Learning from scarce data by combining machine learning and fundamental ecological knowledge

University of Fribourg

Victor Boussange

Swiss Federal Research Institute for Forest, Snow and Landscape Research (WSL)

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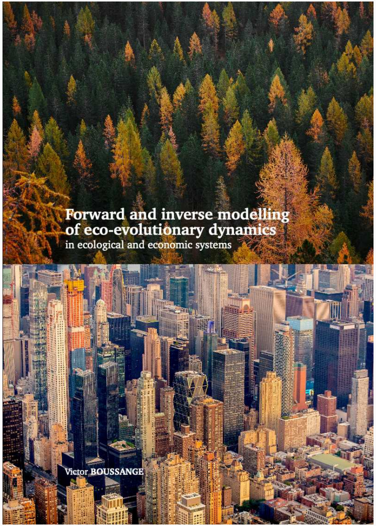

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SPEED2ZERO

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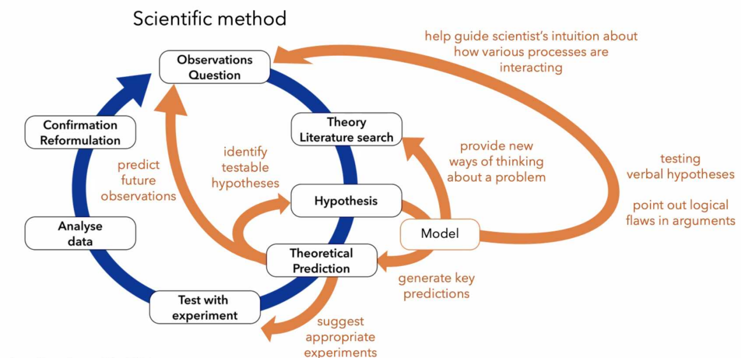
- How can we use this knowledge to benefit society?

Modelling in ecology

Modelling in ecology

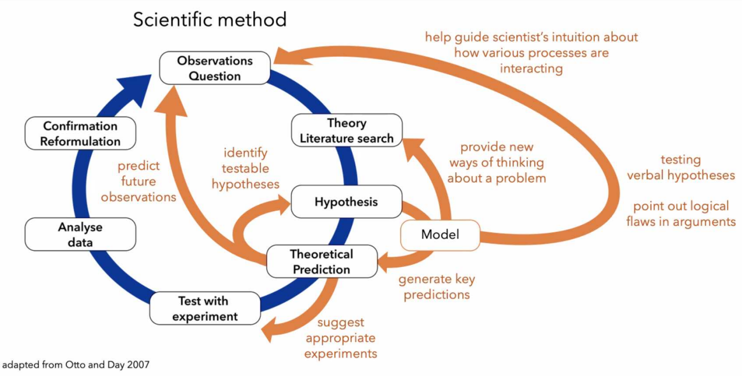
Models to advance ecological theory



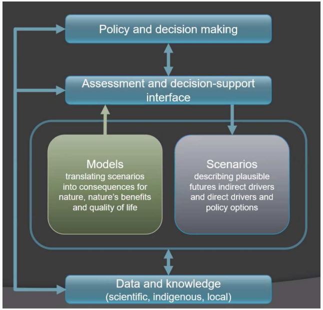
adapted from Otto and Day 2007

Modelling in ecology

Models to advance ecological theory



Models are useful for society



Typology of models

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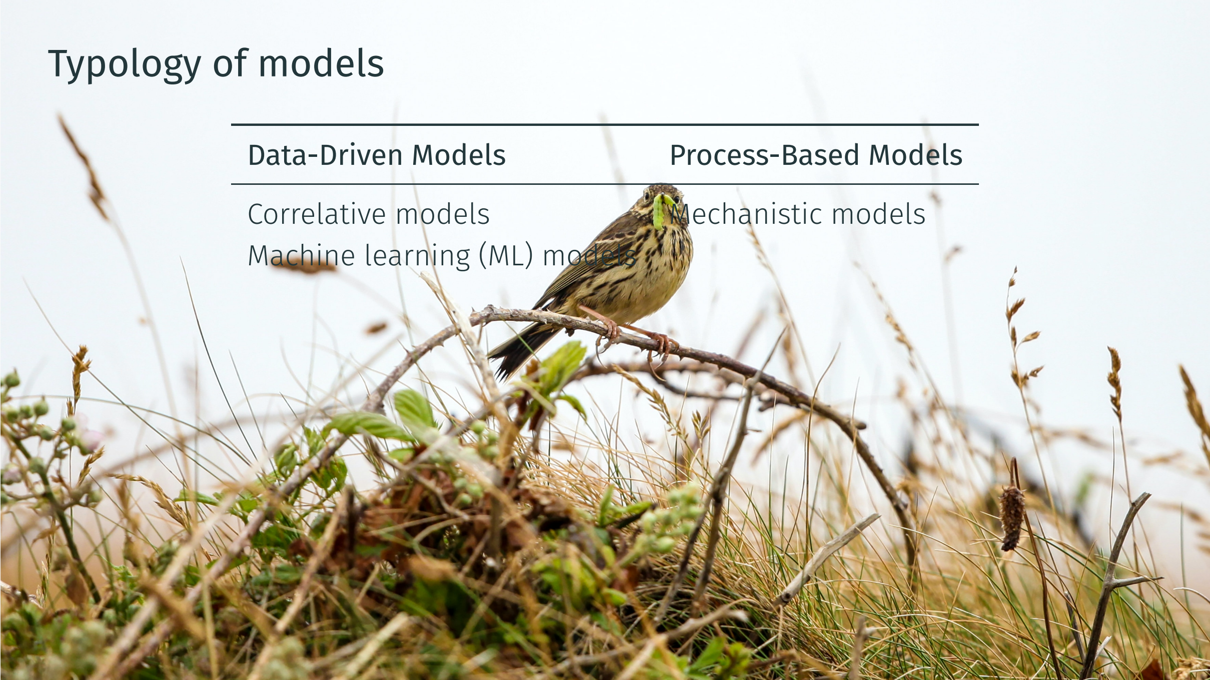
Data-Driven Models	Process-Based Models
Correlative models	Mechanistic models
Machine learning (ML) models	



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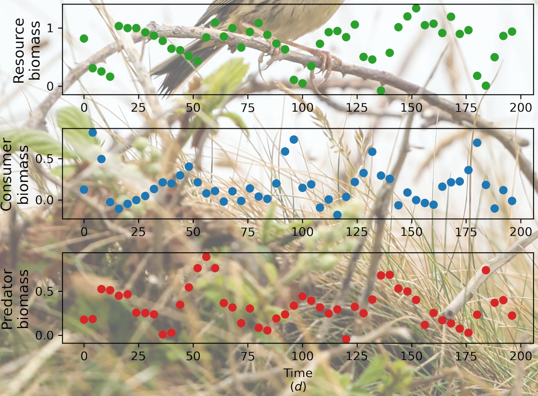
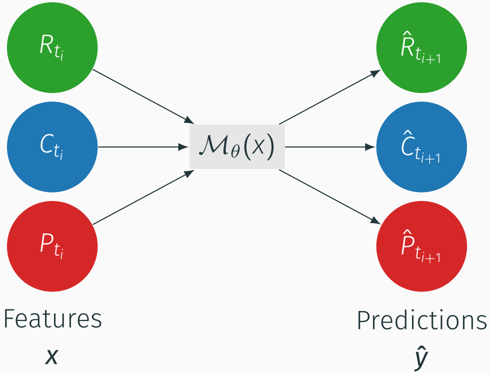


Data-based modelling



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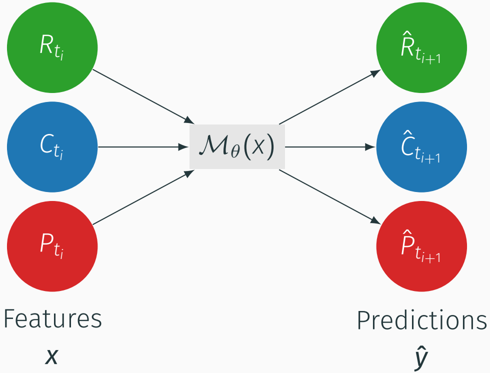
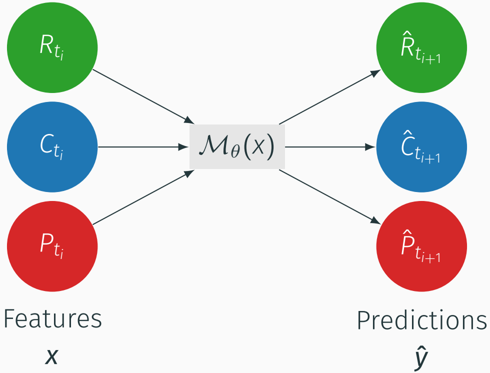


Loss function

$$
\begin{aligned}
L(\theta, \mathbf{y}) &= \sum_{k=1}^{K} ||y_k - \mathcal{M}_\theta(x_k)||^2 \\
&\propto -\log p(\mathbf{y}|\theta)
\end{aligned}
$$

Data-based modelling



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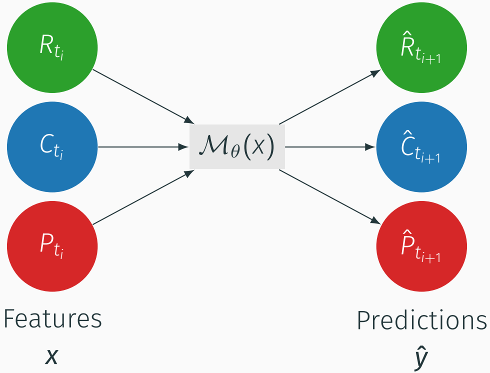
Find the parameters $\hat{\theta}$ that minimize the negative logarithm of the posterior

$$\hat{\theta} = \arg\min_\theta L(\theta, \mathbf{y})$$

Data-based modelling



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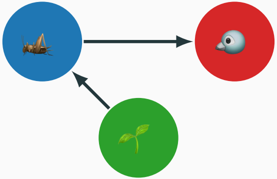
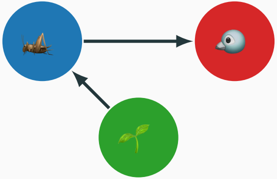


Process-based modelling

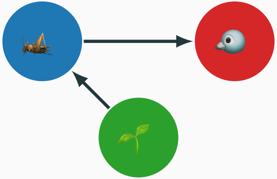


net growth rate 🌱 = basal growth − competition − grazing − death

net rowth rate 🦗 = grazing − predation − death

net growth rate 🐦 = predation − death

Process-based modelling



$$\frac{dy}{dt} = f(y, t)$$

$$\frac{d}{dt} R_t = \overbrace{R_t(1 - R_t)}^{\text{logistic growth}} - x_c y_c \underbrace{\frac{C_t R_t}{R_t + R_0}}_{\substack{\text{functional response} \\ \text{(intake rate of consumers)}}}$$

$$\frac{d}{dt} C_t = x_c C_t \left[-1 + y_c \frac{R_t}{R_t + R_0} \right] - x_p y_p \underbrace{\frac{P_t C_t}{C_t + C_0}}_{\substack{\text{functional response} \\ \text{(intake rate of predators)}}}$$

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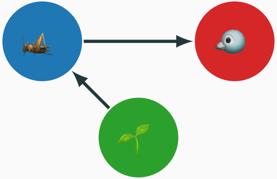

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$$y_{t+1} = \int_t^{t+1} f(y_s, s) ds + y_t$$

Pros and cons

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- – Suffer from inaccuracies, which make them less predictive than their data-based counterparts

I. From the mechanistic world to the ML world

Constraining NN with process-based models

Journal of Computational Physics 378 (2019) 686–707

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

ELSEVIER

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

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NN complies both with data and knowledge

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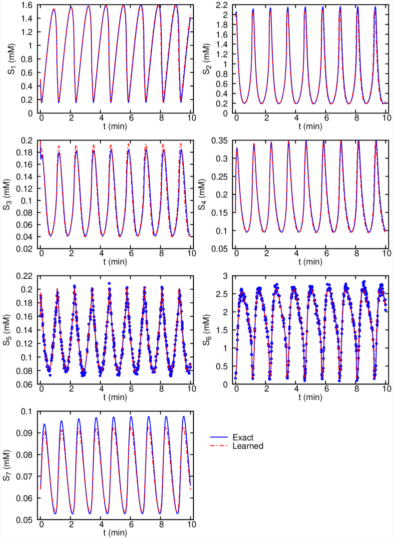
where

$$L^{\mathrm{ODE}}(\theta) = \sum_i \left|\left| \frac{d\,\mathrm{NN}_\theta(t_i)}{dt} - f(\mathrm{NN}_\theta(t_i), t_i) \right|\right|^2$$

Constraining NN with process-based models

Constraining NN with process-based models

NN_θ can predict variables for which it has never seen data!

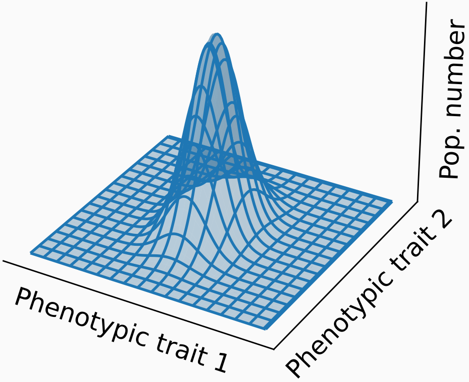


Yazdani et al., 2020

Using neural networks to solve high-dimensional PDEs

Using neural networks to solve high-dimensional PDEs

Modelling population number y as a function of continuous traits z



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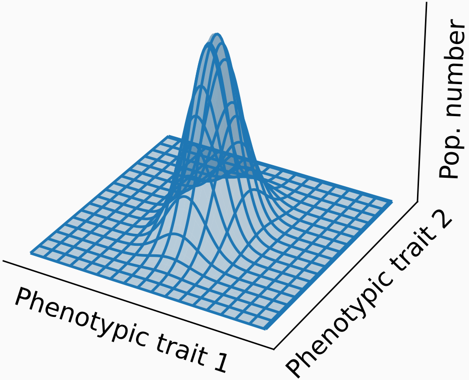
Modelling population number y as a function of continuous traits z

- population height



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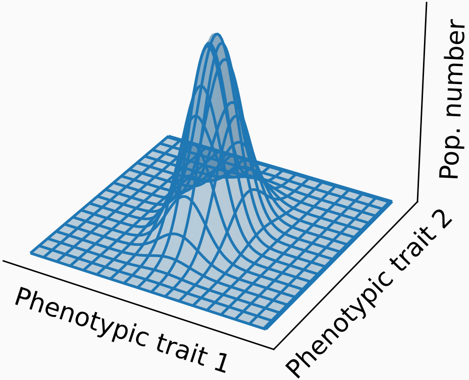

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Modelling population number y as a function of continuous traits z

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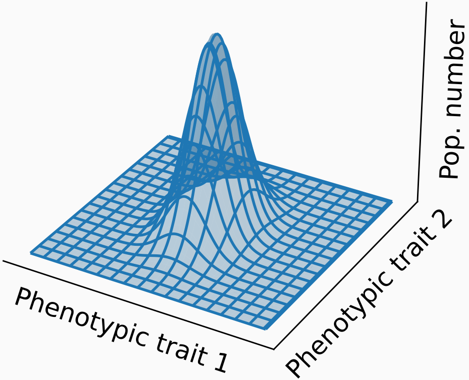

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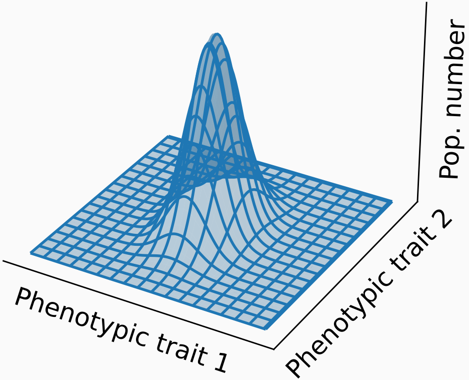

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Modelling population number y as a function of continuous traits z

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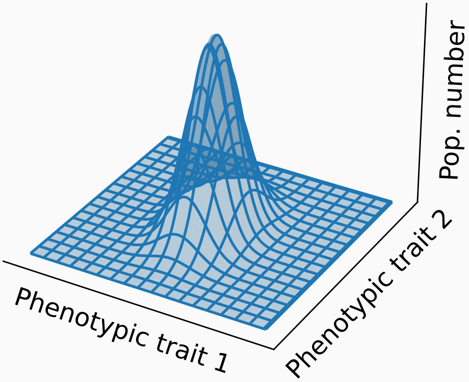
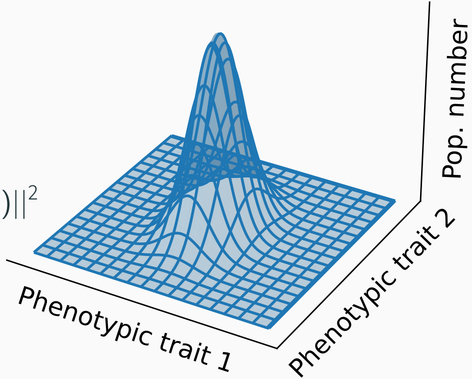
$$\frac{d}{dt} \underbrace{y(t,z)}_{\text{Population number for trait } z} = f(t, y, \partial_z y, \partial_{zz} y, \int y(t, \mathbf{z}) d\mathbf{z})$$



Using neural networks to solve high-dimensional PDEs

$$\mathrm{NN}(t, z) \approx x(t, z)$$

$$L^{\mathrm{ODE}}(\theta) = \sum_i \sum_j || \frac{d\,\mathrm{NN}(t_i, z_j)}{dt} - f(t_i, \mathrm{NN}(t_i, z_j), \ldots) ||^2$$



Curse of dimensionality

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- **Computational complexity** of standard numerical schemes

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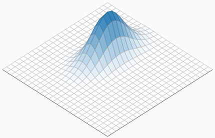
$$z \in \mathbb{R}$$
$$\mathcal{O}(N)$$

Curse of dimensionality

- **Computational complexity** of standard numerical schemes

$z \in \mathbb{R}$	$z \in \mathbb{R}^2$
$\mathcal{O}(N)$	$\mathcal{O}(N^2)$



Curse of dimensionality

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$z \in \mathbb{R}^2$

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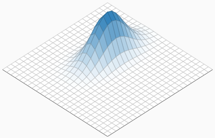
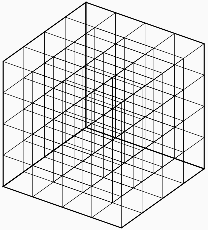


$z \in \mathbb{R}^3$

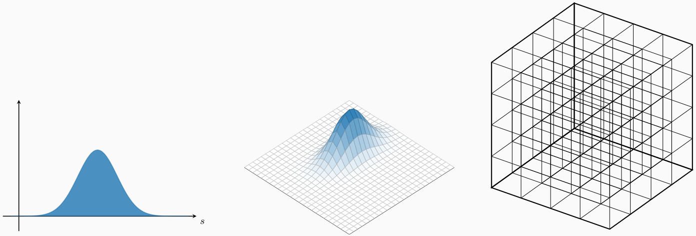
$\mathcal{O}(N^3)$



Curse of dimensionality

- **Computational complexity** of standard numerical schemes

$z \in \mathbb{R}$	$z \in \mathbb{R}^2$	$z \in \mathbb{R}^3$
$\mathcal{O}(N)$	$\mathcal{O}(N^2)$	$\mathcal{O}(N^3)$



- Standard numerical schemes for solving PDEs suffer the **curse of dimensionality**.

Mesh-free deep-learning methods for simulating high-dimensional models

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Machine learning-based method

Partial Differential Equations and Applications (2023) 4:51
https://doi.org/10.1007/s42985-023-00244-0

ORIGINAL PAPER

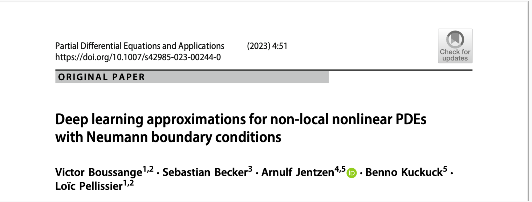
Deep learning approximations for non-local nonlinear PDEs with Neumann boundary conditions

Victor Boussange[1,2] · Sebastian Becker[3] · Arnulf Jentzen[4,5] · Benno Kuckuck[5] · Loïc Pellissier[1,2]

Mesh-free deep-learning methods for simulating high-dimensional models

Machine learning-based method

- Approximation of the solution with NNs
- NNs trained through **Monte Carlo approximation** of a **stochastic reformulation** of the PDE problem (Feynman–Kac)



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Intuition of mesh-free numerical methods

PDE Problem

$$\partial_t u(t,x) = \mu(t,x)\nabla_x u(t,x) + \frac{1}{2}\sigma^2(t,x)\Delta_x u(t,x)$$

with initial conditions $u(0,x) = g(x)$, where
$u\colon \mathbb{R}^d \to \mathbb{R}$.

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Stochastic reformulation through Feynman–Kac formula

$$u(t,x) = \mathbb{E}\left[g(X_t^x)\right]$$

with X_t^x a stochastic process

$$X_t^x = \int_0^t \mu(X_s^x)ds + \int_0^t \sigma(X_s^x)dB_s + x.$$

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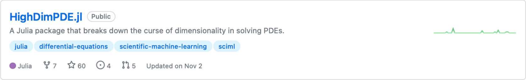
Monte Carlo approximation

$$u(t,x) \approx \frac{1}{N}\sum_i g(X_t^x)$$

`HighDimPDE.jl`: A package implementing recent solver algorithms that break down the curse of dimensionality



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HighDimPDE.jl Public
A Julia package that breaks down the curse of dimensionality in solving PDEs.
julia differential-equations scientific-machine-learning sciml
Julia 7 60 4 5 Updated on Nov 2

`HighDimPDE.jl` belongs to the SciML ecosystem

SciML Open Source Scientific Machine Learning
Open source software for scientific machine learning
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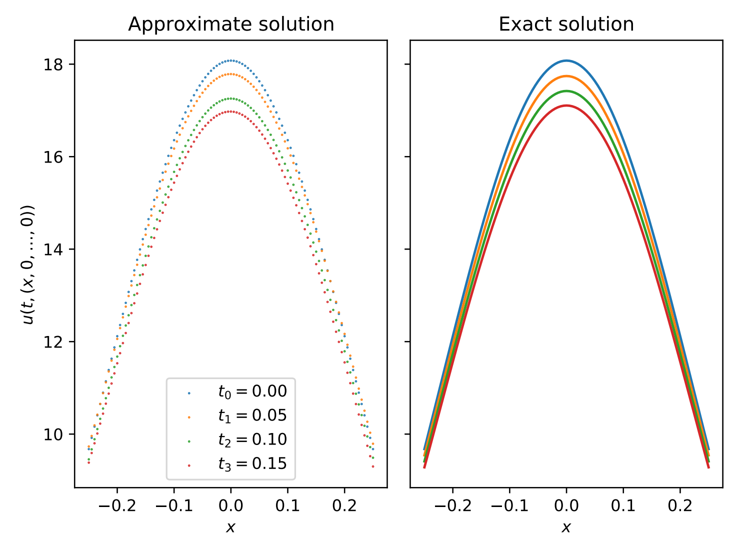
```julia
using HighDimPDE
alg = DeepSplitting(kwargs...)
prob = PIDEProblem(kwargs...)
sol = solve(prob, alg, kwargs...)
```

We are now able to simulate **10-dimensional eco-evolutionary models**!



- Scientific Machine Learning

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- We can constrain NNs with ecological knowledge by adding additional constraints in the loss function

- Scientific Machine Learning
- We can constrain NNs with ecological knowledge by adding additional constraints in the loss function
- Not only can physics-informed NNs facilitate data assimilation, but they can facilitate the simulation of high dimensional process-based models

Using ecological knowledge to augment data for the training of a NN

Using ecological knowledge to augment data for the training of a NN

```
data_augmentation = keras.Sequential(
[
    layers.RandomFlip("horizontal",
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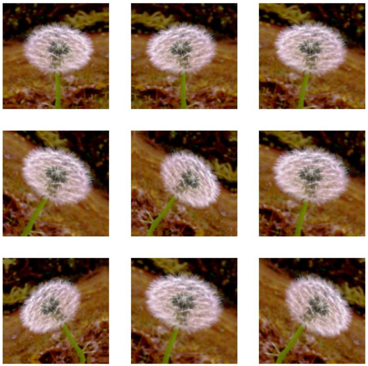

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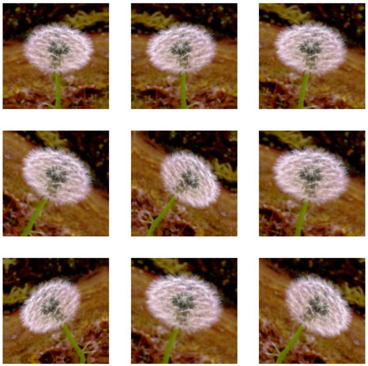

- An image of a flower will still be an image of a flower under small rotation, flip, and zooming

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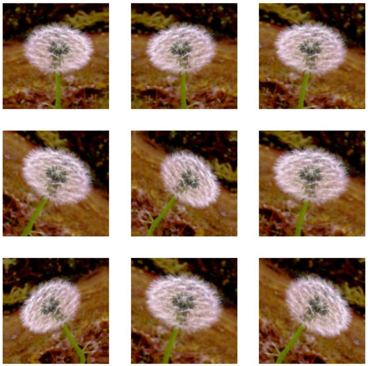

- An image of a flower will still be an image of a flower under small rotation, flip, and zooming
- Augmenting data helps the ML model to **generalize better**

Attribution of biodiversity change to climate change and land-use

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natural climate variations 🌦️

anthropogenic climate change ✈️

changes in land use and land cover 🌐

🦋 biodiversity change

Attribution of biodiversity change to climate change and land-use

?

natural climate variations 🌦️

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Building a macro-ecological model accounting for habitat area

Species-Area models have been central
to predict extinctions due to habitat loss

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Extinction risk from climate change

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$$\log SR = \overbrace{\log c}^{\text{intercept}} + \underbrace{z}_{\text{slope}} \log A$$

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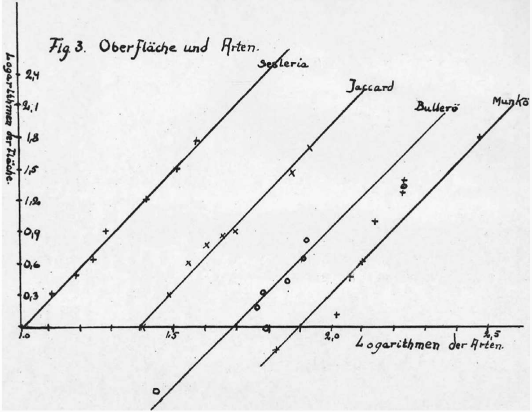
$$\overbrace{SR}^{\text{Species richness}} = c \underbrace{A^z}_{\text{Habitat area}}$$



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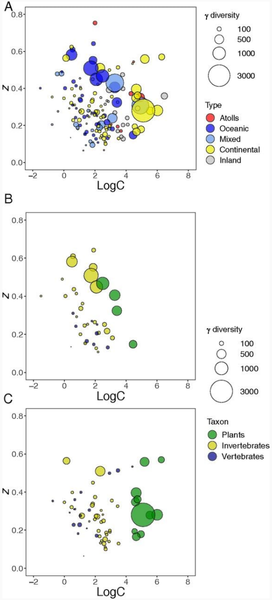

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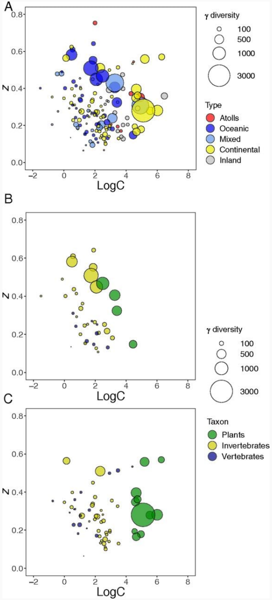
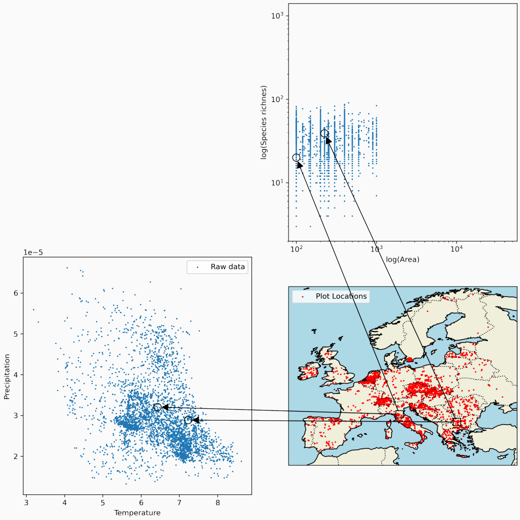


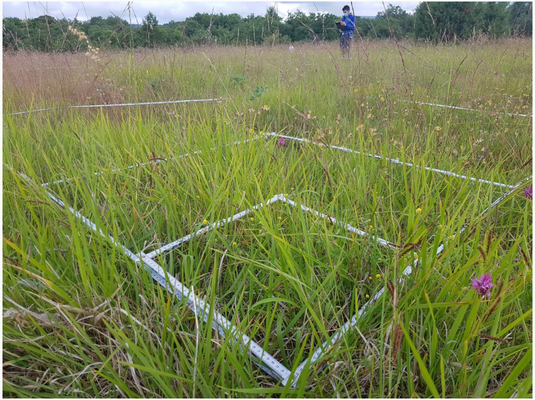
💡

$$SR = c(u)A^{z(u)}$$

where u are additional features corresponding to **environmental conditions**

Building a macro-ecological model accounting for habitat area





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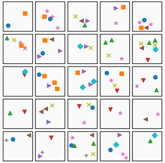

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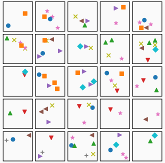
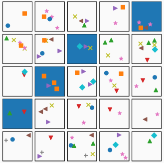
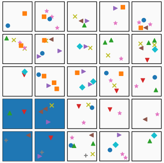


As a first approximation

$\mathbb{E}\Big[\mathrm{SR}\Big($  $\Big)\Big] = \mathbb{E}\Big[\mathrm{SR}\Big($  $\Big)\Big]$

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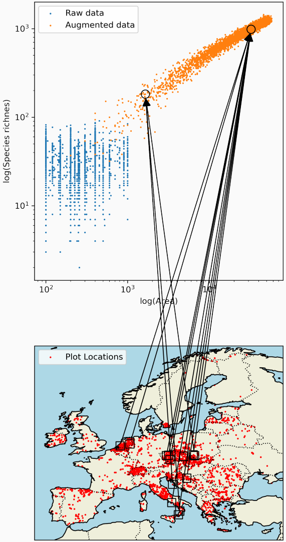

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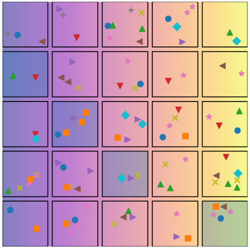

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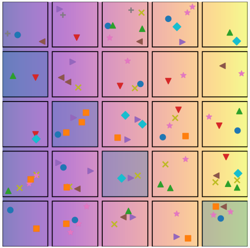

How to account for

- Spatial auto-correlation (limited dispersal)

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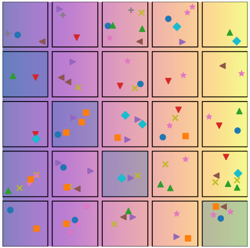

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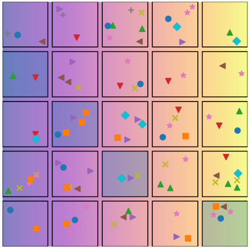

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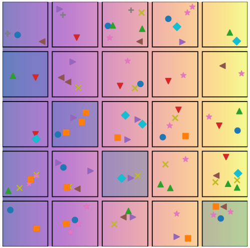

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$$\hat{y} = \mathcal{M}\left(A, \begin{array}{c} \begin{array}{ccc}\text{Site 1} & \quad\quad & \text{Site 4}\end{array} \\ \begin{pmatrix} u_{11} & & u_{14} \\ & \vdots & \\ u_{21} & & u_{24} \\ u_{31} & & u_{34} \end{pmatrix}\end{array}, \begin{array}{c} \begin{array}{ccc}\text{Site 1} & \quad\quad & \text{Site 4}\end{array} \\ \begin{pmatrix} d_{11} & & d_{14} \\ & \vdots & \\ d_{21} & & d_{24} \\ d_{31} & & d_{34} \end{pmatrix}\end{array}\right)$$

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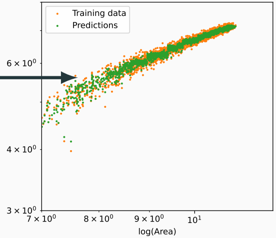

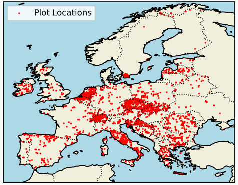

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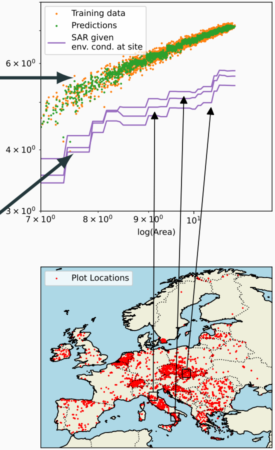
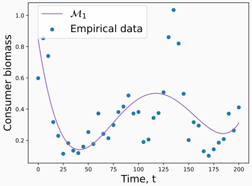


- We can augment the dataset used to train a ML model with ecological knowledge

From the ML world to the mechanistic world

After all, process-based models can be seen as regressors $\mathcal{M}_\theta$!

$$\frac{d}{dt}y = f_p(y, t)$$



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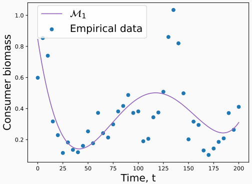
$$\frac{d}{dt}y = f_p(y, t)$$

$$\hat{y} = \underbrace{\int_{t_0}^{t} f_p(y_s, s)ds}_{\text{Numerical integration of the model}} + y_0$$



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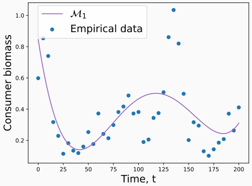
$$= \mathcal{M}_\theta(t)$$

where $\theta = (y_0, p)$



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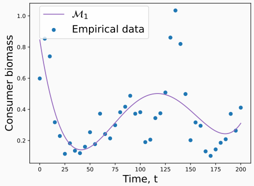

- In principle, process-based models can be trained similarly to ML models

$$L(\theta, \mathbf{y}) = \sum_{k=1}^{K} ||y_k - \mathcal{M}_\theta(x_k)||^2$$

Available methods to minimize L

- Global optimization
  - Markov Chain Monte Carlo
  - Approximate Bayesian Computation
- Local optimization
  - Variational optimizers

Global optimization with MCMC

- Sample L with a Markov chain $\theta^1, \theta^2, \ldots$ which equilibrium distribution is proportional to L

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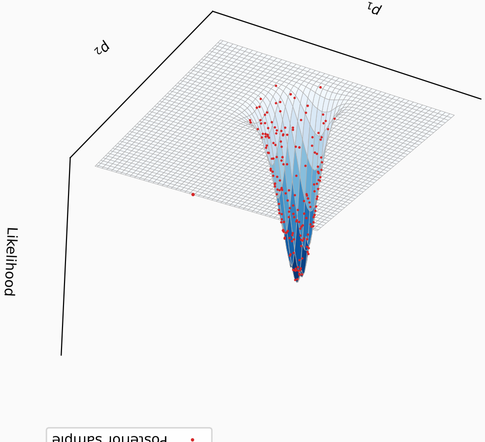
+ Provide uncertainty estimations
− Suffer from the curse of dimensionality

❌ Not suited for training complex process-based models



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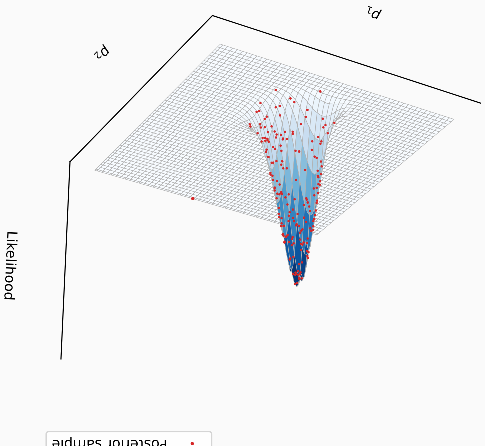
+ Provide uncertainty estimations
− Suffer from the curse of dimensionality
− Process-based models are costly to evaluate

❌ Not suited for training complex process-based models

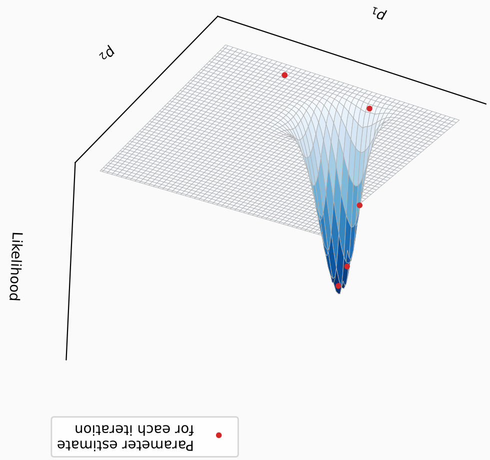


Local optimization with gradient descent

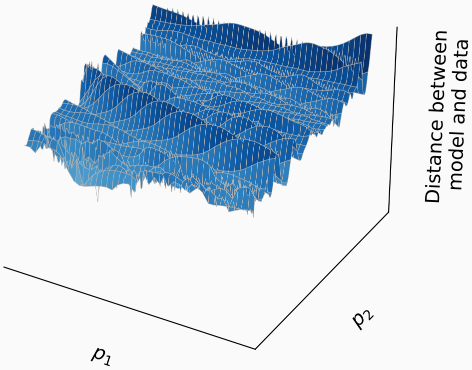
- Follow the steepest slope $\nabla_\theta L(\theta, \mathbf{y})$

$$\theta^{m+1} = \underbrace{\theta^m}_{\text{parameter at iteration } m} - \overbrace{\lambda}^{\text{learning rate}} \underbrace{\nabla_\theta L(\theta^{(m)}, \mathbf{y})}_{\text{gradient w.r.t parameters}}$$

+Less prone to the curse of dimensionality
−Parameter point estimates
−Convergence to local minima
−Require parameter sensitivity

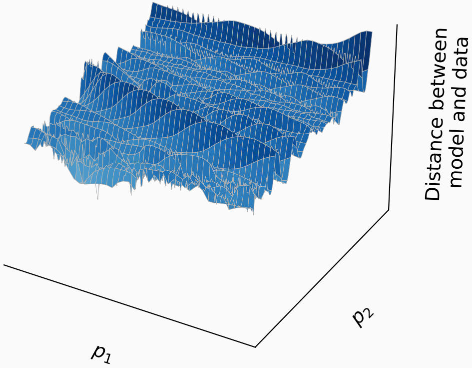


The specificities of ecological models



The specificities of ecological models

❌ Forward pass is expensive



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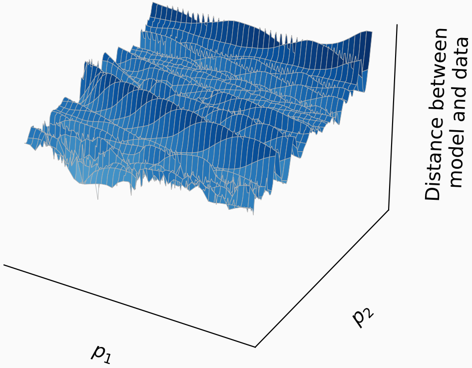

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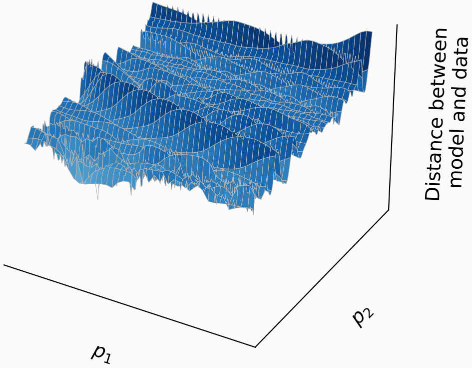
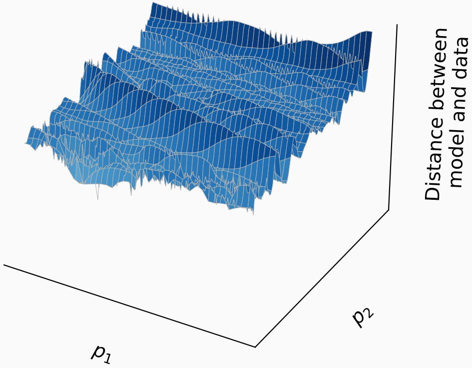


The specificities of ecological models

- ❌ Forward pass is expensive
- ❌ Many local minima
- ❌ Require the sensitivity to the model parameters, $\nabla_\theta \mathcal{M}_\theta$



`PiecewiseInference.jl`: Inverse modelling framework for dynamical systems with highly non-linear dynamics.

Boussange, V., Vilimelis-Aceituno, P., Schäfer, F., Pellissier, L., *Partitioning ecological time series to improve process-based models with machine learning* [bioRxiv] (2022), 46 pages. In review.

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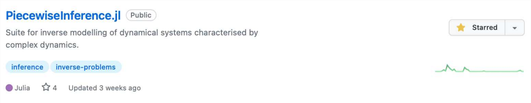

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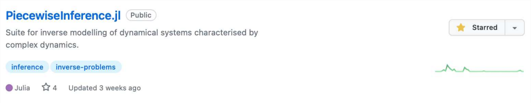

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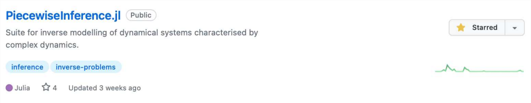
- sensitivity analysis methods based on **Automatic Differentiation**
- use of **deep learning variational optimizers**



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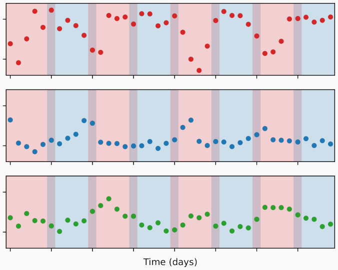

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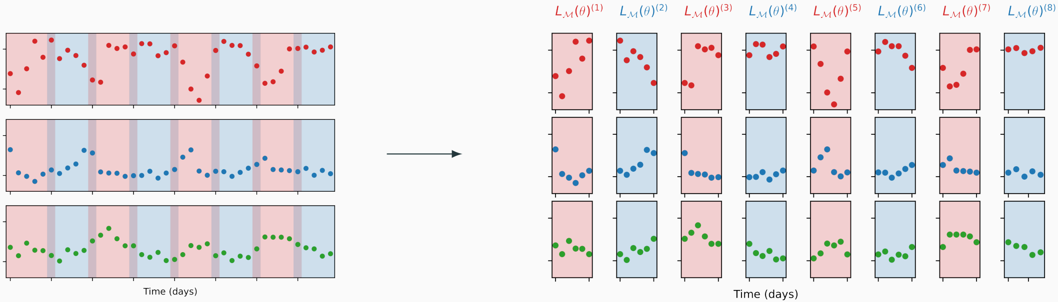

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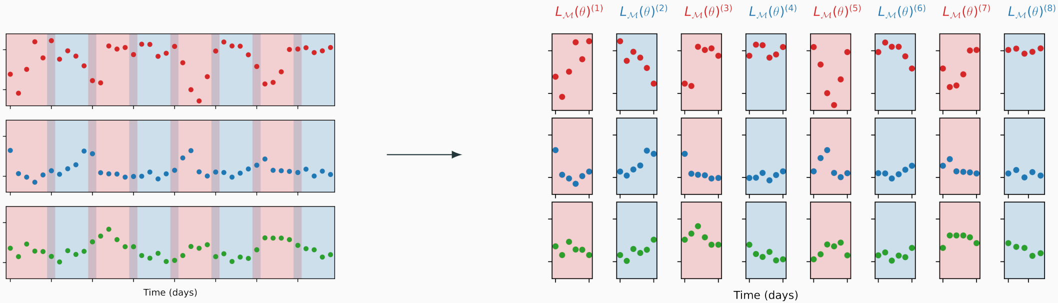

$$L_{\mathcal{M}}(\theta) = L_{\mathcal{M}}^{(1)}(\theta) + L_{\mathcal{M}}^{(2)}(\theta) + \dots \tag{1}$$

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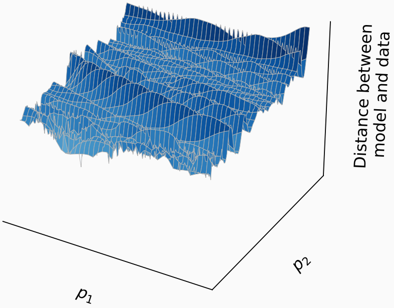

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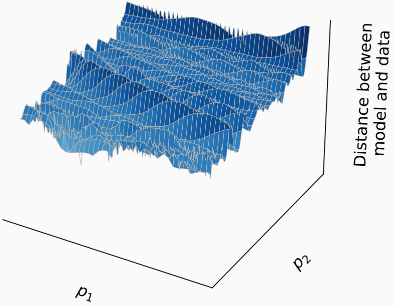

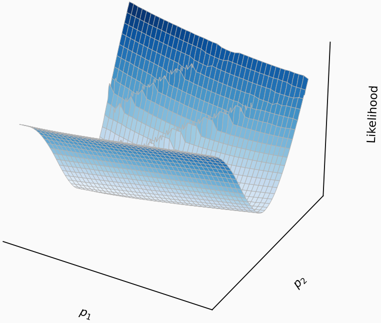

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- Deep learning optimizers

Adam: A method for stochastic optimization [PDF] arxiv.org
DP Kingma, J Ba - arXiv preprint arXiv:1412.6980, 2014 - arxiv.org
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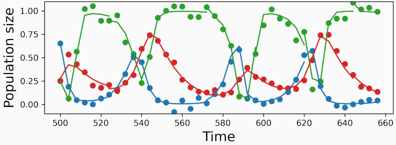
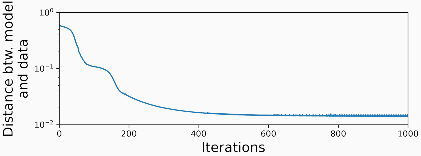
- **Sensitivity analysis** based on **automatic differentiation**

```julia
using ForwardDiff
ForwardDiff.gradient(sin, 0.1) == cos(0.1) # true
```

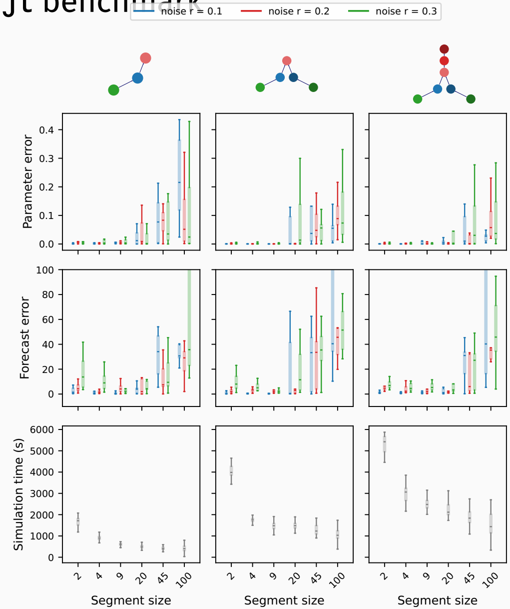
`PiecewiseInference.jl`: Inverse modelling framework for dynamical systems with highly non-linear dynamics.

```julia
using PiecewiseInference

model = MyModel(ModelParams(...))

infprob = InferenceProblem(model, p_init)

res = inference(infprob,
group_nb = 2,
data,
tsteps = tsteps,
epochs = [5000],
optimizers = [ADAM(0.001)],
batchsizes = [1])
```

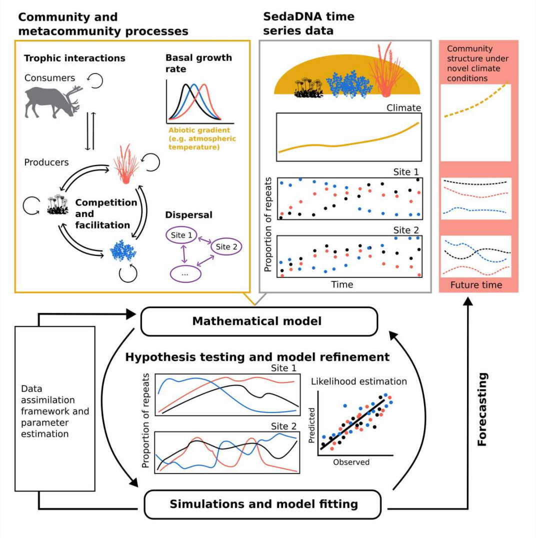




PiecewiseInference.jl benchmark

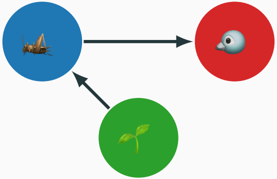


Dynamic forecast of future changes



Alsos, I.G., **Boussange, V.**, ... *Using ancient sedimentary DNA to forecast ecosystem trajectories under climate change* (2023). Accepted in Philosophical Transactions of the Royal Society B

Neural network-based parametrization



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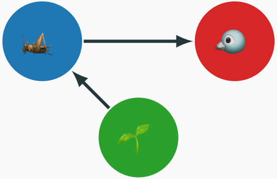
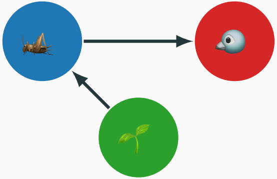


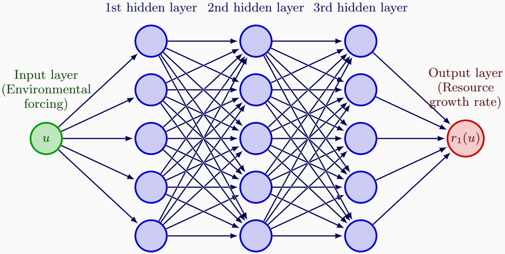
net growth rate 🌱 = basal growth(environmental conditions) − competition − grazing − death

net rowth rate 🦗 = grazing − predation − death

net growth rate 🐦 = predation − death

Neural network-based parametrization



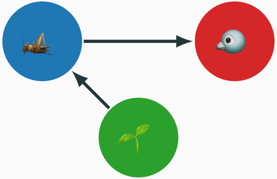


net growth rate 🌱 = NN(environmental conditions) − competition − grazing − death

net rowth rate 🦗 = grazing − predation − death

net growth rate 🐦 = predation − death

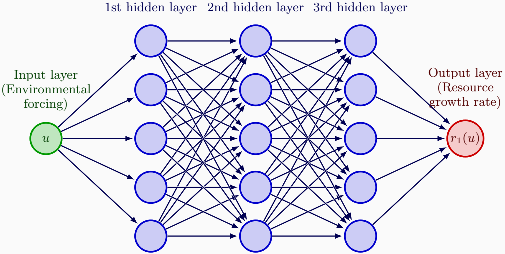
Neural network-based parametrization



$$\frac{d}{dt}R_t = \mathrm{NN(u)}\, \overbrace{R_t(1 - R_t)}^{\text{logistic growth}} - x_c y_c \underbrace{\frac{C_t R_t}{R_t + R_0}}_{\substack{\text{functional response} \\ \text{(intake rate of consumers)}}}$$

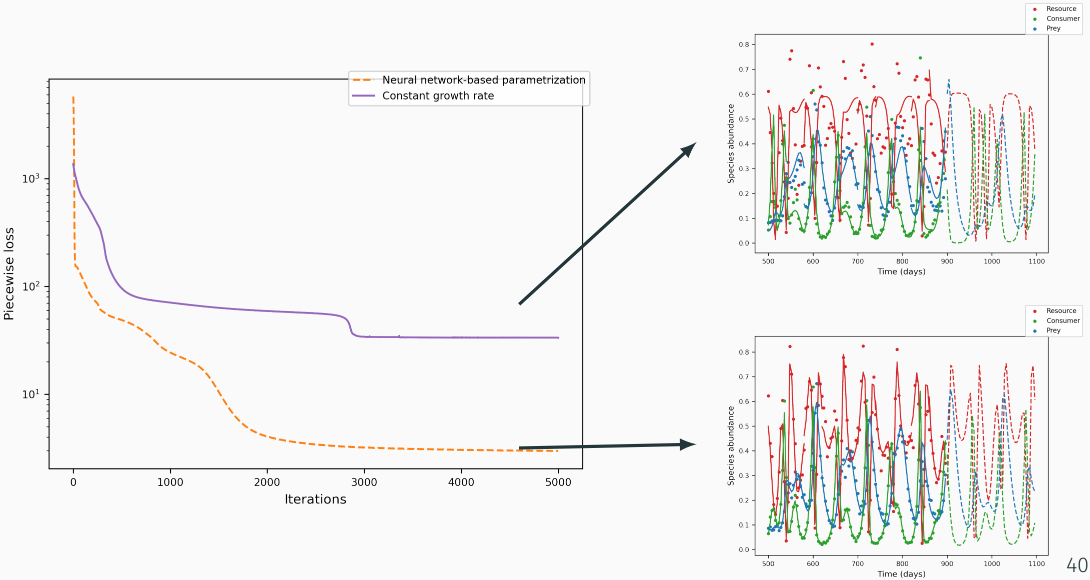
$$\frac{d}{dt}C_t = x_c C_t \left[-1 + y_c \frac{R_t}{R_t + R_0}\right] - x_p y_p \underbrace{\frac{P_t C_t}{C_t + C_0}}_{\substack{\text{functional response} \\ \text{(intake rate of predators)}}}$$

$$\frac{d}{dt}P_t = x_p P_t \left[-1 + y_p \frac{C_t}{C_t + C_0}\right]$$

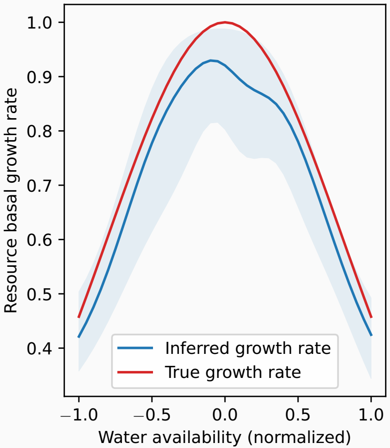


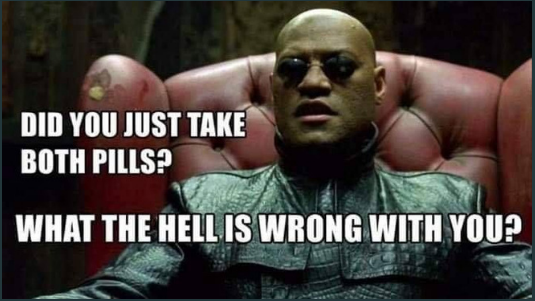
$$\theta = (x_c, y_c, x_p, y_p, C_0, R_0, \underbrace{\mathrm{W}_1, \mathrm{W}_2, \mathrm{W}_3, \mathrm{b}_1, \mathrm{b}_2, \mathrm{b}_3}_{\substack{\text{Weight and biases} \\ \text{of neural network}}})$$

Neural network-based parametrization



Offline interpretation of the neural network-based parametrization




DID YOU JUST TAKE
BOTH PILLS?
WHAT THE HELL IS WRONG WITH YOU?

Paradigm shift

Paradigm shift

github.com/vboussange/WSLJuliaWorkshop2023

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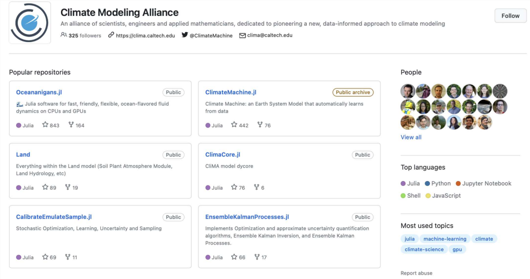

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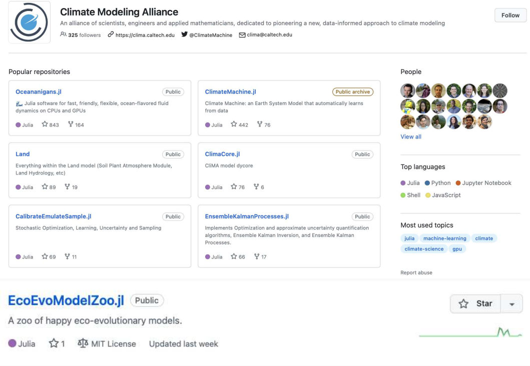

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