Scientific Machine Learning - Theoretical aspects

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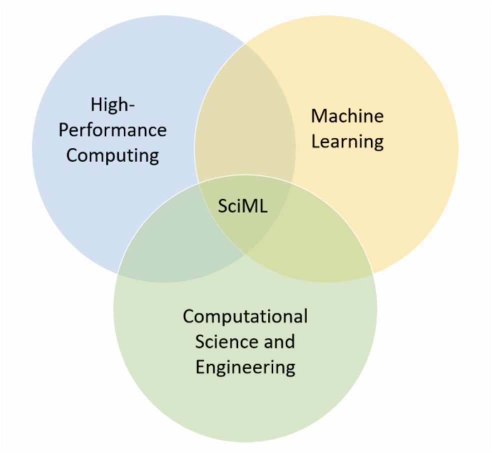
Outline

1. Introduction to Scientific Machine Learning (SciML)
2. Several partial differential equations
3. Approximation of functions by neural networks

Outline

Introduction to SciML



In recent years, the combination of numerical methods and machine learning has gained an ever increasing interest as a research field within Numerical Mathematics and Scientific Computing

Introduction to SciML

What is Scientific Machine Learning ?

- SciML is an emerging discipline within the data science community
- SciML seeks to address domain-specific data challenges and extract insights from scientific data sets through innovative methodological solutions
- SciML draws on tools from both Machine Learning (ML) and scientific computing to develop new methods for robust learning and data analysis
- SciML will be critical in driving the next wave of data-driven scientific discovery in the physical and engineering sciences
- SciML is multidisciplinary and leverages expertise from applied and computational mathematics, computer science, and the physical sciences

Introduction to SciML

Why Scientific Machine Learning ?

- New innovations in ML and Big Data are beginning to drive advances in scientific disciplines
- But the full potential of these techniques for data-driven discovery has yet to be fully realized
- One barrier to data-driven discovery is that existing methods often do not meet the needs of scientific users
- Application-agnostic algorithms, or those designed for more traditional ML applications such as image or natural language processing, can not typically be directly applied to scientific data sets and require non-trivial, task-specific modifications

Introduction to SciML

Why Scientific Machine Learning?

- In many applications only limited or low-quality labels are available, while massive unlabeled (often class imbalanced) data sets are common
- Scientific data are often high-dimensional, noisy, heterogeneous, low-signal-to-noise, and multiscale
- Models should respect or incorporate physical laws, constraints, and other scientific domain knowledge
- Robust methods and an ability to quantify uncertainty are required for scientific rigor

Outline

Poisson equation

- Dirichlet boundary conditions

$$\begin{cases} -u''(x) + c(x)u(x) = f(x), \; x \in]-1, 1[, \\ u(-1) = 0, \; u(1) = 0. \end{cases}$$

Exact solution for $c = 0$ and $f(x) = \pi^2 \sin(\pi x)$, $-1 \leq x \leq 1$,

$$u(x) = \sin(\pi x), \; -1 \leq x \leq 1.$$

- Dirichlet/Neumann boundary conditions

$$\begin{cases} -u''(x) + c(x)u(x) = f(x), \; x \in]-1, 1[, \\ u(-1) = 0, \; u'(1) = 4. \end{cases}$$

Exact solution for $c = 0$ and $f(x) = -2$, $-1 \leq x \leq 1$,

$$u(x) = (x+1)^2, \; -1 \leq x \leq 1.$$

- Dirichlet/Robin boundary conditions

$$\begin{cases} -u''(x) = f(x), \; x \in]0, 1[, \\ u(-1) = 0, \; u'(1) = u(1). \end{cases}$$

Same exact solution for $c = 0$ and $f(x) = -2$, $-1 \leq x \leq 1$.

Heat equation

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) - \dfrac{\partial^2 u}{\partial x^2}(t,x) = 0, x \in]-1,1[,\ t > 0, \\ u(t,-1) = u(t,1) = 0, t > 0, \\ u(0,x) = u_0(x),\ x \in]-1,1[. \end{cases}$$

u_0 is the initial condition

Advection equation

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) + a\dfrac{\partial u}{\partial x}(t,x) = 0,\ (t,x) \in \mathbb{R}^+ \times \mathbb{R} \\ u(0,x) = u_0(x),\ x \in \mathbb{R}, \end{cases}$$

u_0 is the initial condition, a is a constant, $a > 0$.

- If u_0 belongs to $C^1(\mathbb{R})$, existence and uniqueness of a classical solution u belonging to $C^1(\mathbb{R}^+ \times \mathbb{R})$

$$u(t,x) = u_0(x - at).$$

Inviscid Burgers equation / Viscid Burgers equation

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) + u(t,x)\dfrac{\partial u}{\partial x}(t,x) = 0,\ (t,x) \in \mathbb{R}^+ \times \mathbb{R} \\ u(0,x) = u_0(x),\ x \in \mathbb{R}, \end{cases}$$

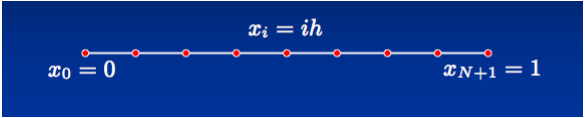
u_0 is the initial condition.

- If u_0 belongs to $C^1(\mathbb{R})$, bounded over $\mathbb{R}$ with a derivative bounded over $\mathbb{R}$, if $u_0' \geq 0$: existence and uniqueness of a classical solution u belonging to $C^1(\mathbb{R}^+ \times \mathbb{R})$.

$$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) + u(t,x)\dfrac{\partial u}{\partial x}(t,x) = \nu \dfrac{\partial^2 u}{\partial x^2}(t,x),\ (t,x) \in \mathbb{R}^+ \times \mathbb{R} \\ u(0,x) = u_0(x),\ x \in \mathbb{R}, \end{cases}$$

u_0 is the initial condition, ν is a constant, $\nu > 0$.
Hopf-Cole transformation, transform the viscid Burgers equation into a linear heat equation.

Forward Euler scheme

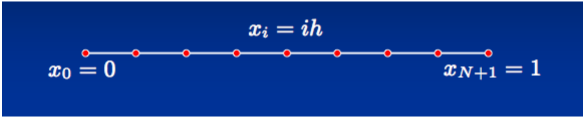


Forward Euler scheme

1

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2} = 0,\ i = 1, \cdots, N,\ n = 0, \cdots, M-1,$$

Forward Euler scheme



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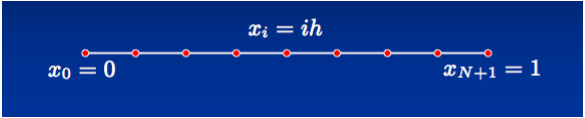
2.
$$u_i^0 = u_0(x_i), i = 1, \cdots, N,$$

Forward Euler scheme



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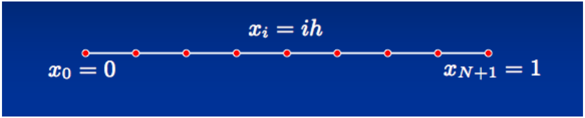
2.
$$u_i^0 = u_0(x_i), i = 1, \cdots, N,$$

3.
$$u_0^n = u_{N+1}^n = 0, n = 0, \cdots, M.$$

Forward Euler scheme



Forward Euler scheme

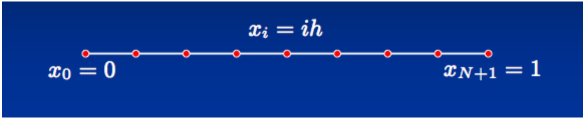
1. $$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{h^2} = 0,\ i = 1, \cdots, N,\ n = 0, \cdots, M-1,$$

2. $$u_i^0 = u_0(x_i), i = 1, \cdots, N,$$

3. $$u_0^n = u_{N+1}^n = 0, n = 0, \cdots, M.$$

$$\lambda = \frac{\Delta t}{h^2}$$

Backward Euler scheme

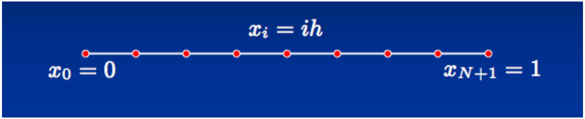


Backward Euler scheme

1.

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{h^2} = 0, \ i = 1, \cdots, N, \ n = 1, \cdots, M-1,$$

Backward Euler scheme

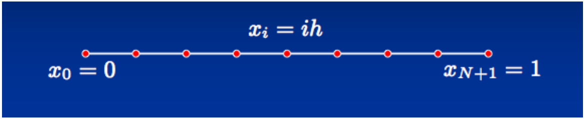


Backward Euler scheme

1.
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{h^2} = 0,\ i = 1, \cdots, N,\ n = 1, \cdots, M-1,$$

2.
$$u_i^0 = u_0(x_i), i = 1, \cdots, N,$$

Backward Euler scheme



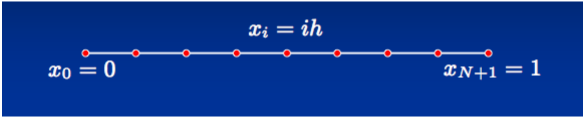
Backward Euler scheme

1. $$\frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{h^2} = 0,\ i = 1, \cdots, N,\ n = 1, \cdots, M-1,$$

2. $$u_i^0 = u_0(x_i), i = 1, \cdots, N,$$

3. $$u_0^n = u_{N+1}^n = 0, n = 0, \cdots, M.$$

Upwind scheme / Lax-Wendroff scheme



1

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_j^n - u_{j-1}^n}{h} = 0,$$

2

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2h} - \frac{a^2\Delta t}{2}\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2} = 0.$$

L^2 stability analysis

1. Let u be a 1-periodic function, the Fourier coefficients $\hat{u}(k)$, $k \in \mathbb{Z}$ are complex numbers defined by the integrals

$$\hat{u}(k) = \int_0^1 u(x) e^{-2\pi ikx} dx.$$

2. Parseval formula

$$\|u\|_2^2 = \sum_{k\in\mathbb{Z}} |\hat{u}(k)|^2.$$

3. Von Neumann analysis, there exists a constant $K > 0$ independent of Δt and h such that for all n, $1 \le n \le M$,

$$\|u^n\|_2 = \left(\sum_{j=1}^{N} h|u_j^n|^2\right)^{1/2} \le K\|u^0\|_2 = \left(\sum_{j=1}^{N} h|u_j^0|^2\right)^{1/2}.$$

4. Stability, consistency, convergence - Lax-Richtmyer theorem.

Outline

1. Introduction to Scientific Machine Learning (SciML)
2. Several partial differential equations
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Back to the future

Let n in $\mathbb{N}^*$, σ a function from $\mathbb{R}$ to $\mathbb{R}$, $M([0,1]^n)$ the space of finite, signed regular Borel measures and $C([0,1]^n)$ the space of continuous functions on $[0,1]^n$.

Definition.

We say that σ is **sigmoidal** if

$$\lim_{t \to -\infty} \sigma(t) = 0, \lim_{t \to +\infty} \sigma(t) = 1,$$

we say that σ is **discriminatory** if for a measure μ in $M([0,1]^n)$

$$\int_{[0,1]^n} \sigma\left(y^t x + \theta\right) d\mu(x) = 0$$

for all y in $\mathbb{R}^n$ and θ in $\mathbb{R}$ implies that $\mu = 0$. □

A sigmoidal function can not be a polynomial function.

Back to the future

Let n in $\mathbb{N}^*$, σ a function from $\mathbb{R}$ to $\mathbb{R}$, $M([0,1]^n)$ the space of finite, signed regular Borel measures and $C([0,1]^n)$ the space of continuous functions on $[0,1]^n$.

Theorem 1, Cybenko (1989).

Let σ be any continuous discriminatory function. The finite sums of the form

$$G(x) = \sum_{j=1}^{N} \alpha_j \sigma \left(y_j^t x + \theta_j \right)$$

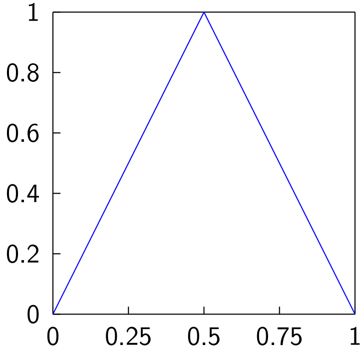
are dense in $C([0,1]^n)$. □

Lemma 1, Cybenko (1989).

Any bounded, measurable sigmoidal function, σ, is discriminatory. In particular, any continuous sigmoidal function is discriminatory. □

Approximation by ReLU Neural Networks

$$g(x) = \begin{cases} 2x, & 0 \leq x \leq 1/2, \\ 2(1-x), & 1/2 < x < 1. \end{cases}$$



Approximation of a one dimensional function by a Neural Networks (NN)

Let us suppose we want to approximate a one dimensional function $f \in C^n([0,1])$ with to simplify $\|f^{(k)}\|_\infty \leq 1$, $0 \leq k \leq n$, by Neural Networks. The main idea with the ReLU is to replace the piecewise linear functions by piecewise polynomials and we need the following ingredients :

- A NN f_1^* approximating linear functions

$$\sup_{x\in[0,1]} |f_1^*(x) - x| \leq \varepsilon$$

- A NN f_2^* approximating quadratic functions

$$\sup_{x\in[0,1]} |f_2^*(x) - x^2| \leq \varepsilon$$

- Approximate a partition of unity :

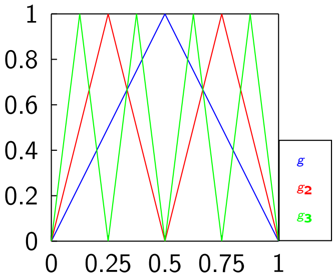
$$\psi_j \geq 0, \sum_{j=1}^{N} \psi_j = 1, \operatorname{supp} \psi_j \subset \left[\frac{j-1}{N}, \frac{j+1}{N}\right] \cap [0,1], \, j = 0, \cdots, N.$$

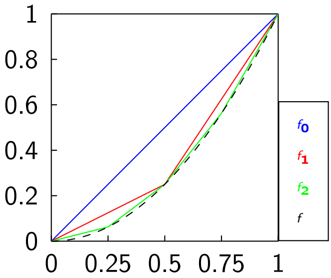
Approximation by ReLU Neural Networks

Step 1 : $x = \max(x, 0) - \max(-x, 0) = ReLU(x) - ReLU(-x) = \sigma(x) - \sigma(-x)$.
Remark : $\max(x, 0) + \max(-x, 0) = |x|$.
Step 2 :

Proposition 1, Yarotsky (2017).

The function $x \mapsto f(x) = x^2$ on the segment $[0, 1]$ can be approximated with any error $\varepsilon > 0$ by a ReLU network. □





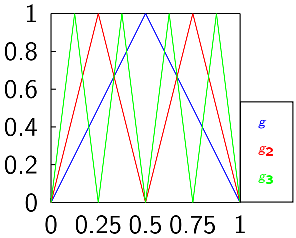
Approximation by ReLU Neural Networks

Lemma 2, Telgarsky (2015).

Let real $x \in [0,1]$ and positive integer m be given, and choose the unique nonnegative integer $i_m \in \{0, \cdots, 2^{m-1}\}$ and real $x_m \in [0,1[$ so that $x = (i_m + x_m)2^{1-m}$. Then

$$g_m(x) = \begin{cases} 2x_m, & 0 \leq x_m \leq 1/2, \\ 2(1 - x_m), & 1/2 < x_m < 1. \end{cases}$$

$\square$

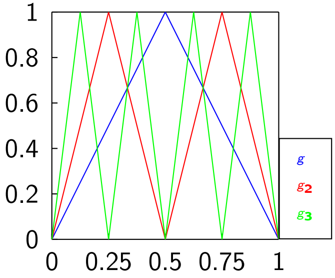


Approximation by ReLU Neural Networks

Lemma 3, Telgarsky (2015).

$$g_m(x) = \begin{cases} 2^m\left(x - \frac{2k}{2^m}\right), & x \in \left[\frac{2k}{2^m}, \frac{2k+1}{2^m}\right], k = 0, 1, \cdots, 2^{m-1} - 1 \\ 2^m\left(\frac{2k}{2^m} - x\right), & x \in \left[\frac{2k-1}{2^m}, \frac{2k}{2^m}\right], k = 1, 2, \cdots, 2^{m-1}. \end{cases}$$

□



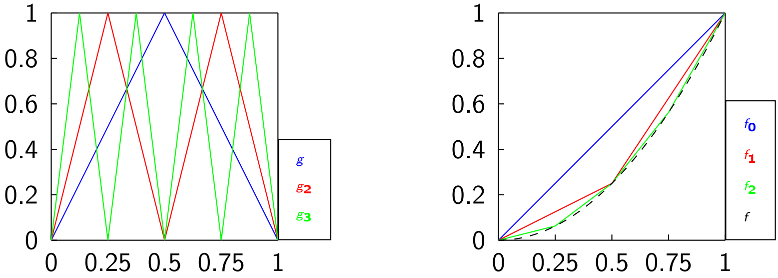
Approximation by ReLU Neural Networks

Let f_m be the piecewise linear interpolation of f with $2^m + 1$ uniformly distributed breakpoints $k/2^m$, $k = 0, \cdots, 2^m$,

$$f_m\left(\frac{k}{2^m}\right) = \left(\frac{k}{2^m}\right)^2, \; k = 0, \cdots, 2^m.$$

We have for all $x \in [0, 1]$

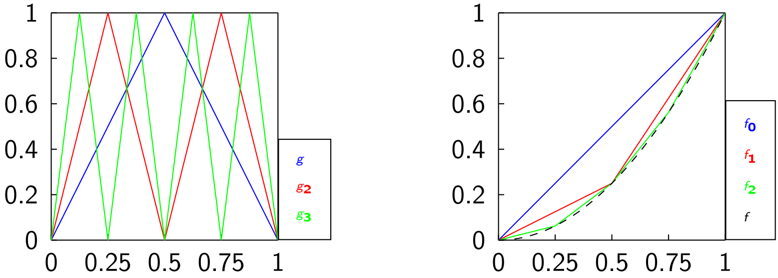
$$f_{m-1}(x) - f_m(x) = \frac{g_m(x)}{2^{2m}}, \; f_m(x) = x - \sum_{\ell=1}^{m} \frac{g_\ell(x)}{2^{2\ell}}$$



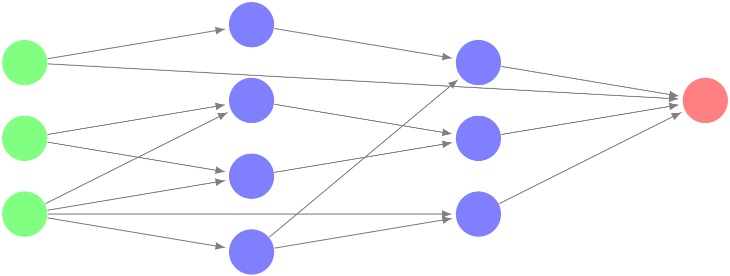
Approximation by ReLU Neural Networks

We have (for all $x \in [0,1]$) - (Exercices)

- $$\|f_m - f\|_{[0,1]} \le 2^{-2m},$$
- $$g(x) = 2\sigma(x) - 4\sigma\left(x - \frac{1}{2}\right) + 2\sigma(x-1).$$



Approximation by ReLU Neural Networks



A feedforward neural network having 3 input units, 1 output unit, and 7 computation units with nonlinear activation. The network has 4 layers and $16 + 8 = 24$ weights.

Proposition 2, Yarotsky (2017).

Given $M > 0$ and $\varepsilon \in]0, 1[$, there exists a ReLU network η with two input units that implements a function $\omega : \mathbb{R}^2 \to \mathbb{R}$ such that

1. for any inputs x, y if $|x| \leq M$ and $|y| \leq M$, then $|\omega(x, y) - xy| \leq \varepsilon$,
2. if $x = 0$ or $y = 0$ then $\omega(x, y) = 0$.

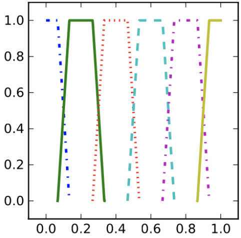
Approximation by ReLU Neural Networks

Step 3 : Partition of unity

$$\psi(x) = \begin{cases} 1 & |x| < 1, \\ 0 & 2 < |x|, \\ 2 - |x| & 1 \le |x| \le 2. \end{cases}$$

Let $N \in \mathbb{N}^*$, $x \in [0,1]$, $\psi_j(x) = \psi(3N(x - j/N))$, $j = 0, \cdots, N$,

$$\sum_{j=0}^{N} \psi_j(x) = 1.$$



Approximation by ReLU Neural Networks

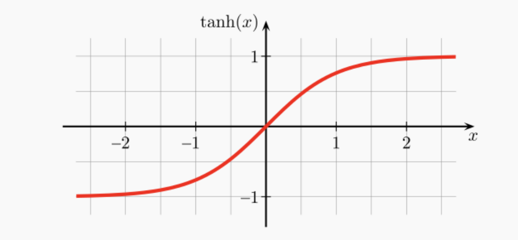
Theorem 2, Yarotsky (2017) - Upper bounds.

For any $n \in \mathbb{N}^*$ and $\varepsilon \in [0,1]$, a function f belonging to $C^n([0,1])$ can be approximated by a ReLU network with error ε. Moreover there exists a constant $c(n)$ such that this ReLU network has the depth at most $c(n)(\ln(1/\varepsilon)+1)$ and at most $c(n)\varepsilon^{-1/n}(\ln(1/\varepsilon)+1)$ weights and computation units. $\square$

Towards PINNs : Approximation by tanh Neural Networks

New activation function defined for all x in $\mathbb{R}$ by

$$\sigma(x) = \tanh(x).$$



σ is a C^∞ function satisfying for x in $\mathbb{R}$,

$$\sigma'(x) = 1 - \sigma^2(x) = \frac{4}{(e^x + e^{-x})^2}$$

Towards PINNs : Approximation by tanh Neural Networks

Theorem 3, De Ryck, Lanthaler, Mishra (2021).

For any $n \in \mathbb{N}^*$ and $\varepsilon \in [0,1]$, a function f belonging to $C^n([0,1])$ can be approximated by a tanh network with error ε. Moreover the tanh network has two hidden layers and there exists a constant $c(n,f)$ such that one is of width at most

$$3 \min \left(p \in \mathbb{N} | p \geq \frac{n}{2} \right) + \frac{c(n,f)}{\sqrt[n]{\varepsilon}} - 1$$

and the other of width at most

$$\frac{6c(n,f)}{\sqrt[n]{\varepsilon}}.$$

$\square$

Towards PINNs : Approximation by tanh Neural Networks

Proposition 3, De Ryck, Lanthaler, Mishra (2021).

Let $p \in \mathbb{N}^*$, the function defined for all x in $[0,1]$ by x^p can be approximated with any error $\varepsilon > 0$ by a tanh network. □

- $p = 1$, exercice
- p odd, use pth order central finite difference approximation with y in $[0,1]$, $h > 0$,

$$\delta^p_{y,h}[\sigma] = \sum_{i=0}^{p} (-1)^i C_p^i \sigma\left(\left(\frac{p}{2} - i\right) yh\right).$$

- p even, $\sigma^{(p)}(0) = 0$, use for y in $\mathbb{R}$ and $\alpha > 0$,

$$y^p = \frac{1}{2\alpha(p+1)}\left((y+\alpha)^{p+1} - (y-\alpha)^{p+1} - 2\sum_{k=0}^{p/2-1} C_{p+1}^{2k}\alpha^{p-2k+1} y^{2k}\right)$$

Towards PINNs : Approximation by tanh Neural Networks

Proposition 3, De Ryck, Lanthaler, Mishra (2021).

Let $p \in \mathbb{N}^*$, the function defined for all x in $[0,1]$ by x^p can be approximated with any error $\varepsilon > 0$ by a tanh network. $\square$

Consequence.

Proposition 3 + Stone-Weirstrass theorem : A continuous function on $[0,1]$ by x^p can be approximated with any error $\varepsilon > 0$ by a tanh network. $\square$

Consequence 2.

Approximation with error ε of the product of two reals x and y by a tanh network. $\square$

Towards PINNs : Approximation by tanh Neural Networks

Step 3 : from "Partition of unity" to "Approximation of partition of unity"
Let $\varepsilon > 0$ and $N \in \mathbb{N}^*$,

$$[0,1] = \bigcup_{j=1}^{N} \left[\frac{j-1}{N}, \frac{j}{N}\right].$$

We fix $\alpha > 0$ large enough such that

$$1 - \sigma\left(\frac{\alpha}{N}\right) \leq \varepsilon.$$

For j, $2 \leq j \leq N-1$ and y in $\mathbb{R}$, we define

$$\rho_j^N(y) = \frac{1}{2}\sigma\left(\alpha\left(y - \frac{j-1}{N}\right)\right) - \frac{1}{2}\sigma\left(\alpha\left(y - \frac{j}{N}\right)\right)$$

and

$$\rho_1^N(y) = \frac{1}{2} - \frac{1}{2}\sigma\left(\alpha\left(y - \frac{1}{N}\right)\right),$$

$$\rho_N^N(y) = \frac{1}{2}\sigma\left(\alpha\left(y - \frac{N-1}{N}\right)\right) + \frac{1}{2}.$$

Towards PINNs : Approximation by tanh Neural Networks

Step 3 : from "Partition of unity" to "Approximation of partition of unity"
Let $\varepsilon >$ and $N \in \mathbb{N}^*$,

$$[0,1] = \bigcup_{j=1}^{N} \left[\frac{j-1}{N}, \frac{j}{N} \right].$$

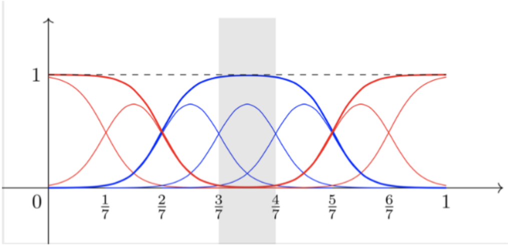


Figure – An example with $N = 7$

Towards PINNs : Approximation by tanh Neural Networks

Lemma 3, De Ryck, Lanthaler, Mishra (2021).

For a fixed j and $\varepsilon > 0$,

$$\left\| \sum_{\ell=j-1}^{j+1} \rho_\ell^N - 1 \right\|_{[\frac{j-1}{N}, \frac{j}{N}]} \leq \varepsilon$$

and for $\ell \neq j-1, j, j+1$,

$$\left\| \rho_\ell^N \right\|_{[\frac{j-1}{N}, \frac{j}{N}]} \leq \varepsilon.$$

□

Almost the same properties as the family of functions ψ_i, $0 \leq i \leq N$.

PINNs : Two disappointing results

Back to the model of dynamics with frictions.

- $mu'' + \mu u' = 0$ on $]0, T[$, $T > 0$.
- Challenge : the physical model is incomplete because the initial conditions are unknown but we have n noisy observations y_i at the points x_i, $1 \leq i \leq n$.
- Other data : a sample of independent and identically distributed random variables $x_j^{(r)}$, $1 \leq j \leq n_r$, uniformly distributed on $]0, T[$.
- Loss function :

$$R_{n,n_r}(u_{NN}(.,\theta)) = \frac{1}{n}\sum_{i=1}^{n} |u_{NN}(x_i,\theta) - y_i|^2 + \frac{1}{n_r}\sum_{j=1}^{n_r}\left((mu''_{NN} + \mu u'_{NN})\left(x_j^{(r)},\theta\right)\right)^2$$

PINNs : Two disappointing results

Theorem 3 (overfitting), Doumèche, Biau, Boyer (2023).

Consider the dynamics with friction model and assume that there are two observations such that $y_i \neq y_j$, $i \neq j$. Then, whenever one hidden size L of the neural network satisfies $L \geq n - 1$, for any integer n_r, for all $x_i^{(r)}$, $1 \leq i \leq n_r$, there exists a minimizing sequence $(u_{NN}(., \theta_p))_{p \in \mathbb{N}}$ such that

$$\lim_{p \to +\infty} R_{n,n_r}(u_{NN}(., \theta_p)) = 0$$

but

$$\lim_{p \to +\infty} \int_0^T \Big((m u''_{NN} + \mu u'_{NN})(x, \theta_p) \Big)^2 dx = +\infty$$

So, this PINN estimator is not consistent. $\square$

PINNs : Two disappointing results

Key ingredient : For θ in $\mathbb{R}$ and x in $\mathbb{R}$

$$\tanh_\theta(x) = \tanh(\theta x).$$

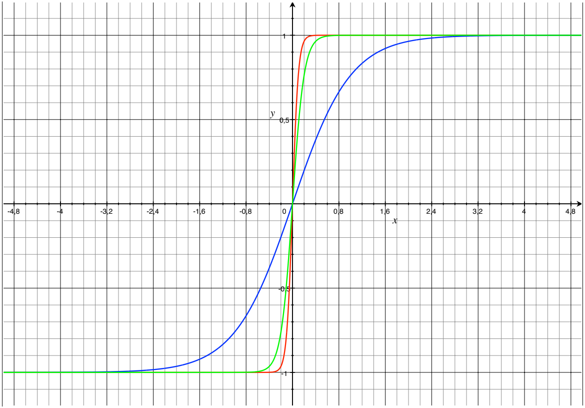


Figure – Graphs of $\tanh_\theta$ for $\theta = 1, 5, 10$

PINNs : Two disappointing results

Lemma 4, Doumèche, Biau, Boyer (2023).

Let the sign function defined for x in $\mathbb{R}$ by $\mathrm{sign}(x) = \mathbb{1}_{\{x>0\}} - \mathbb{1}_{\{x<0\}}$. Let K in $\mathbb{N}$ and H in $\mathbb{N}$, then for all $\varepsilon > 0$,

$$\lim_{\theta \to +\infty} \| \tanh_\theta^{\circ H} - \mathrm{sign} \|_{C^K(\mathbb{R} \setminus]-\varepsilon, \varepsilon[)} = 0.$$

□

Proof :

- $H = 1$ Exercice
- $H \geq 2$, by induction with the Faà di Bruno's formula (here with two regular functions f and g)

$$(D^n(f \circ g))(t) = \sum \frac{n!}{k_1! \dots k_n!} (D^k f)(g(t)) \left(\frac{(Dg)(t)}{1!} \right)^{k_1} \cdots \left(\frac{(D^n g)(t)}{n!} \right)^{k_n}$$

where $k = k_1 + \dots + k_n$ and the sum is over all partitions of n, i.e., values of $k_1, \cdots, k_n$ such that $k_1 + 2k_2 + \dots + nk_n = n$.

PINNs : Two disappointing results

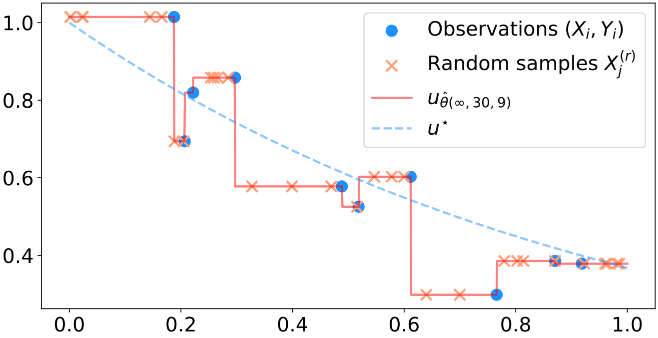


Figure – One example of an inconsistant PINNs in the model of dynamics with frictions

PINNs : Two disappointing results

Back to the heat equation.

- $\Omega =]-1, 1[\cup]0, T[$.
- $$\begin{cases} \dfrac{\partial u}{\partial t}(t,x) - \dfrac{\partial^2 u}{\partial x^2}(t,x) = 0, x \in \Omega, \\ u(t,-1) = u(t,1) = 0, t > 0, \\ u(0,x) = u_0(x),\ x \in [-1,1]. \end{cases}$$
- For $x \in [-1, 1]$,

$$u(x,0) = \tanh^{\circ H}(x+0.5) - \tanh^{\circ H}(x-0.5) + \tanh^{\circ H}(0.5) - \tanh^{\circ H}(1.5).$$

$\square$

PINNs : Two disappointing results

Back to the heat equation.

- Data 1 : a sample of independent and identically distributed random variables $x_i^{(e)}$, $1 \leq i \leq n_e$, on $E = [-1,1] \times \{0\} \cup (\{-1,1\} \times [0,T])$ distributed according to μ.
- Data 2 : a sample of independent and identically distributed random variables $x_i^{(r)}$, $1 \leq i \leq n_r$, uniformly distributed on Ω.
- Loss function : $R_{n_e,n_r}(u_{NN}(.,\theta)) =$

$$\frac{\lambda_e}{n_e}\sum_{j=1}^{n_e} |u_{NN}(x_j^{(e)},\theta) - h(x_j^{(e)})|^2 + \frac{1}{n_r}\sum_{\ell=1}^{n_r}\left(\left(\frac{\partial u_{NN}}{\partial t} - \frac{\partial^2 u_{NN}}{\partial x^2}\right)\left(x_j^{(r)},\theta\right)\right)^2$$

□

PINNs : Two disappointing results

Theorem 4 (overfitting), Doumèche, Biau, Boyer (2023).

Consider the heat equation, then, whenever $D > 4$, for any pair (n_e, n_r), for all $x_1^{(e)}, \cdots, x_{n_e}^{(e)}$ and for all $x_1^{(r)}, \cdots, x_{n_r}^{(r)}$, there exists a minimizing sequence $(u_{NN}(., \theta_p))_{p \in \mathbb{N}}$ such that

$$\lim_{p \to +\infty} R_{n_e, n_r}(u_{NN}(., \theta_p)) = 0$$

but

$$\lim_{p \to +\infty} \int_{\Omega} \left(\left(\frac{\partial u_{NN}}{\partial t} - \frac{\partial^2 u_{NN}}{\partial x^2} \right) (t, x, \theta_p) \right)^2 dt\, dx = +\infty$$

So, this PINN estimator is not consistent. □

PINNs : Two disappointing results

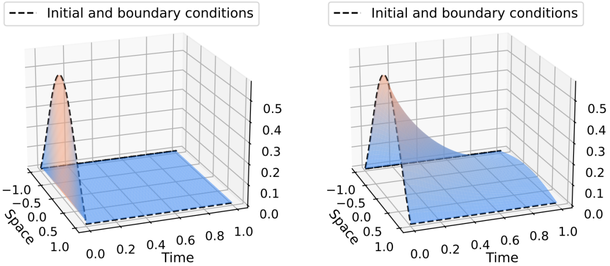


Figure – One example of an inconsistant PINNs with the heat equation