pumas AI

DeepPumas
DeepNLME

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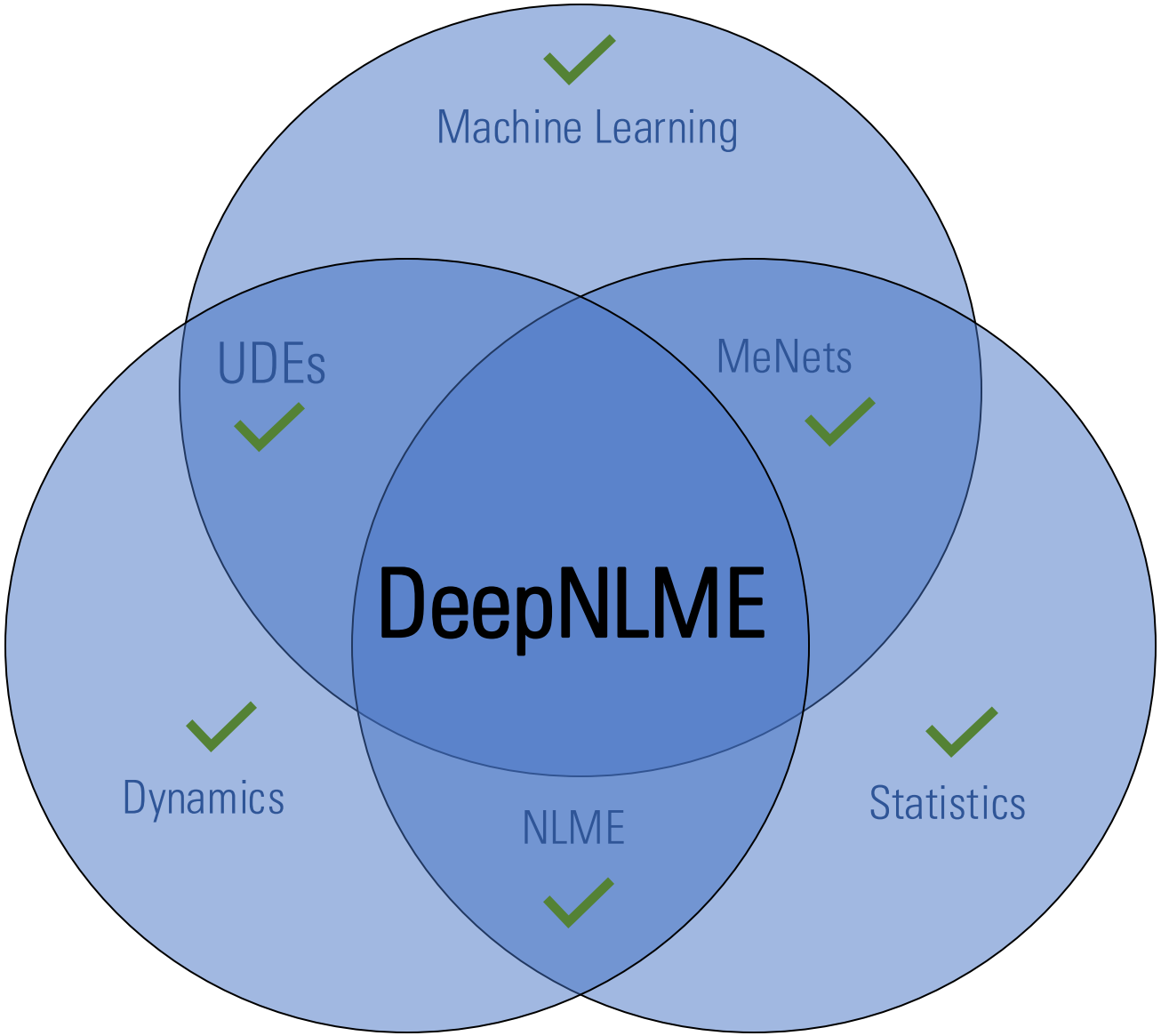

Machine Learning
UDEs
MeNets
DeepNLME
Dynamics
NLME
Statistics

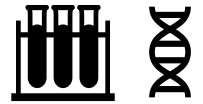
NLME with DeepPumas

Typical values

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

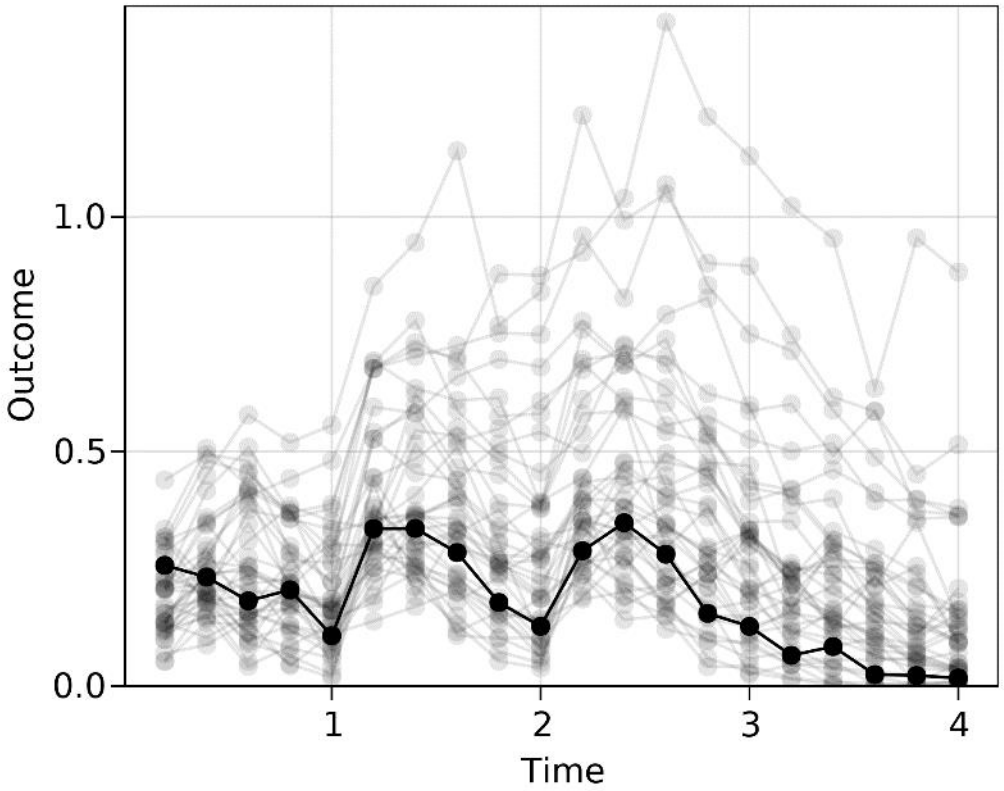
Patient data

Age
Weight



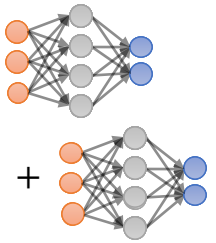
Random effects

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



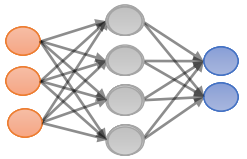
Individual parameters

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



Dynamics

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



Error model

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

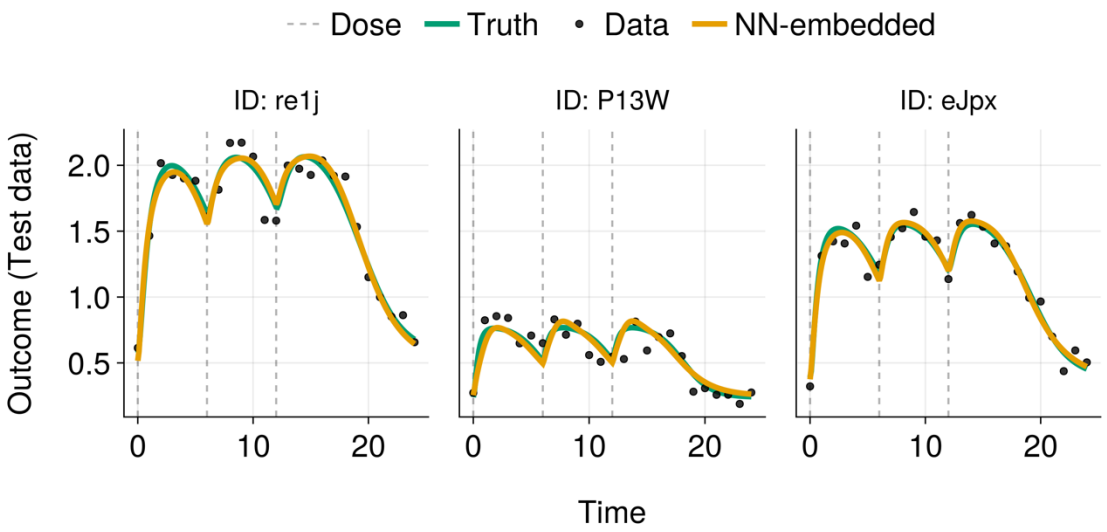
DeepPumas

Let's just dive into the deep end.

Exercise time!

Open up 04_DeepNLME.jl

What did we just see?



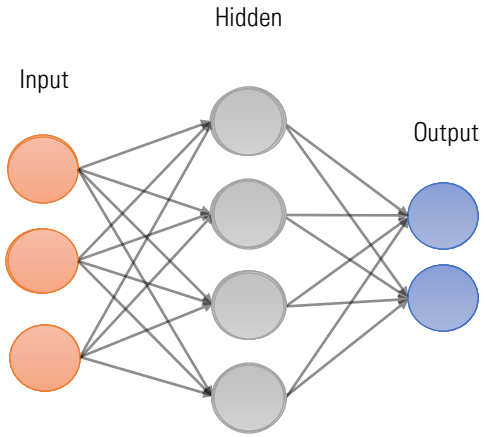
Where Smax, SC50, Vc, and Kout all have different "true" values for each patient

Very similar results on test data.

What must the DeepPumas model have discovered?

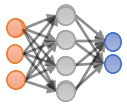
DeepPumas

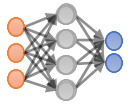
Flexible local information processing



Dynamic variables
Drug PK
Random effects
Covariate data
Time

DiffEQ terms
Outcome transformations
Individualized parameters
Longitudinal biomarkers

Dynamic variables  Dynamics term

Dynamic variables
Random effects

Individualizable dynamics term

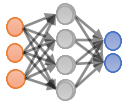
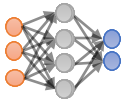
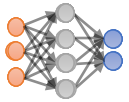
Receptor drug occupancy
Random effect

Pain score

Image  Parameter contribution

Time after first dose
Random effects

Individualizable longitudinal biomarkers

DeepPumas

Sharing information

- Direct mechanistic dependencies
- Shared random effects
- Random effect covariances

Look at code for examples