot n|dv\right)^{-1}$ and $\mu(v) = e^{-\frac{v^2}{2}}$ for both $\mathrm{n} = \hat{x}$ and $-\hat{x}$

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- **Using PINN to the kinetic Fokker-Planck equation.**
  - Easily changing the varied types of the physical boundary conditions.
  - Include a term regarding the conservation of the total mass of the system in the t otal loss function
  - Long time behaviors of neural network solution and its physical quantities
    - Apply various initial conditions and coefficients.
    - Convergence to the global Maxwellian.
  - Providing the theoretical supports for the pointwise convergence of the neural ne twork solutions to the a priori analytic solutions.

My interest [1]

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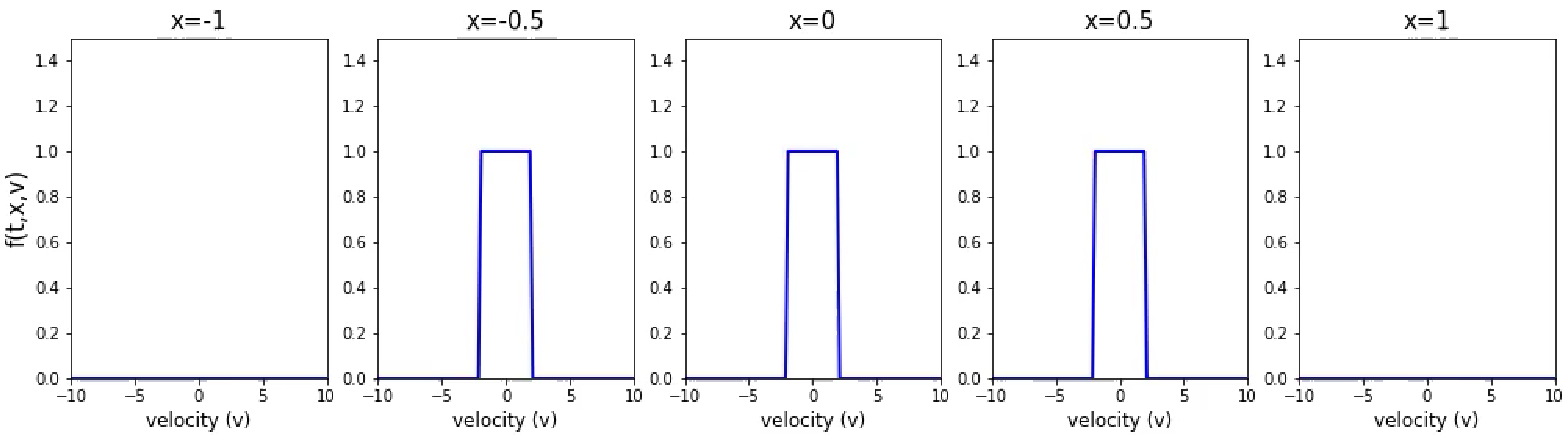
- **Results : Specular boundary conditions which conserve the total mass**



Video: The pointwise values of $f^{nn}(t,x,v)$ as t varies at each x's for the **specular boundary condition**. x = ±1 stand for the boundary points, and x = ±0.5 and = 0 are the points away from the boundary.

Part 2. Operator learning

- **Operator learning**
  - Learning a mapping from the parameters (e.g. external force, initial, and boundary conditions) of the PDEs to the corresponding solution.
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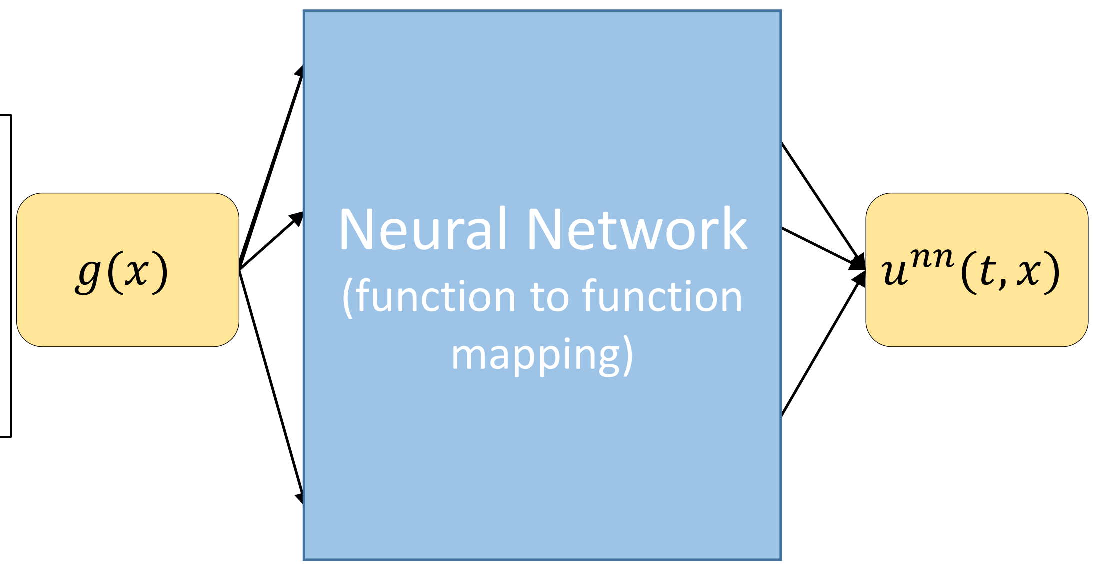
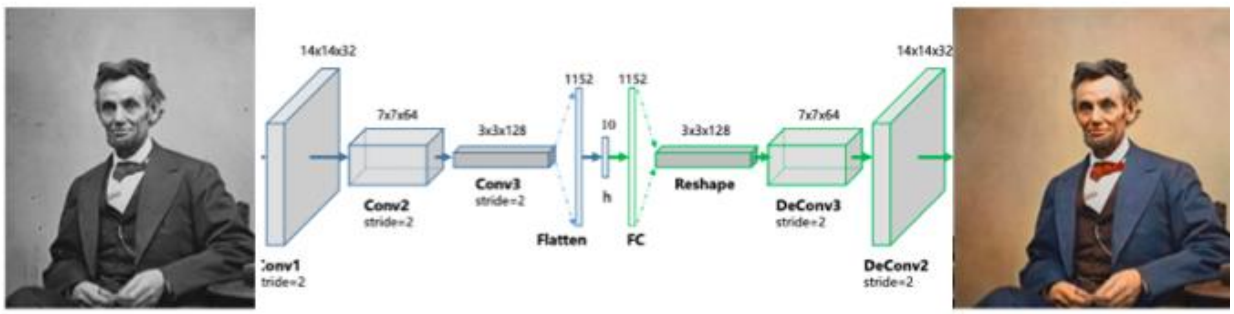


Data-driven operator learning

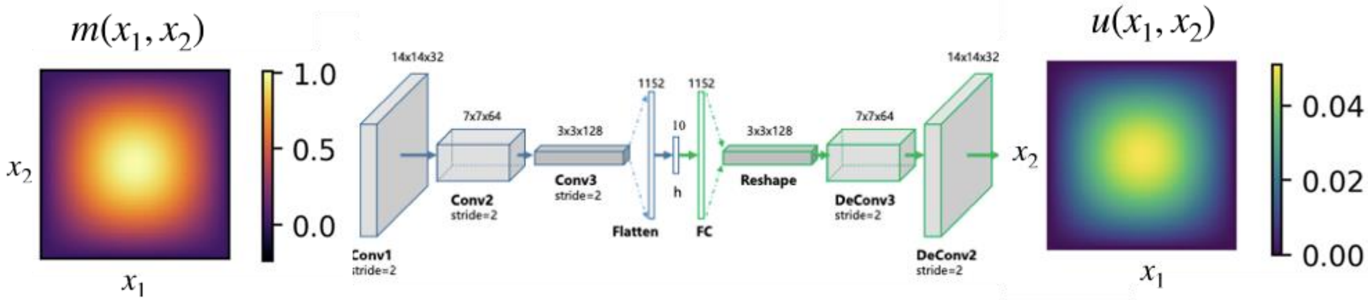
- **CNN encoder-decoder (Image-to-image regression)**
  - Image segmentation, Image Noise Reduction, Image coloring



https://towardsdatascience.com/convolutional-autoencoders-for-image-noise-reduction-32fce9fc1763

Data-driven operator learning

- **Operator learning (function-to-function regression)**



Ex) Poisson equation

$$-\Delta u - m = 0 \text{ in } \Omega \subset \mathbb{R}^2$$
$$u = 0 \text{ in } \partial\Omega$$

Goal) Find a solution $u(x_1, x_2)$ for different source term $m(x_1, x_2)$.
(Learning operator from the source term to the solution)

$$m(x_1, x_2) \mapsto u(x_1, x_2)$$

Ex) Burgers' equation

$$u_t + uu_x = \nu u_{xx}$$
$$u(x,0) = u_0(x)$$

Goal) For a fixed coefficient ν, find a solution $u(t, x)$ for different initial condition $u_0(x)$.
(Learning operator from the initial condition to the solution)

$u_0(x) \mapsto u(x, t = T)$ or $u_0(x) \mapsto u(x, t)$

New models for operator learning : DeepONet(2019), Fourier Neural Operator (FNO) [2020]

My interest [2]

Hwang, R., **Lee, J. Y.**, Shin, J. Y., & Hwang, H. J. (2022, June). Solving pde-constrained control problems using operator learning. In *Proceedings of the AAAI Conference on Artificial Intelligence* (Vol. 36, No. 4, pp. 4504-4512).

- **Solving control problems using operator learning.**

Poisson equation with zero Dirichlet boundary conditions

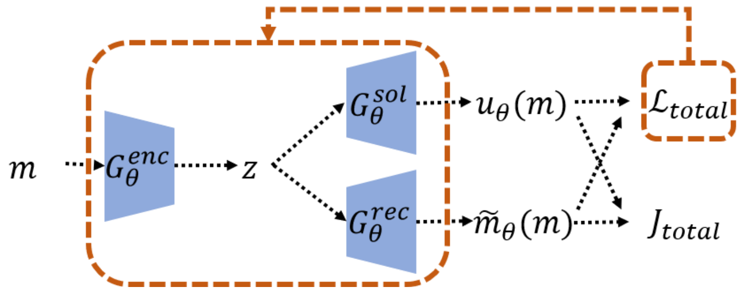
$$\begin{cases} -\Delta u(x) - m(x) = 0, & x \in \Omega, \\ u = 0, & x \in \partial\Omega, \\ m_a \leq m \leq m_b, & x \in \Omega, \end{cases}$$

- Ω : domain of interest
- $u : \Omega \to \mathbb{R}$ (unknown temperature)
- $u_d : \Omega \to \mathbb{R}$ (desired temperature)
- α : (unknown temperature)
- $m : \Omega \to \mathbb{R}$ (source term : control function)

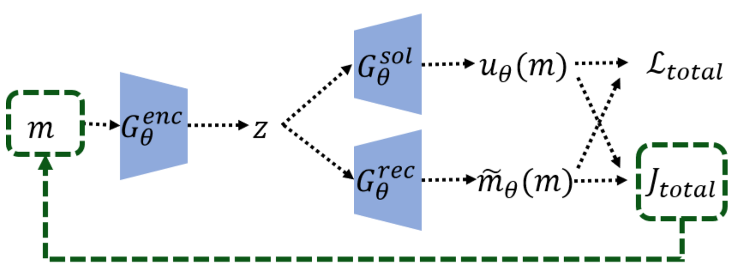
- We want to control $m(x)$ which minimize

$$J_{total}(m(x), u(x))$$

$$= \min \frac{1}{2}\int_\Omega (u - u_d)^2\, dx + \frac{\alpha}{2}\int_\Omega m^2 dx$$



Phase 1 : Operator learning
(Learning $m(x) \mapsto u(x)$)



Phase 2 : Solving control problem
(Minimize J_{total} to find optimal $m(x)$)

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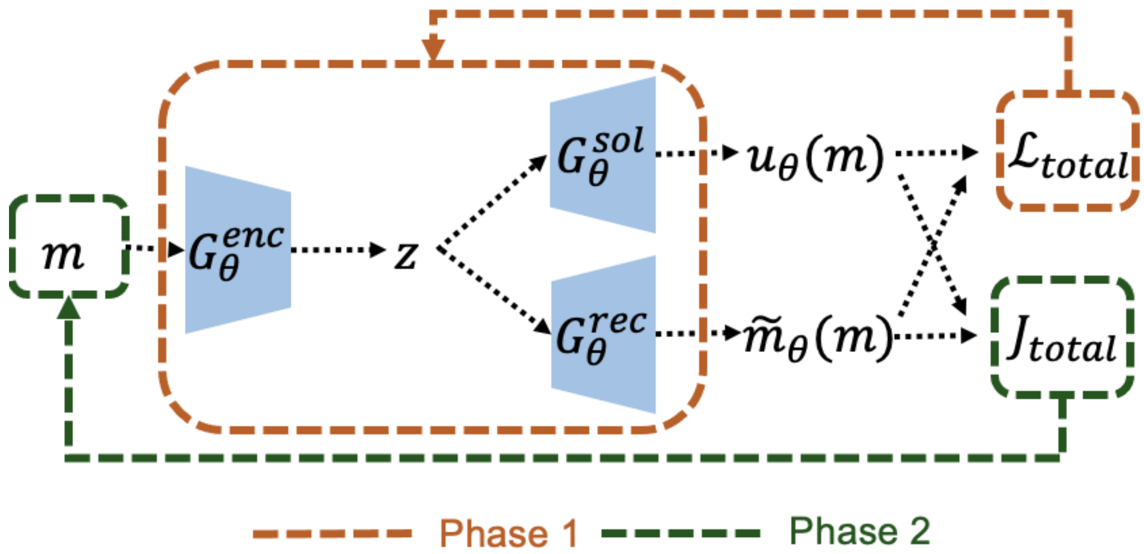
- **Solving control problems using operator learning.**
  - Our framework approximates a PDE solution with **sufficiently high accuracy** to search optimal controls while taking significantly **less time for inference.**



Conclusion

- **PDE solver**

Find $\boldsymbol{u(t,x)}$ satisfying

$$\mathcal{L}_{PDE} = f(u, u_t, u_x, u_{xx}, \dots) = 0$$
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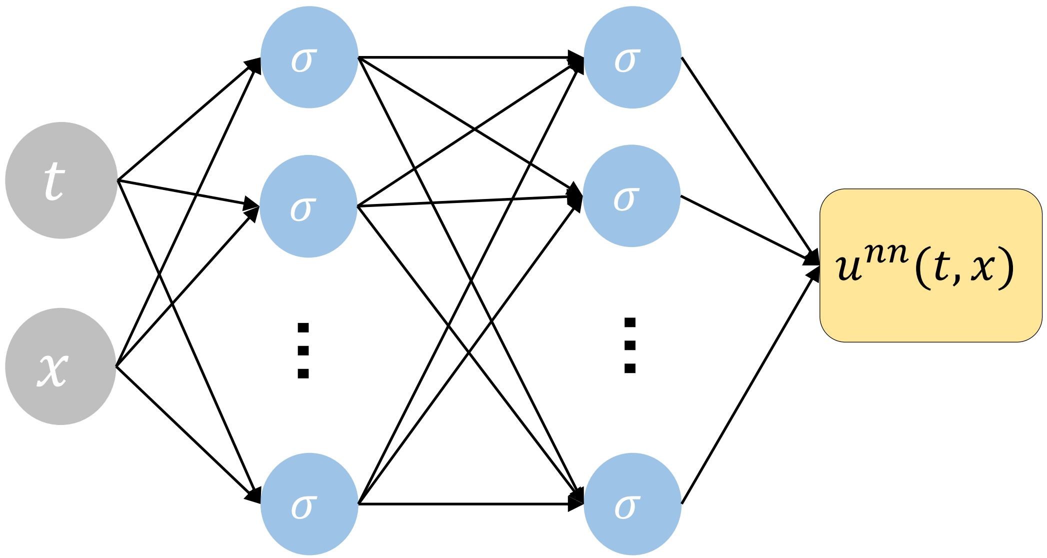

- **Operator learning**

Find a map $\boldsymbol{\mathcal{G}}$: $\boldsymbol{g(x) \mapsto u(t,x)}$ satisfying

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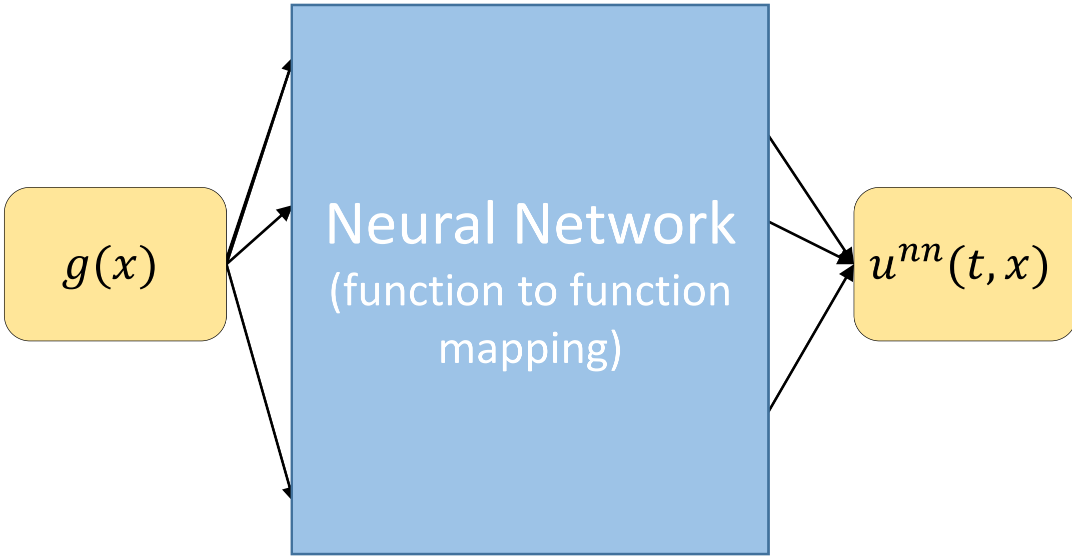

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Thank you