

Lecture 2: Approximation and expressivity of NNs

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Some papers/books to look at

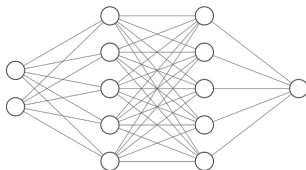
- Grohs and Kutyniok, Mathematical aspects of deep learning, (2022)
- Korylev

Overview

All of Scientific Machine Learning is based on Neural Networks of some architecture. Regardless of the architecture these all have one thing in common

A Deep Neural Net (NN) of width W and depth L gives a **nonlinear functional approximation to $u(x)$ with **input** $x \in R^n$ (or even $x \in H^1$) given by**

$$y(\mathbf{x}) = DNN(\mathbf{x}) \in R^m$$



Big Question

To understand the use of NN's to solve (for example) differential equations, we must first understand how well they can approximate a function

A NN of width W , depth L , and activation functions σ with parameter set θ describes a set of functions. These lie in a **nonlinear space** Y .

Suppose that we have a function $u(x)$ that we want to approximate. Have two questions

- ① **Expressivity**: What is the best approximation $y^* \in Y$ that we can find for u :
- ② **Trainability**: Can we train the NN, i.e. find the optimal θ^*
 - At all?
 - In a reasonable computational time?

We have good answers to Question 1, and few answers to Question 2!

$y(\mathbf{x})$ is constructed via a combination of linear transformations and nonlinear/semi-linear activation functions.

Example: Shallow 1D neural net

$$y(\mathbf{x}) = \sum_{i=0}^{W-1} c_i \sigma(a_i \mathbf{x} + \mathbf{b}_i)$$

Often take

$$\sigma(z) = \text{ReLU}(z) \equiv z_+,$$

Then

$$y(\mathbf{x}) = \sum_{i=0}^{W-1} c_i (a_i \mathbf{x} + \mathbf{b}_i)_+$$

In 1-dimension this is a **piece-wise linear function** with N **free knots** at

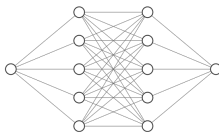
$$k_i = -b_i/a_i.$$

Expressivity 1

Convergence of a NN relies on understanding both approximation and training

A feed-forward **Deep Neural Network** (DNN) can be 'in principle' trained to approximate a target function $u(x)$

$$y_j = \sum_{i=0}^{W-1} c_{i,j} \sigma(a_{i,j} y_i + b_{i,j}) \quad j = 1, \dots, L \quad y_0 \equiv x, \quad y(x) = y_L$$



Expressivity 2

There are a **lot of results** on the **theoretical expressivity** of a DNN [Grohs and Kutyniok, Mathematical aspects of deep learning, (2022)].

Universal approximation theorem, [Hornick et. al., 1989] *If $u(\mathbf{x})$ is a continuous function with $\mathbf{x} \in K \subset \mathbb{R}^d$ (compact), and σ a continuous activation function. Then for any $\epsilon > 0$ there exists a (shallow) neural network $y(\mathbf{x}, \theta)$ such that*

$$\|u(\mathbf{x}) - y(\mathbf{x})\|_{\infty} < \epsilon.$$

Expressivity 3

Theorem [Yarotsky (2017)]

Let

$$F_{n,d} = \{u \in W^{n,\infty}([0,1]^d) : \|u\|_{W^{n,\infty}} \leq 1\}$$

For any d, n and $\epsilon \in (0,1)$ there is a ReLU network architecture that

- ① Is capable of expressing any function from $F_{d,n}$ with error ϵ
- ② Has depth

$$\text{depth: } L < c(\log(1/\epsilon) + 1) \quad \text{width: } W < c\epsilon^{-d/n}(\log(1/\epsilon) + 1)$$

for some constant $c(d, n)$.

Implies exponential rates of convergence with increasing depth L

But how well do we do in practice?

Other approximation methods: Linear splines

Express $u(x)$ as:

$$u(x) = \sum_{i=0}^N a_i \phi_i(x).$$

Here $\phi_i(x)$ are **known functions**. eg. **B-splines (Finite element)**, **Fourier modes**, **Wavelets etc.**

Advantages: Linear in a_i , Convex optimisation problem, easy to use, guaranteed error bounds

Disadvantages: Poor expressivity, slow convergence as N increases, results depend on the form of the function $u(x)$ (hard to approximate rapidly changing functions), **Curse of dimensionality**

Example: Direct Learned Univariate NN Function Approximation

For a learned function $y(x)$ approximate target function $u(x)$ by minimising the 'usual' loss function L over parameters θ

$$\min_{\theta} L(\theta) \equiv \sum_{k=1}^M |y(X_k) - u(X_k)|^2$$

Use the shallow ReLU network

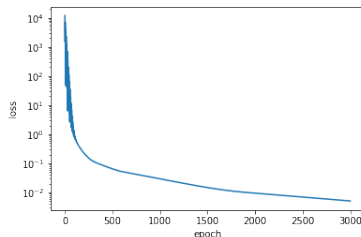
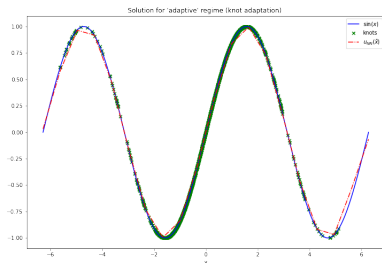
$$y(x) = \sum_{j=0}^{W-1} c_j (a_j x + b_j)_+, \quad \theta = [\mathbf{a}, \mathbf{b}, \mathbf{c}].$$

Find the optimal set of coefficients a, b, c

Use an ADAM SGD (over the quadrature points) optimiser

Approximation of: $u(x) = \sin(x)$ using ReLU network

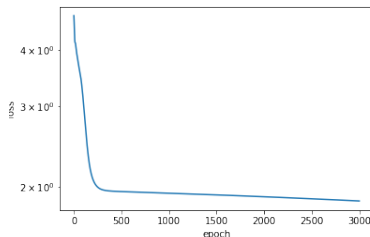
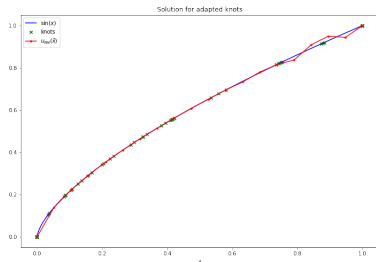
Uniform quadrature points:



Results **poor**. Depend crucially on the starting values. Even then poor.

Approximation of: $u(x) = x^{2/3}$

Uniform quadrature points:



Results even worse! Depend crucially on the starting values. Even then very bad!

Problems with:

- the loss function,
- training,
- and conditioning,

of the ReLU NN.

REASON: Trying to train a_i, b_i, c_i together, whereas they play very different role in the approximation.

This leads to a very non-convex and ill conditioned optimisation problem. Either very slow convergence to the optimum approximation, or convergence to a (very) sub-optimal solution

RESOLUTION:

- **First** solve the *nonlinear* problem of finding nearly optimal (knots) a_i, b_i first
- **Then** Solve the *nearly linear but ill-conditioned* problem of finding the (weights) c_i next by *pre-conditioning the system*
- **Iterate** if needed (it's not needed)

Compare with other univariate approximation methods:

- Linear spline

$$y(x) = \sum_{i=0}^N w_i \phi_i(x - X_i), \quad X_i \text{ fixed}$$

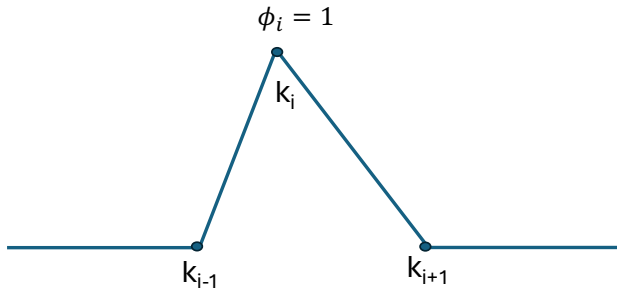
w_i to be determined **Linear**

- Free Knot Spline (FKS)

$$y(x) = \sum_{i=0}^N w_i \phi_i(x - k_i).$$

Knots k_i also to be determined **Nonlinear**

Basic linear spline on free knots



Comparison between approximation methods

Linear spline

- Less expressive (lower accuracy for a given N)
- Non-adaptive (problems with singular functions)
- Not Equivariant (fixed mesh imposes a-priori structure)
- Good error estimates
- **Linear space:** Essential to the use of the FE method

FKS/NN

- Very expressive (high accuracy for a given N)
- Self-adaptive (can work for singular functions, adaptive FE)
- Equivariant (eg. to Galilean transformations, scalings)
- Good error estimates
- **Nonlinear space:** Addition of two FKS with N knots is not a FKS with N knots

ReLU NN and Free Knot Splines (FKS)

[deVore] Any 1D ReLU network of width W and depth L is formally equivalent to a piecewise linear free knot spline (FKS) with N free knots k_i , where

$$N \leq W^L,$$
$$y(x) = \sum_{i=0}^N w_i \phi_i(x - k_i).$$

Note usually $N \ll W^L$.

Proof ReLU \implies FKS

The combination of two piecewise linear functions is a piecewise linear function. Therefore a ReLU network is a piecewise linear function with knot points that depend in a subtle way on the coefficients of the network.

Proof FKS \implies ReLU

The linear spline functions $\phi_i(z)$ can be expressed as a combination of ReLU functions with coefficients *nonlinear functions* of k_i

$$\phi_i(z) = \frac{\text{ReLu}(z - k_{i-1})}{k_i - k_{i-1}} - \frac{(k_{i+1} - k_{i-1}) \text{ReLu}(z - k_i)}{(k_{i+1} - k_i)(k_i - k_{i-1})} + \frac{\text{ReLu}(z - k_{i+1})}{k_{i+1} - k_i}.$$

Therefore

$$\sum w_i \phi_i(x - k_i) = \sum c_i \text{ReLu}(x - k_i)$$

$$c_i = \frac{w_{i-1}}{k_i - k_{i-1}} - \frac{(k_{i+1} - k_{i-1})w_i}{(k_{i+1} - k_i)(k_i - k_{i-1})} + \frac{w_{i+1}}{k_{i+1} - k_i} \approx \frac{k_{i+1} - k_{i-1}}{2} w_i''.$$

SO .. in principle a ReLU network has the **same expressivity** as a FKS and **vice-versa**

But this often does not seem to be the case in practice when training the network

We will explore

- The theoretical and practical expressivity of the FKS
Correct loss function and **train knots then weights**
- Whether the ReLU network can be **trained stably and efficiently** to give the same result as the FKS! **Pre-conditioning**
- Extensions to deep networks and higher dimensions

Analysis of a FKS

Can compare ReLU expressivity results to those of

- Using a **free knot linear spline** (FKS):

$$y(x) = \sum_{i=0}^N w_i \phi_i(x - k_i).$$

Optimise over $\theta = [\mathbf{w}, \mathbf{k}]$

- Using an **interpolating free knot linear spline** (IFKS):

$$y(x) \equiv \Pi_1 u(x) = \sum_{i=0}^N u(k_i) \phi_i(x - k_i).$$

Optimise over $\theta = \mathbf{k}$

Expressivity of a (I)FKS

The expressivity of a (I)FKS can be very good. Full theory [see deVore (1998),(2022)] uses results from Besov spaces.

In summary: for both regular (eg. $\sin(x)$) and quite irregular target functions $u(x)$ (eg. $x^{2/3}$) expect to see

$$\|u - y_{FKS}\|_p < C_{FKS}/N^2, \quad p = 2, \quad \infty$$

$$\|u - y_{IFKS}\|_p < C_{IFKS}/N^2, \quad p = 2, \quad \infty$$

With $C_{FKS} < C_{IFKS}$ but with very similar knot locations

A little theory on linear spline IFKS

If we know $u''(x)$ we can develop a theory for the best knot location for an IFKS (and hence for a FKS). [Huang + Russell (2010)]. Using the local interpolation over the knot intervals we have:

$$\|u - y_{IFKS}\|_2^2 = \frac{1}{120} \sum_i (k_{i+1} - k_i)^5 (u''(\xi_i))^2, \quad \xi_i \in (k_i, k_{i+1}).$$

$$\|u - y_{IFKS}\|_\infty = \frac{1}{4} \max_i (k_{i+1} - k_i)^2 |u''(\xi_i)|, \quad \xi_i \in (k_i, k_{i+1}).$$

Equidistribution

It can be shown [de Boor, Huang + Russell] that the *best knot location* for the IFKS **equidistributes** $\rho_{i+1/2}$ given by:

$$\rho_{i+1/2} = (k_{i+1} - k_i)(u'')^{2/5}, \quad p = 2$$

or

$$\rho_{i+1/2} = (k_{i+1} - k_i)(u'')^{1/2}, \quad p = \infty$$

Motivates the **equidistribution loss function** to train the **knots** of the IFKS:

$$L_E(\mathbf{k}) = \sum (\rho_{i+1/2} - \sigma)^2, \quad \sigma = \text{mean}(\rho).$$

Some analytical results

Can sometimes solve the equidistribution equations by quadrature (and a bit of care at the singularity). Useful for comparison with the numerical computations.

Set $x = x(\xi)$, with $x \in [0, 1]$, $\xi \in [0, 1]$ and set

$$k_0 = 0, k_N = 1, \quad k_i = x(i/N).$$

Then

$$\rho_{i+1/2} \approx \frac{1}{N} x_\xi (u'')^{2/5} = \sigma \quad (*)$$

Solve (*) and apply the boundary conditions to find x and σ

Example: $u(x) = x^{2/3}$.

$$u_{xx} = -(2/9)x^{-4/3} \implies \frac{1}{N}(2/9)^{2/5} x_{\xi}^{-8/15} = \sigma.$$

Solve and apply the BC to give *optimal knots*

$$x = \xi^{15/7}, \quad k_i = (i/N)^{15/7}.$$

With optimal L_2^2 error:

$$L_2^2 = \sum_{i=0}^{N-1} \frac{1}{120} \frac{1}{N^5} x_{\xi}^5 (u'')^2 = \frac{1}{120 N^5} \sum_{i=0}^{N-1} \left(\frac{15}{7}\right)^5 \frac{4}{81} = \frac{1.859 \times 10^{-2}}{N^4}.$$

NOTE The L_2^2 error for a PWL interpolant with *uniform knots* has:

$$L_2^2 = \frac{C}{N^{7/3}}.$$

Training the FKS for $x^{2/3}$ directly

Consider training the FKS with:

- Random start
- Starting from the PWL interpolant with *uniform knots* $k_i = i/N$
- Starting from the PWL interpolant with *optimal knots* $k_i = (i/N)^{15/7}$.

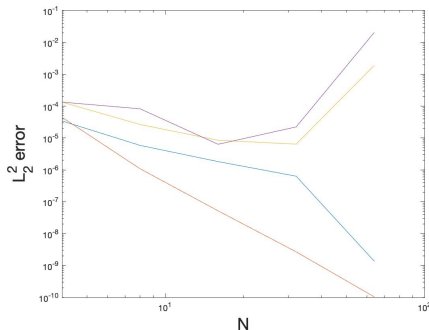


Figure: (Blue) Uniform, (Red) Optimal, (Others) Random

Comparison of the splines for $x^{2/3}$

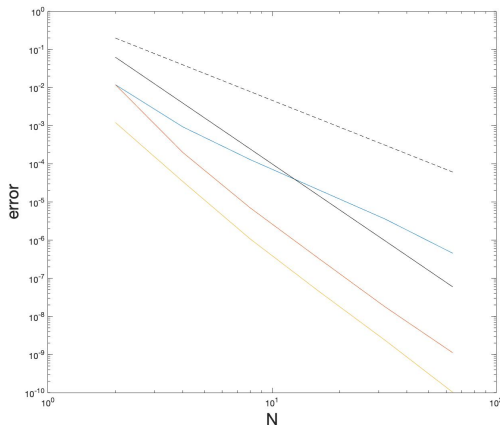


Figure: (Red) Optimal IFKS, (Yellow) Optimal FKS, (Blue) Uniform interpolating spline, (Black) $1/N^4$, (Black dashed) $1/N^{7/3}$

Approximation form for $u(x) = x^{2/3}$ (singularity at $x = 0$)

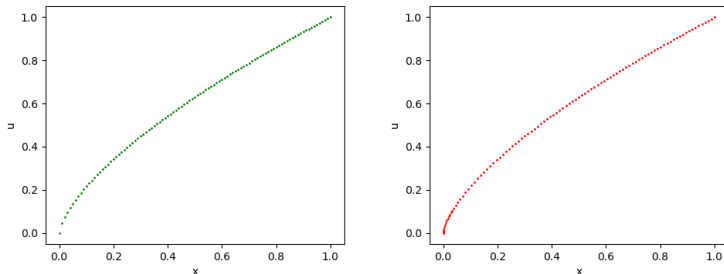


Figure: Comparison between uniform and optimal spline for $N = 100$. Note that the optimal knots cluster towards $x = 0$, where the solution exhibits a singular behaviour.

Two-level training for a general FKS

Find knots a_i, b_i then the weights c_i

- Construct a *mixed* loss function

$$L = \lambda L_2^2(\theta) + (1 - \lambda)L_E(\mathbf{k}).$$

- From a set of uniform knots $k_i = i/N$ set $\lambda = 0.1$ and train to find **optimal IFKS knots** and y_{IFKS}
- Set $\lambda = 0.9$ and use Adam to optimise y_{FKS} from y_{IFKS} by finding optimal *weights*
Almost linear and well-conditioned as IFKS knots close to optimal FKS knots

Training a shallow ReLU NN

Motivated by this we can modify the **training** of a *shallow* ReLU NN.

- Take shallow ReNN with parameters $\theta = [\mathbf{a}, \mathbf{b}, \mathbf{c}]$
- Compute the implicit knot locations \mathbf{k}
- Construct a *mixed* loss function

$$L = \lambda L_2^2(\theta) + (1 - \lambda) L_E(\mathbf{k}).$$

- Use two-layer training as above.

This improves the training results for the ReLU NN knot location, but there are still strong ill-conditioning problems with finding the ReLU weights c_i

Results I : $W = 30$: ReLU NN approximation

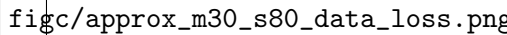
figc/approx_m30_s80_data_loss.png

Figure: L_2^2 Loss function

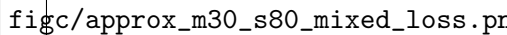
figc/approx_m30_s80_mixed_loss.png

Figure: Mixed loss function

Results $W = 30$: Knot location

`figc/30nodes_80pts_hist_data_loss`

Figure: L_2^2 Loss function

`figc/30nodes_80pts_hist_mixed_loss`

Figure: Mixed loss function

Results $W = 30$: Knot evolution during training

`figc/knot_evolution_30nodes_80pts`

Figure: L_2^2 Loss function. Note knot coalescence and irregularity

`figc/knot_evolution_30nodes_80pts`

Figure: Mixed loss function

Comparison between the ReLU NN and the FKS I

`figc/plots_x(1-x).png`

`figc/plots_sin(pi_x).png`

`figc/plots_x_23.png`

Figure: $u(x) = x(1 - x), \sin(\pi x), x^{2/3},$

Comparison between the ReLU NN and the FKS II

`figc/plots_tanh.png`
`figc/plots_oscillatory(1).png`

Figure: $u(x) = \tanh(100(x - 1/4), \exp(500(x - 3/4)^2) \sin(20\pi x)$.

It is clear that the FKS significantly outperforms the ReLU NN

Timing and ill-conditioning

WHY: The training of the ReLU NN network is **much slower** than for the FKS due to the ill conditioning of the ReLU coefficients c_i (high condition number of the matrices) compared to the weights w_i of the FKS.

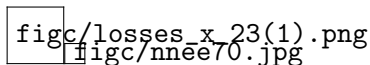


Figure: Two-level training ReLU NN and FKS for $u(x) = x^{2/3}$
(left) timings (right) ReLU coefficients.

Conditioning and pre-conditioning

Can establish the following

Theorem *Given known N knots, the condition number of the normal equation matrices solving for the weights is*

$\mathcal{O}(1)$ for FKS architectures

$\mathcal{O}(N^4)$ for ReLU architectures

Conclusion: To get optimal expressivity for ReLU training

- Train the knots
- Pre-condition the ReLU NN to have same architecture as the FKS.

Then get expressivity equivalent to that of the FKS

Other activation functions

The L_2^2 error of directly training a shallow network with the **tanh** activation function, without preconditioning, to approximate the test functions $u_i(x)$.

N	u_1	u_2	u_3	u_4	u_5	P
8	4.6×10^{-9}	1.70×10^{-6}	3.55×10^{-4}	1.08×10^{-3}	1.77×10^{-2}	25
16	1.56×10^{-9}	1.20×10^{-8}	1.62×10^{-7}	8.01×10^{-4}	1.53×10^{-2}	49
32	1.21×10^{-8}	1.41×10^{-8}	1.50×10^{-7}	6.17×10^{-4}	1.64×10^{-2}	97
64	5.25×10^{-9}	8.88×10^{-9}	2.15×10^{-7}	5.54×10^{-4}	1.77×10^{-2}	193
128	2.21×10^{-8}	8.00×10^{-9}	2.15×10^{-7}	4.40×10^{-4}	1.90×10^{-2}	385

Error is better than the ReLU NN as the system is much better conditioned. But still not as good as the two-layer trained FKS

Deep networks

Consider 2-layer neural network, with ReLU activation, width $W = 5$ and 46 trainable parameters.

	u_1	u_2	u_3	u_4	u_5
L_2^2 error	4.2×10^{-3}	5.47×10^{-2}	3.45×10^{-2}	1.8×10^{-1}	1.85×10^{-2}
Variance	9.71×10^{-5}	1.42×10^{-2}	1.35×10^{-2}	5.40×10^{-2}	1.09×10^{-4}

Compare with FKS with $N = 20$ knots and 42 trainable parameters.

FKS error of 10^{-6} or less on each of these problems.

Solving PDEs with Deep Learning

Can now apply these ideas in the context of PINNs

Rezoning method: learned collocation points

Apply alternatively

- Train PINN to solving PDE on given collocation points $X_i \rightarrow y(x)$
- Use DNN and $y(x)$ to find new points (X_i)

Semi-Lagrangian framework

Train a single PINN to learn **simultaneously** both y and the collocation points X_i [Pardo, David et. al.] **In progress but semi-promising.**

Good news: Singular Reaction-Diffusion Equation

Solve $-\varepsilon^2 u_{xx} + u = 1 - x$ on $[0, 1]$ $u(0) = u(1) = 0$

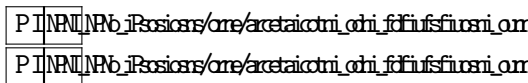
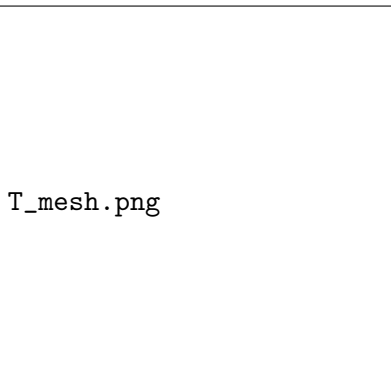


Figure: PINN (tanh) trained for 20000 epochs, $N_r = 101$, Adam optimizer with $lr = 1e - 3$. (left) Uniform collocation points (right) Adapted collocation points **much faster training**

Higher dimensions

- Much harder to make comparisons in higher dimensions
- ReLU NN is still a piecewise linear function, but it is 'defined' over a very complex space of linear polytopes
- This have a much more irregular structure than a conventional 'adaptive mesh'



Deep Galerkin Method for the Poisson equation (PVP)

The **Deep Galerkin Method** (DGM) [Sirignano J. and Spiliopoulos K., (2018)] mimics the action of a PINN

$$y = \arg \min_{v \in H} \mathcal{I}(v),$$

where H is the set of admissible functions (trial functions)

$$\mathcal{I}(v) = \int_{\Omega} (\Delta v(\mathbf{x}) + f(\mathbf{x}))^2 d\mathbf{x} + \beta \int_{\partial\Omega} (v(\mathbf{x}) - u_D)^2 ds$$

- $y(\mathbf{x})$ is a DNN based approximation of $u\mathbf{x}$ which is in C^2
- A numerical quadrature rule for the functional using chosen quadrature points
- An algorithm for solving the optimization problem

Deep Ritz method for the Poisson equation

The **Deep Ritz Method** (DRM) [Weinan E and Bing Yu, (2017)] seeks the solution u satisfying

$$y = \arg \min_{v \in H} \mathcal{I}(v),$$

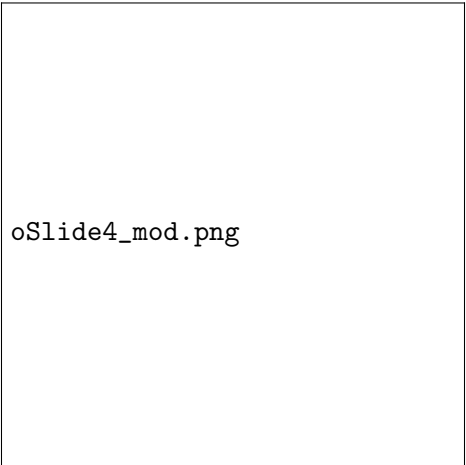
where H is the set of admissible functions (trial functions) and

$$\mathcal{I}(v) = \int_{\Omega} \left(\frac{1}{2} |\nabla v(\mathbf{x})|^2 - f(\mathbf{x})v(\mathbf{x}) \right) d\mathbf{x} + \beta \int_{\partial\Omega} (v(\mathbf{x}) - u_D)^2 ds$$

The Deep Ritz method is based of the following assumptions:

- $y(\mathbf{x})$ is DNN based approximation of u which is in H^1 eg. ReLU
- A numerical quadrature rule for the functional using chosen quadrature points eg. random, optimal
- An algorithm for solving the optimization problem eg. ADAM on random quadrature points

Poisson Problem on an L-shaped domain



oSlide4_mod.png

Singular solution

- Solution $u(\mathbf{x})$ has a **gradient singularity at the interior corner** A_i
- If the interior angle is ω and the distance from the corner is r then

$$u(r, \theta) \sim r^\alpha f(\theta), \quad \alpha = \frac{\pi}{\omega}$$

where $f(\theta)$ is a **regular function of θ**

- Corner problem

$$u(r, \theta) \sim r^{2/3}, \quad r \rightarrow 0.$$

Numerical results: **random** quadrature points

Solve $\Delta u(x) = 0$ on Ω_L $u(r, \theta) = r^{2/3} \sin(2\theta/3)$ on $\Gamma = \partial\Omega_L$

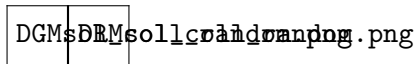


Figure: Left: DGM Right: DRM

Can we improve the accuracy by a better choice of quadrature points?

Optimal interpolation points for the L-shaped domain

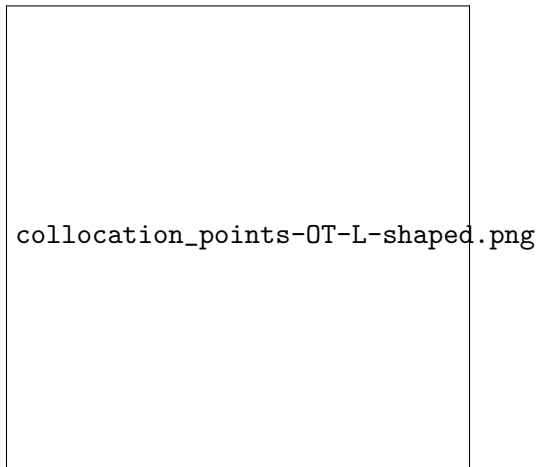


Figure: Optimal points for interpolating $u(r, \theta) \sim r^{2/3}$

Optimal and Deep Galerkin/Ritz

Solutions with Optimal quadrature points

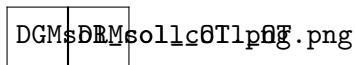


Figure: L^2 error - randomly sampled points: 0.468 | Optimal: 0.0639

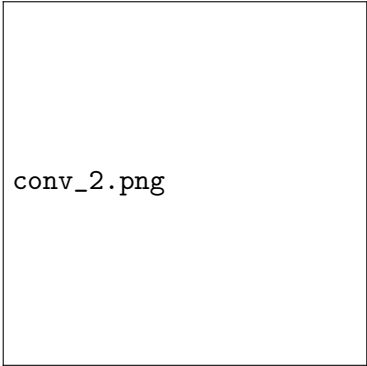
Left: Deep Galerkin, Right: Deep Ritz

Good choice of quadrature points makes a big difference

Convergence:

DRM method works well for small DOF

dG is **much** better for more DOF



conv_2.png

Pattern consistent with the ill-conditioning issues seen earlier
To resolve need to address the ReLU approximation problem in higher dimensions

Summary

- There is often a gap between theoretical expressivity of a ReLU NN and what we see in practice
- FKS and ReLU NN are formally equivalent
- We can train an FKS effectively using an equidistribution based loss function and two-level training
- Finding the coefficients of a ReLU NN is **ill conditioned** and the network cannot be easily trained with a standard loss function **unless two-layer training and pre-conditioning** is used
- This impacts directly on the training and accuracy of PINNS
- Long way to go before we understand the convergence and reliability of PINNS!

For full results see: <https://arxiv.org/abs/2407.02153v1>