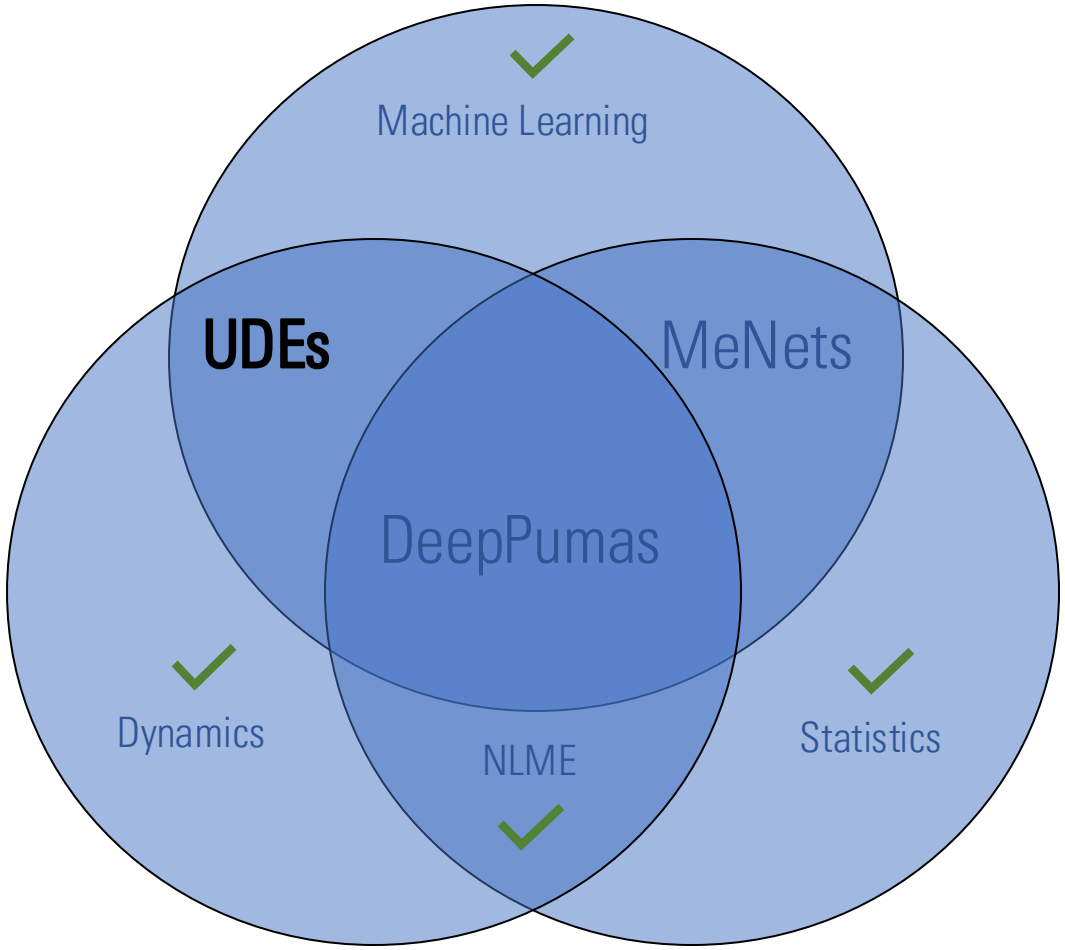
pumas AI

NeuralODEs and UDEs

Niklas Korsbo

DeepPumas

What to make of embedded ML?



NLME with DeepPumas

Typical values

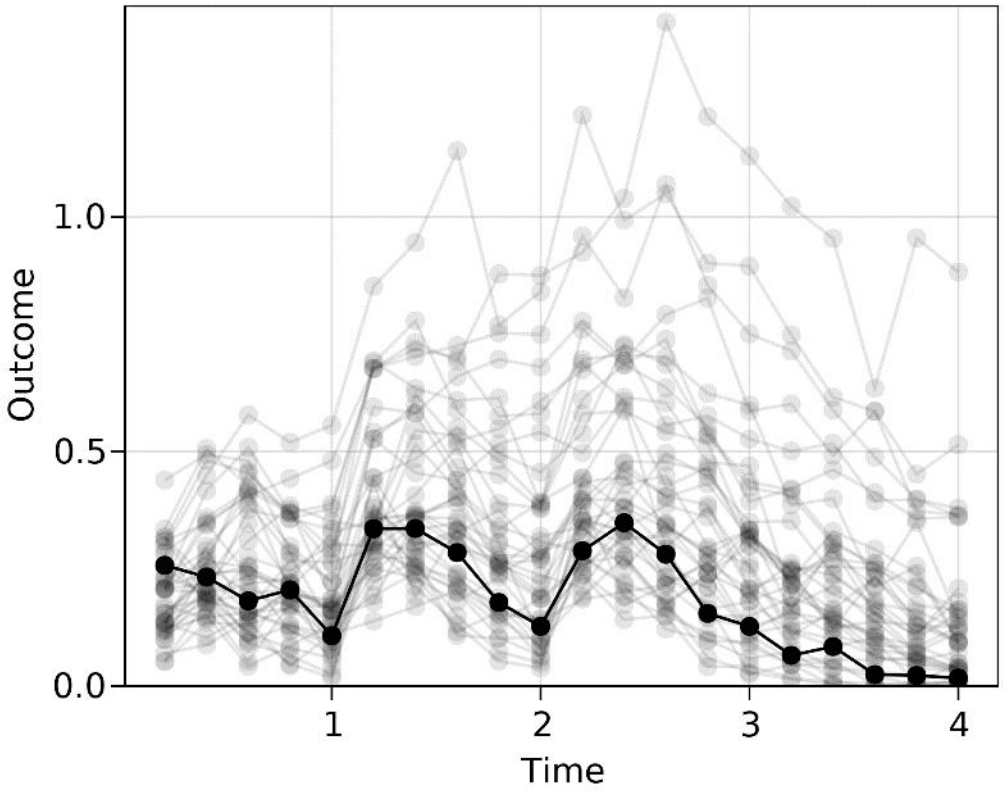
$$\theta \in \mathbb{R}^3_+$$
$$\Omega \in \mathbb{R}^3_+$$

Patient data

Age
Weight

Random effects

$$\eta \sim \text{MvNormal}(\Omega)$$



Universal differential equations (UDEs)

Individual parameters

$$Ka_i = \theta_1 \cdot e^{\eta_{i,1}} + c_1 \cdot Age_i +$$
$$CL_i = \theta_2 \cdot e^{\eta_{i,2}}$$
$$V_i = \theta_3 \cdot e^{\eta_{i,3}} + c_2 \cdot Weight_1^{c_3} +$$

Dynamics

$$\frac{d[\text{Depot}]}{dt} = -Ka[\text{Depot}],$$
$$\frac{d[\text{Central}]}{dt} = Ka[\text{Depot}] -$$

Error model

$$Outcome \sim \text{Normal}\left(Central, \sqrt{Central} \cdot \sigma\right)$$

DeepPumas

Universal Differential Equations and friends

2018 - "Neural Ordinary Differential Equations", Chen et al.

2020 - "Universal Differential Equations for Scientific Machine Learning", Rackauckas et al.

Neural ODE

$$\frac{d\boldsymbol{X}}{dt} = NN(\boldsymbol{X}(t), t)$$

Use a differential equation solvers as a scaffold for continuous time, continuous depth neural networks.

Similar to recurrent neural networks and ResNets

Universal differential equation (UDE)

$$\frac{dx}{dt} = x \cdot y \; - NN(x)$$
$$\frac{dy}{dt} = p \; - x \cdot y$$

Insert universal approximators (like NNs) to capture terms in dynamical systems.

Scientific Machine Learning (SciML)

An abstract concept of mixing scientific modeling with machine learning.

Different encoded knowledge

- Number of states.

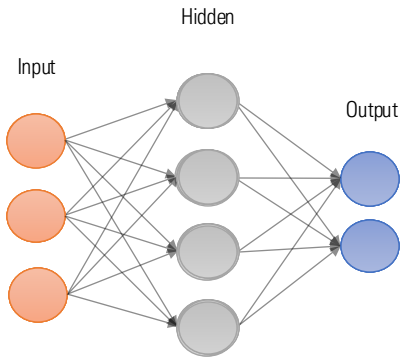
- Explicit knowledge of some terms
- Relationships (R independent of Depot!)

- Number of states.
- Relationships
- Dependence/independence of terms
- Conservation between Depot and Central

- Precise position of the unknown function.
- Precise input to the unknown function.
- Lots of knowledge!

DeepPumas

UDEs – pretty simple, really



Mathematically: Just a function!

NNs are useable anywhere where you'd use a function!

- Decide where in the dynamics you have an unknown function.
- Decide what inputs this function may have.
- Fit everything in concert

The only hard part is building software for fitting but, with DeepPumas, that's not your problem!

DeepPumas