Phd-teach-PhD: Approaching science with AI

An introduction to scientific machine learning

Guilherme Zagatti
PhD candidate NUS NGS/IDS
gzagatti@u.nus.edu

Outline

1. Motivation: Dynamical systems describe changes we observe
2. Julia

   Intro to the language and ecosystem
3. A formal introduction to ODEs and SciML

   The initial value problem

   `DifferentialEquations.jl`

   Fitting data to ODEs, classical approaches
4. NeuralODE

   The initial value problem reviewed

   `Flux.jl`
5. Exercises

Motivation

Dynamical systems describe changes we observe

”It is then by cause that we define time” (Poincaré 1903)

How do we learn about cause and effect if not by how we observe things evolving?

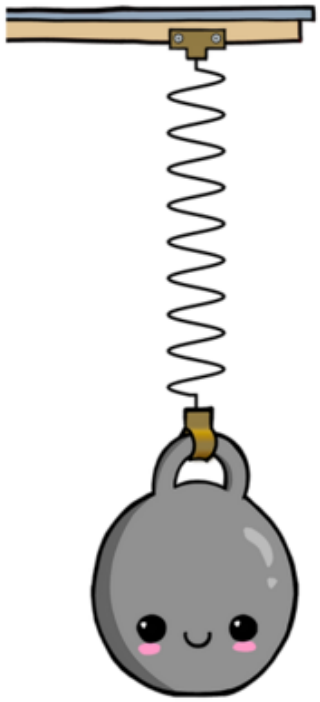
Dynamical systems are an evolution rule that defines a trajectory as a map (Meiss 2007):

$$\text{time} \mapsto \text{set of states}$$

As a mathematics discipline, the study of dynamical systems originates at the end of 19th century spearheaded by Henri Poincaré who also developed an extensive theory of sciences.

Physics: coupled oscillator

Describes the movement of an object with mass m attached to a spring under force F.



$$F = ma \Rightarrow \frac{d^2x}{dt^2} = -\frac{kx}{m}$$

Ecology: Lotka-Volterra

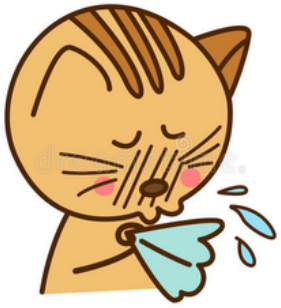
Describes the dynamics of two-competing species, the prey x and predator y.

$$\frac{dx}{dt} = \alpha x - \beta xy$$

$$\frac{dy}{dt} = \delta xy - \gamma y$$

Epidemiology: SIR

Susceptible-infected-recovered. Describes the evolution of an infectious disease which is transmitted with rate β when a susceptible and an infected individual come into contact and disappears with rate γ.



$$\frac{ds}{dt} = -\beta si$$
$$\frac{di}{dt} = \beta si - \gamma i$$
$$\frac{dr}{dt} = \gamma i$$

Economics: Solow growth model

The production function $f(.)$ describes growth as a function of k. The rate of capital growth is constrained by the savings rate s and the depreciation rate of capital δ.

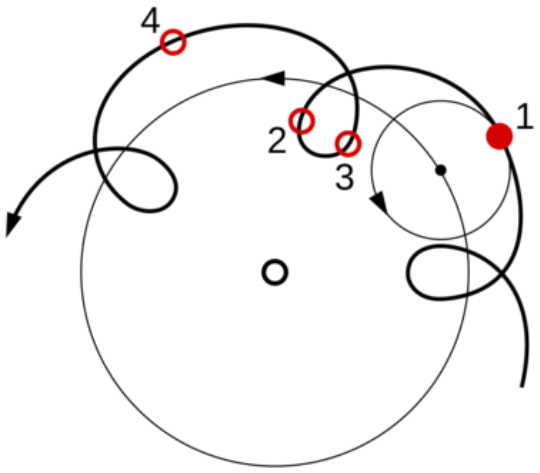
$$\frac{dk}{dt} = sf(k) - \delta k$$

Describing nature with models

A lot ingenuity and observation is required to develop models that are both **consistent with reality and existing theory**.

Science is a combination of **marginal revolutions and paradigm shifts**.

Scientific machine learning is a **set of tools for automated model discovery** to support the development of models from data.



"*It is not sufficient for each elementary phenomenon to obey simple laws, all those to be combined must obey the same law as well.* "
Poincaré 1902

The julia programming language

Fast designed for high-performance, JIT compiled code.

Reproducible environment `Manifest.toml` contains all the instructions to reproduce the environment; like the one in this notebook.

General from data-wrangling through data-analytics to data-reporting

Dynamic feels like Python

Composable multiple dispatch as a paradigm and functional programming, not quite like Python

Open source MIT license and active developer community in the scientific machine learning field.

Visit Julia's website to get started.

Installation

To follow the course, make sure to install the latest stable version of `Julia` from its official page.

Then, clone this repository:

```
> git clone git@github.com:gzagatti/phdteachphd-sciml.git
```

After downloading the repository, activate the Julia environment and install all the dependencies:

```
> cd phdteachphd-sciml/
> julia
                _
   _       _ _(_)_     |  Documentation: https://docs.julialang.org
  (_)     | (_) (_)    |
   _ _   _| |_  __ _   |  Type "?" for help, "]?" for Pkg help.
  | | | | | | |/ _` |  |
  | | |_| | | | (_| |  |  Version 1.6.1 (2021-04-23)
 _/ |\__'_|_|_|\__'_|  |  Official https://julialang.org/ release
|__/                   |

julia> ]
(@v1.6) pkg> activate .
  Activating environment at `./phdteachphd-sciml/Project.toml`
(@v1.6) pkg> instantiate
  Resolving package versions...
  ...
```