

# NPDE Project 3: Solving the Biharmonic Equation by Deep Neural Network



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# Outline

## 1 Prerequisite knowledge

- Learning theory
- Neural network
- Optimization
- Backward propagation and forward propagation

## 2 Poisson equation

- Deep Galerkin Method
- Numerical result
- Deep Ritz Method
- Numerical result

## 3 Biharmonic equation

- Deep Galerkin Method
- Numerical result

# Problem

## Poisson equation:

$$\begin{cases} \Delta u = f, & \text{in } \Omega, \\ u = g, & \text{on } \partial\Omega \end{cases}$$

# Problem

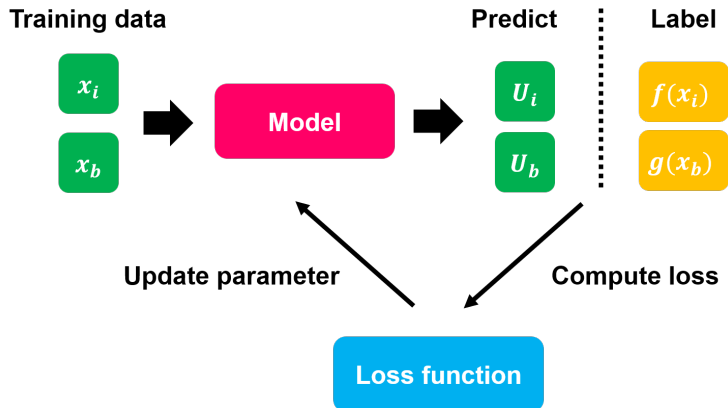
## Poisson equation:

$$\begin{cases} \Delta u = f, & \text{in } \Omega, \\ u = g, & \text{on } \partial\Omega \end{cases}$$

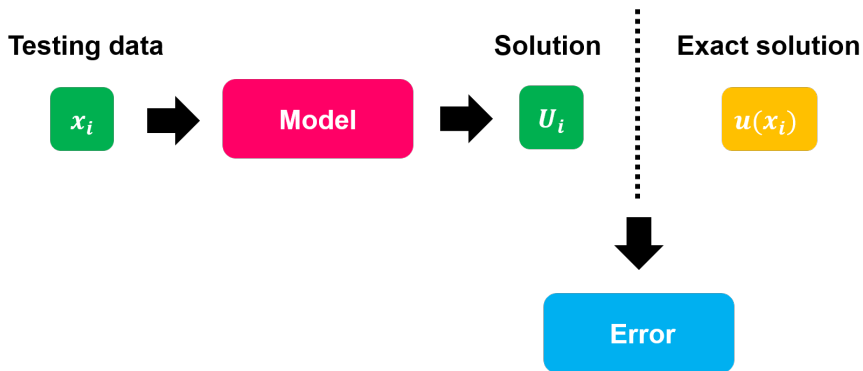
## Biharmonic equation:

$$\begin{cases} \Delta^2 u = f, & \text{in } \Omega, \\ u = g_0, & \text{on } \partial\Omega, \\ \frac{\partial u}{\partial n} = g_1, & \text{on } \partial\Omega \end{cases} \implies \begin{cases} \Delta u = p, & \text{in } \Omega, \\ \Delta p = f, & \text{in } \Omega, \\ u = g_0, & \text{on } \partial\Omega, \\ \frac{\partial u}{\partial n} = g_1, & \text{on } \partial\Omega \end{cases}$$

# Training process



# Testing process



# Neural network (NN)

**Question:** Why functions can be approximated by neural network? <sup>1</sup>

## Theorem (Universal Approximation Theorem With ReLU Network)

*For any Lebesgue-integrable function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  and any  $\varepsilon > 0$ , there exists a fully-connected ReLU network  $\mathcal{Q}$  with width  $\leq n + 4$  and depth  $\leq 4n + 1$  such that the function  $F_{\mathcal{Q}}$  represented by this network satisfies*

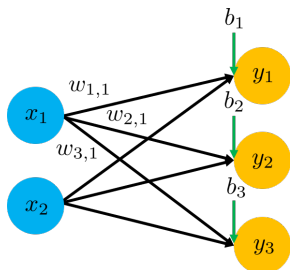
$$\int_{\mathbb{R}^n} |f(x) - F_{\mathcal{Q}}| dx < \varepsilon$$

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<sup>1</sup>Lu et al., The Expressive power of Neural Networks: A View from the Width, NIPS 2017

# Fully connected layer

## Version 1:

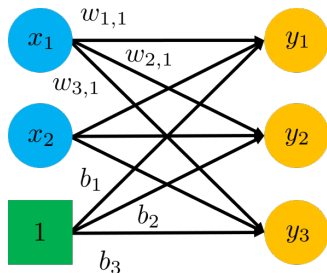


$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} w_{1,1} & w_{1,2} \\ w_{2,1} & w_{2,2} \\ w_{3,1} & w_{3,2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$



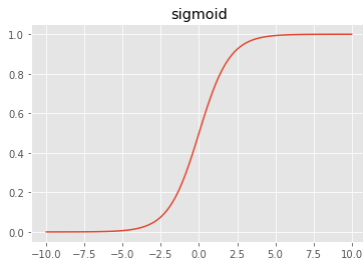
# Fully connected layer

## Version 2:

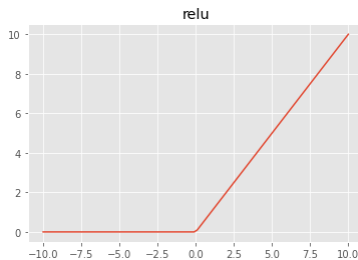


$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} w_{1,1} & w_{1,2} & b_1 \\ w_{2,1} & w_{2,2} & b_2 \\ w_{3,1} & w_{3,2} & b_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ 1 \end{bmatrix}$$

# Activation function

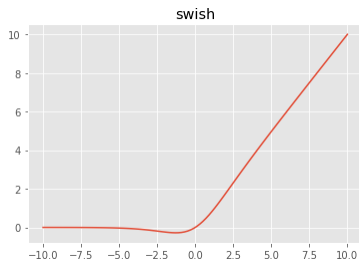


$$\text{Sigmoid}(x) = \frac{1}{1 + e^{-x}}$$

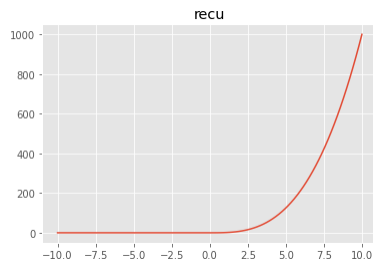


$$\text{ReLU}(x) = \max(x, 0)$$

# Activation function

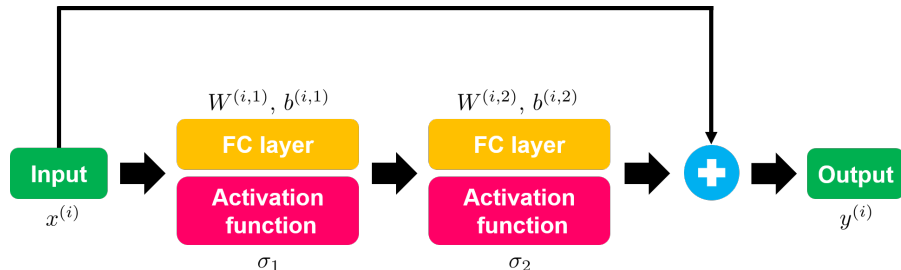


$$\text{Swish}(x) = \frac{x}{1 + e^{-x}}$$



$$\text{ReCU}(x) = \max(x^3, 0)$$

# Residual Network



$$y^{(i)} = \sigma_2 \left( W^{(i,2)} \cdot \sigma_1(W^{(i,1)}x + b^{(i,1)}) + b^{(i,2)} \right) + x^{(i)}$$

# Optimization

## Gradient decent:

$$\theta_t = \theta_{t-1} - \gamma \nabla_{\theta} \mathcal{L}(u; \theta)$$

where

- $\mathcal{L}$  : loss function.
- $\theta$  : parameters in the Neural Network.
- $\gamma$  : learning rate.

# Optimization

## Adam algorithm (ICLR 2015)

Let  $\mathcal{L}(\theta)$  be the objective function with parameters  $\theta$ ,  $\beta_1, \beta_2$  be the exponential decay rates for the moment estimates,  $\gamma$  be the learning rate and  $\varepsilon = 10^{-8}$ .

$$\textcircled{1} \quad m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla_{\theta} \mathcal{L}(\theta_{t-1})$$

$$\textcircled{2} \quad v_t = \beta_2 v_{t-1} + (1 - \beta_2) (\nabla_{\theta} \mathcal{L}(\theta_{t-1}))^2$$

$$\textcircled{3} \quad \hat{m}_t = \frac{m_{t-1}}{1 - \beta_1^t}$$

$$\textcircled{4} \quad \hat{v}_t = \frac{v_{t-1}}{1 - \beta_2^t}$$

$$\textcircled{5} \quad \theta_t = \theta_{t-1} - \gamma \frac{\hat{m}_t}{\sqrt{\hat{v}_t} + \varepsilon}$$

# Forward propagation and backward propagation

## Motivation:

- Minimize the loss function by using gradient descent.

# Forward propagation and backward propagation

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## Approach:

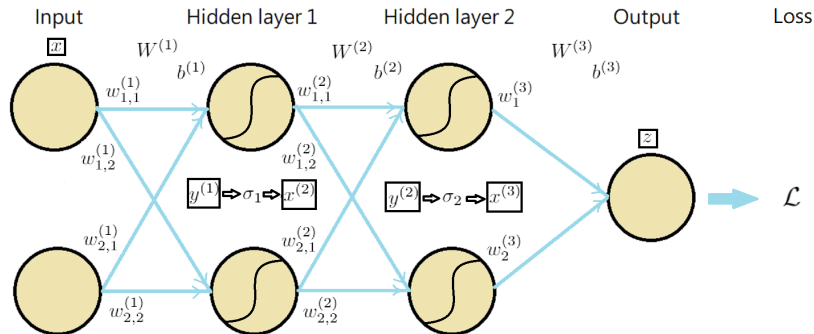
- Build a small neural network as defined in the architecture below.
- Use forward propagation to get predicted value and calculate the loss.
- Use backward propagation and adjust weights and bias accordingly.
- Repeat forward and backward steps until the stop criterion is satisfied.

## Architecture:

- Build a Feed Forward neural network with 2 hidden layers.  
All layers have 2 Neurons.

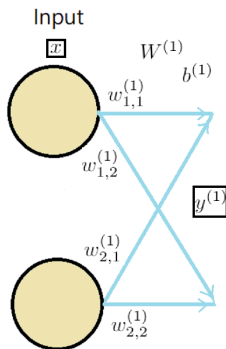


# Forward propagation



# Forward propagation

Matrix operation  $W^{(1)}$  and  $b^{(1)}$ :



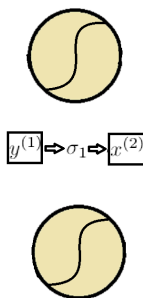
$$y^{(1)} = W^{(1)}x + b^{(1)}$$

$$\begin{bmatrix} y_1^{(1)} \\ y_2^{(1)} \end{bmatrix} = \begin{bmatrix} w_{1,1}^{(1)} & w_{1,2}^{(1)} \\ w_{2,1}^{(1)} & w_{2,2}^{(1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \end{bmatrix}$$

# Forward propagation

## Activation function $\sigma_1$ :

Hidden layer 1

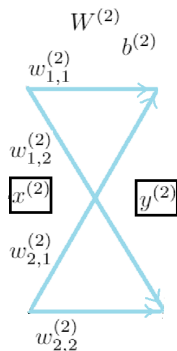


$$x^{(2)} = \sigma_1(y^{(1)})$$

$$\begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \end{bmatrix} = \begin{bmatrix} \sigma_1(y_1^{(1)}) \\ \sigma_1(y_2^{(1)}) \end{bmatrix}$$

# Forward propagation

## Matrix operation $W^{(2)}$ and $b^{(2)}$ :



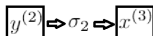
$$y^{(2)} = W^{(2)}x^{(2)} + b^{(2)}$$

$$\begin{bmatrix} y_1^{(2)} \\ y_2^{(2)} \end{bmatrix} = \begin{bmatrix} w_{1,1}^{(2)} & w_{1,2}^{(2)} \\ w_{2,1}^{(2)} & w_{2,2}^{(2)} \end{bmatrix} \begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \end{bmatrix} + \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix}$$

# Forward propagation

## Activation function $\sigma_2$ :

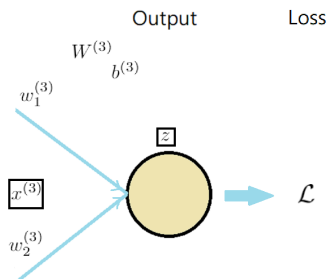
Hidden layer 2



$$x^{(3)} = \sigma_2(y^{(2)})$$
$$\begin{bmatrix} x_1^{(3)} \\ x_2^{(3)} \end{bmatrix} = \begin{bmatrix} \sigma_2(y_1^{(2)}) \\ \sigma_2(y_2^{(2)}) \end{bmatrix}$$

# Forward propagation

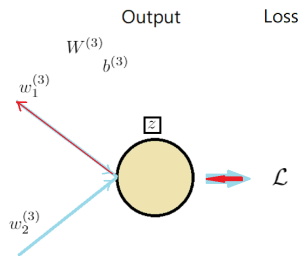
## Matrix operation $W^{(3)}$ and $b^{(3)}$ :



$$z = W^{(3)}x^{(3)} + b^{(3)}$$

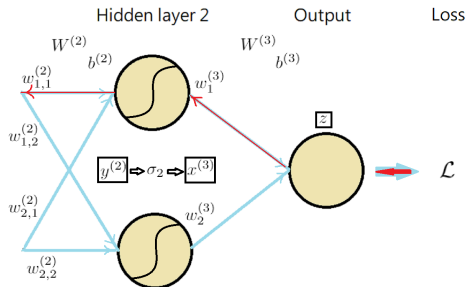
$$z = \begin{bmatrix} w_1^{(3)} & w_2^{(3)} \end{bmatrix} \begin{bmatrix} x_1^{(3)} \\ x_2^{(3)} \end{bmatrix} + b^{(3)}$$

# Backward propagation



$$\begin{cases} \frac{\partial \mathcal{L}}{\partial w_i^{(3)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot \frac{\partial z}{\partial w_i^{(3)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot x_i^{(3)} \\ \frac{\partial \mathcal{L}}{\partial b^{(3)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot \frac{\partial z}{\partial b^{(3)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot 1 \end{cases}$$

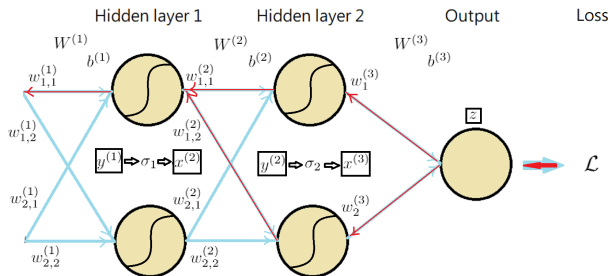
# Backward propagation



$$\begin{cases} \frac{\partial \mathcal{L}}{\partial w_{ij}^{(2)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot \frac{\partial z}{\partial x_j^{(3)}} \cdot \frac{\partial x_j^{(3)}}{\partial y_j^{(2)}} \cdot \frac{\partial y_j^{(2)}}{\partial w_{ij}^{(2)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot w_j^{(3)} \cdot \sigma_2'(y_j^{(2)}) \cdot x_i^{(2)} \\ \frac{\partial \mathcal{L}}{\partial b_i^{(2)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot \frac{\partial z}{\partial x_i^{(3)}} \cdot \frac{\partial x_i^{(3)}}{\partial y_i^{(2)}} \cdot \frac{\partial y_i^{(2)}}{\partial b_i^{(2)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot w_i^{(3)} \cdot \sigma_2'(y_i^{(2)}) \cdot 1 \end{cases}$$



# Backward propagation



$$\begin{cases} \frac{\partial \mathcal{L}}{\partial w_{i,j}^{(1)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot \frac{\partial z}{\partial x_*^{(3)}} \cdot \frac{\partial x_*^{(3)}}{\partial y^{(2)}} \cdot \frac{\partial y^{(2)}}{\partial x^{(2)}} \cdot \frac{\partial x^{(2)}}{\partial y^{(1)}} \cdot \frac{\partial y^{(1)}}{\partial w_{i,j}^{(1)}} \\ \frac{\partial \mathcal{L}}{\partial b_i^{(1)}} = \frac{\partial \mathcal{L}}{\partial z} \cdot \frac{\partial z}{\partial x_*^{(3)}} \cdot \frac{\partial x_*^{(3)}}{\partial y^{(2)}} \cdot \frac{\partial y^{(2)}}{\partial x^{(2)}} \cdot \frac{\partial x^{(2)}}{\partial y^{(1)}} \cdot \frac{\partial y^{(1)}}{\partial b_i^{(1)}} \end{cases}$$

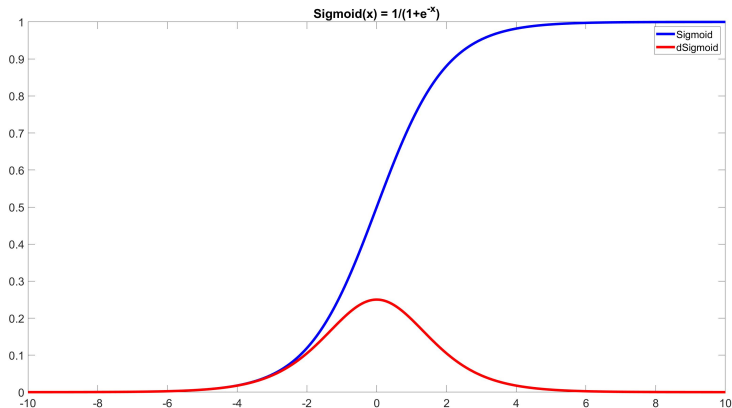
# Backward propagation

From the results in previous pages, we can have

$$\begin{aligned}
 \frac{\partial \mathcal{L}}{\partial w_{i,j}^{(1)}} &= \frac{\partial \mathcal{L}}{\partial z} \cdot \frac{\partial z}{\partial x_*^{(3)}} \cdot \frac{\partial x_*^{(3)}}{\partial y^{(2)}} \cdot \frac{\partial y^{(2)}}{\partial x^{(2)}} \cdot \frac{\partial x^{(2)}}{\partial y^{(1)}} \cdot \frac{\partial y^{(1)}}{\partial w_{i,j}^{(1)}} \\
 &= \frac{\partial \mathcal{L}}{\partial z} \cdot \left[ \left( w_1^{(3)} \cdot \sigma'_2(y_1^{(2)}) \cdot w_{1,1}^{(2)} + w_2^{(3)} \cdot \sigma'_2(y_2^{(2)}) \cdot w_{1,2}^{(2)} \right) \cdot \sigma'_1(y_1^{(1)}) \cdot x_1 \right] \\
 \frac{\partial \mathcal{L}}{\partial b_i^{(1)}} &= \frac{\partial \mathcal{L}}{\partial z} \cdot \frac{\partial z}{\partial x_*^{(3)}} \cdot \frac{\partial x_*^{(3)}}{\partial y^{(2)}} \cdot \frac{\partial y^{(2)}}{\partial x^{(2)}} \cdot \frac{\partial x^{(2)}}{\partial y^{(1)}} \cdot \frac{\partial y^{(1)}}{\partial b_i^{(1)}} \\
 &= \frac{\partial \mathcal{L}}{\partial z} \cdot \left[ \left( w_1^{(3)} \cdot \sigma'_2(y_1^{(2)}) \cdot w_{1,1}^{(2)} + w_2^{(3)} \cdot \sigma'_2(y_2^{(2)}) \cdot w_{1,2}^{(2)} \right) \cdot \sigma'_1(y_1^{(1)}) \cdot 1 \right]
 \end{aligned}$$

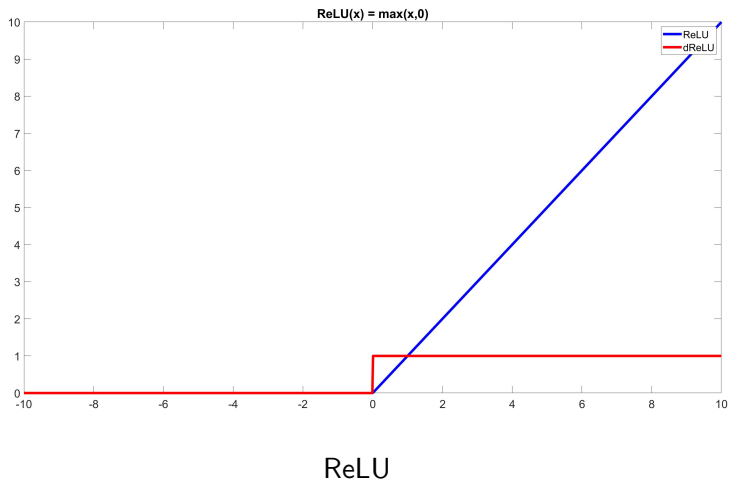
Finally, we can update the weights and biases by previous optimization method.

# Revisit activation functions

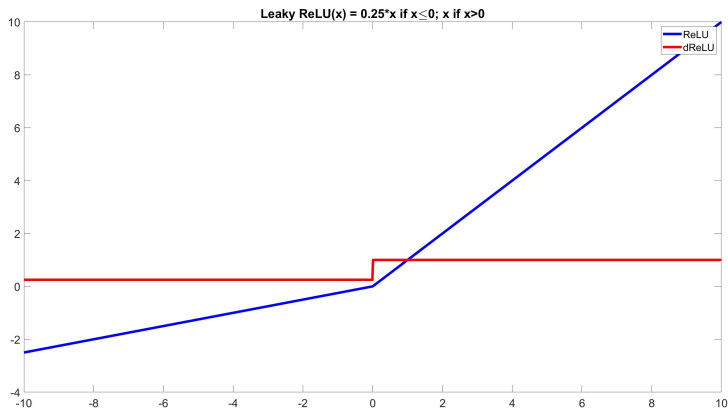


Sigmoid

# Revisit activation functions

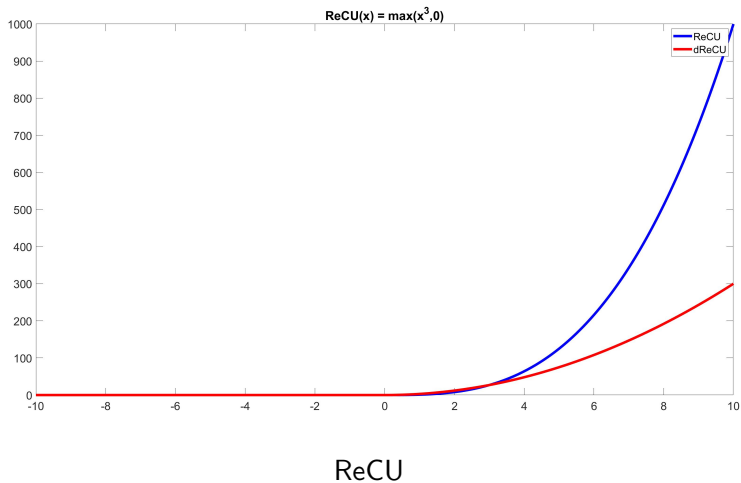


# Revisit activation functions

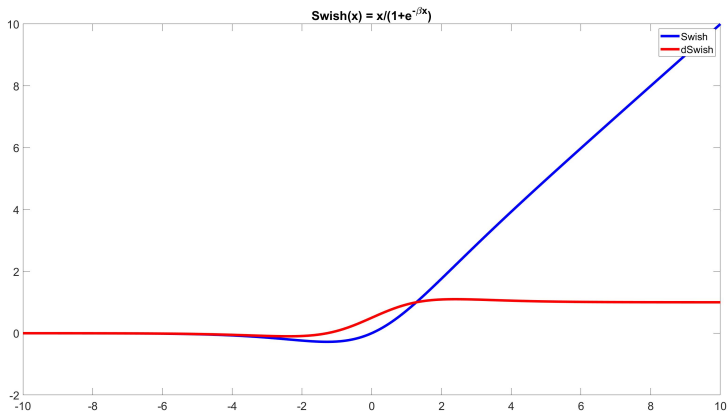


Leaky ReLU

# Revisit activation functions



# Revisit activation functions



Swish

# Poisson equation

Consider the Poisson equation with Dirichlet boundary conditions

$$\begin{cases} \Delta u = f, & \text{in } \Omega, \\ u = g, & \text{on } \partial\Omega \end{cases}$$

We implement following methods to solve the Poisson equation

- Deep Galerkin Method (DGM)
- Deep Ritz Method (DRM)



# Deep Galerkin Method (DGM)

## Loss function:

$$\begin{aligned}\mathcal{L}[u] &= \|\Delta u - f\|_{2,\Omega}^2 + \lambda \|u - g\|_{2,\partial\Omega}^2 \\ &= \int_{\Omega} (\Delta u - f)^2 dx + \lambda \int_{\partial\Omega} (u - g)^2 dx\end{aligned}$$

## Goal:

$$\min_{u \in \mathcal{F}} \mathcal{L}[u]$$

where  $\mathcal{F}$  is the class of neural networks.

# Monte Carlo approach

## Monte Carlo approach

$$I := \int_a^b f(x) dx = (b-a) \int_a^b f(x) \cdot \frac{1}{b-a} dx = (b-a) \mathbb{E}[f(X)]$$

where  $X \sim U(a, b)$ .

- 1 Generate  $X_1, \dots, X_N \stackrel{iid}{\sim} U(a, b)$
- 2 Compute  $\hat{I}_N = \frac{b-a}{N} \sum_{i=1}^N f(X_i)$

# Monte Carlo approach

- **Unbiased estimation:**

$$\mathbb{E}[\hat{I}_N] = \mathbb{E}\left[\frac{b-a}{N} \sum_{i=1}^N f(X_i)\right] = \frac{1}{N} \sum_{i=1}^N (b-a) \mathbb{E}[f(X_i)] = I$$

- **Probability convergence:**

By Law of Large Number, for any  $\varepsilon > 0$ , there exists  $N \in \mathbb{N}$  such that

$$\mathbb{P}(|\hat{I}_N - I| > \varepsilon) = 0$$

- **Convergent rate:** By Center Limit Theorem,

$$\frac{\hat{I}_N - I}{\frac{\sigma}{\sqrt{N}}} \xrightarrow{\mathcal{D}} \mathcal{N}(0, 1)$$

where  $\sigma$  is population standard deviation. The error convergence rate is  $\mathcal{O}(\frac{1}{\sqrt{N}})$ .

# Deep Galerkin Method (DGM)

$$\mathcal{L}[u] = |\Omega| \mathbb{E}_{x \sim p(x)} [(\Delta u(x) - f(x))^2] + \lambda |\partial\Omega| \mathbb{E}_{x \sim q(x)} [(u(x) - g(x))^2]$$

where  $p(x)$  is a uniform distribution on  $\Omega$  and  $q(x)$  is a uniform distribution on  $\partial\Omega$ .

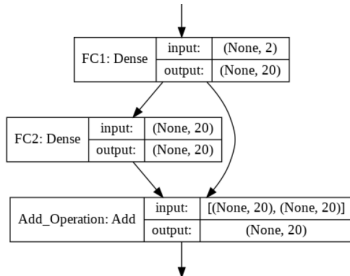
$$\mathcal{L}[u] = \frac{|\Omega|}{N} \sum_{i=1}^N [\Delta u(x_i) - f(x_i)]^2 + \lambda \frac{|\partial\Omega|}{M} \sum_{j=1}^M [u(t_j) - g(t_j)]^2$$

where  $x_i \in \Omega$  and  $t_j \in \partial\Omega$ , for all  $i = 1, 2, \dots, N$ ,  $j = 1, 2, \dots, M$ .

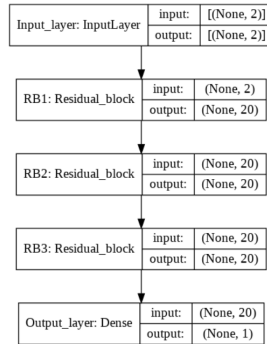
# Numerical result of DGM

## Information:

- Network: ResNet
- Activation function: Swish



Residual block structure



Model structure

# Numerical result of DGM

## Information (continue):

### Residual block (RB1)

Layer	Input shape	Output shape	parameters
FC1	(batch size, 2)	(batch size, 20)	60
FC2	(batch size, 20)	(batch size, 20)	420

### ResNet model

Layer	Input shape	Output shape	parameters
RB1	(batch size, 2)	(batch size, 20)	480
RB2	(batch size, 20)	(batch size, 20)	840
RB3	(batch size, 20)	(batch size, 20)	840
Output layer	(batch size, 20)	(batch size, 1)	21

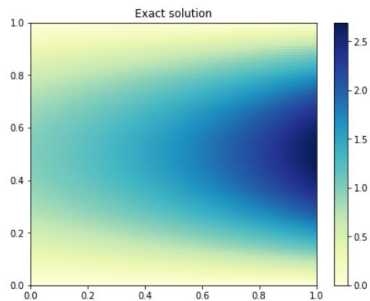
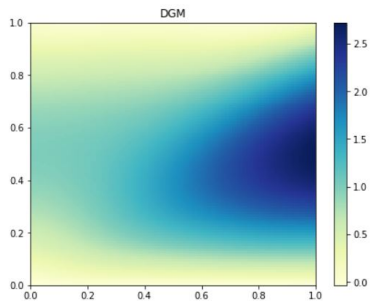
- Total parameters : 2181

# Numerical result of DGM

## Information (continue):

- Exact solution:  $u = e^x \sin(\pi y)$
- Epochs: 20000
- Learning rate:  $5e - 4$
- Penalty term:  $\lambda = 1$
- Number of training points: 110 (interior: 100 / boundary: 10)
- Number of testing points: 10000 (uniform mesh by  $100 \times 100$ )
- Device: Google Colab (GPU accelerated)
- Total time: 1200s (0.06 s/ep)

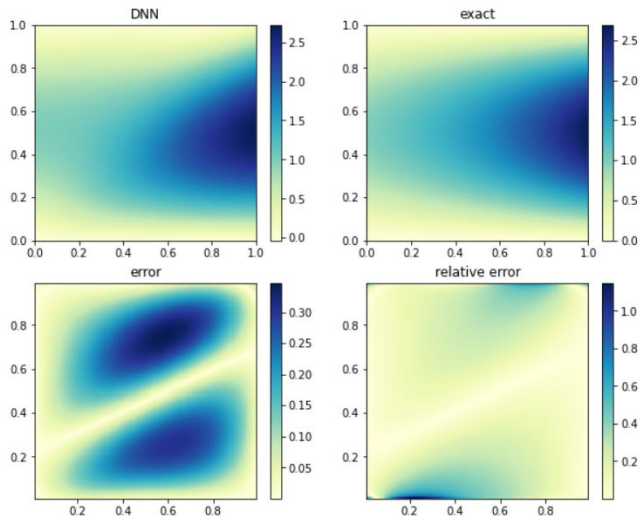
# Numerical result of DGM



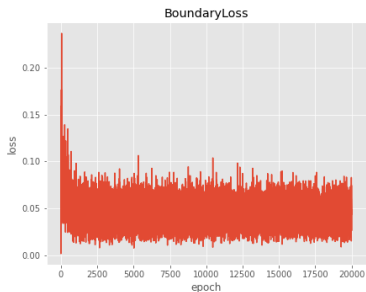
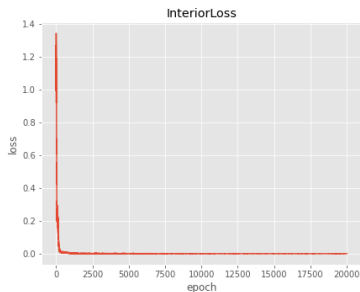
uniform mesh by  $100 \times 100$



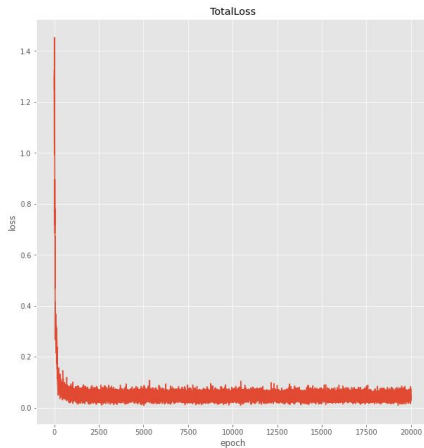
# Numerical result of DGM



# Numerical result of DGM



# Numerical result of DGM



# Numerical result of DGM

- Number of testing points:  $100 \times 100$

error \ epoch	5000	10000	20000
$\ U - u\ _{\infty}$	0.3253	0.3461	0.3668
$\ U - u\ _2$	0.1633	0.1657	0.1725
$\frac{\ U - u\ _2}{\ u\ _2}$	0.1296	0.1315	0.1369

# Deep Ritz Method (DRM)

## Loss function:

$$\mathcal{L}[u] = \int_{\Omega} \left( \frac{1}{2} |\nabla u|^2 + fu \right) dx + \lambda \int_{\partial\Omega} (u - g)^2 dx$$

## Goal:

$$\min_{u \in \mathcal{F}} \mathcal{L}[u]$$

where  $\mathcal{F}$  is the class of neural networks.

# Energy functional

Consider the functional

$$\mathcal{J}[v] = \int_{\Omega} \left( \frac{1}{2} |\nabla v|^2 + f v \right) dx =: \int_{\Omega} F[v] dx.$$

Suppose  $\mathcal{J}[v]$  has local minimum at  $u$ . Then for any  $w \in \mathcal{C}_0^{\infty}(\Omega)$ , we have

$$\mathcal{J}[u] \leq \mathcal{J}[u + \varepsilon w]$$

as  $\varepsilon$  closed to 0. Define  $\Phi(\varepsilon) = \mathcal{J}[u + \varepsilon w]$ . Then

$$\Phi'(0) = \left. \frac{d\Phi(\varepsilon)}{d\varepsilon} \right|_{\varepsilon=0} = \int_{\Omega} \left. \frac{dF[u + \varepsilon w]}{d\varepsilon} \right|_{\varepsilon=0} dx = 0$$

# Energy functional

Note that

$$F[u + \varepsilon w] = F[u] + \frac{1}{2}\varepsilon^2 |\nabla w|^2 + \varepsilon \nabla u \cdot \nabla w + \varepsilon f w$$

Then

$$\Phi'(0) = \int_{\Omega} (\varepsilon |\nabla w|^2 + \nabla u \cdot \nabla w + f w) \Big|_{\varepsilon=0} dx = 0$$

that is,

$$\int_{\Omega} (\nabla u \cdot \nabla w + f w) dx = 0$$

# Energy functional

## Green's first identity

$$\int_{\Omega} \Delta u w dx = \int_{\partial\Omega} \frac{\partial u}{\partial n} \cdot w ds - \int_{\Omega} \nabla u \cdot \nabla w dx$$

Since  $w \in C_0^\infty(\Omega)$ ,

$$\int_{\Omega} (-\Delta u + f) w dx = 0$$

Hence we can get

$$\Delta u = f.$$



# Deep Ritz Method (DRM)

$$\mathcal{L}[u] = |\Omega| \mathbb{E}_{x \sim p} \left[ \frac{1}{2} |\nabla u(x)|^2 + f(x)u(x) \right] + \lambda |\partial\Omega| \mathbb{E}_{x \sim q} [(u(x) - g(x))^2]$$

where  $p(x)$  is a uniform distribution on  $\Omega$  and  $q(x)$  is a uniform distribution on  $\partial\Omega$ .

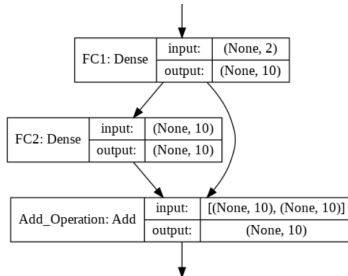
$$\mathcal{L}[u] = \frac{|\Omega|}{N} \sum_{i=1}^N \left[ \frac{1}{2} |\nabla u(x_i)|^2 + f(x_i)u(x_i) \right] + \lambda \frac{|\partial\Omega|}{M} \sum_{j=1}^M [u(t_j) - g(t_j)]^2$$

where  $x_i \in \Omega$  and  $t_j \in \partial\Omega$ , for all  $i = 1, 2, \dots, N$ ,  $j = 1, 2, \dots, M$ .

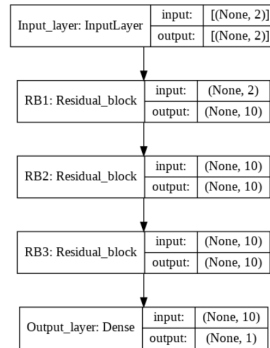
# Numerical result of DRM

## Information:

- Network: ResNet
- Activation function: ReCU



Residual block structure



Model structure

# Numerical result of DRM

## Information (continue):

### Residual block (RB1)

Layer	Input shape	Output shape	parameters
FC1	(batch size, 2)	(batch size, 10)	30
FC2	(batch size, 10)	(batch size, 10)	110

### ResNet model

Layer	Input shape	Output shape	parameters
RB1	(batch size, 2)	(batch size, 10)	140
RB2	(batch size, 10)	(batch size, 10)	220
RB3	(batch size, 10)	(batch size, 10)	220
Output layer	(batch size, 10)	(batch size, 1)	11

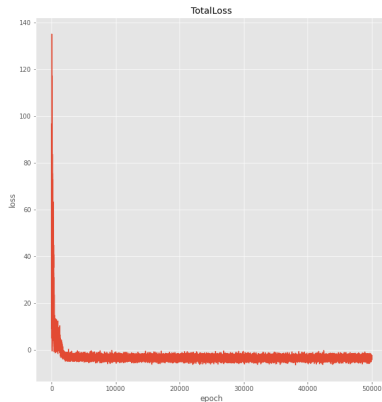
- Total parameters : 591

# Numerical result of DRM

## Information (continue):

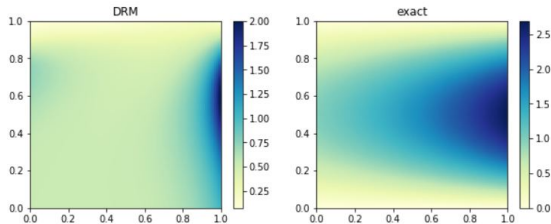
- Exact solution:  $u = e^x \sin(\pi y)$
- Epochs: 20000
- Learning rate:  $5e - 4$
- Penalty term:  $\lambda = 5000$
- Number of training points: 600 (interior: 500 / boundary: 100)
- Number of testing points: 10000 (uniform mesh by  $100 \times 100$ )
- Device: Google Colab (GPU accelerated)
- Total time: 400s (0.02 s/ep)

# Numerical result for DRM

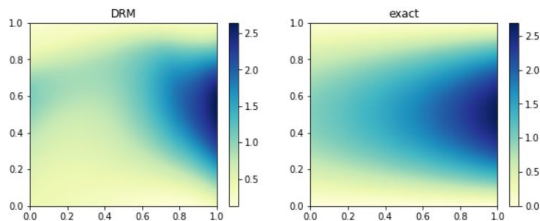


# Numerical result of DRM

epoch 1000

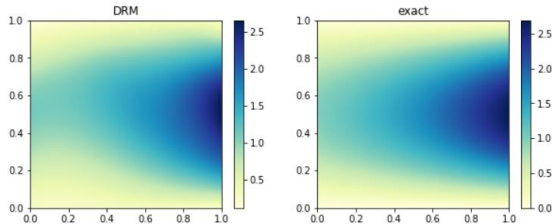


epoch 2500

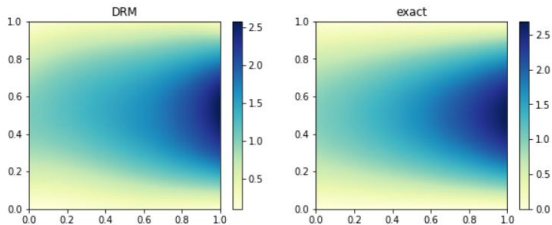


# Numerical result of DRM

epoch 5000

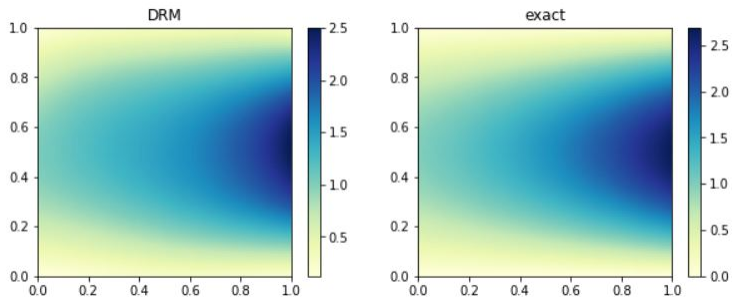


epoch 10000



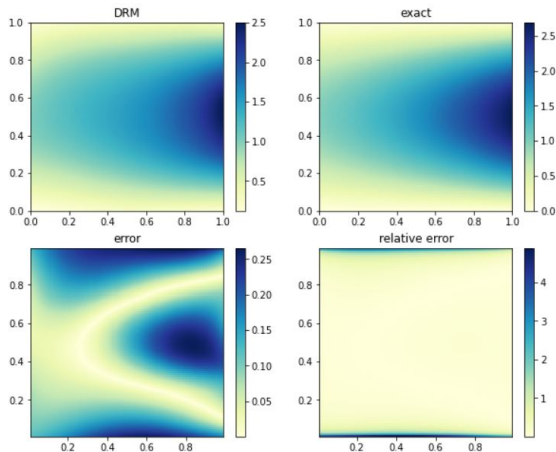
# Numerical result of DRM

epoch 20000





# Numerical result



# Numerical result of DRM

- Number of testing points:  $100 \times 100$

error \ epoch	5000	10000	20000
$\ U - u\ _{\infty}$	0.3329	0.2908	0.2911
$\ U - u\ _2$	0.1128	0.1112	0.1233
$\frac{\ U - u\ _2}{\ u\ _2}$	0.0896	0.0883	0.0979

# Biharmonic equation

Consider the Biharmonic equation with boundary conditions

$$\begin{cases} \Delta^2 u = f, & \text{in } \Omega, \\ u = g_0, & \text{on } \partial\Omega, \\ \frac{\partial u}{\partial n} = g_1, & \text{on } \partial\Omega \end{cases}$$

To make the calculation easier, we rewrite the equation as following,

$$\begin{cases} \Delta u = p, & \text{in } \Omega, \\ \Delta p = f, & \text{in } \Omega, \\ u = g_0, & \text{on } \partial\Omega, \\ \frac{\partial u}{\partial n} = g_1, & \text{on } \partial\Omega \end{cases}$$

# DGM for biharmonic equation

## Loss function:

$$\begin{aligned}\mathcal{L}[u] = & \|\Delta u - p\|_{2,\Omega}^2 + \|\Delta p - f\|_{2,\Omega}^2 \\ & + \alpha \|u - g_0\|_{2,\partial\Omega}^2 + \beta \|(\nabla u \cdot n) - g_1\|_{2,\partial\Omega}^2\end{aligned}$$

By Monte Carlo approach,

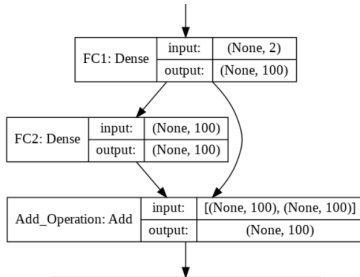
$$\begin{aligned}\mathcal{L}[u] = & \frac{|\Omega|}{N} \sum_{i=1}^N [\Delta u(x_i) - p(x_i)]^2 + \frac{|\Omega|}{N} \sum_{i=1}^N [\Delta p(x_i) - f(x_i)]^2 \\ & + \alpha \frac{|\partial\Omega|}{M} \sum_{j=1}^M [u(t_j) - g_0(t_j)]^2 + \beta \frac{|\partial\Omega|}{M} \sum_{j=1}^M [\nabla u(t_j) \cdot n(t_j) - g_1(t_j)]^2\end{aligned}$$

where  $x_i \in \Omega$  and  $t_j \in \partial\Omega$ , for all  $i = 1, 2, \dots, N$ ,  $j = 1, 2, \dots, M$ .

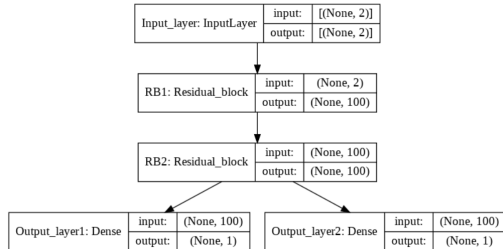
# Numerical result of DGM

## Information:

- Network: ResNet
- Activation function: Swish



Residual block structure



Model structure

# Numerical result of DGM

## Information (continue):

### Residual block (RB1)

Layer	Input shape	Output shape	parameters
FC1	(batch size, 2)	(batch size, 100)	300
FC2	(batch size, 100)	(batch size, 100)	10100

### ResNet model

Layer	Input shape	Output shape	parameters
RB1	(batch size, 2)	(batch size, 100)	10400
RB2	(batch size, 100)	(batch size, 100)	20200
Output layer1	(batch size, 100)	(batch size, 1)	101
Output layer2	(batch size, 100)	(batch size, 1)	101

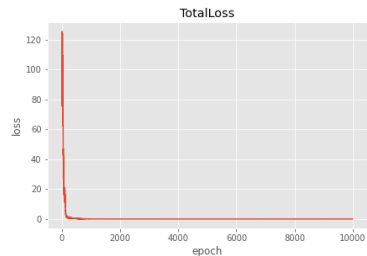
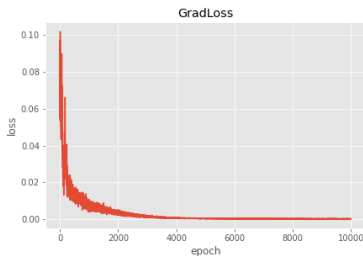
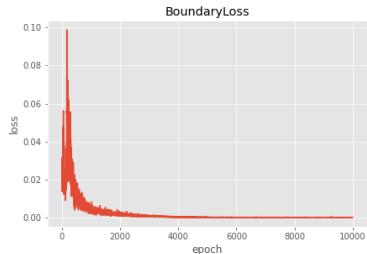
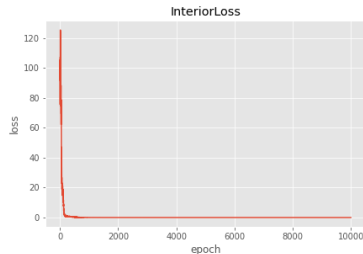
- Total parameters : 30802

# Numerical result of DGM

## Information (continue):

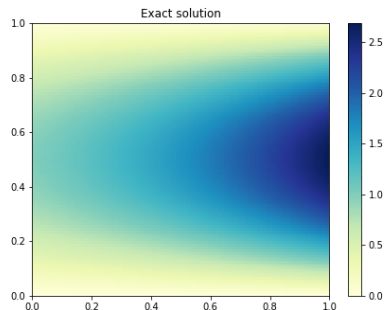
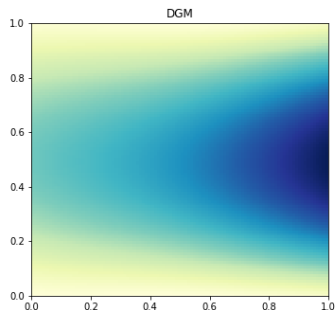
- Exact solution:  $u = e^x \sin(\pi y)$
- Epochs: 10000
- Learning rate:  $5e - 4$
- Penalty term:  $\lambda = 1$
- Number of training points: 130 (interior: 100 / boundary: 30)
- Number of testing points: 10000 (uniform mesh by  $100 \times 100$ )
- Device: Google Colab (GPU accelerated)
- Total time: 1040s (0.1 s/ep)

# Numerical result of DGM



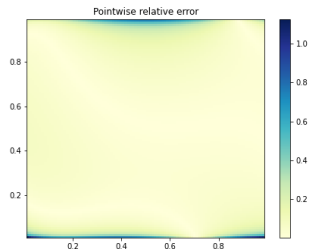
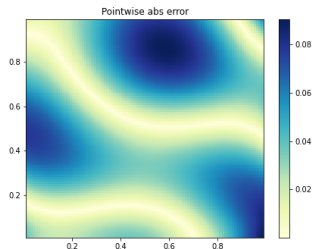
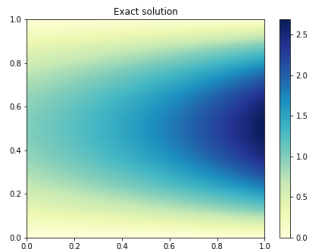
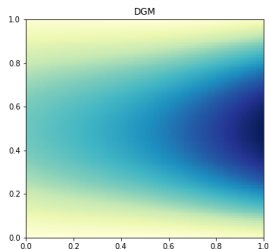


# Numerical result of DGM



uniform mesh by  $100 \times 100$

# Numerical result of DGM



# Numerical result of DGM

- Number of training points:  $100 + 30 / \text{ep}$
- Number of testing points:  $100 \times 100$

error \ epoch	2000	4000	6000	8000	10000
$\ U - u\ _\infty$	0.4190	0.1517	0.1456	0.1085	0.0993
$\ U - u\ _2$	0.1419	0.0701	0.0542	0.0519	0.0452
$\frac{\ U - u\ _2}{\ u\ _2}$	0.1126	0.0556	0.0430	0.0412	0.0359

# Numerical result of DGM

- Number of testing points:  $100 \times 100$
- Error: relative error of two norm

$T_p \setminus \text{epoch}$	2000	4000	6000	8000	10000
100/10	0.0619	0.0426	0.0408	0.0421	0.0391
400/20	0.0417	0.0316	0.0357	0.0331	0.0270
900/30	0.0363	0.0257	0.0347	0.0278	0.0264

# Numerical result of DGM

- Epochs: 10000
- Number of training points:  $100 + 30 / \text{ep}$
- Number of testing points:  $100 \times 100$

error	Swish	Sigmoid	ReLU
$\ U - u\ _\infty$	0.0993	0.2292	0.0723
$\ U - u\ _2$	0.0452	0.0897	0.0220
$\frac{\ U - u\ _2}{\ u\ _2}$	0.0359	0.0712	0.0175

# Code on Github

- Poisson DGM:

[https://github.com/Jia-wei-liao/NPDE\\_final\\_project/blob/main/DGM\\_Poisson2D.ipynb](https://github.com/Jia-wei-liao/NPDE_final_project/blob/main/DGM_Poisson2D.ipynb)

- Possion DRM:

[https://github.com/Jia-wei-liao/NPDE\\_final\\_project/blob/main/DRM\\_Poisson2D.ipynb](https://github.com/Jia-wei-liao/NPDE_final_project/blob/main/DRM_Poisson2D.ipynb)

- Biharmonic DGM:

[https://github.com/Jia-wei-liao/NPDE\\_final\\_project/blob/main/DGM\\_Biharmonic2D.ipynb](https://github.com/Jia-wei-liao/NPDE_final_project/blob/main/DGM_Biharmonic2D.ipynb)

# References

- Jingrun Chen, Rui Du and Keke Wu, A Comparison Study of Deep Galerkin Method and Deep Ritz Method for Elliptic Problems with Different Boundary Conditions (2020).
- Liyao Lyu, Zhen Zhangc, Minxin Chen, Jingrun Chen, MIM: A deep mixed residual method for solving high-order partial differential equations (2020).
- Weinan E and Bing Yu, The Deep Ritz method: A deep learning-based numerical algorithm for solving variational problems (2017).

THE END

**Thanks for listening!**