Neural networks and isogeometric analysis



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Physics Informed Neural Networks Variational Physics Informed Neural Networks

- M. Raissi, P. Perdikaris, G.E.Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear PDEs, **Journal of Computational Physics** 378(1) (2019)
- E. Kharazmi, Z. Zhang, G. E. Karniadakis, Variational Physics-Informed Neural Networks For Solving PDEs arxiv.org/abs/1912.00873 (2019)
- K. Doległo, A. Paszyńska, M. Paszyński, L. Demkowicz, Deep neural networks for smooth approximation of physics with higher order and continuity B-spline base functions, https://arxiv.org/abs/2201.00904 (2022)

Physics Informed Neural Networks for strong form of PDE

Strong form: Find $u \in C^2(0,1)$:

$$\underbrace{-\epsilon \frac{d^2 u(x)}{dx^2}}_{\text{diffusion} = \epsilon} \underbrace{+1 \frac{du(x)}{dx}}_{\text{advection"wind"} = 1} = 0, x \in (0, 1), -\epsilon \frac{du}{dx}(0) + u(0) = 1.0, \ u(1) = 0$$

Now, neural network IS the solution

$$u(x) = NN(x) = A_n \sigma (A_{n-1} \sigma (... \sigma (A_1 x + B_1)... + B_{n-1}) + B_n$$

$$LOSS_{PDE}(x) = \left(-\epsilon \frac{d^{2}NN(x)(x)}{dx^{2}} + \frac{dNN(x)(x)}{dx}\right)^{2},$$

$$LOSS_{BC0} = \left(-\epsilon \frac{dNN(0)}{dx} + NN(0) - 1.0\right)^{2},$$

$$LOSS_{BC1} = (NN(1)s)^{2},$$

$$LOSS(x) = (LOSS_{PDE}(x)^{2} + LOSS_{BC0}^{2} + LOSS_{BC1}^{2}).$$

- $\epsilon = 1.0$, #N = number of points = 10 (selected randomly at beginning of each epoch)
 - One epoch is: random selection of 10 points, evaluation of LOSS functions at the 10 points. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis $= x \in (0, 1)$, vertical axis = NN(x)).
- ② $\epsilon = 1.0$, #N = number of points = 100 (selected randomly at beginning of each epoch)
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- $\epsilon = 0.1$, #N = number of points = 10 (selected randomly at beginning of each epoch)
 - One epoch is: random selection of 10 points, evaluation of LOSS functions at the 10 points. Please run 100 epochs.
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- $\epsilon = 0.01$, #N = number of points = 10 (selected randomly at beginning of each epoch)
 - One epoch is: random selection of 10 points, evaluation of LOSS functions at the 10 points. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
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- $\epsilon = 1.0$, #N = number of points = 10 (now, 10 points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. (0, 0.5, 0.75, 0,875, 0,9375, 0,96875, 0,984375, 0,9921875, 0,99609375, 1.0)
 - One epoch is: 10 adaptive points, evaluation of LOSS functions at the 10 points. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

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 - One epoch is: 100 adaptive points, evaluation of LOSS functions at the 100 points. Please run 100 epochs.
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- **1** $\epsilon = 0.1$, #N = number of points = 10 (now, 10 points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. (0, 0.5, 0.75, 0,875, 0,9375, 0,96875, 0,984375, 0,9921875, 0,99609375, 1.0)
 - One epoch is: 10 adaptive points, evaluation of LOSS functions at the 10 points. Please run 100 epochs.
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 - One epoch is: 100 adaptive points, evaluation of LOSS functions at the 100 points. Please run 100 epochs.
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Variational Physics Informed Neural Networks for weak form of PDE

Weak form: Find $u \in H^1(0,1)$:

$$\int_0^1 \epsilon \frac{du(x)}{dx} \frac{dv(x)}{dx} dx + \int_0^1 \frac{du(x)}{dx} v(x) dx + u(0)v(0) = v(0)$$

$$\forall v \in V$$

Now, neural network IS the solution

$$u(x) = NN(x) = A_{n}\sigma (A_{n-1}\sigma(...\sigma(A_{1}x + B_{1})... + B_{n-1}) + B_{n}$$

$$b_{weak}(v) = \int \left(\epsilon \frac{dNN(x)}{dx} \frac{dv}{dx} + \frac{dNN(x)}{dx}v\right) dx + NN(0)v(0),$$

$$l_{weak}(v) = v(0), LOSS_{weak}(v) = (b_{weak}(v) - l_{weak}(v))^{2},$$

$$LOSS_{BC0} = (-\epsilon \frac{dNN(0)}{dx} + NN(0) - 1.0)^{2}, \quad LOSS_{BC1} = (NN(1))^{2},$$

$$LOSS(v) = LOSS_{strong}(x) + LOSS_{weak} + LOSS_{BC0} + LOSS_{BC1}.$$

- **1** $\epsilon = 1.0$, #N = number of intervals = 10 [0 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.0] (linear B-splines based on 11 knot points)
 - One epoch is: test with 11 test functions build from 11 knot points, evaluation of LOSS functions with 11 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).
- ② $\epsilon = 1.0$, #N = number of intervals = 100 [0 0 0.01 0.02 0.03 ... 0.98 0.99 1.0 1.0] (linear B-splines based on 101 knot points)
 - One epoch is: test with 101 test functions build from 101 knot points, evaluation of LOSS functions with 101 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)

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• Please measure the total time of training

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• Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0, 1)$, vertical axis = NN(x)).

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- **1** $\epsilon = 1.0$, #N = number of intervals = 1000 [0 0 0.001 0.002 0.003 ... 0.998 0.999 1.0 1.0] (linear B-splines based on 1001 knot points)
 - One epoch is: test with 1001 test functions build from 1001 knot points, evaluation of LOSS functions with 1001 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis $= x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon = 1.0$, #N = number of intervals = 10 [0 0 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.0 1.0] (quadratic B-splines based on 11 knot points)
 - One epoch is: test with 12 test functions build from 11 knot points, evaluation of LOSS functions with 12 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).
- ② $\epsilon = 1.0$, #N = number of intervals = 100 [0 0 0 0.01 0.02 0.03 ... 0.98 0.99 1.0 1.0 1.0] (quadratic B-splines based on 101 knot points)
 - One epoch is: test with 102 test functions build from 101 knot points, evaluation of LOSS functions with 102 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)

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• Please measure the total time of training

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• Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0, 1)$, vertical axis = NN(x)).

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- ϵ = 1.0, #N = number of intervals = 1000 [0 0 0.001 0.002 0.003 ... 0.998 0.999 1.0 1.0 1.0] (quadratic B-splines based on 1002 knot points)
 - One epoch is: test with 1002 test functions build from 1002 knot points, evaluation of LOSS functions with 1002 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon = 1.0$, #N = number of intervals = 10 [0 0 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.0 1.0 1.0] (cubic B-splines based on 11 knot points)
 - One epoch is: test with 11 test functions build from 13 knot points, evaluation of LOSS functions with 13 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis $= x \in (0,1)$, vertical axis = NN(x)).
- ② $\epsilon = 1.0$, #N = number of intervals = 100 [0 0 0 0.01 0.02 0.03 ... 0.98 0.99 1.0 1.0 1.0 1.0] (cubic B-splines based on 101 knot points)
 - One epoch is: test with 103 test functions build from 101 knot points, evaluation of LOSS functions with 103 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best

- ϵ = 1.0, #N = number of intervals = 1000 [0 0 0 0.001 0.002 0.003 ... 0.998 0.999 1.0 1.0 1.0 1.0] (cubic B-splines based on 1003 knot points)
 - One epoch is: test with 1003 test functions build from 1003 knot points, evaluation of LOSS functions with 1003 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon = 0.1$, #N = number of points = 10 (now, 11 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. [0 0 0.5 0.75 0.875 0.9375 0.96875 0.984375 0.9921875 0,99609375 0,998046875 1.0 1.0] We use linear B-splines
 - One epoch is: 11 linear B-splines, evaluation of LOSS functions with 11 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon = 0.1$, #N = number of points = 100 (now, 101 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i - x_{i-1})/2$, e.g. (99 intervals) [0 0 0.5 0.75 0.875 0.9375 0.96875 0.984375 0.9921875 0.99609375 0.998046875 ... 1.0 1.0] We use linear B-splines
 - One epoch is: 101 linear B-splines, evaluation of LOSS functions with 101 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).
- \bullet $\epsilon = 0.1$, #N = number of points = 1000 (now, 1001 test functions are distributed as x_i , where $x_0 = 0$, $x_i = x_{i-1} + (x_i - x_{i-1})/2$, e.g. (999 intervals) [0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0] We use linear B-splines
 - One epoch is: 1001 linear B-splines, evaluation of LOSS functions at the 1001 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training

- **1** $\epsilon = 0.1$, #N = number of points = 10 (now, 11 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. [0 0 0 0.5 0.75 0.875 0.9375 0.96875 0.984375 0.9921875 0.99609375 0.998046875 1.0 1.0 1.0] We use quadratic B-splines
 - One epoch is: 12 quadratic B-splines, evaluation of LOSS functions with 12 test functions. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
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- $\epsilon=0.1$, #N= number of points =101 (now, 101 knot points are distributed as x_i , where $x_0=0$, $x_1=\frac{1}{2}$, $x_i=x_{i-1}+(x_i-x_{i-1})/2$, e.g. (100 intervals) [0 0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0 1.0] We use quadratic B-splines
 - One epoch is: 102 quadratic B-splines, evaluation of LOSS functions with 102 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).
- ② $\epsilon = 0.1$, #N = number of points = 1001 (now, 1001 knot points are distributed as x_i , where $x_0 = 0$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. (999 intervals) [0 0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0 1.0] We use quadratic B-splines
 - One epoch is: 1002 quadratic B-splines, evaluation of LOSS functions with 1002 test functions. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training

- $\epsilon = 0.1$, #N = number of points = 10 (now, 11 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. [0 0 0 0.5 0.75 0.875 0.9375 0.96875 0.984375 0.9921875 0.99609375 0.998046875 1.0 1.0 1.0 1.0] We use cubic B-splines
 - One epoch is: 13 cubic B-splines, evaluation of LOSS functions with 13 test functions. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon = 0.1$, #N = number of points = 101 (now, 101 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i - x_{i-1})/2$, e.g. (100 intervals) [0 0 0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0 1.0 1.0] We use cubic B-splines
 - One epoch is: 103 cubic B-splines, evaluation of LOSS functions with 103 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).
- \bullet $\epsilon = 0.1$, #N = number of points = 1001 (now, 1001 knot points are distributed as x_i , where $x_0 = 0$, $x_i = x_{i-1} + (x_i - x_{i-1})/2$, e.g. (999) intervals) [0 0 0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0 1.0 1.0] We use cubic B-splines
 - One epoch is: 1003 cubic B-splines, evaluation of LOSS functions with 1003 test functions. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training

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- **1** $\epsilon = 0.01$, #N = number of points = 10 (now, 11 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. [0 0 0.5 0.75 0.875 0.9375 0.96875 0.984375 0.9921875 0,99609375 0,998046875 1.0 1.0] We use linear B-splines
 - One epoch is: 11 linear B-splines, evaluation of LOSS functions with 11 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- $\epsilon = 0.01$, #N = number of points = 100 (now, 101 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i - x_{i-1})/2$, e.g. (99 intervals) [0 0 0.5 0.75 0.875 0.9375 0.96875 0.984375 0.9921875 0.99609375 0.998046875 ... 1.0 1.0] We use linear B-splines
 - One epoch is: 101 linear B-splines, evaluation of LOSS functions with 101 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).
- \bullet $\epsilon = 0.01$, #N = number of points = 1000 (now, 1001 test functions are distributed as x_i , where $x_0 = 0$, $x_i = x_{i-1} + (x_i - x_{i-1})/2$, e.g. (999 intervals) [0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0] We use linear B-splines
 - One epoch is: 1001 linear B-splines, evaluation of LOSS functions at the 1001 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)

Please measure the total time of training

- $\epsilon = 0.01$, #N = number of points = 10 (now, 11 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. [0 0 0 0.5 0.75 0.875 0.9375 0.96875 0.984375 0.9921875 0.99609375 0.998046875 1.0 1.0 1.0] We use quadratic B-splines
 - One epoch is: 12 quadratic B-splines, evaluation of LOSS functions with 12 test functions. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon = 0.01$, #N = number of points = 101 (now, 101 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i - x_{i-1})/2$, e.g. (100 intervals) [0 0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0 1.0] We use quadratic B-splines
 - One epoch is: 102 quadratic B-splines, evaluation of LOSS functions with 102 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).
- \bullet $\epsilon = 0.01$, #N = number of points = 1001 (now, 1001 knot points are distributed as x_i , where $x_0 = 0$, $x_i = x_{i-1} + (x_i - x_{i-1})/2$, e.g. (999) intervals) [0 0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0 1.0] We use quadratic B-splines
 - One epoch is: 1002 quadratic B-splines, evaluation of LOSS functions with 1002 test functions. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training

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- $\epsilon = 0.01$, #N = number of points = 10 (now, 11 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. [0 0 0 0.5 0.75 0.875 0.9375 0.96875 0.984375 0.9921875 0.99609375 0.998046875 1.0 1.0 1.0 1.0] We use cubic B-splines
 - One epoch is: 13 cubic B-splines, evaluation of LOSS functions with 13 test functions. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- $\epsilon = 0.01$, #N = number of points = 101 (now, 101 knot points are distributed as x_i , where $x_0 = 0$, $x_1 = \frac{1}{2}$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. (100 intervals) [0 0 0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0 1.0 1.0] We use cubic B-splines
 - One epoch is: 103 cubic B-splines, evaluation of LOSS functions with 103 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).
- ② $\epsilon = 0.01$, #N = number of points = 1001 (now, 1001 knot points are distributed as x_i , where $x_0 = 0$, $x_i = x_{i-1} + (x_i x_{i-1})/2$, e.g. (999 intervals) [0 0 0 0 0.5 0.75 0.875 0.9375 ... 1.0 1.0 1.0 1.0] We use cubic B-splines
 - One epoch is: 1003 cubic B-splines, evaluation of LOSS functions with 1003 test functions. Please run 100 epochs.
 - Please plot the convergence of PINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)

Neural networks and isogeometric analysis

Please measure the total time of training

Maciej Paszyński et.al.

Select a single hest solution (where the loss functions was minimial)

May 5, 2023

IGA-DNN-VPINN

Weak form: Find $u \in H^1(0,1)$:

$$\int_0^1 \epsilon \frac{du(x)}{dx} \frac{dv(x)}{dx} dx + \int_0^1 \frac{du(x)}{dx} v(x) dx + u(0)v(0) = v(0)$$

$$\forall v \in V$$

Now, we plug a combination of B-splines in place of the solution $u(x) = \sum_{i=1,...,N} u_i B_{i,p}(x)$

$$\begin{split} b_{weak}(v) &= \int \left(\epsilon \sum_{i} u_{i} \frac{dB_{i,p}(x)}{dx} \frac{dv}{dx} + \sum_{i} u_{i} \frac{dB_{i,p}(x)}{dx} v \right) dx + u_{1}v(0), \\ I_{weak}(v) &= v(0), LOSS_{weak}(v) = (b_{weak}(v) - I_{weak}(v))^{2}, \\ LOSS_{BC0} &= (-\epsilon u_{1} \frac{dB_{i,p}(0)}{dx} + u_{1} - 1.0)^{2}, LOSS_{BC1} = (u_{N})^{2}, \\ LOSS(v) &= LOSS_{strong}(x) + LOSS_{weak} + LOSS_{BC0} + LOSS_{BC1}. \end{split}$$

Experiments

All the experiments like in VPINN

Parametric-IGA-VPINN

Weak form: Find $u \in H^1(0,1)$:

$$\int_0^1 \epsilon \frac{du(x)}{dx} \frac{dv(x)}{dx} dx + \int_0^1 \frac{du(x)}{dx} v(x) dx + u(0)v(0) = v(0)$$

$$\forall v \in V$$

Now, NN input is ϵ , NN output are N coefficients of B-splines $\epsilon \to NN(\epsilon)_i \quad u(x) = \sum_{i=1,\dots,N} NN(\epsilon)_i B_{i,p}(x)$

$$b_{weak}(v) = \int \left(\epsilon \sum_{i} NN(\epsilon)_{i} \frac{dB_{i,p}(x)}{dx} \frac{dv}{dx} + \sum_{i} NN(\epsilon)_{i} \frac{dB_{i,p}(x)}{dx} v \right) dx + NN(\epsilon)_{1} v(0), \quad I_{weak}(v) = v(0)$$

$$LOSS_{weak}(v) = (b_{weak}(v) - l_{weak}(v))^{2}.$$

$$LOSS_{BC0} = (-\epsilon NN(\epsilon)_1 \frac{dB_{1,p}(0)}{d\epsilon} + NN(\epsilon)_1 - 1.0)^2, LOSS_{BC1} = (NN(\epsilon)_N)^2,$$

$$LOSS(v) = LOSS_{strong}(x) + LOSS_{weak} + LOSS_{BC0} + LOSS_{BC1}.$$

- **1** $\epsilon \in (0.01, 1.0)$, #N = number of intervals = 10 [0 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.0] (linear B-splines based on 11 knot points)
 - One epoch is: test with 11 test functions build from 11 knot points, evaluation of LOSS functions with 11 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solutions for $\epsilon = 0.01$, for $\epsilon = 0.1$, and for $\epsilon = 1.0$ (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon \in (0.01, 1.0), \#N = \text{number of intervals} = 100 [0 \ 0.01 \ 0.02 \ 0.03 \ ... \ 0.98 \ 0.99 \ 1.0 \ 1.0]$ (linear B-splines based on 101 knot points)
 - One epoch is: test with 101 test functions build from 101 knot points, evaluation of LOSS functions with 101 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution for $\epsilon = 0.01$, for $\epsilon = 0.1$, and for $\epsilon = 1.0$ (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon \in (0.01, 1.0), \#N = \text{number of intervals} = 1000 [0 \ 0.001 \ 0.002 \ 0.003 \dots 0.998 \ 0.999 \ 1.0 \ 1.0]$ (linear B-splines based on 1001 knot points)
 - One epoch is: test with 1001 test functions build from 1001 knot points, evaluation of LOSS functions with 1001 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution for $\epsilon=0.01$, for $\epsilon=0.1$, and for $\epsilon=1.0$ (horizontal axis = $x\in(0,1)$, vertical axis = NN(x)).

- $\epsilon \in (0.01, 1.0)$, #N = number of intervals = 10 [0 0 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.0 1.0] (quadratic B-splines based on 11 knot points)
 - One epoch is: test with 12 test functions build from 11 knot points, evaluation of LOSS functions with 12 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solutions for $\epsilon=0.01$, for $\epsilon=0.1$, and for $\epsilon=1.0$ (horizontal axis = $x\in(0,1)$, vertical axis = NN(x)).

- **1** $\epsilon \in (0.01, 1.0)$, #N = number of intervals = 100 [0 0 0.01 0.02 0.03 ... 0.98 0.99 1.0 1.0 1.0] (quadratic B-splines based on 101 knot points)
 - One epoch is: test with 102 test functions build from 101 knot points, evaluation of LOSS functions with 102 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution for $\epsilon=0.01$, for $\epsilon=0.1$, and for $\epsilon=1.0$ (horizontal axis = $x\in(0,1)$, vertical axis = NN(x)).

- $\epsilon \in (0.01, 1.0)$, #N = number of intervals = 1000 [0 0 0 0.001 0.002 0.003 ... 0.998 0.999 1.0 1.0 1.0] (quadratic B-splines based on 1001 knot points)
 - One epoch is: test with 1002 test functions build from 1001 knot points, evaluation of LOSS functions with 1002 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution for $\epsilon=0.01$, for $\epsilon=0.1$, and for $\epsilon=1.0$ (horizontal axis = $x\in(0,1)$, vertical axis = NN(x)).

- $\epsilon \in (0.01, 1.0)$, #N = number of intervals = 10 [0 0 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.0 1.0 1.0] (cubic B-splines based on 11 knot points)
 - One epoch is: test with 13 test functions build from 11 knot points, evaluation of LOSS functions with 13 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solutions for $\epsilon=0.01$, for $\epsilon=0.1$, and for $\epsilon=1.0$ (horizontal axis = $x \in (0,1)$, vertical axis = NN(x)).

- **1** $\epsilon \in (0.01, 1.0)$, #N = number of intervals = 100 [0 0 0 0.01 0.02 0.03 ... 0.98 0.99 1.0 1.0 1.0 1.0] (cubic B-splines based on 101 knot points)
 - One epoch is: test with 103 test functions build from 101 knot points, evaluation of LOSS functions with 103 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution for $\epsilon=0.01$, for $\epsilon=0.1$, and for $\epsilon=1.0$ (horizontal axis = $x\in(0,1)$, vertical axis = NN(x)).

- **1** $\epsilon \in (0.01, 1.0)$, #N = number of intervals = 1000 [0 0 0 0 0.001 0.002 0.003 ... 0.998 0.999 1.0 1.0 1.0 1.0] (cubic B-splines based on 1001 knot points)
 - One epoch is: test with 1003 test functions build from 1001 knot points, evaluation of LOSS functions with 1003 test functions. Please run 100 epochs.
 - Please plot the convergence of VPINN training (horizontal axis = number of epochs, vertical axis = LOSS function value)
 - Please measure the total time of training
 - Select a single best solution (where the loss functions was minimial). It does not have to be the last point of training! Please plot the best solution for $\epsilon=0.01$, for $\epsilon=0.1$, and for $\epsilon=1.0$ (horizontal axis = $x\in(0,1)$, vertical axis = NN(x)).

Eriksson-Johnson model problem

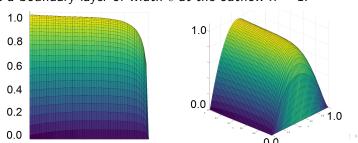
Given $\Omega = (0,1)^2$, $\beta = (1,0)^T$, we seek the solution of the advection-diffusion problem

$$\frac{\partial u}{\partial x} - \epsilon \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0$$

with Dirichlet boundary conditions

$$u = 0 \text{ for } x \in (0,1), y \in \{0,1\}$$
 $u = sin(\Pi y) \text{ for } x = 0$

The problem is driven by the inflow Dirichlet boundary condition. It develops a boundary layer of width ϵ at the outflow x=1.



Experiments'

All the methods and experiments as for 1D problem, but for VPINN experiments we use knot vector $[0\ 0\ 0.25\ 0.5\ 0.75\ 1.0\ 1.0]$ in y direction for linear B-splines, $[0\ 0\ 0\ 0.25\ 0.5\ 0.75\ 1.0\ 1.0\ 1.0]$ in y direction for quadratic B-splines, and $[0\ 0\ 0\ 0.25\ 0.5\ 0.75\ 1.0\ 1.0\ 1.0\ 1.0]$ in y direction for cubic B-splines. The knot vectors in x directions identical as for 1D problem.

Physics Informed Neural Networks for strong form of PDE

Strong form: Given
$$\Omega = (0,1)^2$$
, $\beta = (1,0)^T$, we seek $\Omega \ni (x,y) \to u(x,y)$ such that $\frac{\partial u}{\partial x} - \epsilon \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0$ with Dirichlet boundary conditions $u = 0$ for $x \in (0,1), y \in \{0,1\}$ $u = sin(\Pi y)$ for $x = 0$

Now, neural network IS the solution

$$u(x,y) = NN(x,y) = A_{n}\sigma \left(A_{n-1}\sigma(...\sigma(A_{1} \begin{bmatrix} x \\ y \end{bmatrix} + B_{1})... + B_{n-1} \right) + B_{n}$$

$$LOSS_{PDE}(x,y) = \left(\frac{\partial NN(x,y)}{\partial x} - \epsilon \frac{\partial^{2}NN(x,y)(x)}{\partial x^{2}} + -\epsilon \frac{\partial^{2}NN(x,y)(x)}{\partial y^{2}} \right)^{2},$$

$$LOSS_{BC0y}(0,y) = \left(NN(0,y) - \sin(\Pi y) \right)^{2}, LOSS_{BC1y}(1,y) = \left(NN(1,y) \right)^{2},$$

$$LOSS_{BCx0}(x,0) = \left(NN(x,0) \right)^{2}, LOSS_{BCx1}(x,1) = \left(NN(x,1) \right)^{2},$$

$$LOSS(x,y) = LOSS_{PDE}(x,y) + LOSS_{BC0y}(0,y) + LOSS_{BC1y}(1,y) +$$

$$+ LOSS_{BCx0}(x,0) + LOSS_{BCx1}(x,1)$$

Variational Physics Informed Neural Networks for weak form of PDE

Weak form: Find
$$u \in H^1([0,1]^2)$$
: $b(u,v) = l(v)$

$$b(u,v) = \int_{[0,1]^2} \epsilon \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} dx dy + \int_{[0,1]^2} \epsilon \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} dx dy + \int_{[0,1]^2} \frac{\partial u}{\partial x} v dx dy$$

$$I(v) = \int_{[0,1]^2} \left[\epsilon \left(\sin(\Pi y) \frac{\partial v}{\partial x} dx dy - \Pi \cos(\Pi y) \frac{\partial v}{\partial y} \right) + \sin(\Pi y) v \right] dx dy, \forall v \in V$$

$$u(x,y) = NN(x,y) = A_n \sigma \left(A_{n-1} \sigma (...\sigma (A_1 \begin{bmatrix} x \\ y \end{bmatrix} + B_1)... + B_{n-1} \right) + B_n$$

$$LOSS_{strong} = \left(\int_{[0,1]^2} \left[\frac{\partial NN(x,y)}{\partial x} - \epsilon \left(\frac{\partial^2 NN(x,y)}{\partial x^2} + \frac{\partial^2 NN(x,y)}{\partial y^2} \right) \right] v dx dy \right)^2$$

$$LOSS_{weak}(v) = (b(NN(x, y), v) - l(NN(x, y), v))^{2},$$

$$LOSS_{BC}(x, y) = (NN(0, y) - \sin(\Pi y))^{2} + (NN(1, y))^{2} + (NN(x, 1))^{2}$$

$$(NN(x, 0))^{2} + (NN(x, 1))^{2} = 0$$

IGA-DNN-VPINN

Weak form: Find $u \in H^1([0,1]^2)$: b(u,v) = I(v)

$$b(u,v) = \int_{[0,1]^2} \epsilon \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} dx dy + \int_{[0,1]^2} \epsilon \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} dx dy + \int_{[0,1]^2} \frac{\partial u}{\partial x} v dx dy$$

$$I(v) = \int_{[0,1]^2} \left[\epsilon \left(\sin(\Pi y) \frac{\partial v}{\partial x} dx dy - \Pi \cos(\Pi y) \frac{\partial v}{\partial y} \right) + \sin(\Pi y) v \right] dx dy, \forall v \in V$$

Now, we plug a combination of B-splines in place of the solution $u(x,y) = \sum_{i=1,...,N_x; j=1,...,N_y} u_{ij}B_i(x)B_j(y)$

$$LOSS_{strong} = \left(\int_{[0,1]^2} \left[\frac{\partial \sum u_{ij} B_i B_j}{\partial x} - \epsilon \left(\frac{\partial^2 \sum u_{ij} B_i B_j}{\partial x^2} + \frac{\partial^2 \sum u_{ij} B_i B_j}{\partial y^2} \right) \right] v \right)^2$$

$$LOSS_{weak}(v) = \left(b(\sum u_{ij}B_{i}B_{j}, v) - I(\sum u_{ij}B_{i}B_{j}, v)\right)^{2},$$

$$LOSS_{BC}(x, y) = (\sum u_{ij}B_{i}(0)B_{j}(y) - \sin(\Pi y))^{2} + (\sum u_{ij}B_{i}(1)B_{j}(y))^{2} + (\sum u_{ij}B_{i}(x)B_{j}(0))^{2} + (\sum u_{ij}B_{i}(x)B_{j}(1))^{2}$$

Parametric-IGA-VPINN

Weak form: Find $u \in H^1([0,1]^2)$: b(u,v) = I(v)

$$b(u,v) = \int_{[0,1]^2} \epsilon \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} dx dy + \int_{[0,1]^2} \epsilon \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} dx dy + \int_{[0,1]^2} \frac{\partial u}{\partial x} v dx dy$$

$$I(v) = \int_{[0,1]^2} \left[\epsilon \left(\sin(\Pi y) \frac{\partial v}{\partial x} dx dy - \Pi \cos(\Pi y) \frac{\partial v}{\partial y} \right) + \sin(\Pi y) v \right] dx dy, \forall v \in V$$

Now, NN input is ϵ , NN output are N coefficients of B-splines $\epsilon \to NN(\epsilon)_{ij}$ $u(x,y) = \sum_{i=1,\dots,N_x; j=1,\dots,N_y} NN(\epsilon)_{ij} B_{i,p}(x) B_{j,p}(y)$

$$(A_{ij}) = (A_{ij}) \left(\partial B_{ij} B_{ij} - (\partial^{2} B_{ij} B_{ij} - \partial^{2} B_{ij} B_{ij}) \right)$$

$$LOSS_{strong} = \left(\int_{[0,1]^2} \sum N(\epsilon)_{ij} \left(\frac{\partial B_i B_j}{\partial x} - \epsilon \left(\frac{\partial^2 B_i B_j}{\partial x^2} + \frac{\partial^2 B_i B_j}{\partial y^2} \right) \right) v \right)^2$$

$$LOSS_{weak}(v) = \left(b(\sum u_{ij}B_{i}B_{j},v) - I(\sum u_{ij}B_{i}B_{j},v)\right)^{2}, LOSS_{BC}(x,y) =$$

$$(\sum NN(\epsilon)_{ij}B_{i}(0)B_{j}(y) - \sin(\Pi y))^{2} + (\sum NN(\epsilon)_{ij}B_{i}(1)B_{j}(y))^{2} +$$

$$(\sum NN(\epsilon)_{ij}B_{i}(x)B_{j}(0))^{2} + (\sum NN(\epsilon)_{ij}B_{i}(x)B_{j}(1))^{2}$$