Designing and fitting neural ODEs
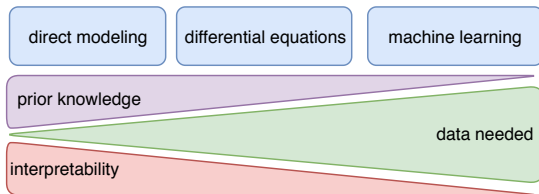## Background and preliminary results

Elisabeth Rösch

University of Melbourne

24 June 2019

Motivation

Ordinary Differential Equation (ODE)

$$\frac{\delta u}{\delta t} = f(u)$$

u: Species, t: Time, f: Function
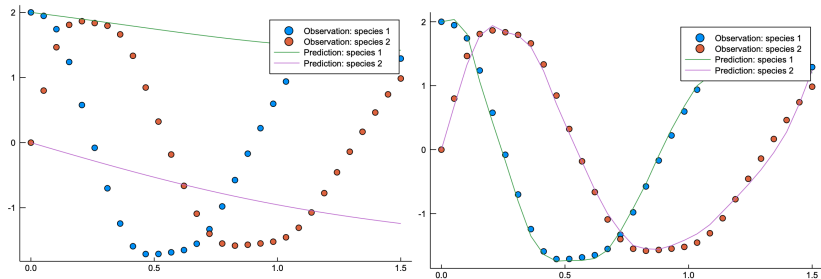
Neural ODE [Chen et al., 2018]

$$\frac{\delta u}{\delta t} = f(u)$$

u: Species, t: Time, f: **Neural net**

In Julia: DiffEqFlux.jl [Rackauckas et al., 2019]

```julia
# Derivative is modeled by a neural net.
dudt = Chain(x -> x.^3,
        Dense(2,50,tanh),
        Dense(50,2))
# Parameters of the model which are to be learnt.
ps = Flux.params(dudt)
```

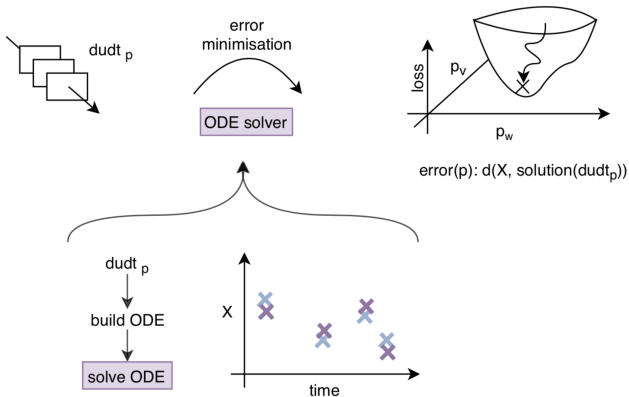# Fitting neural ODEs: Optimize loss functions

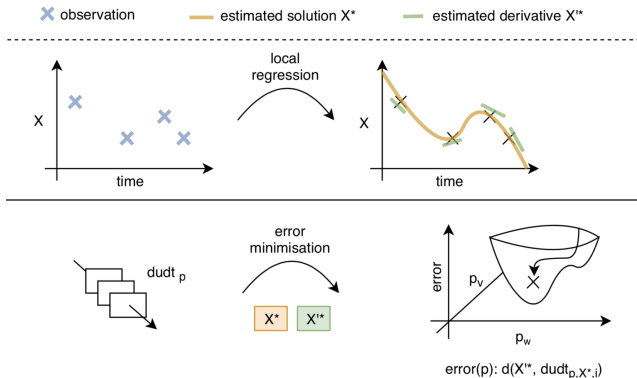Before and after training: Observed and predicted species over time
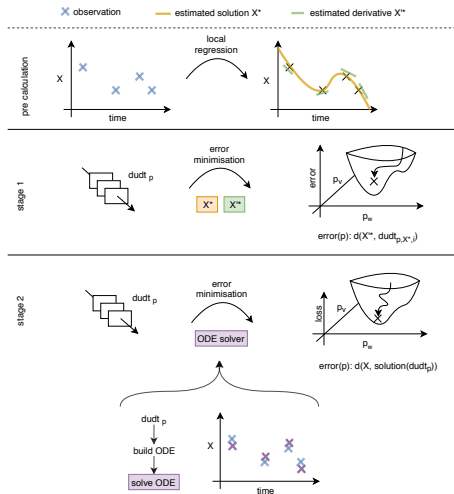
Loss functions

1. L2
2. Collocation based
3. Mixtures

Loss function: L2

Loss function: Collocation based [Liang and Wu, 2008]

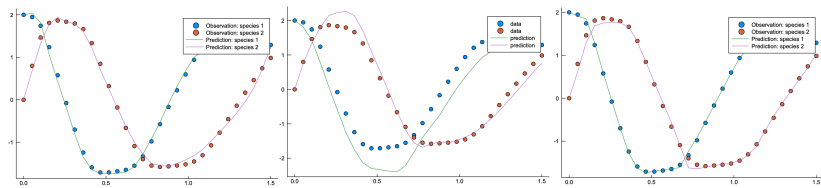error(p): d(X'*, dudt$_{p,X^*,i}$)
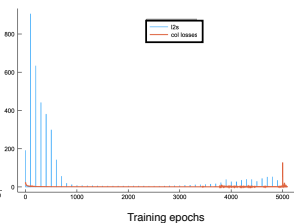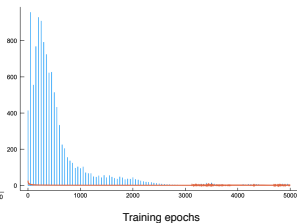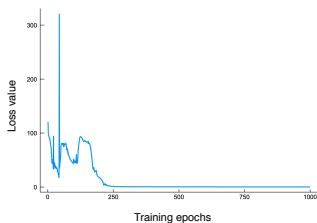
Loss function: Mixture

Performance: Accuracy

a. L2 norm as loss function b. Collocation as loss c. Mixture loss function
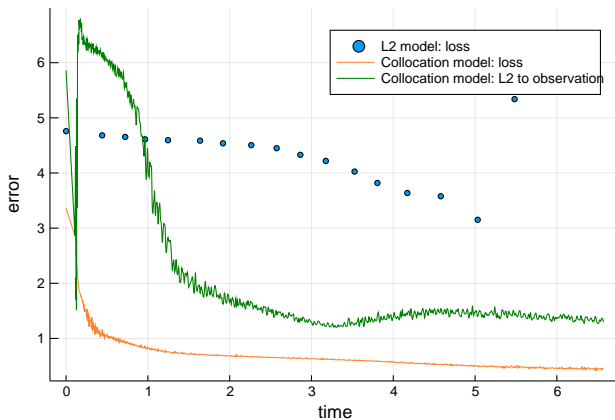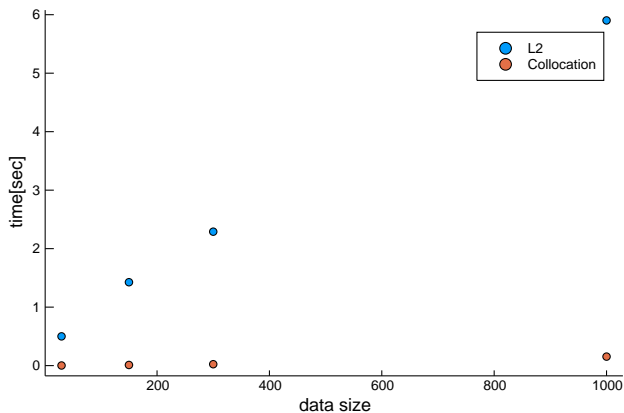
Performance: Convergence

a. L2 norm as loss function b. Collocation as loss c. Mixture loss function
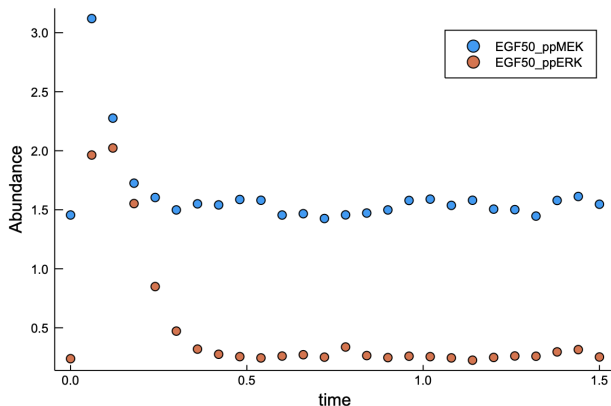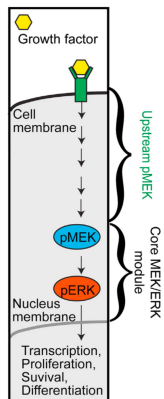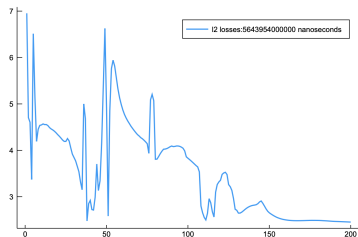
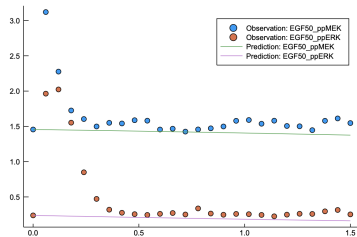# Performance: Time

Effect on performance: Data size
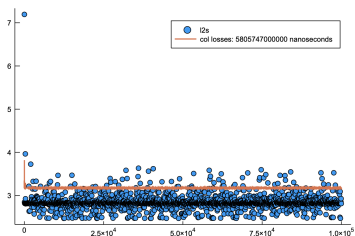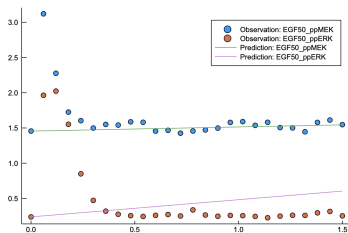
Application to biological data [Filippi et al., 2016]

Application to biological data: L2

Application to biological data: Collocation based

Next steps

1. try other neural nets for biological data
2. quantify results (GPU)
3. multiple shooting
4. noise effect

Acknowledgements

Supervision/Mentoring – Michael, Heejung, Chris.
Support/Discussions – Lucy, Anissa, Megan, Leo.

Bibliography

📄 Chen, T. Q., Rubanova, Y., Bettencourt, J., and Duvenaud, D. K. (2018).
Neural ordinary differential equations.
CoRR.

📄 Filippi, S. et al. (2016).
Robustness of MEK-ERK Dynamics and Origins of Cell-to-Cell Variability in MAPK Signaling.
Cell Reports, 15(11):2524–2535.

📄 Liang, H. and Wu, H. (2008).
Parameter estimation for differential equation models using a framework of measurement error in regression models.
Journal of the American Statistical Association.

📄 Rackauckas, C., Innes, M., Ma, Y., Bettencourt, J., White, L., and Dixit, V. (2019).
Diffeqflux.jl - a julia library for neural differential equations.
CoRR.