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JACOBS SCHOOL OF ENGINEERING

ECE/SIOC 228 Machine Learning for Physical Applications
Lecture 11: Physics Informed Machine Learning II

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University of California, San Diego

Reference: Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equation: https://www.sciencedirect.com/science/article/pii/S0021999118307125
A First Course in the Numerical Analysis of Differential Equations, https://www.uaar.edu.pk/fs/books/28.pdf

Logistics

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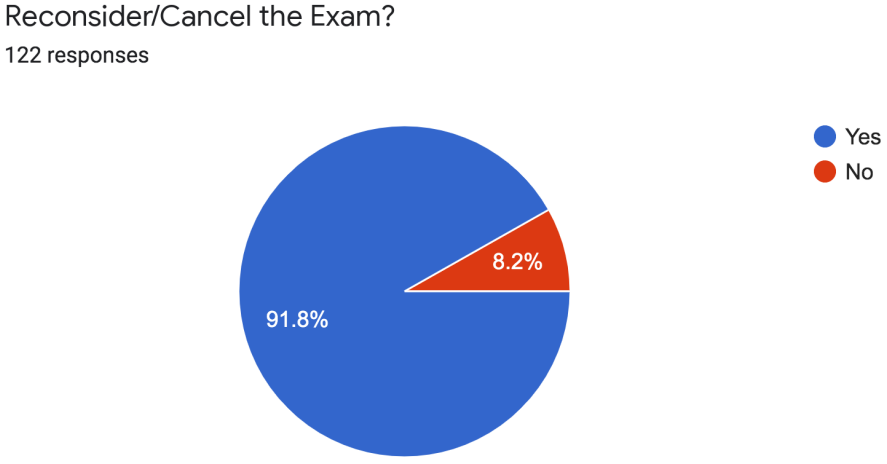

We will cancel the exam on May 17th, and have regular lecture for that day. Final grade will only depend on 40% Homework, 40% Project and 5% Participation → scale them to 100% as the final grades

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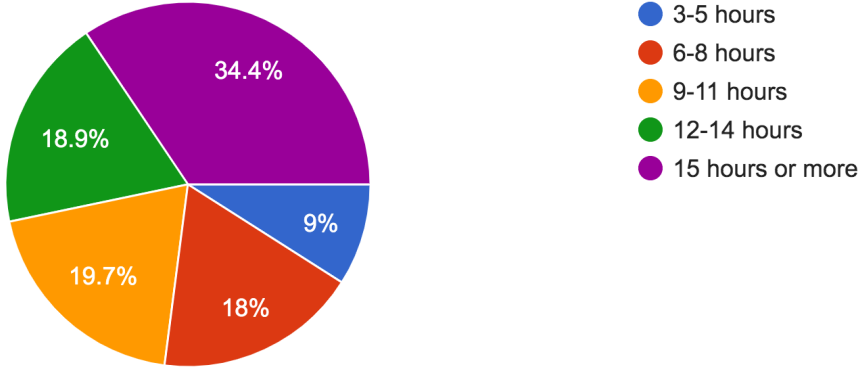
How many hours did you spend on HW1 Written part?

122 responses



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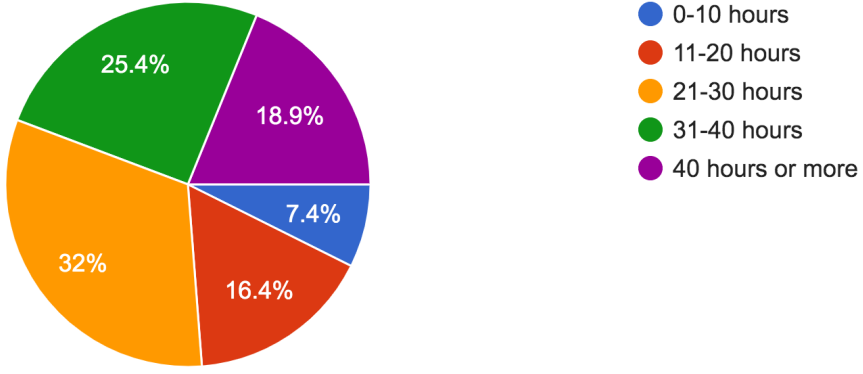
How many hours did you spend on HW1 Coding part?

122 responses



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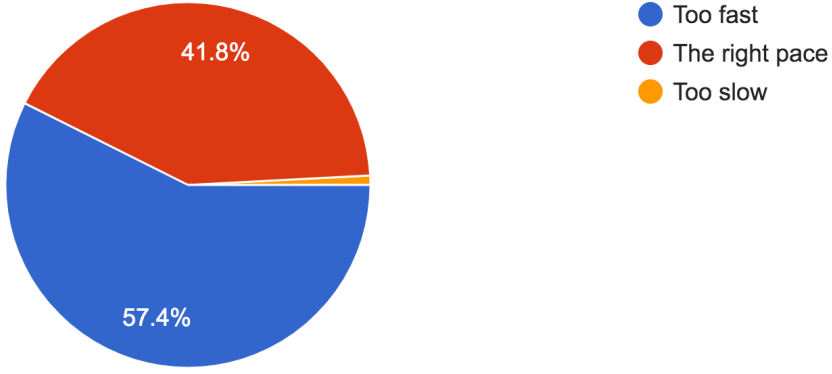
The speed with which we cover the material covered in lecture is

122 responses



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- We'll try to improve based on the feedbacks.
- **Please respect to the rules and final deadlines, for fairness of the entire class.**
- We really appreciate all the helpful suggestions. Keep in mind we have a **good diversity** in this class. Everyone brings in different ideas and experiences, everyone potentially also has different learning objectives and goals. Please be kind and patient, and try to understand each other.

Review: Pipeline of Operator Learning

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- Heat equation: $u_t = u_{xx}$ (The change in time is equal to 2nd-order difference in space.)
- Numerical solver to generate training data under different initial conditions $u(0, x) \longrightarrow u(T, x)$

Supervised learning

Get a dataset {(a , u)} (existing solvers or experiments)

- Initialize NN, F: a->u
- For N epoch, For batches of data pairs (a, u)
- Compute the prediction F(a)
- Minimize ||F(a)-u||

Review: Operator learning

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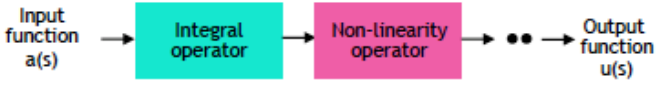
- Operator learning

$$F:\ a(s) \rightarrow u(s)$$
$$(R^n \rightarrow R^m) \rightarrow (R^n \rightarrow R^m)$$



$$v_0(s) = P(x(s), s)$$
$$v_{l+1}(s) = \sigma\left(W_l v_l(s) + \int_D \kappa_l(s,z) v_l(z)\, dz + b_l(s)\right), \quad l = 0, \ldots, L-1$$
$$y(s) = Q(v_L(s))$$
$$P : \mathbb{R}^{m+n} \rightarrow \mathbb{R}^{d_0}, \quad W_l \in \mathbb{R}^{d_{l+1} \times d_l}, \quad \kappa_l : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{d_{l+1} \times d_l}, \quad b_l : \mathbb{R}^n \rightarrow \mathbb{R}^{d_{l+1}}, \quad Q : \mathbb{R}^L \rightarrow \mathbb{R}^r$$

Review: Operator learning

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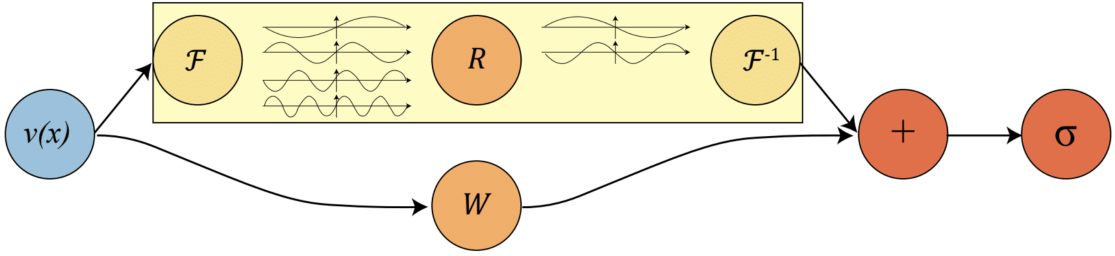
- **Operator learning**
  - Graph-based Neural Operator
  - Deep Operator Network (DeepONet)
  - Fourier Neural Operator



https://arxiv.org/abs/2006.09535

Supervised learning

Get a dataset {(a , u)} (existing solvers or experiments)

- Initialize NN, F: a->u
- For N epoch, For batches of data pairs (a, u)
- Compute the prediction F(a)
- Minimize ||F(a)-u||

What if there is no existing solvers or data available?

Outline

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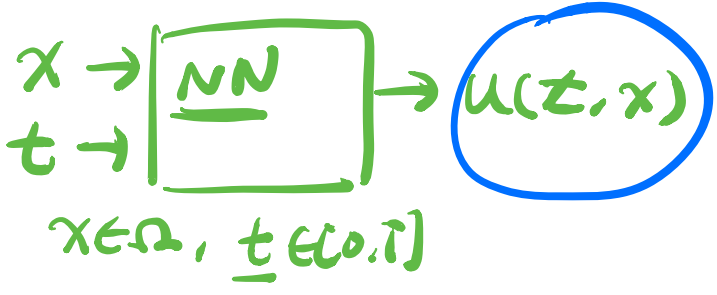
- Continuous Time Physics Informed Neural Network (PINN)
- Discrete Time PINN
- Extensions
  - Data driven parameter discovery via PINN
  - PINN + Neural Operator (PINO)
  - Applications: ML-Accelerated PDE Observers

- Suppose we want to solve a partial differential equations of the general form

$$u_t = -\mathcal{N}[u]$$

where $x \in \Omega$, $t \in [0, T]$. $u(t, x)$ denotes the solution. $\mathcal{N}[u]$ is a nonlinear differential operator.

Example: 1D heat equation $u_t = u_{xx}$ $\mathcal{N}[u] = -u_{xx}$

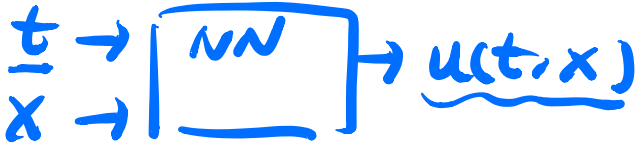


Any requirement for the solution u(t, x)?

- We define $f(t, x)$ to be given by

$$f := u_t + \mathcal{N}[u]$$

- We appromate the PDE solution $u(t, x)$ by a deep neural network.
- Thus, we will have $f(t, x)$ a physics informed neural network (PINN). This neural network can be defined by computing the involved gradients via backpropagation.



PINN (Physics laws on NN)

$f(t,x) = u_t - u_{xx} \equiv 0$ $\forall x \in \Omega$, $t \in [0,T]$

heat equation

Example: Burgers' Equation

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- As a more complete example, we consider the 1D Burgers' Equation.

X

$$u_t + uu_x = \frac{0.01}{\pi} u_{xx}, x \in [-1,1], t \in [0,1]$$

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

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

✓

- A fundamental partial differential equation occurring in various areas of applied mathematics, such as fluid mechanics, nonlinear acoustics, gas dynamics, and traffic flow. https://en.wikipedia.org/wiki/Burgers%27_equation

Example: Burgers' Equation

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- As a more complete example, we consider the 1D Burgers' Equation.

$$u_t + uu_x = \frac{0.01}{\pi} u_{xx}, x \in [-1,1], t \in [0,1]$$

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

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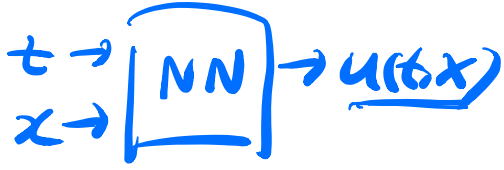

- Define Solution $u(t,x)$ as a neural network
- Define a PINN $f(t,x)$

$$f(t,x) := u_t + u \cdot u_x - \frac{0.01}{2} u_{xx}$$

Example: PINN for Burgers' Equation

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```
def u(t, x):
    u = neural_net(tf.concat([t,x],1), weights, biases)
    return u
```

Correspondingly, the physics informed neural network $f(t, x)$ takes the form

```
def f(t, x):
    u = u(t, x)
    u_t = tf.gradients(u, t)
    u_x = tf.gradients(u, x)
    u_xx = tf.gradients(u_x, x)
    f = u_t + u*u_x - (0.01/tf.pi)*u_xx
    return f
```

Example: PINN for Burgers' Equation

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- The shared parameters between the neural network $u(t, x)$ and the physics informed neural network $f(t, x)$ can be learned by minimizing the mean squared error loss

Question:

- **What should $f(t, x)$ be for physical system $u_t + uu_x = \frac{0.01}{\pi} u_{xx}$?**

$f(t,x)=0$, $\forall x \in [-1,1]$, $t \in [0,1]$

- **Any other constraints?**

$u(0,x) = -\sin(\pi x)$ ← initial

$u(t,-1) = u(t,1)$ ← boundary condition

$\{t^i, x^i, u^i\}$

Example: PINN for Burgers' Equation

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- The shared parameters between the neural network $u(t, x)$ and the physics informed neural network $f(t, x)$ can be learned by minimizing the mean squared error loss

$$MSE_f = \frac{1}{N_f} \sum_{i=1}^{N_f} |f(t_f^i, x_f^i)|^2$$

$$MSE_u = \frac{1}{N_u} \sum_{i=1}^{N_u} |u^i(t^i, x^i) - u^i|^2$$

$$MSE = MSE_f + MSE_u$$

physics law

initial & boundary conditions

$\min MSE$
weights, biases

$x \rightarrow$
$t \rightarrow$ $\tilde{u}(W, b)$ $\rightarrow u(t, x)$

Example: PINN for Burgers' Equation

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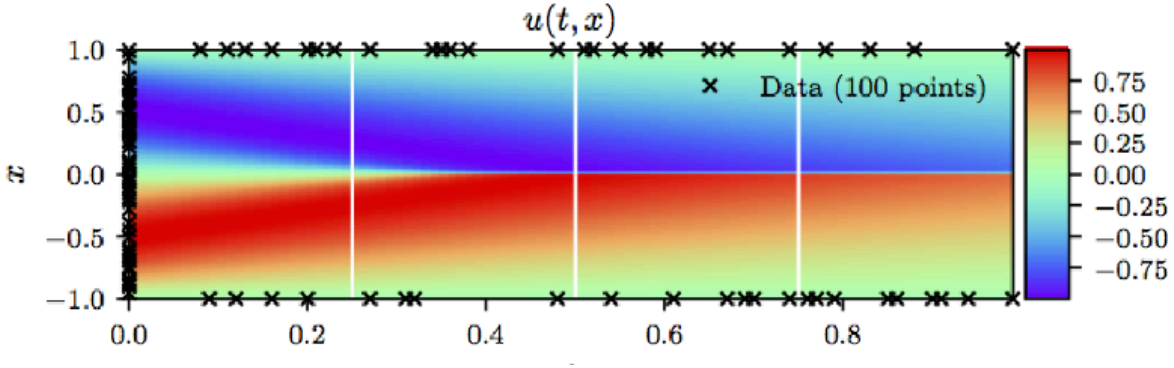
- The shared parameters between the neural network $u(t, x)$ and the physics informed neural network $f(t, x)$ can be learned by minimizing the mean squared error loss



+ 10,000 (x, t) points for enforcing the physics law $f(t, x) = 0$

PINNs v.s. Classic PDE Solvers

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PINNs is like a PDE solver

- Give a PDE instance: with certain initial and boundary condition → Solution for that instance
- Compared to classic numerical solvers (e.g. FDM, FEM)
  - ✓ Simple and flexible
  - ✓ Complex geometry, high dim, etc
  - X optimization can be tricky
  - X no guarantee for convergence

less accurate than classic solvers

PINNs (solve) v.s. Operator Learning (learn)

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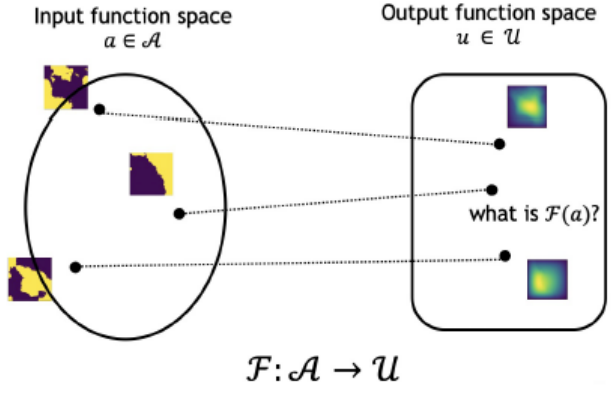
PINNs is like a PDE solver

- Give a PDE instance: with certain initial and boundary condition →
- Compared to classic numerical solvers (e.g. FDM, FEM)
  - ✓ Simple and flexible
  - ✓ Complex geometry, high dim, etc
  - X .
  - X .

Operator Learning

learn the solution operator $\mathcal{F}$
interpolate u in the function space.



but requires existing solvers or experiment data that contains solutions under different initial/boundary conditions or PDE parameters

What's Next…

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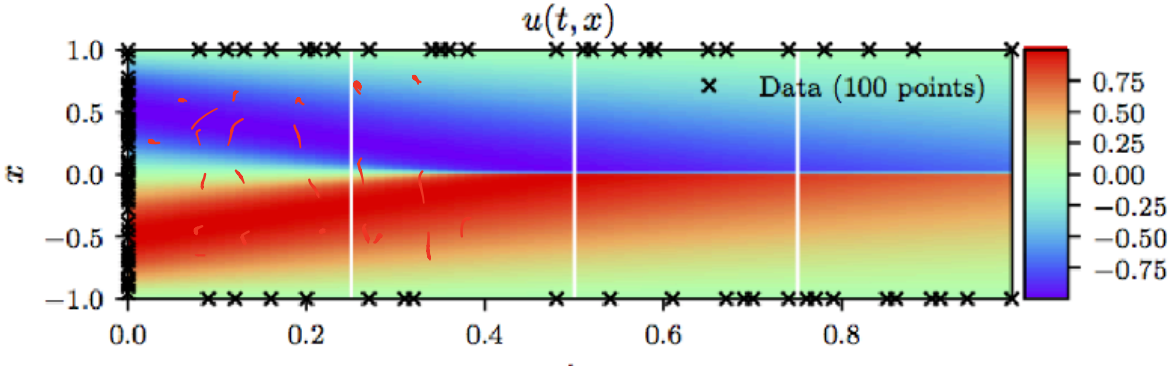

+ 10,000 (x,t) points for enforcing the physics law $f(t,x)=0$

- **A large number of points** in order to enforce physics constraints in the **entire spatio-temporal domain**
- May introduce a severe bottleneck in higher dimensional problems, as the total number of points needed to globally enforce a physics informed constrain will increase exponentially.
- **What can we do to improve this?**

Outline

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- Continuous Time Physics Informed Neural Network (PINN)
- **Discrete Time PINN**
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Numerical Solutions of PDEs

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- The discrete time PINN models are built upon the **numerical methods (i.e., Runge-Kutta Method)**
- Numerical methods to approximate the solution of the following ODEs

$$\frac{dy}{dt} = f(t, y), y(t^0) = y^0$$

and you want to solve for $y(t), t \geq t^0$

- We know the value of y at a single point t=to
- Given any t≥to, y, we can tell the slope from the differential equation

Can we predict the value of y at t^0+h, t^0+2h, t^0+3h, ...

0.1s
0.01s

$\Rightarrow$ $y(t)$ by making the following Approximation

$$f(t,y) \approx f(t^0, y^0), \text{ for } t \in [t^0, t^0+h]$$

Sufficient small h

$$y(t) = y^0 + \int_{t^0}^{t} f(z, y(z))\, dz$$

$$= y^0 + f(t^0, y^0)\,(t-t^0), \quad t \in [t^0, t^0+h]$$

$t^1 = t^0+h, \quad y^1 = y^0 + hf(t^0, y^0)$

$t^2 = t^0+2h, \quad y^2 = y^1 + hf(t^1, y^1)$

$\vdots$

Continue to produce $t^3, t^4, \ldots$

$$y^{n+1} = y^n + hf(t^n, y^n), \quad n=0,1,\ldots$$

Euler Method

Explicit/Implicit Runge-Kutta Method

$$y^{n+1} = y^n + h\sum_{j=1}^{q} b_j f(t^n + c_j h, y(t^n + c_j h))$$

$t^n + c_1 h, t^n + c_2 h \cdots t^n + c_q h$: RK nodes

$b_1, b_2, \cdots, b_q$ RK weights

Runge-Kutta expresses $y(t^n + c_j h)$

by updating y^n with a linear combination

of $f(t^n + c_i h, y(t^n + c_i h)), \forall i = 1, \cdots, q$

$$y(t^n + c_j h) = y^n + h \sum_{i=1}^{q} a_{j,i} f(t^n + c_i h, y^{n+c_i})$$

denotes as y^{n+c_j}

$$\sum_{i=1}^{q} a_{j,i} = c_j$$

$A = (a_{j,i})_{j,i=1,2,\cdots,q}$ $\Leftarrow$ RK matrix

Explicit RK: A is lower triangular matrix

Implicit RK: A can be arbitrary matrix

See Reference "A first course in the Numerical Analysis of Differential Equations" for more info.

Runge-Kutta Methods

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- The family of Runge–Kutta methods is a generalization of the RK4 method, given by

$$y^{n+1} = y^n + h\sum_{j=1}^{q} b_j f(t^n + c_j h, y(t^n + c_j h))$$

we express the value of y^{n+1} as combination of values of y at nodes $t^n + c_1 h, t^n + c_2 h, \dots, t^n + c_q h$.

- But we don't know the value of $y(t^n + c_j h)$, need to have an approximation!

$$y(t^n + c_j h) = y^n + h\sum_{i=1}^{q} a_{j,i} f(t^n + c_i h, y(t^n + c_i h))$$

$A = (a_{j,i})_{i,j=1,2,\dots,q}$ RK matrix; $b = \begin{bmatrix} b_1 \\ \vdots \\ b_q \end{bmatrix}$ RK weights

$c = \begin{bmatrix} c_1 \\ \vdots \\ c_q \end{bmatrix}$ RK nodes $\quad \sum_{i=1}^{q} a_{j,i} = c_j$

(Note: the above equations may have different but equivalent definitions in other texts)

Runge-Kutta Methods

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4-th order Runge-Kutta Method

$$y^{n+1} = y^n + h\left(\frac{1}{6}f(t^{n+c_1}, y^{n+c_1}) + \frac{1}{3}f(t^{n+c_2}, y^{n+c_2}) + \frac{1}{3}f(t^{n+c_3}, y^{n+c_3}) + \frac{1}{6}f(t^{n+c_4}, y^{n+c_4})\right)$$

0				
$\frac{1}{2}$	$\frac{1}{2}$			
$\frac{1}{2}$	0	$\frac{1}{2}$		
1	0	0	1	
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

c	A
	$b^\top$

- $t^{n+c_1} = t^n + c_1 h = t^n$ $\quad y^{n+c_1} = y^n$
- $t^{n+c_2} = t^n + c_2 h = t^n + \frac{1}{2}h$, $\quad y^{n+c_2} = y^n + \frac{h}{2}f(t^{n+c_1}, y^{n+c_1})$
- $t^{n+c_3} = t^n + c_3 h = t^n + \frac{1}{2}h$ $\quad y^{n+c_3} = y^n + \frac{h}{2}f(t^{n+c_2}, y^{n+c_2})$
- $t^{n+c_4} = t^n + h$ $\quad y^{n+c_4} = y^n + hf(t^{n+c_3}, y^{n+c_3})$

(Note: the above equations may have different but equivalent definitions in other texts)

Discrete Time PINNs

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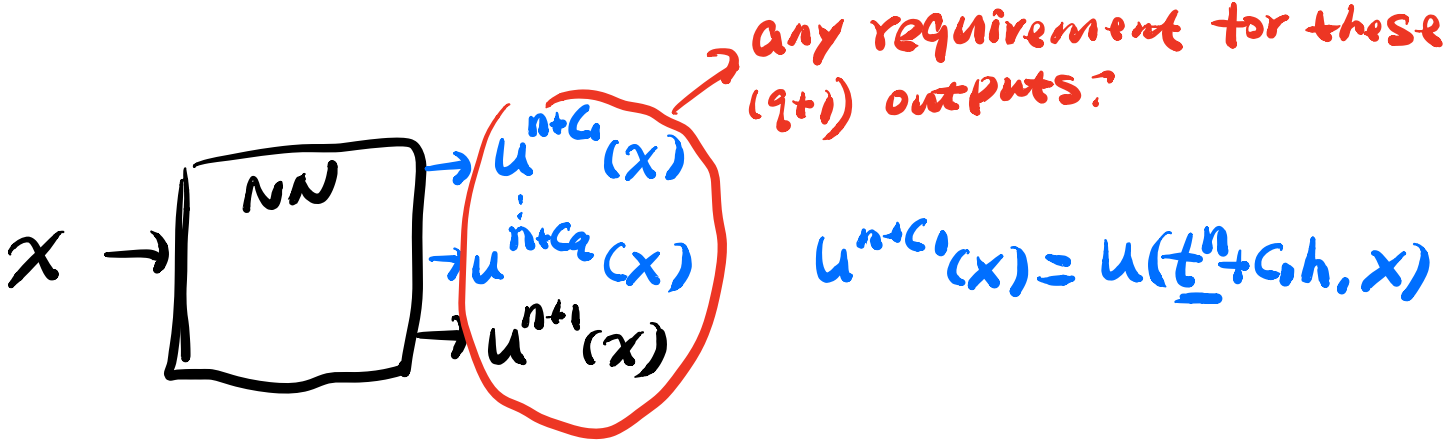
- Suppose we want to solve a partial differential equations of the general form

$$u_t = -\mathcal{N}[u]$$

where $x \in \Omega$, $t \in [0, T]$. $\mathcal{N}[u]$ is a nonlinear differential operator.

- Denote $u^n(x) = u(t^n, x), u^{n+1}(x) = u(t^{n+1}, x)$. We know: $u^n(x) \rightarrow$ want to predict $u^{n+1}(x)$



$$u^{n+c_j} = u^n + h\sum_{i=1}^{q} a_{j,i}\,(-\mathcal{N}[u^{n+c_i}]),\quad j=1,2,\cdots,q$$

$$u^{n+1} = u^n + h\sum_{i=1}^{q} b_i\,(-\mathcal{N}[u^{n+c_i}])$$

Rearrangement:

$$u^n = \underbrace{u^{n+c_j} + h\sum_{i=1}^{q} a_{j,i}\,\mathcal{N}[u^{n+c_i}]}_{\text{PINN}} \quad \swarrow\ u_j^n,\ j=1,\cdots,q$$

$$u^n = \underbrace{u^{n+1} + h\sum_{i=1}^{q} b_i\,\mathcal{N}[u^{n+c_i}]}_{\text{PINN}} \quad \swarrow\ u_{q+1}^n$$

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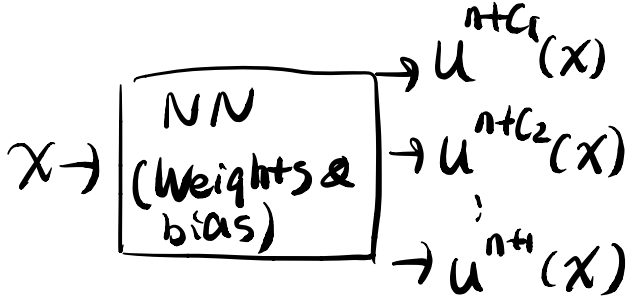
At step t^n, we have $u(t^n, x)$, want to predict $u(t^{n+1}, x)$

Neural Network



- multi-output NN with $(q+1)$ outputs

Physics Informed NN with $(q+1)$ outputs

$$u_1^n(x) = u^{n+c_1}(x) + h\sum_{i=1}^{q} a_{1,i}\, N[u^{n+c_i}(x)]$$

$$\vdots$$

$$u_{q+1}^n(x) = u^{n+1}(x) + h\sum_{i=1}^{q} b_i\, N[u^{n+c_i}(x)]$$

- use $u^n(x)$ as label

Example: Allen–Cahn Equation

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- Consider the Allen–Cahn equation along with periodic boundary conditions

$$u_t - 0.0001u_{xx} + 5u^3 - 5u = 0, x \in [-1,1], t \in [0,1]$$
$$u(0,x) = \mathrm{x}^2\cos(\pi x)$$
$$u(t,-1) = u(t,1)$$
$$u_x(t,-1) = u_x(t,1)$$

- For the Allen–Cahn equation, the nonlinear operator is given by

$$\mathcal{N}[u] = -0.0001u_{xx} + 5u^3 - 5u$$

- Define a deep neural network, takes x as input and output $(q+1)$ items

$$[u^{n+c_1}(x), u^{n+c_2}(x), \cdots, u^{n+1}(x)]$$

- Define a PINN also with $(q+1)$ outputs

$$u_i^n(x) = u^{n+c_i}(x) + h\sum_{j=1}^{q} a_{i,j} N[u^{n+c_j}(x)], \quad i=1,\cdots,q+1$$

$$N[u^{n+c_i}(x)] = -0.0001 u_{xx}^{n+c_i}(x) + 5(u^{n+c_i}(x))^3 - 5u^{n+c_i}(x)$$

- Use $u^n(x)$ as supervised label for the PINN outputs $u_1^n(x), u_2^n(x) \cdots u_{q+1}^n(x)$

$$SSE_n = \sum_{j=1}^{q+1} \sum_{i=1}^{N_n} |u_j^n(x_i) - u^n(x_i)|^2$$

Here $\{x_i, u^n(x_i)\}$ corresponding to data at time t^n

Example: Allen–Cahn Equation

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- Similarly, we add a loss for the boundary and initial conditions

$$SSE_b = \sum_{i=1}^{q} |u^{n+c_i}(-1) - u^{n+c_i}(1)|^2 + |u^{n+1}(-1) - u^{n+1}(1)|^2$$
$$+ \sum_{i=1}^{q} |u_x^{n+c_i}(-1) - u_x^{n+c_i}(1)|^2 + |u_x^{n+1}(-1) - u_x^{n+1}(1)|^2.$$

- Therefore, we can train the shared parameters of multi-output neural network $u(x)$ and multi-output PINN by minimizing the sum of squared loss (or MSE loss):

$$SSE = SSE_n + SSE_b$$

Example: Allen–Cahn equation

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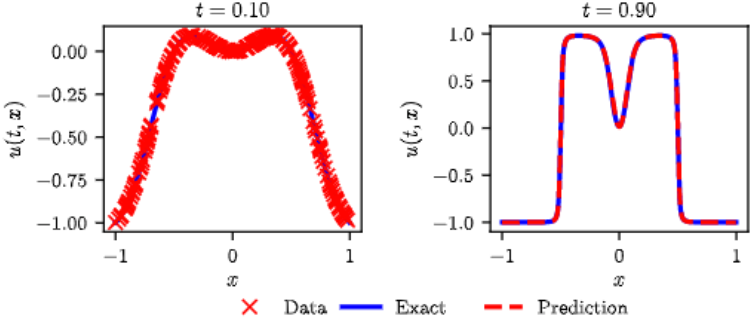
- For classic Runge–Kutta methods, the time step Δt (or h) are usually confined to be small in order to ensure numerical stability and obtain accurate solution
- For PINNs, we can choose an arbitrarily large number of stages (q). This enables us to take very large time steps while retaining stability and high predictive accuracy.
- For example, choose $t^n = 0.1, t^{n+1} = 0.9$ with q=100 Runge–Kutta stages (NN has in total 101 output quantities), allowing us to resolve the entire spatio-temporal solution **in a single step**.



- 4 hidden layers and 200 neurons per layer
- 200 training data points for $\mathrm{u}(0.1, \mathrm{x})$ randomly sampled from $\mathrm{x} \in [-1,1]$