Lecture 2: Introduction to PINNS

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Some papers to look at

- Raissi, M., P. Perdikaris, and G. E. Karniadakis. 2019. "Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations." Journal of Computational Physics 378: 686–707. https://doi.org/https://doi.org/10.1016/j.jcp.2018.10.045.
- Grossman et. al. *Can PINNS beat the FE method?*
- Shin et. al. *On the convergence of PINNS for linear elliptic and parabolic PDEs*
- Wang et. al. *When and why PINNS fail to train: a neural tangent kernel perspective*
- Kiyani *Which Optimizer Works Best for Physics-Informed Neural Networks and Kolmogorov-Arnold Networks?*
- Chen et. al. *Sidecar: A Structure-Preserving Framework for Solving Partial Differential Equations with Neural Networks*
- Russell et. al. *Two-point boundary value problems*

Motivation: Solving ODEs and PDEs

Seek to solve ODE/PDE problems of the form

$$\mathbf{u}_t = F(\mathbf{x}, u, \nabla u, \nabla^2 u) \quad \text{with BC}$$

eg. ODE (IVP or BVP)

$$\frac{du}{dt} = u^2, u(0) = 1, \quad -\epsilon^2 \frac{d^2 u}{dx^2} + u = 1, \quad u(0) = u(1) = 0.$$

eg. PDE

$$-\Delta u = f(x), \quad iu_t + \Delta u + u|u|^2 = 0, \quad u_t = \Delta u + f(x, u) \quad x \in R^n$$

Classical Method 1. Finite Differences

Work with a set of point values for a function never with a function directly IVP/BVP:

$$U_j^n \approx u(n\Delta t, j\Delta x), \quad \Delta t, \Delta x \ll 1$$

eg.

$$u_t = u_{xx} + u^3$$

IMEX Crank-Nicholson method:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} =$$

$$\frac{1}{2\Delta x^2}\left(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1} + U_{j+1}^n - 2U_j^n + U_{j-1}^n\right) + \left(U_j^n\right)^3.$$

- Have error estimates of the form

$$\|U_j^n - u(n\Delta t, j\Delta x)\| < C(u)\Delta t^p \Delta x^q, \quad \Delta t, \Delta x \to 0$$

- Can reduce $C(u)$ and increase p, q using an adaptive approach.
- Lots of software
- Have to recover the function from the point values
- Awkward in higher dimensions!

Classical Method 2: Finite Elements

Express $u(x, t)$ as a Galerkin approximation:

$$u(t, x) \approx U(t, x) = \sum_{i=0}^{N} U_i(t)\, \phi_i(x)$$

with $\phi_i(x)$ **Not** globally differentiable *locally supported, piece-wise polynomial spline functions*

- Work with a function $U(x) \in H^1$
- Require U to satisfy a *weak form* of the PDE (see Lecture 4)
- Have guaranteed error estimates of the form

$$\|u - U\|_{H^1} < C(u) N^{-\alpha}$$

- Lots of software (see Lecture 2b)
- Can reduce $C(u)$ and increase α using an adaptive approach.
- Awkward in higher dimensions!

Classical Method 3: Collocation

Express $u(x,t)$ as a function approximation:

$$u(t,x) \approx U(t,x) = \sum_{i=0}^{N} U_i(t)\, \phi_i(x)$$

with $\phi_i(x)$:

Locally differentiable locally supported, piece-wise polynomial spline functions such as Lagrange polynomial interpolants

- Work with a function $U(x) \in C^n_{loc}$
- Require U to satisfy the PDE exactly at a carefully chosen set of **collocation points**

- Have guaranteed error estimates of the form

$$\|u - U\|_{C_2} < C(u)N^{-\alpha}$$

- Can reduce $C(u)$ and increase α using VERY carefully chosen collocation points
- Implemented in `python` as $solve_bvp$, Colsys
- Impossible in higher dimensions!

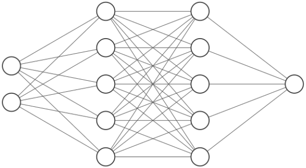
Issues with classical methods

- Well tested and good convergence theories
- Accuracy of the computation depends crucially on the choice and shape of the mesh points
- Generally require **time and practice** to implement (although FireDrake etc. makes this easier)
- Two-fold curse of dimensionality

PINNS

Physics Informed Neural Networks for solving PDEs: advertised as ”Mesh free methods”.
Use a Deep Neural Net of width W and depth L to give a nonlinear functional approximation to $u(\mathbf{x})$ with input x.

$$y(\mathbf{x}) = DNN(\mathbf{x})$$



$y(\mathbf{x})$ 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

$$\sigma(z) = \mathrm{ReLU}^3(z) \equiv z_+^3, \quad \text{or} \quad \sigma(z) = \tanh(z)$$

As a result we can define y_{zz} for every point z

Operation of a 'traditional' PINN

Want to solve a ODE/PDE in $\mathbf{x}$

- PINNS are similar to collocation methods
- Assume that $y(\mathbf{x})$ has strong regularity eg. C^2
- Differentiate $y(\mathbf{x})$ exactly using the chain rule
- Evaluate the PDE residual at N_r collocation points $\mathbf{X}_i$, :chosen to be uniformly spaced, or samples from a random distribution
- Train the neural net to minimise a **loss function** L combining the PDE residual and boundary and initial conditions. May use Epochs linked to the random training samples.

Eg 1. Solution of regular two-point BVPs by PINNs

Consider the two-point BVP with Dirichlet boundary conditions:

$$-u_{xx} = f(x, u, u_x),\ x \in [0,1] \quad u(0) = a,\ u(1) = b.$$

Define output of the PINN by $y(x)$ and residual $r(x) := y_{xx} + f(x, y, y_x)$. Train the coefficients θ of the NN by minimising the loss function

$$L = \frac{1}{N_r}\sum_{i}^{N_r} |r(X_i^r)|^2 + \frac{\beta}{2}\left(|y(0) - a|^2 + |y(1) - b|^2\right),$$

where $\{X_i^r\}_i^{N_r}$ are the collocation points (possibly randomly) placed in $(0,1)$.

Eg 2. Solution of regular second order IVPs by PINNs

Consider the second order IVP with initial conditions:

$$-u_{xx} = f(x, u, u_x), \ x \in [0, 1] \quad u(0) = a, \ u'(0) = b.$$

Define output of the PINN by $y(x)$ and residual $r(x) := y_{xx} + f(x, y, y_x)$. Train the coefficients θ of the NN by minimising the loss function

$$L = \frac{1}{N_r} \sum_{i}^{N_r} |r(X_i^r)|^2 + \frac{\beta}{2} \left(|y(0) - a|^2 + |y'(0) - b|^2 \right),$$

where $\{X_i^r\}_i^{N_r}$ are the collocation points (possibly randomly) placed in $(0, 1)$.

Eg 3. Solution of regular parabolic PDEs by time-stepping PINNs

Consider the semilinear parabolic PDE with Dirichlet boundary conditions:

$$u_t = u_{xx} + f(x, u, u_x), \; x \in [0, 1] \quad u(0) = a, \; u(1) = b$$

and initial condition

$$u(x, 0) = u_0(x).$$

Implicit time-stepping scheme $U^n(x) \approx u(n\Delta t, x)$.

$$\frac{U^{n+1}(x) - U^n(x)}{\Delta t} = U_{xx}^{n+1} + f\left(x, U^{n+1}, U_x^{n+1}\right) \equiv F(U^{n+1}).$$

- Start with $U^0(x) = u_0(x)$
- For $n > 0$: Define output of the PINN by $y(x)$ and residual

$$r(x) := U^n(x) + \Delta t F(y).$$

- The PINN is trained by minimising the loss function

$$L = \frac{1}{N_r} \sum_{i}^{N_r} |r(X_i^r)|^2 + \frac{1}{2} \left(|y(0) - a|^2 + |y(1) - b|^2 \right),$$

  where $\{X_i^r\}_i^{N_r}$ are the collocation points placed in $(0, 1)$.
- Set $U^{n+1} = y(x)$ and repeat.

Eg 4. Solution of regular parabolic PDEs by a full PINN

Consider the same semilinear parabolic PDE

$$u_t = u_{xx} + f(x, u, u_x), \; x \in [0, 1] \quad u(0) = a, \; u(1) = b.$$

Bold approach!

- Have NN with $y(t, x)$ a function of t and x
- Take N_r collocation points Z_i in space and time
- Residual $r = u_t - u_{xx} - f(x, u, u_x)$
- Minimise

$$L = \frac{1}{N_r} \sum_{i}^{N_r} |r(Z_i^r)|^2 + \frac{\beta}{2} \left(|y(0) - a|^2 + |y(1) - b|^2 \right)$$

$$+\gamma \|y(0, x) - u_0(x)\|^2.$$

Problematic as space and time play very different roles in the PDE

Numerical results for: $-u'' = \pi^2 sin(\pi x)$.

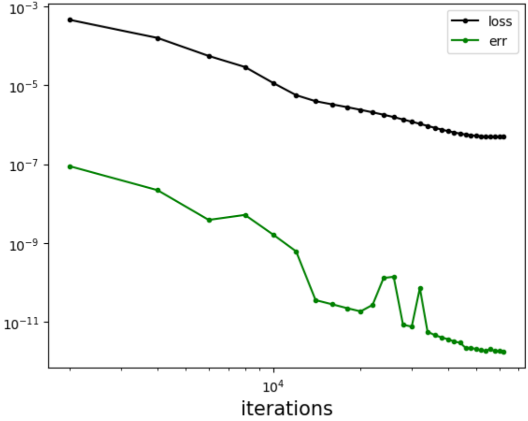


Figure: Residual based Loss and L^2 error of the PINN solution for $N_r = 100$

Numerical results: $u(x) = sin(\pi x)$

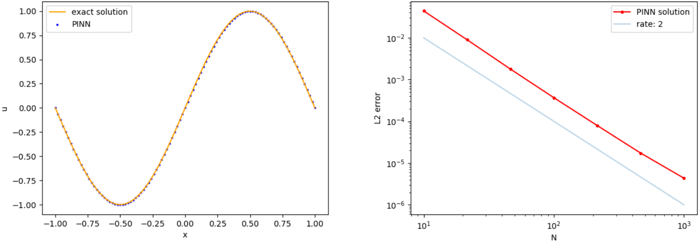


Figure: (Left) PINN with depth $L = 2$ and width $W = 30$. $N_r = 100$ uniformly distributed quadrature points, activation function: tanh, optimizer: Adam with $lr = 1e - 3$ (Right) Convergence rate for 1st order interpolant

Eg 2. Singular Reaction-Diffusion Equation

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

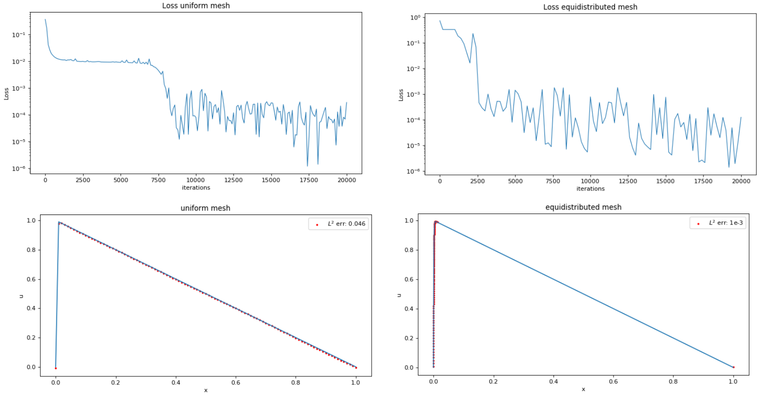


Figure: PINN (tanh) trained for 20000 epochs, $N_r = 101$, Adam optimizer with $lr = 1e-3$. (left) Uniform collocation points (right) Adapted collocation points **much faster training**

Eg 3. Bad news: Convection-dominated equation

PINNs often fail to train when the solution of the BVP exhibits singular and convective behaviour [Krishnapriyan, Aditi et. al., (2021)]:

$$-\varepsilon u_{xx} + \left(1 - \frac{\varepsilon}{2}\right) u_x + \frac{1}{4}\left(1 - \frac{1}{4}\varepsilon\right) u = e^{-x/4} \text{ on } [0,1] \quad u(0) = u(1) = 0$$

$$u(x) = exp^{\frac{-x}{4}} \left(x - \frac{exp^{-\frac{1-x}{\varepsilon}} - exp^{-\frac{1}{\varepsilon}}}{1 - exp^{-\frac{1}{\varepsilon}}} \right)$$

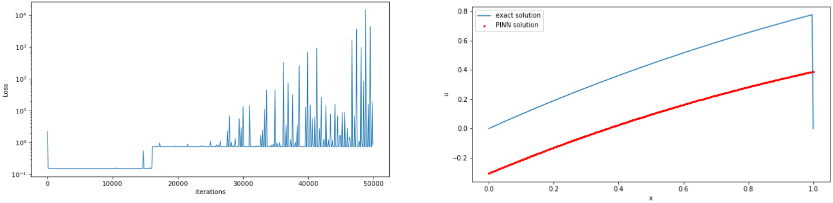
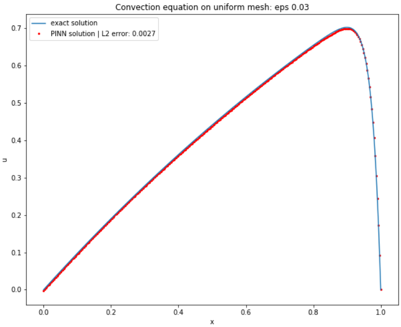
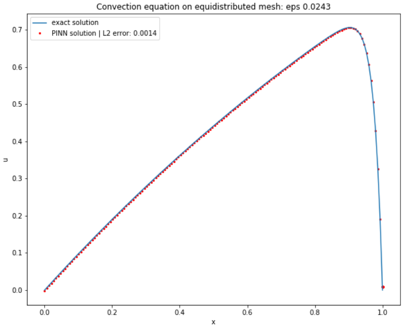


Figure: PINN trained for 50000 epochs with Adam optimizer ($l = 1, n = 2$)

Numerical results: Convection Equation





General questions for consideration

A PINN is based on a NN so we can expect in theory to achieve the expressivity and highly accurate approximation results. But do we see this in practice?

1. When do and don't PINNs work, and why?
2. How do these answers depend on (i) the problem (ii) choice of activation function, optimisation, collocation points, conditioning etc
3. Can we develop a useful convergence theory for a PINN using tools from approximations theory, bifurcation theory, numerical analysis etc.
4. How does a PINN compare to a finite element method?

Convergence theory for PINNS

[Shin, Darbon and Kaniardarkis, 2020], [Jiao, Lai, Lo, Wang, Yang, 2024]

- PINN error is a combination of approximation error and training/optimization error
- Show that a PINN (depth L width W) can be constructed with low approximation error which reduces as the complexity of the PINN increases.
- Hope that the optimization error can be reduced to acceptable levels.
- Try things out on simple problems

BUT

- **Non convex (no guarantee of uniqueness or convergence of training)**
- PINNs are nonlinear function approximators. No equivalent of Cea's lemma giving a bound on the solution error.
- Solutions can sometimes have no connection to reality!

Simple convergence theory for any collocation method including a PINN

Consider the DE:

$$-u_{xx} = f(x), \quad u(0) = f, u(1) = g.$$

There exists an exact solution using a Green's function $G(x, y)$

$$u(x) = G * f = \int_0^1 G(x, y) f(y)\, dy.$$

Suppose we have N collocation points Y_i then we can approximate the integral by a quadrature

$$u(x) = \sum_{i=1}^{N} w_i G(x, Y_i) f(Y_i) + \mathcal{O}(N^{-\alpha})$$

for some α depending on the weights w_i and the smoothness of u.

Now let $U(x)$ be any solution of the collocation problem

$$-U_{xx}(Y_i) = f(Y_i).$$

It follows that

$$\sum_{i=1}^{N} w_i G(x, Y_i) f(Y_i) = -\sum_{i=1}^{N} w_i G(x, Y_i) U_{xx}(Y_i) = U(x) + \mathcal{O}(N^{-\beta})$$

for some β depending on the weights w_i and the smoothness of u.
Hence we have the convergence result

$$u(x) = U(x) + \mathcal{O}(N^{-\alpha}) + \mathcal{O}(N^{-\beta}).$$

Can do better .. see [Russell et. al.]

Implementation of collocation methods and PINNS

A standard collocation method for the problem $-u_{xx} = f(x)$ is a linear approximation of the form:

$$u(x) \approx U(x) = \sum a_j \phi_j(x).$$

The collocation conditions at the points X_i lead to a linear equation:

$$\sum_j A_{i,j} a_j = f_i$$

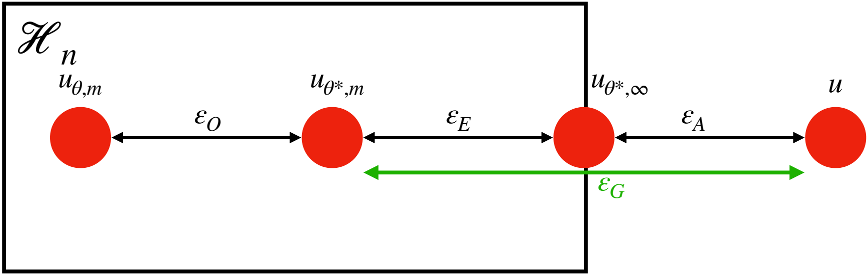
$$A_{i,j} = -\epsilon^2 \phi_j(X_i) + \phi_j(X_i), \quad f_i = f(X_i).$$

These linear equations are (in general) well conditioned and have a unique solution

Compare with the PINN formulation for the same problem

- PINN is a nonlinear approximation
- It may have better expressivity
- The collocation equations become an optimisation problem
- We may not find a good optimum

Detailed PINN Convergence Theory 1



Detailed PINN Convergence Theory 2

Underlying solution: $u(x)$

H_n: Class of functions approximated by NN with n degrees of freedom

- $u_{\theta,m}$: Approximation found in practice after some training. Is less accurate than
- $u_{\theta^*_m}$: Approximation obtained by perfect optimisation with finite collocation points. Is less accurate than
- $u_{\theta^*,\infty}$: Approximation obtained by perfect optimisation with infinite collocation points.

Measured error is $\|u_{\theta,m} - u\|$

- $\|u_{\theta,m} - u_{\theta^*,m}\|$: Optimisation error $\mathcal{E}_O$: Hard to contol and depends on the optimiser and the initialisation: See Lecture 2
- $\|u_{\theta^*,m} - u_{\theta^*,\infty}\|$: Estimation error $\mathcal{E}_E$: Main results on this
- $\|u_{\theta^*,\infty} - u^*\|$: Approximation error $\mathcal{E}_A$: See Lecture 2

Training data

[Shin et. al] prove

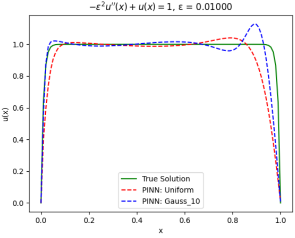
Theorem *If there is a random set of training data and n samples are chosen for training. Then the optimal minimiser h_n over this set converges to the best approximation $\hat{h}$ as $n \to \infty$.*

Results on a mildly singular BVP

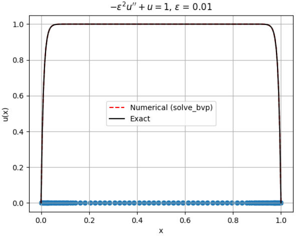
Compare standard collocation and a PINN for the ODE using ADAM

$$-\epsilon^2 u_{xx} + u = 1, \quad u(0) = u(1) = 0, \quad 0 < \epsilon \ll 1$$

This has a boundary layer at $x = 0, x = 1$ of width ϵ.

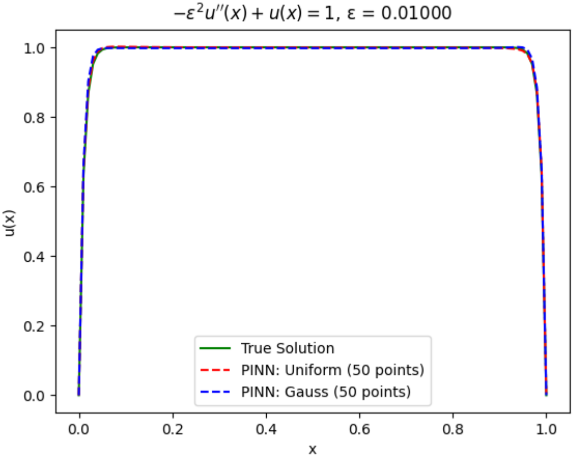


PINN



Collocation

Using the LBFGS optimiser



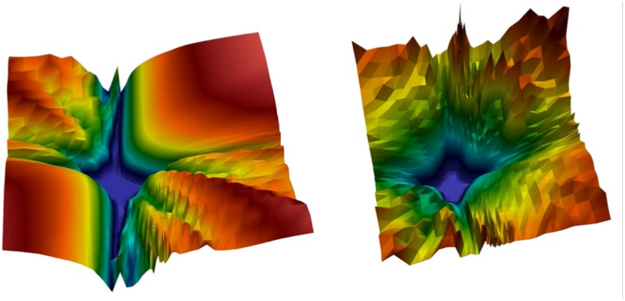
How and why do PINNS struggle to train .. and how can we fix this?

A subject of intensive research! See [Wang et. al.] for a summary: Observe

- PINNS train especially badly when they have high frequency features
- Loss function has multi-scale interactions, leading to ill-conditioning and stiffness in the gradient flow dynamics and a stringent stability requirement on the loss rate
- Standard networks show spectral bias and cannot learn high frequencies. This has been see for example in weather forecasting

They advocate the use of Neural Tanjent Kernels in the optimisation process. [Kiyani et. al.] extend this with the development of better optimisers eg. Broyden methods, for PINNS

Loss landscape is highly non-convex, [Kiyani et. al.]



Also Issues with **conditioning** as in the last lecture on approximation.

Can fix for shallow networks by **preconditioning**