Designing and fitting neural ODEs

Background and preliminary results

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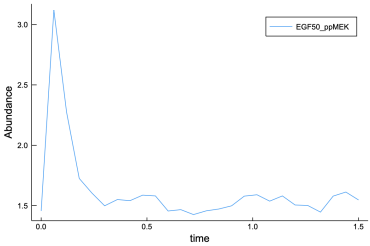
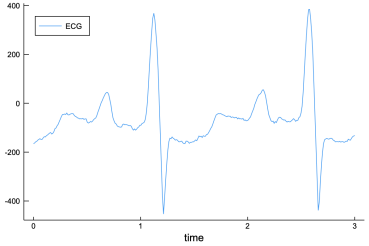
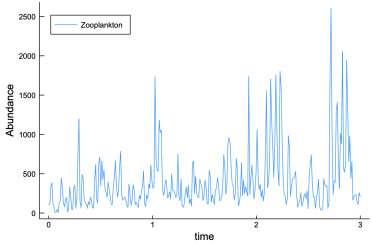
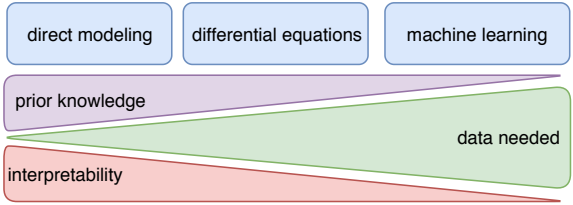
Example


EGF50_ppMEK
Abundance
time
3.0
2.5
2.0
1.5
0.0
0.5
1.0
1.5


ECG
time
400
200
0
-200
-400
0
1
2
3


Zooplankton
Abundance
time
2500
2000
1500
1000
500
0
0
1
2
3

Motivation


direct modeling
differential equations
machine learning
prior knowledge
data needed
interpretability

Ordinary Differential Equation (ODE)

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

u: Species, t: Time, f: Function

Neural ODE [Chen et al., 2018]

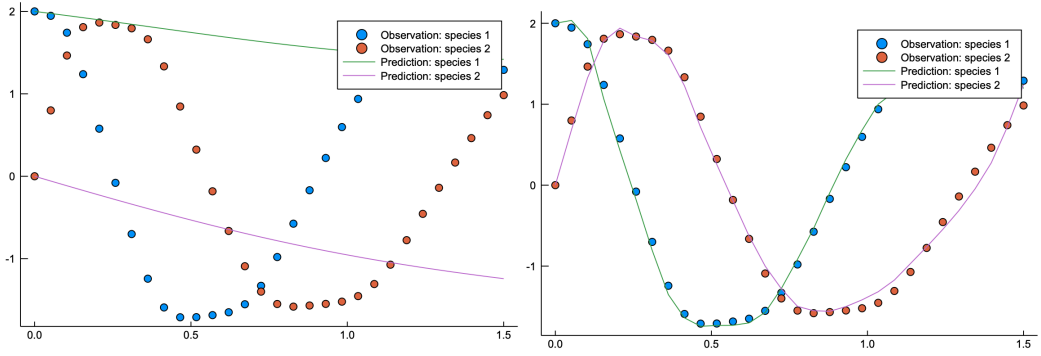
$$\frac{\delta u}{\delta t} = f(u)$$

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

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

```
# 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

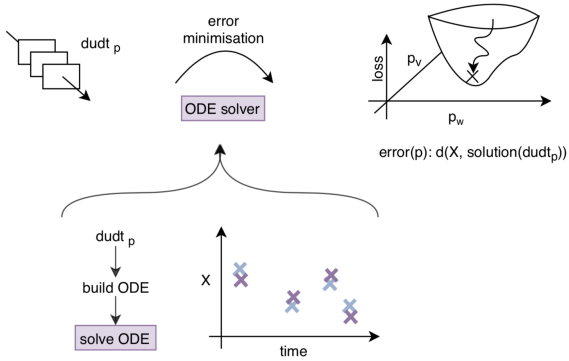


Before and after training: Observed and predicted species over time

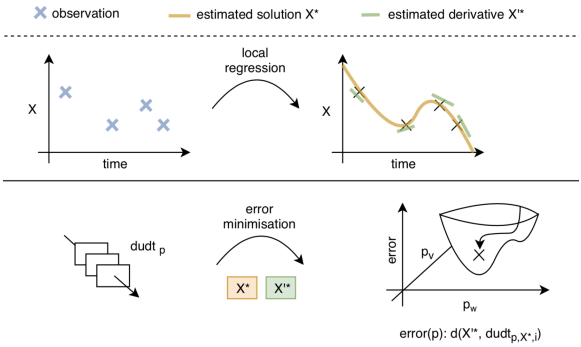
Loss functions

1. L2
2. Collocation based
3. Mixtures

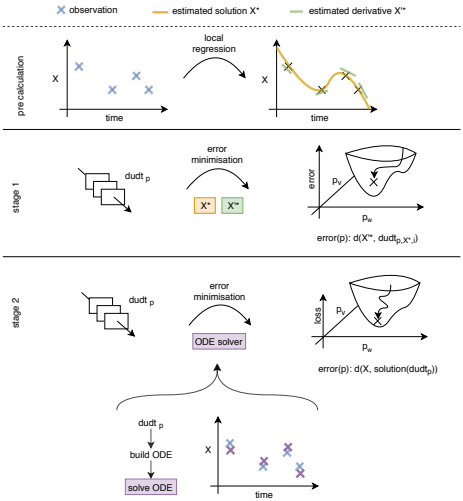
Loss function: L2



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

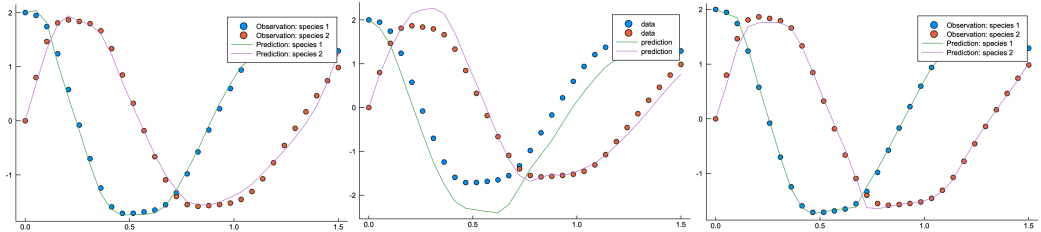


Loss function: Mixture



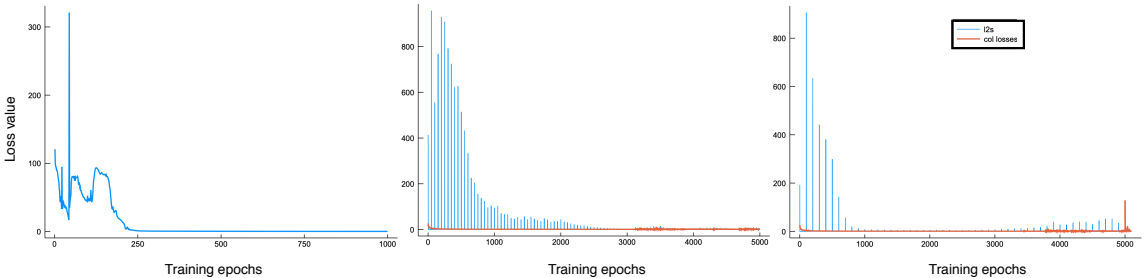
Performance: Accuracy

a. L2 norm as loss function b. Collocation as loss c. Mixture loss function

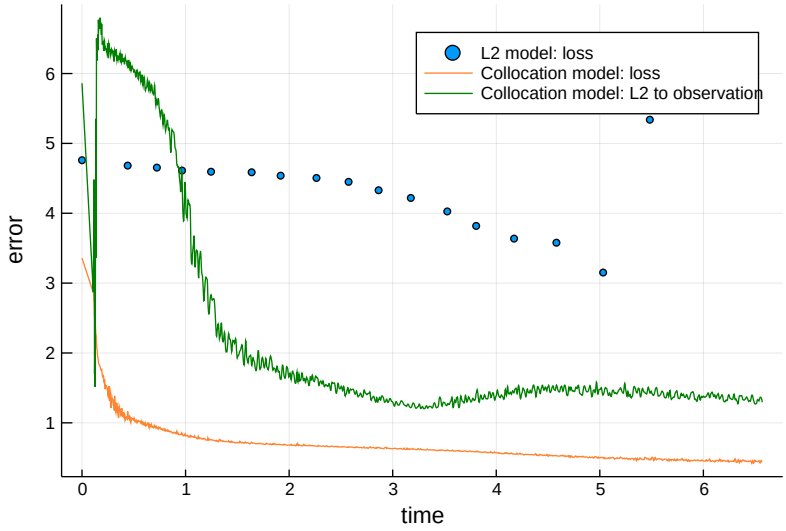


Performance: Convergence

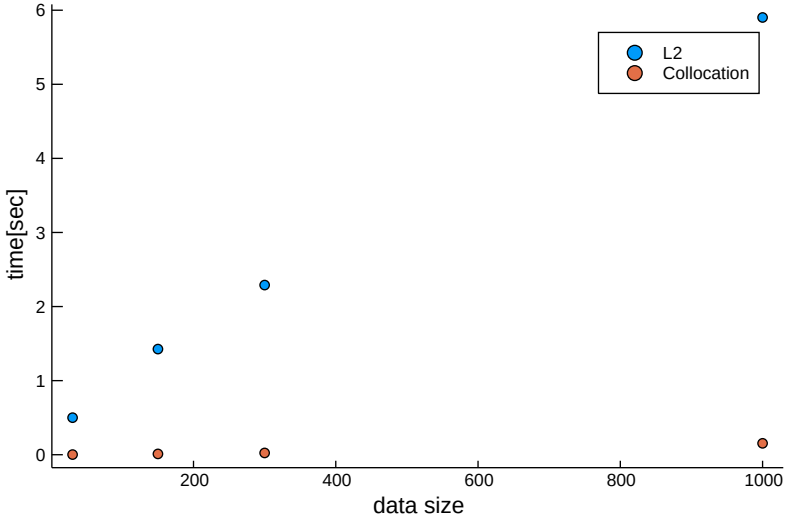
a. L2 norm as loss function b. Collocation as loss c. Mixture loss function



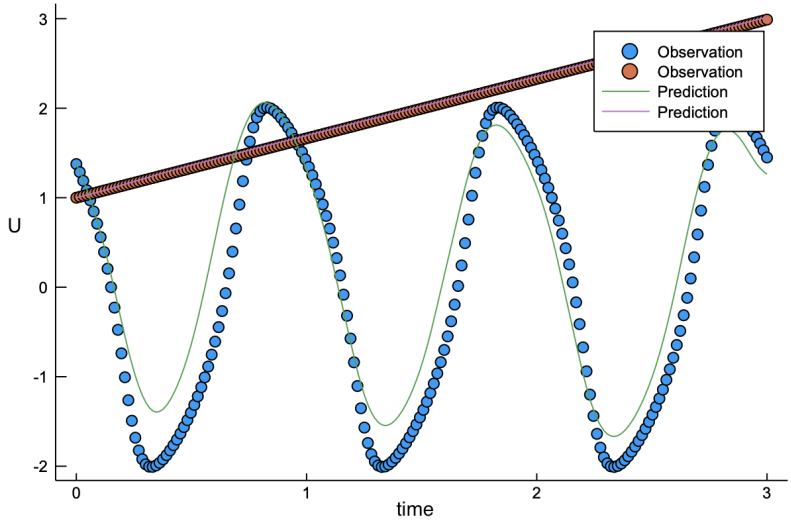
Performance: Time



Effect on performance: Data size



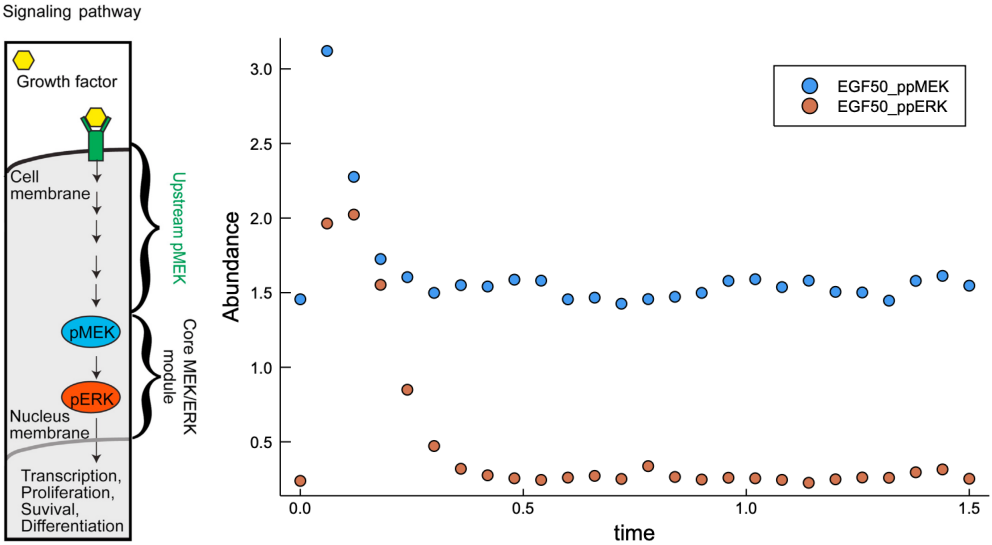
Biological application: Van der Pol Oscillator



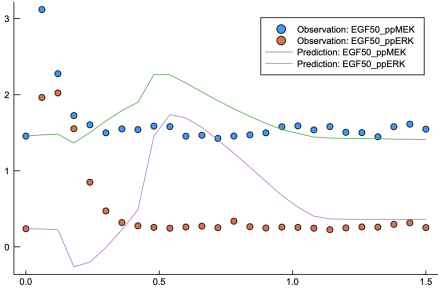
Biological application: FIND EASY

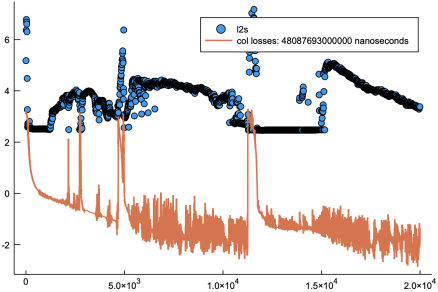
to add

Biological application: MEK-ERK dynamics [Filippi et al., 2016]



Biological application: Collocation based model

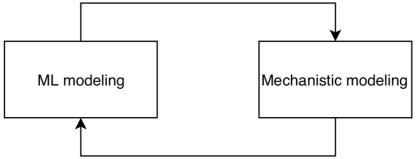




Biological application: Collocation based model with multiple shooting

to add

Outlook: Hybrid modeling



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