The Symbiosis of Neural Networks and Differential Equations: From PINNs to Neural ODEs

by

Cecília Coelho[1] **and Luís Ferrás**[1,2]

[1]Centre of Mathematics (CMAT), University of Minho, Portugal
[2]CEFT and DEMec (Section of Mathematics) - FEUP, University of Porto, Portugal
cmartins@cmat.uminho.pt, lferras@fe.up.pt

Outline of the Tutorial

- Introduction to Differential Equations
  - What are Differential Equations
  - Solving Differential Equations
  - Differential Equations in Real life
- Neural Networks for Solving Differential Equations
  - Challenges of Numerical Methods
  - Physics-Informed Neural Networks
  - Hands-on with the DeepXDE Library
- Neural Networks for Modelling Differential Equations
  - Challenges on Differential Equations Formulation for Describing Real-world Systems
  - Neural Ordinary Differential Equations
  - Hands-on with the Torchdiffeq Library
- Wrap-up
  - Physics-Informed Neural Networks versus Neural Ordinary Differential Equations
  - What's Next?

Availability of the Materials

All material can be found at the official tutorial's website, including a jupyter notebook with the coding examples and hands-on that will be used.

https://symbiosisnn-des.github.io/

Introduction to Differential Equations

- What are Differential Equations
- Solving Differential Equations
- Differential Equations in Real life

What are Differential Equations

Let's look at a simple, classic example of building a mathematical model to describe the evolution over time of a certain population (human, animal species, bacterial, etc.).
Suppose that the number of individuals in a certain population at a given time t is given by

$$P(t), \tag{1}$$

that is, $P(t)$ represents a function of time (the population as a function of time). To develop the model, let's fix a certain time interval

$$[t, t + \Delta t]. \tag{2}$$

For example, if $t = 1 hour$ and $\Delta t = 4$ *hours*, the interval would be $[1;\ 5]$. We will try to find a relationship between the population at time t ($P(t)$) and the population at time $t + \Delta t$ ($P(t + \Delta t)$).

What are Differential Equations

What happens during this time interval is that there was a certain number of deaths (M) and a certain number of births (N).
Our common sense suggests that:

- The larger the population, the higher the number of deaths and births (e.g., if in a population of 1000 individuals we have 10 deaths, then in a population of 2000 individuals we would expect 20 deaths). In other words, the number of deaths (M) and births (N) is proportional to the number of individuals ($P(t)$):

$$N = \alpha P(t), \quad M = \beta P(t) \tag{3}$$

  where α and β ($\in \mathbb{R}^+$) are the proportionality constants, which may vary from population to population.
- It is also expected that N and M depend on the time interval Δt. That is, the longer the time interval, the greater the number of births and deaths.

What are Differential Equations

This double dependency of N and M on $P(t)$ and Δt can then be expressed as:

$$N = \alpha P(t)\Delta t, \qquad M = \beta P(t)\Delta t. \tag{4}$$

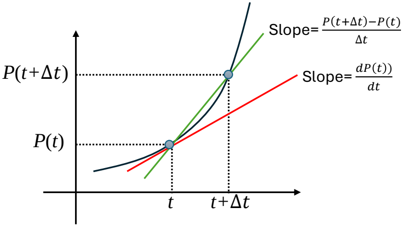
Consequently, the change in population over the time interval $[t,\ t+\Delta t]$ is given by $P(t+\Delta t) - P(t) = N - M$, that is:

$$P(t+\Delta t) - P(t) = (\alpha - \beta)P(t)\Delta t. \tag{5}$$

Dividing both sides by Δt, we obtain the following equation:

$$\frac{P(t+\Delta t) - P(t)}{\Delta t} = (\alpha - \beta)P(t). \tag{6}$$

What are Differential Equations



Taking the limit as $\Delta t \to 0$, we obtain the following differential equation:

$$\frac{dP}{dt} = (\alpha - \beta)P(t), \tag{7}$$

which is the well-known Malthusian equation, describing the *expected* variation (model) of population growth ($\alpha > \beta$) or decline ($\alpha < \beta$). Often, the notation $P'(t)$ is used instead of $\frac{dP}{dt}$.

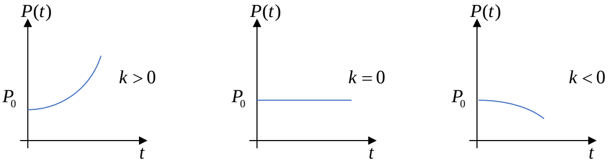
What are Differential Equations

Let $k = \alpha - \beta$, then ce^{kt} with $c \in \mathbb{R}$ an arbitrary constant, is the solution of our problem:

$$\frac{dP}{dt} = kP(t), \tag{8}$$

If we denote by P_0 the number of individuals at the beginning of the study ($t_0 = 0$), $P(0) = P_0$, then the solution to the model is given by (the arbitrary constant become a specific value: P_0):

$$P(t) = P_0 e^{kt} \tag{9}$$



What are Differential Equations

The differential equation $\frac{dP}{dt} = kP(t)$ together with the initial condition $P(0) = P_0$ is known as an **Initial Value Problem**.

This differential equation, which represents the Malthusian model, can also be written in the form:

$$\frac{dy(x)}{dx} = ky(x) \quad \text{or} \quad y' = ky$$

where the typical notation of x and y is used. From now on, we will preferably use this notation, where y is a function of x, with x being the independent variable.

What are Differential Equations

A differential equation is an equality that involves a function of one or more variables and its derivatives up to a certain order.

Example

$$x^2\frac{d^2y}{dx^2} - xy\left(\frac{dy}{dx}\right)^4 = 0 \quad \text{or} \quad x^2y'' - xy(y')^4 = 0 \tag{10}$$

$$y' = y \tag{11}$$

$$y'' + 2yy' = 3x \tag{12}$$

$$\frac{d^3v}{dt^3} + 5v\frac{dv}{dt} = \cos t \quad \text{or} \quad v''' + 5vv' = \cos t \tag{13}$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + 2\frac{\partial^2 u}{\partial z^2} = 0 \tag{14}$$

What are Differential Equations

Definition (Ordinary Differential Equation (ODE))

A differential equation involving derivatives of one or more dependent variables with respect to an independent variable is called an ordinary differential equation (ODE).

Definition (Partial Differential Equation (PDE))

is a differential equation that involves partial derivatives of a multivariable function. A **PDE** involves one or more dependent variables and their partial derivatives with respect to two or more independent variables.

Example: For a function $u(x, y)$, a PDE might look like:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

This is known as the **Laplace equation**, which appears in heat conduction, fluid flow, and electrostatics.

Solving Differential Equations

- The theory of differential equations began in the late 17th century, influenced by the works of G.W. Leibniz, I. Barrow, I. Newton, and the Bernoulli brothers, who solved simple first and second-order equations in mechanics and geometry. A notable milestone occurred on November 11, 1675, when Leibniz solved the equation $\frac{dy}{dx} = x$, using the integral symbol ($\int$).
  - The Malthus model is a simple ODE known as a separable variable differential equation. Its solution can be easily derived, as described in the following equations.
    Assuming that $P \neq 0$, we start with:
    $$\frac{dP}{dt} = kP \Leftrightarrow \frac{1}{P}\,dP = k\,dt, \tag{15}$$
    Next, we apply the integral to both sides of the equation:
    $$\int \frac{1}{P}\,dP = \int k\,dt \Rightarrow \ln|P| = kt + c_1 \Rightarrow P(t) = c_2 e^{kt}, \tag{16}$$
    where c_1 and c_2 are constants, with $c_2 \in \mathbb{R}_0^+$.

Solving Differential Equations

- Newton's equation of motion was pivotal in developing calculus, categorizing first-order equations into forms such as $\frac{dy}{dx} = f(x, y)$. Leibniz introduced the notation for derivatives and integral, and he developed the theory of **separable differential equations** and discovered methods for solving **linear first-order equations**.
- The 18th century saw significant advancements in the theory of differential equations, with contributions from Jacob and Johann Bernoulli, as well as prominent mathematicians like Clairaut, D'Alembert, and Euler. Euler established conditions for **exact first-order equations** and developed the theory of **integrating factors**.
- In the 19th century, Dirichlet proved the convergence of Fourier series, and Cauchy rigorously defined convergence concepts. Liouville established the limitations of solving differential equations using elementary functions, while the works of Picard and Peano addressed the existence and uniqueness of solutions for initial value problems.
- The second half of the 20th century witnessed advancements in **computational methods for solving differential equations**, thanks to the contributions of Carl Runge and Martin Kutta.

Solving Differential Equations

Engineering

Engineers apply scientific and mathematical principles to design, build and analyze systems. Their work is mostly practical and oriented towards solving real-world problems.

Applied Mathematics

Applied mathematicians use mathematical techniques and theories to solve practical problems in various fields. They focus on modeling real-world phenomena and finding numerical solutions.

Pure Mathematics

Pure mathematicians study mathematical concepts for their intrinsic value, without necessarily considering practical applications. They are more concerned with exploring theoretical aspects of mathematics.

The three fields are all essential because they approach problems differently.

- Pure mathematicians focus on determining whether a mathematical solution exists and under what conditions it can be applied.
- In contrast, engineers assume that a solution exists and immediately begin working on finding an exact or approximate solution to the problem.

Solving Differential Equations

For example, mathematicians are concerned with the following type of results for differential equations:

Theorem (Existence and Uniqueness of Solution)

Consider the differential equation

$$\frac{dy}{dx} = f(x, y)$$

where

1. *The function f is continuous in a domain D of the xy-plane;*
2. *The partial derivative* $\frac{\partial f}{\partial y}$ *is also continuous in D.*

Let (x_0, y_0) *be a point in D. Then the differential equation has a unique solution* ϕ *in the interval* $]x_0 - h, x_0 + h[$ *(or* $|x - x_0| < h$*), for sufficiently small h, which satisfies the condition*

$$\phi\left(x_0\right) = y_0.$$

Solving Differential Equations

We previously discussed how to find the analytical solution to the equation

$$\frac{dP}{dt} = kP(t)$$

with the initial condition $P(0) = P_0$.

However, not all differential equations are this straightforward. In many cases, we must rely on **numerical solutions** to solve more complex equations!

Solving Differential Equations

Scientists

SOLVER

Physical phenomenon

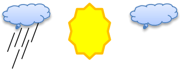
Mathematical Model

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \nabla \cdot (\mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}$$

Physical phenomena described by a mathematical model (differential equation).

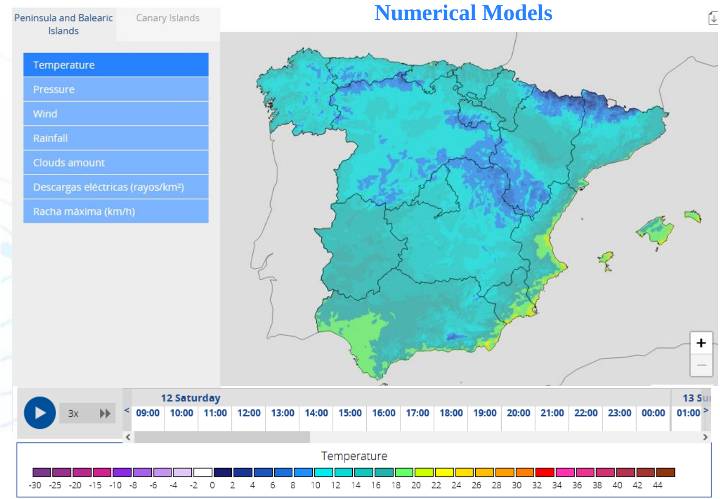
Numerical Solution

Monday Tuesday Wednesday



Prediction of the evolution of physical phenomena by numerical solution of the differential equations.

Solving Differential Equations



Please note that while we can obtain weather forecasts for every hour, we cannot provide a forecast for a specific time, such as 10:36.

Solving Differential Equations

Consider the simple differential equation,

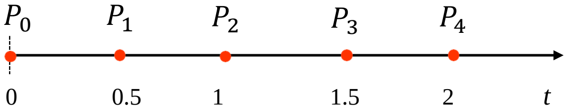
$$\frac{dP}{dt} = kP(t)$$

with the initial condition $P(0) = P_0$. We will now obtain its numerical solution!
For that we need to define the kind of approximation we will use, that is, the numerical method:

- Finite Difference (FD)
- Finite Volume (FV)
- Finite Elements (FE)
- other methods ...

Solving Differential Equations - FD

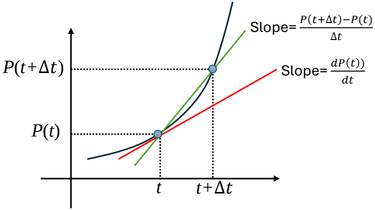
- Define an interval: $[0, 2]$
- Create a mesh: we will consider 5 mesh elements (4 intervals of 0.5) $\Delta t = 0.5$



- Initial condition: $P(0) = P_0 = 2$
- Let: $k = 1$
- **Objective**: determine the discrete solution $P_1,\ P_2,\ P_3,\ P_4$

Solving Differential Equations - FD

- Obtain approximations for $\dfrac{dP}{dt}$ at $t_1 = 0.5,\ t_2 = 1,\ t_3 = 1.5,\ t_4 = 2$



- $\dfrac{dP(t_i)}{dt} \approx \dfrac{P_i - P_{i-1}}{\Delta t}, i = 1, .., 4$
- Solve the system of equations (**Explicit Euler Method**):

$$\frac{P_1 - Po}{\Delta t} = P_0 \Leftrightarrow P_1 = P_0 + \Delta t P_0$$

$$P_2 = P_1 + \Delta t P_1$$

$$P_3 = P_2 + \Delta t P_2$$

$$P_4 = P_3 + \Delta t P_3$$

Solving Differential Equations - FD

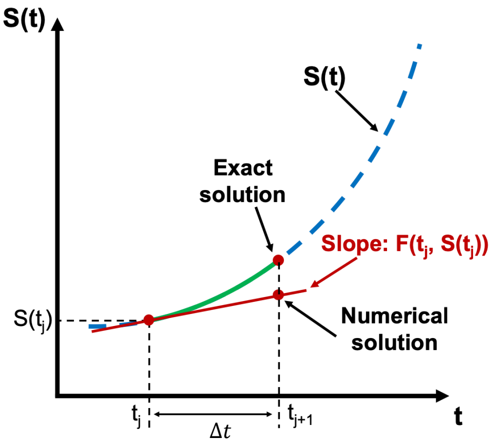
Let $\frac{dS(t)}{dt} = F(t, S(t))$ be an explicitly defined first order ODE. That is, F is a function that returns the derivative, or change, of a state given a time and state value. Also, let t_i be a numerical grid point of the interval $[t_0, t_f]$ with spacing Δt. Without loss of generality, we assume that $t_0 = 0$, and that $t_f = N\Delta t$ for some positive integer, N. We then approximate the solution at $S(t_{j+1})$ by:

$$S(t_{j+1}) = S(t_j) + (t_{j+1} - t_j)\frac{dS(t_j)}{dt}$$

which can also be written as

$$S(t_{j+1}) = S(t_j) + \Delta t \, F(t_j, S(t_j))$$

Solving Differential Equations - FD



https://pythonnumericalmethods.studentorg.berkeley.edu

Solving Differential Equations - FD

Implicit Euler Method:

$$S(t_{j+1}) = S(t_j) + \Delta t \, F(t_{j+1}, S(t_{j+1}))$$

- for our previous example, we obtain the following system of equations:

$$\frac{P_1 - P_0}{\Delta t} = kP_1$$
$$\frac{P_2 - P_1}{\Delta t} = kP_2$$
$$\frac{P_3 - P_2}{\Delta t} = kP_3$$
$$\frac{P_4 - P_3}{\Delta t} = kP_4$$

Solving Differential Equations - Hands On

Its now time for you to do it by yourselves (Part I)!

The differential equation $\frac{df(t)}{dt} = e^{-t}$ with initial condition $f(0) = -1$ has the exact solution $f(t) = -e^{-t}$. Approximate the solution to this initial value problem between 0 and 1 in increments of 0.1 using the **Explicit Euler method**. Plot the difference between the approximated solution and the exact solution.

Play with the **solver**, **model parameters** and the **number of mesh elements**.
https://www.kaggle.com/code/cici118/ecai24-tutorial

Solving Differential Equations - Hands On

Its now time for you to do it by yourselves (Part I)!

```python
import numpy as np
import matplotlib.pyplot as plt

# Define parameters
f = lambda t, s: np.exp(-t) # ODE
h = 0.3 # Step size
t = np.arange(0, 1 + h, h) # Numerical grid
s0 = -1 # Initial Condition

# Explicit Euler Method
s = np.zeros(len(t))
s[0] = s0

for i in range(0, len(t) - 1):
s[i + 1] = s[i] + h*f(t[i], s[i])
```

Solving Differential Equations - Hands On

Cont.

```
plt.figure(figsize = (6, 5))
plt.plot(t, s, 'bo--', label='Approximate')
plt.plot(t, -np.exp(-t), 'g', label='Exact')
plt.title('Approximate and Exact Solution \
for Simple ODE')
plt.xlabel('t')
plt.ylabel('f(t)')
plt.grid()
plt.legend(loc='lower right')
plt.show()
```

Solving Differential Equations - Hands On

Its now time for you to do it by yourselves (Part II)! You do not need to implement the numerical solver, Python can easily deal with that:

```
sol = solve_ivp(ODE, [0, 5], y0, t_eval=t)
```

Consider a population of organisms that follows a logistic growth. The population size $P(t)$ at time t is governed by the following differential equation:

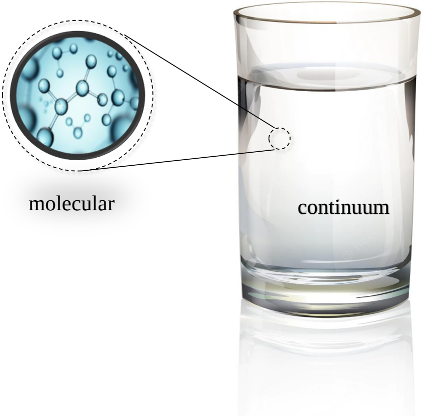
$$P'(t) = rP(t)\left(1 - \frac{P(t)}{K}\right), \quad P(t_0) = 100, \tag{17}$$

where r is the growth rate, and K is the carrying capacity of the environment. Consider $r = 0.1, K = 1000$. Also, consider a mesh of 200 points.

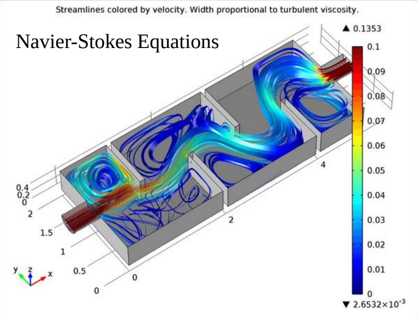
Play with the **solver**, **model parameters** and the **number of mesh elements**.

Differential Equations in Real Life

Most interesting real life applications are modelled by the **Partial Differential Equations**



Most interesting real life applications are modelled by the **Partial Differential Equations**



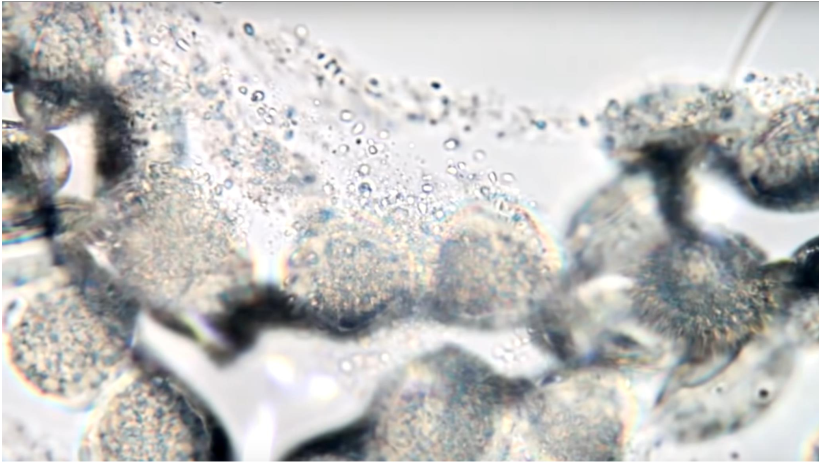
They are used by engineers and physicists all over the world in many fields, which go from aircraft design to blood circulation. They are also very complicated to solve and that is why they are one of the seven *Millennium Prize Problem*. Solving one of these problems will win you a million dollars

$$\nabla \cdot \overline{u} = 0$$

$$\rho \frac{D\overline{u}}{Dt} = -\nabla p + \mu \nabla^2 \overline{u} + \rho \overline{F}$$

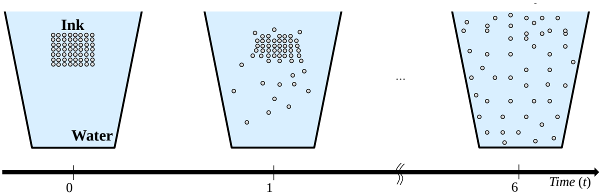
Navier-Stokes equations

Differential Equations in Real Life



Differential Equations in Real Life

Diffusion can be seen as a transport phenomena where distribution, mixing or transport of mass/particles occurs without requiring bulk motion (the spreading of something more widely).



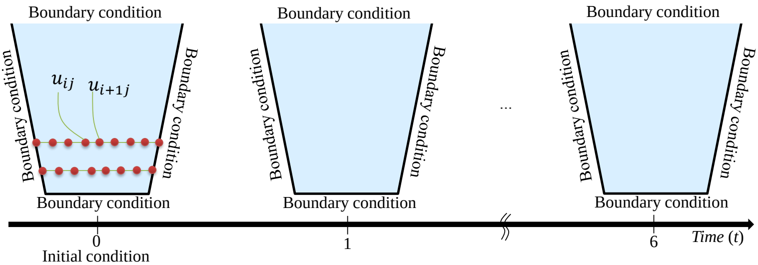
$$\frac{\partial u(t,x)}{\partial t} = D\frac{\partial^2 u(t,x)}{\partial x^2} \quad (1D) \tag{18}$$

$$\frac{\partial u(t,x,y)}{\partial t} = D\left(\frac{\partial^2 u(t,x,y)}{\partial x^2} + \frac{\partial^2 u(t,x,y)}{\partial y^2}\right) \quad (2D) \tag{19}$$

Neural Networks for Solving DE

- Challenges of Numerical Methods
- Physics-Informed Neural Networks
- Hands-on with the DeepXDE Library

Challenges of Numerical Methods



$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

Explicit

$$\frac{u_{ij}^{n+1} - u_{ij}^{n}}{\triangle t} = D\left(\frac{u_{i+1j}^{n} - 2u_{ij}^{n} + u_{i-1j}^{n}}{\triangle x^2} + \frac{u_{ij+1}^{n} - 2u_{ij}^{n} + u_{ij-1}^{n}}{\triangle y^2}\right)$$

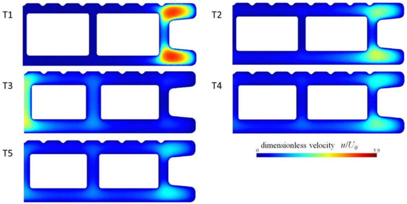
Implicit

$$\frac{u_{ij}^{n+1} - u_{ij}^{n}}{\triangle t} = D\left(\frac{u_{i+1j}^{n+1} - 2u_{ij}^{n+1} + u_{i-1j}^{n+1}}{\triangle x^2} + \frac{u_{ij+1}^{n+1} - 2u_{ij}^{n+1} + u_{ij-1}^{n+1}}{\triangle y^2}\right)$$

Solve a system of equations for each time step

Challenges of Numerical Methods

There are several numerical methods and different solvers for solving differential equations, but nearly all of them share one major drawback — **they are time and memory-consuming!** Simulations can sometimes take months to complete.



N. Gonçalves, P. Teixeira, L.L. Ferrás, A. Afonso, Innovative approach to the design of profile extrusion dies, Society of Plastic Engineers – Plastic Research Online (2014) 10.2417/spepro.005733.

Two Paradigms

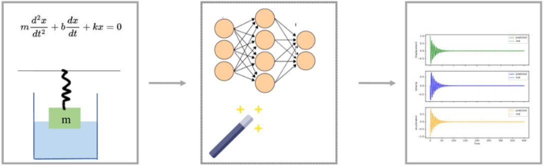
Solving differential equations

- Complete knowledge of the system;
- Exact solutions can be found but not often;
- Numerical solutions involve numerical methods;
- Used for finding the exact solutions for ODEs and PDEs in physics and engineering, where the system's behavior is well-defined mathematically.

Modelling differential equations

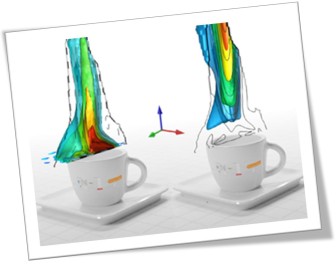
- Fully or partially unknown governing equations;
- Requires observed data to adjust the parameters or functions to match the data;
- Involves traditional optimization methods;
- Used for modeling systems in epidemiology, ecology, finance, and others.

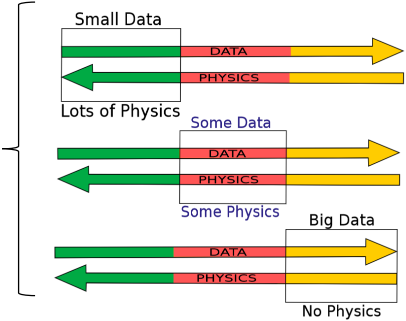
Neural Networks for Solving DEs



- Real systems in physics, chemistry and engineering are typically described by differential equations;
- When differential equations are known, numerically solving them can be computationally prohibitive [8];
- Physics-Informed Neural Networks (PINNs) use a neural network to approximate the curve of solutions [8];
- PINNs offer a faster and more cost-effective alternative to numerical methods when doing predictions [8].

Physics-Informed Neural Networks





Raissi, M., Perdikaris, P., Ahmadi, N., & Karniadakis, G. E. (2024). Physics-informed neural networks and extensions. *arXiv preprint arXiv:2408.16806*.

Cai, S., Wang, Z., Fuest, F., Jeon, Y. J., Gray, C., & Karniadakis, G. E. (2021). Flow over an espresso cup: inferring 3-D velocity and pressure fields from tomographic background oriented Schlieren via physics-informed neural networks. *Journal of Fluid Mechanics*, *915*, A102.

Physics-Informed Neural Networks

Consider a parameterised and nonlinear partial differential equation (PDE) of the general form:

$$\frac{\partial u(t,x)}{\partial t} + \mathcal{N}[u;\lambda] = 0, \quad x \in \Omega, t \in [0,T], \tag{20}$$

where $u(t,x)$ is the solution, $\mathcal{N}[u;\lambda]$ is a differential operator and Ω the domain of x. This setup encapsulates a wide range of problems in mathematical physics including conservation laws, diffusion processes, advection–diffusion–reaction systems, and kinetic equations.

PINNs - 1D Burger's Equation

As a motivating example, take the 1D Burger's equation, corresponding to $\mathcal{N}[u;\lambda] = \lambda_1 u \frac{du}{dx} - \lambda_2 \frac{\partial^2 u}{\partial x^2}$:

$$\frac{\partial u}{\partial t} + \lambda_1 u \frac{\partial u}{\partial x} - \lambda_2 \frac{\partial^2 u}{\partial x^2} = 0, \quad x \in \Omega, t \in [0, T]. \tag{21}$$

This equation arises in various areas of applied mathematics, including fluid mechanics, nonlinear acoustics, gas dynamics, and traffic flow. For small values of the viscosity parameters λ_1, λ_2, it is hard to solve by numerical methods.
Given noisy measurements of the system, we are interested in the solution of two distinct problems: data-driven solutions of PDEs, and data-driven discovery of PDEs [8].

Data-driven Solutions of PDEs

Problem: *Given fixed model parameters λ, what can be said about the unknown $u(t,x)$?*
PINNs approximate the solution $u(t,x)$ using a neural network $\hat{u}(t,x;\boldsymbol{\theta})$, where $\boldsymbol{\theta}$ represents the network parameters. The PINN is trained to fit the data (u_n) and satisfy the PDE, given by Eq. (20) [8]. This can be formulated as a constrained optimisation problem:

$$\begin{aligned} \underset{\boldsymbol{\theta} \in \mathbb{R}^{n_\theta}}{\text{minimize}} \quad & l(\boldsymbol{\theta}) = \frac{1}{N}\sum_{n=1}^{N}(\hat{u}_n(\boldsymbol{\theta}) - u_n)^2 \\ \text{subject to} \quad & \frac{\partial u(t,x)}{\partial t} + \mathcal{N}[u;\lambda] = 0, \quad t = [0,T], \end{aligned} \tag{22}$$

Data-driven Solutions of PDEs

To do this, we can rewrite the constrained problem (22) into an unconstrained problem by using a penalty method [7]:

$$\underset{\boldsymbol{\theta} \in \mathbb{R}^{n_\theta}}{\text{minimize}} \quad l(\boldsymbol{\theta}) = \frac{1}{N}\sum_{n=1}^{N}(\hat{u}_n(\boldsymbol{\theta}) - u_n)^2 + \mu \left(\frac{\partial u(t,x)}{\partial t} + \mathcal{N}[u;\lambda]\right) \tag{23}$$

Then, the loss function of the neural network $\hat{u}(t,x;\boldsymbol{\theta})$ consists of two components: the error of the fit to the data, and the violation of the PDE constraint multiplied by a weighting factor μ [8].

Data-driven Solutions of PDEs

To train the neural network $\hat{u}(x;\boldsymbol{\theta})$, data is needed. Collocation points are crucial in training PINNs and these are taken from locations to enforce the PDE's loss term. Likewise, initial and boundary training data are used to fit the data:

- **Collocation points**, N_{PDE}: scattered points within the domain where the PDE is enforced;
- **Initial/boundary points**, N_u: points where the solution is known to enforce initial and boundary conditions [8].

Example - 1D Burger's Equation

Consider the 1D Burger's Equation with Dirichlet boundary conditions and $\lambda_1 = 1, \lambda_2 = \frac{0.01}{\pi}$ [8]:

$$\begin{aligned} \frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \frac{0.01}{\pi}\frac{\partial^2 u}{\partial x^2} = 0, \quad x \in [-1, 1], t \in [0, 1], \\ u(0, x) = -\sin(\pi x), \\ u(t, -1) = u(t, 1) = 0. \end{aligned}$$

Example - 1D Burger's Equation

First, we define the penalty term as $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \frac{0.01}{\pi}\frac{\partial^2 u}{\partial x^2}$ and build the loss function:

$$\underset{\boldsymbol{\theta} \in \mathbb{R}^{n_\theta}}{\text{minimize}} \quad l(\boldsymbol{\theta}) = \frac{1}{N_u}\sum_{n=1}^{N_u}(\hat{u}_n(\boldsymbol{\theta}) - u_n)^2 + \frac{1}{N_{PDE}}\sum_{n=1}^{N_{PDE}}\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \frac{0.01}{\pi}\frac{\partial^2 u}{\partial x^2}\right) \tag{24}$$

Then we proceed by approximating $u(t, x)$ by a neural network [8].

Example - 1D Burger's Equation

To compute the derivatives of $u(t, x)$, PINNs use backpropagation [8].

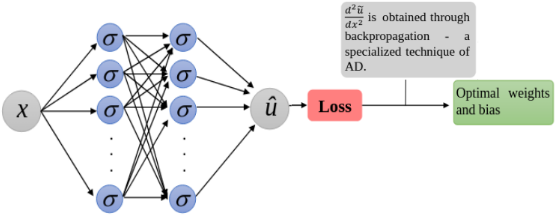


Figure 1: Schematic of the methodology used in the PINN method.

Example - 1D Burger's Equation

First, the DeepXDE and TensorFlow modules are imported:

```
import deepxde as dde
from deepxde.backend import tf
```

Then we start by defining the geometry and time domain of the problem using the built-in classes [8, 6]:

```
geom = dde.geometry.Interval(-1, 1)
timedomain = dde.geometry.TimeDomain(0, 1)
geomtime = dde.geometry.GeometryXTime(geom, timedomain)
```

Example - 1D Burger's Equation

Next, we code the PDE:

```
def pde(x, u):
    du_x = dde.grad.jacobian(u, x, i=0, j=0)
    du_t = dde.grad.jacobian(u, x, i=0, j=1)
    du_xx = dde.grad.hessian(u, x, i=0, j=0)

    return du_t + u * du_x - 0.01 / np.pi * du_xx
```

The first argument *x* is a vector in which the first component is the *x*-coordinate and the second component is the *t*-coordinate. The second argument *u* is the output given by the neural network [8, 6].

Example - 1D Burger's Equation

Then we define the initial and boundary conditions using the geometry and time domains previously defined:

```
bc = dde.icbc.DirichletBC(geomtime, lambda x: 0,
lambda _, on_boundary: on_boundary)
ic = dde.icbc.IC(geomtime, lambda x: -np.sin(np.pi *
x[:, 0:1]), lambda _, on_initial: on_initial)
```

The first argument *x* is a vector in which the first component is the *x*-coordinate and the second component is the *t*-coordinate. The second argument *u* is the output given by the neural network [8, 6].

Example - 1D Burger's Equation

Now, we have specified the geometry, PDE, and initial and boundary conditions. Thus we define the time-dependent PDE problem using the built-in function:

```
data = dde.data.TimePDE(geomtime, pde, [bc, ic],
num_domain=2540, num_boundary=80, num_initial=160)
```

The number 2540 is the number of training points sampled inside the domain, N_{PDE}. The number 80 is the number of training points sampled on the boundary and 160 are the initial points for the initial conditions, N_u [8, 6].

Example - 1D Burger's Equation

Next we define a neural network architecture. Here, we use a fully connected neural network of depth 4 and width 20:

```
net = dde.nn.FNN([2] + [20] * 3 + [1], "tanh",
"Glorot normal")
```

Then we build the network and choose an optimiser [8, 6]:

```
model = dde.Model(data, net)
model.compile("adam", lr=1e-3)
```

Example - 1D Burger's Equation

We then train the model for 15000 iterations:

```
losshistory, train_state = model.train(iterations=15000)
```

After we train the network using Adam, we continue to train the network using L-BFGS to achieve a smaller loss [8, 6]:

```
model.compile("L-BFGS-B")
losshistory, train_state = model.train()
```

Example - 1D Burger's Equation

Having some test data taken from a reference solution of the 1D Burger's Equation, we can compute the testing metrics [8, 6]:

```python
def gen_testdata():
    data = np.load("Burgers.npz")
    t, x, exact = data["t"], data["x"], data["usol"].T
    xx, tt = np.meshgrid(x, t)
    X = np.vstack((np.ravel(xx), np.ravel(tt))).T
    y = exact.flatten()[:, None]
    return X, y

X, y_true = gen_testdata()
y_pred = model.predict(X)
f = model.predict(X, operator=pde)
print("Mean residual:", np.mean(np.absolute(f)))
print("L2 relative error:",
dde.metrics.l2_relative_error(y_true, y_pred))
np.savetxt("test.dat", np.hstack((X, y_true, y_pred)))
```

Hands-On

- What happens if we change the number of training points inside the domain? What about in the inital and boundary conditions?
- Use PINNs to approximate the solution of the following Lotka-Volterra problem to know how the population of rabbits and foxes change over time in a system:

$$\frac{dr}{dt} = \frac{R}{U}(2Ur - 0.04U^2 rf), \quad \frac{df}{dt} = \frac{R}{U}(0.002U^2 rf - 1.06Uf),$$
$$r(0) = \frac{100}{U}, \quad f(0) = \frac{15}{U}$$

with $U = 200$ and $R = 20$.

Data-driven Discovery of PDEs

Problem: *What are the parameters λ that best describe the observed data?*
Again, PINNs approximate the solution $u(x)$ using a neural network $\hat{u}(t, x; \boldsymbol{\theta})$, where $\boldsymbol{\theta}$ represents the network parameters. The PINN is trained to fit the data and satisfy the PDE:

$$\begin{aligned} \underset{\boldsymbol{\theta}, \boldsymbol{\lambda} \in (\mathbb{R}^{n_\theta}, \mathbb{R}^{n_\lambda})}{\text{minimize}} \quad & l(\boldsymbol{\theta}, \boldsymbol{\lambda}) = \frac{1}{N} \sum_{n=1}^{N} (\hat{u}_n(\boldsymbol{\theta}) - u_n)^2 \\ \text{subject to} \quad & \frac{\partial u(t,x)}{\partial t} + \mathcal{N}[u; \lambda] = 0, \quad t = [0, T], \end{aligned} \tag{25}$$

Additionally, the parameters λ turn into parameters of the PINN [9].

Data-driven Discovery of PDEs

The loss function of the neural network $\hat{u}(t, x; \boldsymbol{\theta})$ consists of the two components: the error of the fit to the data, and the violation of the PDE constraint multiplied by a weighting factor μ.

$$\underset{\boldsymbol{\theta}, \boldsymbol{\lambda} \in (\mathbb{R}^{n_\theta}, \mathbb{R}^{n_\lambda})}{\text{minimize}} \quad l(\boldsymbol{\theta}, \boldsymbol{\lambda}) = \frac{1}{N} \sum_{n=1}^{N} (\hat{u}_n(\boldsymbol{\theta}) - u_n)^2 + \mu \left(\frac{\partial u}{\partial t} + \mathcal{N}[u; \lambda] \right) \tag{26}$$

The parameters λ are learnt by being optimised along the neural network parameters [9].

Data-driven Discovery of PDEs

To train the neural network $\hat{u}(t, x; \boldsymbol{\theta})$ and discover the parameters λ, data is needed:

- **Collocation points**, N_{PDE}: scattered points within the domain where the PDE is enforced;
- **Initial/boundary points**, N_u: points where the solution is known to enforce initial and boundary conditions, as well as to discover the unknown parameters λ.

Unlike the problem of ”data-driven solutions”, in this case some training data from the solution is needed, which can be experimental data [9].

Example - Diffusion Equation

Consider a diffusion equation with an unknown parameter C and Dirichlet boundary conditions [9]:

$$\frac{\partial u}{\partial t} = C\frac{\partial^2 u}{\partial x^2} - e^{-t}(\sin(\pi x) - \pi^2 \sin(\pi x)), \quad x \in [-1, 1], t \in [0, 1],$$
$$u(0, x) = \sin(\pi x),$$
$$u(t, -1) = u(t, 1) = 0.$$

Example - Diffusion Equation

First, we define the penalty term by rewriting the PDE and build the loss function [9]:

$$
\begin{aligned}
&\underset{\boldsymbol{\theta} \in \mathbb{R}^{n_\theta}}{\text{minimize}} \quad l(\boldsymbol{\theta}) = \frac{1}{N_u} \sum_{n=1}^{N_u} (\hat{u}_n(\boldsymbol{\theta}) - u_n)^2 + \\
&\frac{1}{N_{PDE}} \sum_{n=1}^{N_{PDE}} \left(\frac{\partial u}{\partial t} - C \frac{\partial^2 u}{\partial x^2} + e^{-t} (\sin(\pi x) + \pi^2 \sin(\pi x)) \right)
\end{aligned} \tag{27}
$$

Then we proceed by approximating $u(t, x)$ by a neural network [9].

Example - Diffusion Equation

Then we start by defining the geometry and time domain of the problem using the built-in classes [9, 6]:

```
geom = dde.geometry.Interval(-1, 1)
timedomain = dde.geometry.TimeDomain(0, 1)
geomtime = dde.geometry.GeometryXTime(geom, timedomain)
```

Example - Diffusion Equation

Next, we code the PDE [9, 6]:

```
def pde(x, u):
    du_t = dde.grad.jacobian(u, x, i=0, j=1)
    du_xx = dde.grad.hessian(u, x, i=0, j=0)

    return (dy_t - C * dy_xx + tf.exp(-x[:, 1:])
    * (tf.sin(np.pi * x[:, 0:1]) - np.pi ** 2
    * tf.sin(np.pi * x[:, 0:1])))
```

The first argument *x* is a vector in which the first component is the *x*-coordinate and the second component is the *t*-coordinate. The second argument *u* is the output given by the neural network. *C* is an unknown parameter that will be initialised as 2.0 [9, 6].

```
C = dde.Variable(2.0)
```

Example - Diffusion Equation

Then we define the initial and boundary conditions using the geometry and time domains previously defined:

```
bc = dde.icbc.DirichletBC(geomtime, func,
lambda _, on_boundary: on_boundary)
ic = dde.icbc.IC(geomtime, func, lambda _,
on_initial: on_initial)
```

The reference solution is [9, 6]:

```
def func(x):
    return np.sin(np.pi * x[:, 0:1]) * np.exp(-x[:, 1:])
```

Example - Diffusion Equation

In this problem, we provide extra information on some training points so the parameter C can be identified from these observations. We generate 10 equally-spaced input points (x, t), with $x \in [-1, 1]$ and $t = 1$, using the corresponding exact solution [9].

```
observe_x = np.vstack((np.linspace(-1, 1, num=10),
np.full((10), 1))).T
observe_y = dde.icbc.PointSetBC(observe_x,
func(observe_x), component=0)
```

Example - Diffusion Equation

Now, we have specified the geometry, PDE, initial and boundary conditions, and extra observations. Thus we define the time-dependent PDE problem using the built-in function [9, 6]:

```
data = dde.data.TimePDE(geomtime, pde,
[bc, ic, observe_y],
num_domain=40, num_boundary=20, num_initial=10,
anchors=observe_x, solution=func, num_test=10000)
```

The number 40 is the number of training points sampled inside the domain, N_{PDE}. The number 20 is the number of training points sampled on the boundary, 10 are the initial points for the initial conditions, furthermore *anchors* is the additional training points N_u [9, 6].

Example - Diffusion Equation

Next we define a neural network architecture. Here, we use a fully connected neural network of depth 4 and width 32 [9, 6]:

```
net = dde.nn.FNN([2] + [32] * 3 + [1], "tanh",
"Glorot normal")
```

Then we build the network, choose an optimiser and pass the unknown parameter C as a trainable variable [9, 6]:

```
model = dde.Model(data, net)
model.compile("adam", lr=1e-3,
metrics=["l2 relative error"],
external_trainable_variables=C)
```

Example - Diffusion Equation

We then train the model for 50000 iterations and output C every 1000 iterations:

```
variable = dde.callbacks.VariableValue(C, period=1000)
losshistory, train_state = model.train(iterations=50000,
callbacks=[variable])
```

We also save and plot the best trained result and loss history [9, 6]:

```
dde.saveplot(losshistory, train_state, issave=True
, isplot=True)
```

Hands-On

- What happens if we change the number of training points inside the domain? What about in the inital and boundary conditions?
- Use PINNs to discover σ, ρ, β for the following Lorenz system:

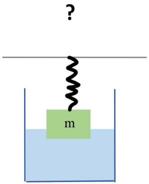
$$\frac{dx}{dt} = \sigma(y - x), \quad \frac{dy}{dt} = x(\rho - z) - y, \quad \frac{dz}{dt} = xy - \beta z, \quad t \in [0, 3]$$
$$x(0) = -8, \quad y(0) = 7, \quad z(0) = 27.$$

The true values are 10, 15, and $\frac{8}{3}$, respectively.

Neural Networks for Modelling DE

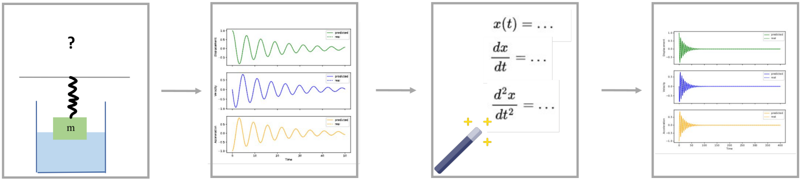
- Challenges on Differential Equations Formulation for Describing Real-world Systems
- Neural Ordinary Differential Equations
- Hands-on with the Torchdiffeq Library

Challenges on Formulating DEs



- Often the equations that model systems are unknown;
- When experimental data is available, mathematical models can be fitted;
- Traditional techniques require expert-knowledge and are a ”trial and error” process.

Neural Networks for Modelling DEs



- Neural networks are universal approximators [4];
- Experimental data can be used to train a neural network to fit the data;
- However, they fit time-independent functions to data [2];
- Data has to be regularly-sampled for training [2];
- Neural Ordinary Differential Equations adjust a time-dependent function to data, an ODE [2].

Neural Ordinary Differential Equations

In Residual Networks, we consider the following transformation of a hidden state from layer t to layer $t+1$:

$$\boldsymbol{h}_{t+1} = \boldsymbol{h}_t + \boldsymbol{f}_t(\boldsymbol{h}_t, \boldsymbol{\theta}_t), \tag{28}$$

where $\boldsymbol{h}_t \in \mathbb{R}^d$ is the hidden state at layer t, $\boldsymbol{\theta}_t$ represents the parameters of the network determined by the learning process (the weights and biases), and $\boldsymbol{f}_t : \mathbb{R}^d \to \mathbb{R}^d$ is a differentiable function. Assuming we have a finite number of layers, for the residual forward problem presented in (28) to be stable, it is recommended to control the variation of $\boldsymbol{f}_t(\boldsymbol{h}_t, \boldsymbol{\theta}_t)$ across iterations. Therefore, introducing a positive constant δ, one can control the variation of $\boldsymbol{f}_t$:

$$\boldsymbol{h}_{t+1} = \boldsymbol{h}_t + \delta \boldsymbol{f}_t(\boldsymbol{h}_t, \boldsymbol{\theta}_t). \tag{29}$$

Neural Ordinary Differential Equations

This equation can be rewritten as:

$$\frac{\boldsymbol{h}_{t+1} - \boldsymbol{h}_t}{\delta} = \boldsymbol{f}_t(\boldsymbol{h}_t, \boldsymbol{\theta}_t), \tag{30}$$

and taking the limit $\delta \to 0$, we obtain the following ODE,

$$\frac{d\boldsymbol{h}(t)}{dt} = \boldsymbol{f}(t, \boldsymbol{h}(t), \boldsymbol{\theta}(t)). \tag{31}$$

defined over a certain time interval $t \in [t_0, T]$ with $T > t_0$. Note that while it is indeed true that the parameter δ provides a means to regulate the stability of the forward problem (29), the stability is not solely determined by δ but also influenced by the variations in the weights.

Eq. (31) extends the discrete nature of the Residual Network, Eq. (29), to a continuous model.

Neural Ordinary Differential Equations

Assume we have a collection of ordered data ($N+1$ ordered observations) $\boldsymbol{x} = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, which represent the state of some dynamical system at discrete instants t_i over the time interval $[t_0, T]$ (with $t_N = T$). Each $\boldsymbol{x}_i = (x_i^1, x_i^2, \ldots, x_i^d) \in \mathbb{R}^d$, $i = 0, \ldots, N$ is associated with instant t_i.

We assume that the given data can be modelled by the initial value problem in Eq. (32). This allows us to determine the behaviour of the dynamical system at any instant within the interval $[t_0, T]$ [2, 3].

$$\begin{cases} \dfrac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{f}(t, \boldsymbol{x}(t)) \\ \boldsymbol{x}(t_0) = \boldsymbol{x}_0, \quad t \in [t_0, T]. \end{cases} \tag{32}$$

Neural Ordinary Differential Equations

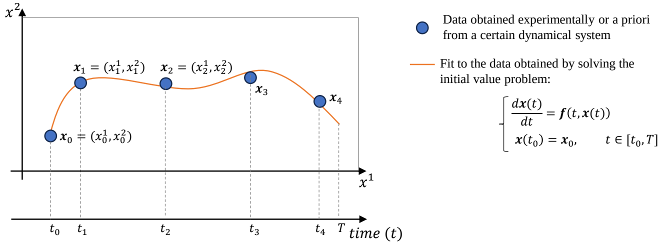


Figure 2: Fit of an ODE to data $\{\boldsymbol{x}_0, \boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4\}$ obtained experimentally or provided by a dynamical system. The blue symbols represent the data points, while the orange line represents the fit obtained from the initial value problem shown on the right. Each vector $\boldsymbol{x}_i$ corresponds to a specific instant t_i. The initial value problem allows us to determine the behaviour of the dynamical system at any instant within the interval $[t_0, T]$ [2, 3].

Neural Ordinary Differential Equations

The problem is that neither the solution $\boldsymbol{x}(t) \in \mathbb{R}^d$ nor the function $\boldsymbol{f}(t, \boldsymbol{x}(t)) : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ are known (the ODE may be linear, nonlinear, etc).

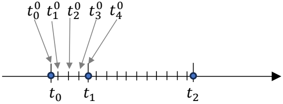
Neural ODEs provide a viable solution to approximate the initial value problem (32) using only the data $\boldsymbol{x} = \{\boldsymbol{x}_0, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ (the ground truth in our Neural ODE).
Let $\boldsymbol{h}(t)$ be an approximation of $\boldsymbol{x}(t)$.

$$\begin{cases} \dfrac{d\boldsymbol{h}(t)}{dt} = \boldsymbol{f}_{\boldsymbol{\theta}}(t, \boldsymbol{h}(t)), \\ \boldsymbol{h}(t_0) = \boldsymbol{x}_0 \quad t \in [t_0, T]. \end{cases} \tag{33}$$

The right-hand side's analytical expression $(\boldsymbol{f}(t, \boldsymbol{x}(t)))$ is replaced by a NN (denoted by $\boldsymbol{f}_{\boldsymbol{\theta}}(t, \boldsymbol{h}(t))$), where $\boldsymbol{\theta}$ represents the weights and biases of the network [2, 3].

Neural Ordinary Differential Equations

To illustrate the Neural ODE, we assume that the numerical method used to solve the initial value problem (33) is the explicit Euler method. A mesh is defined for each interval $[t_i, t_{i+1}]$, $i = 0, \ldots, N-1$. Therefore, given the initial condition $\boldsymbol{h}(t_0) = \boldsymbol{x}_0$, a (uniform) mesh $\{t^i_m = m\Delta t_i : m = 0, 1, ..., M_i\}$ on an interval $[t_i, t_{i+1}]$ with some integer M_i and $\Delta t := (t_{i+1} - t_i)/M_i$, we compute the numerical solution as (for the interval $[t_0, t_1]$) [2, 3],



$$
\begin{aligned}
\hat{\boldsymbol{h}}(t_1^0) &= \boldsymbol{x}_0 + \Delta t \boldsymbol{f}_{\boldsymbol{\theta}}(t_0^0, \boldsymbol{x}_0) \\
\hat{\boldsymbol{h}}(t_2^0) &= \hat{\boldsymbol{h}}(t_1^0) + \Delta t \boldsymbol{f}_{\boldsymbol{\theta}}(t_1^0, \hat{\boldsymbol{h}}(t_1^0)) \\
&\vdots \\
\hat{\boldsymbol{h}}(t_{M_0}^0) &= \hat{\boldsymbol{h}}(t_{M-1}) + \Delta t \boldsymbol{f}_{\boldsymbol{\theta}}(t_{M-1}, \hat{\boldsymbol{h}}(t_{M-1})).
\end{aligned}
$$

Neural Ordinary Differential Equations

We can say that the Neural ODE consists of two main components: a numerical ODE solver, and the neural network $\boldsymbol{f_\theta}(t, \boldsymbol{h}(t))$ [2, 3].

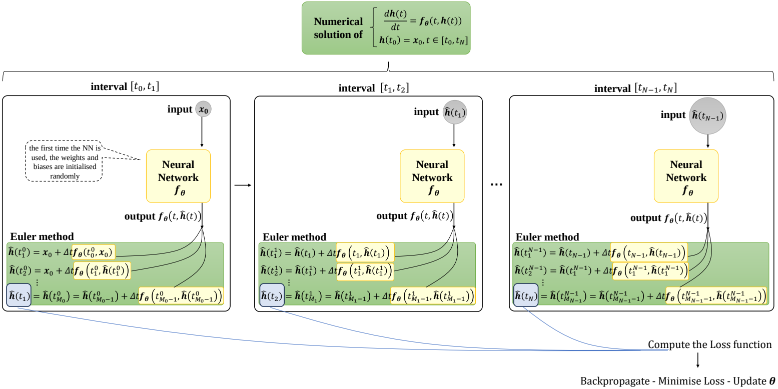


Figure 3: Schematic of a Neural ODE iteration. Note that along the sequence of figures (left to right) the NN $\boldsymbol{f_\theta}(t, \boldsymbol{h}(t))$ doesn't change.

Neural Ordinary Differential Equations

We can use both adaptive and fixed-step ODE solvers. When the step size is explicitly specified Δt, the discretization takes place for each sub-interval of observations $[t_i, t_{i+1}]$ with the specified step size yielding $(t_{i+1} - t_i)/\Delta t$ time steps [2, 3].

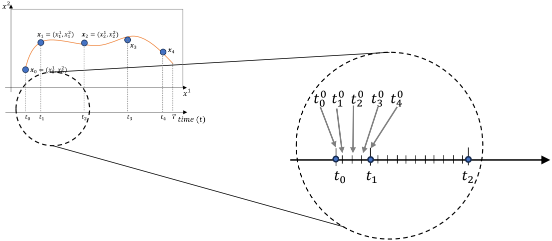


Figure 4: Example of a typical mesh used in the numerical solution of Eq. (33) for each interval $[t_i, t_{i+1}]$, $i = 0, \ldots, N - 1$, where t_i is the time of observation $\boldsymbol{x}_i$ [3].

Neural Ordinary Differential Equations

Different numerical solvers can be used to obtain the numerical solution of (33), for the time being, we will refer to a numerical solver as ODESolve. Assuming $i = 1, \ldots, N$ and that that t_N corresponds to T, each state $\boldsymbol{h}(t_i)$ is then numerically given by [2, 3],

$$\hat{\boldsymbol{h}}(t_i) = \text{ODESolve}(\boldsymbol{f}_{\boldsymbol{\theta}}, \boldsymbol{x}_0, \{t_1, \ldots, t_N\}). \tag{34}$$

Example - Population Growth

Consider you have experimental data from a population growth. Here, we will use the synthetic data fabricated earlier. We want to model the dynamics using a Neural ODE [2, 3].
First, the torchdiffeq and torch modules are imported [3, 1]:

```
import torch
import torch.nn as nn
import torch.optim as optim
from torchdiffeq import odeint
```

With this Neural ODE we will be able to predict the population P at each time instant given the initial condition:

```
true_y0 = torch.tensor([2.518629])
```

Example - Population Growth

Next, we define a neural network to approximate the right-hand side of the ODE [3, 1]:

```
class ODEFunc(nn.Module):
    def __init__(self):
        super(ODEFunc, self).__init__()

        self.net = nn.Sequential(nn.Linear(1, 50),
            nn.Tanh(), nn.Linear(50,50),
            nn.ELU(), nn.Linear(50, 1))

        for m in self.net.modules():
            if isinstance(m, nn.Linear):
                nn.init.normal_(m.weight, mean=0, std=0.1)
                nn.init.constant_(m.bias, val=0)

    def forward(self, t, y):
        return self.net(y)
```

Example - Population Growth

Then we compile the network and choose an optimiser:

```
func = ODEFunc()
optimizer = optim.Adam(func.parameters(), lr=1e-5)
```

We define the time instants in which we want to know the solutions [3, 1]:

```
t = torch.linspace(0., 1, 500)
```

Example - Population Growth

Now, we have specified the network, optimiser and we have training data available. Then we define the training loop:

```
for itr in range(1, 2000):
    pred_y = odeint(func, true_y0, t, method='rk4')
    loss = nn.MSELoss()(pred_y, true_y)

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
    for itr % 100 == 0:
      print('Iter {:04d}|Loss {:.6f}'.format(itr, loss))
```

Here we specify the numerical method to be a fixed-step one and print the loss value every 100 iterations [3, 1].

Hands-On

- What happens if we change the numerical method from a fixed-step solver to an adaptive-solver?
- Choose a known differential equation that is used to model a real system. Solve it to create a synthetic dataset. Try using a Neural ODE to model the data.

Wrap-up

- Physics-Informed Neural Networks versus Neural Ordinary Differential Equations
- What's Next?

PINNs vs Numerical Methods

PINNs

- Mesh-independent;
- Suitable for problems in irregular or complex domains;
- Generalise to unseen data;
- Computes at arbitrary times directly;
- Data-hungry;
- Sensitive to hyperparameter choices and NN architectures;
- Computationally expensive to train;
- Lack transparency and interpretability.

Numerical Methods

- Some methods rely on structured grids;
- Computationally expensive in high dimensions;
- Iterative method;
- Work with limited data;
- Established guidelines;
- Computationally efficient for some problems;
- Well-understood algorithms.

Neural ODEs vs Traditional NNs

Neural ODEs

- Can handle irregularly-sampled data;
- Allows predictions at any point in time and discretisation;
- Computationally intensive due to solving differential equations at each training iteration;
- May be unstable due to the numerical solver inside.

Traditional NNs

- Only handles regularly-sampled data;
- Makes predictions based on discrete time steps;
- More straightforward training process.

What's next?

- Learning families of solutions with Neural Operators [5];
- Neural ODEs combined with other architectures such as ODE-RNN, Latent ODE [2, 10];
- Modelling other types of differential equations to data such as integro-differential equations [11] and fractional differential equations [3].

Thank You!

Thank you for your time and patience!

Acknowledgements

This work was funded by Fundação para a Ciência e Tecnologia (Portuguese Foundation for Science and Technology) through CMAT projects UIDB/00013/2020 and UIDP/00013/2020, the funding by FCT and Google Cloud partnership through projects CPCA-IAC/AV/589164/2023 and CPCA-IAC/AF/589140/2023, through the scholarship with reference 2021.05201.BD, and national funds through the FCT/MCTES (PIDDAC), under the project 2022.06672.PTDC - iMAD - Improving the Modelling of Anomalous Diffusion and Viscoelasticity: solutions to industrial problems.

Google Cloud CMAT Centro de Matemática Universidade do Minho Universidade do Minho Escola de Ciências fct Fundação para a Ciência e a Tecnologia REPÚBLICA PORTUGUESA

References

[1] Ricky T. Q. Chen. *torchdiffeq*. 2018. URL: https://github.com/rtqichen/torchdiffeq.

[2] Ricky TQ Chen et al. "Neural ordinary differential equations". In: *Advances in neural information processing systems* 31 (2018).

[3] C. Coelho, M. Fernanda P. Costa, and L. L. Ferrás. "Neural Fractional Differential Equations". In: *arXiv preprint arXiv:2403.02737* (2024).

[4] Kurt Hornik, Maxwell Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators". In: *Neural networks* 2.5 (1989), pp. 359–366.

[5] Nikola Kovachki et al. "Neural operator: Learning maps between function spaces with applications to pdes". In: *Journal of Machine Learning Research* 24.89 (2023), pp. 1–97.

[6] Lu Lu et al. "DeepXDE: A deep learning library for solving differential equations". In: *SIAM review* 63.1 (2021), pp. 208–228.

[7] Jorge Nocedal and Stephen J Wright. *Numerical optimization*. Springer, 1999.

[8] Maziar Raissi, Paris Perdikaris, and George E Karniadakis. "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations". In: *Journal of Computational physics* 378 (2019), pp. 686–707.

[9] Maziar Raissi, Paris Perdikaris, and George Em Karniadakis. "Physics informed deep learning (part i): Data-driven solutions of nonlinear partial differential equations". In: *arXiv preprint arXiv:1711.10561* (2017).

[10] Yulia Rubanova, Ricky TQ Chen, and David K Duvenaud. "Latent ordinary differential equations for irregularly-sampled time series". In: *Advances in neural information processing systems* 32 (2019).

[11] Emanuele Zappala et al. "Neural integro-differential equations". In: *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 37. 9. 2023, pp. 11104–11112.