Combining eco-evolutionary theory and machine learning to advance our understanding of living systems

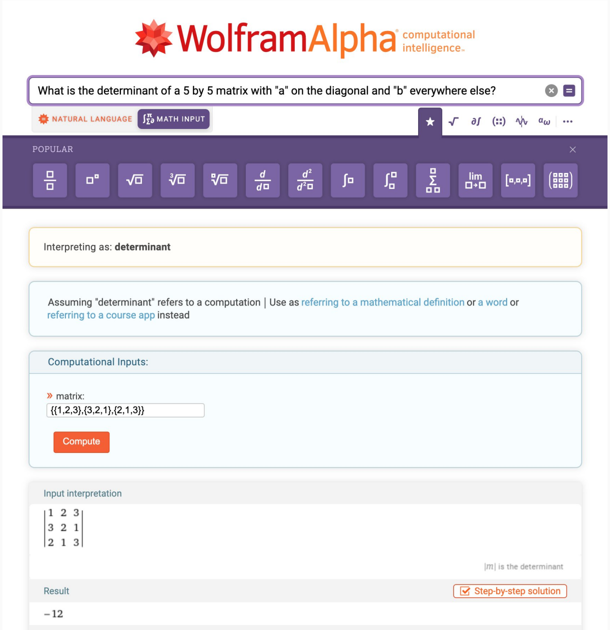
LIPhy seminar

Victor Boussange

What is the determinant of a 5 by 5 matrix with "a" on the diagonal and "b" everywhere else?

The determinant of a 5 by 5 matrix with "a" on the diagonal and "b" everywhere else would be (a^4) * (1-b) where a is the value on the diagonal and b is the value everywhere else. This is because the determinant of a matrix is equal to the product of the diagonal elements multiplied by the determinant of the matrix formed by removing the rows and columns corresponding to those diagonal elements. Since the diagonal elements are all "a" and the remaining elements are "b", the determinant is (a^4) * (1-b).

@DrJimFan


WolframAlpha computational intelligence.
What is the determinant of a 5 by 5 matrix with "a" on the diagonal and "b" everywhere else?
NATURAL LANGUAGE
MATH INPUT
POPULAR
Interpreting as: determinant
Assuming "determinant" refers to a computation | Use as referring to a mathematical definition or a word or referring to a course app instead
Computational Inputs:
» matrix:
{{1,2,3},{3,2,1},{2,1,3}}
Compute
Input interpretation
1 2 3
3 2 1
2 1 3
|m| is the determinant
Result
Step-by-step solution
−12

Translate the following to Wolfram Mathematica code:

The determinant of a 5 by 5 matrix with "a" on the diagonal and "b" everywhere else?

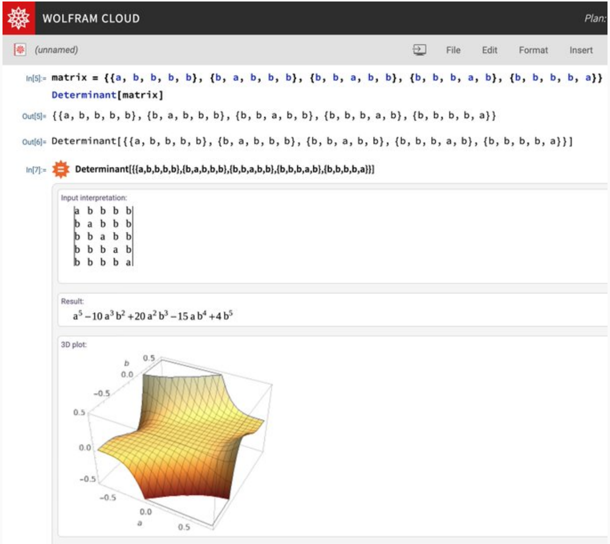
The Wolfram Mathematica code to calculate the determinant of a 5 by 5 matrix with "a" on the diagonal and "b" everywhere else would be:

Copy code

```
matrix = {{a, b, b, b, b}, {b, a, b, b, b}, {b, b, a, b, b}, {b, b, b, a,
b}, {b, b, b, b, a}}
Determinant[matrix]
```

This code creates a 5 by 5 matrix called "matrix" where the diagonal elements are "a" and the remaining elements are "b". Then it calculates the determinant of this matrix using the Determinant[] function.

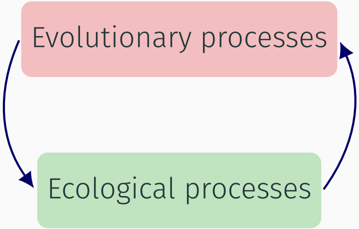
@DrJimFan


WOLFRAM CLOUD
Plan:
(unnamed)
File
Edit
Format
Insert
In[5]:= matrix = {{a, b, b, b, b}, {b, a, b, b, b}, {b, b, a, b, b}, {b, b, b, a, b}, {b, b, b, b, a}}
Determinant[matrix]
Out[5]= {{a, b, b, b, b}, {b, a, b, b, b}, {b, b, a, b, b}, {b, b, b, a, b}, {b, b, b, b, a}}
Out[6]= Determinant[{{a, b, b, b, b}, {b, a, b, b, b}, {b, b, a, b, b}, {b, b, b, a, b}, {b, b, b, b, a}}]
In[7]:= Determinant[{{a,b,b,b,b},{b,a,b,b,b},{b,b,a,b,b},{b,b,b,a,b},{b,b,b,b,a}}]
Input interpretation:
$\begin{vmatrix} a & b & b & b & b \\ b & a & b & b & b \\ b & b & a & b & b \\ b & b & b & a & b \\ b & b & b & b & a \end{vmatrix}$
Result:
$a^5 - 10 a^3 b^2 + 20 a^2 b^3 - 15 a b^4 + 4 b^5$
3D plot:
b
a
0.5
0.0
-0.5

1. Machine learning to simulate high-dimensional eco-evolutionary models

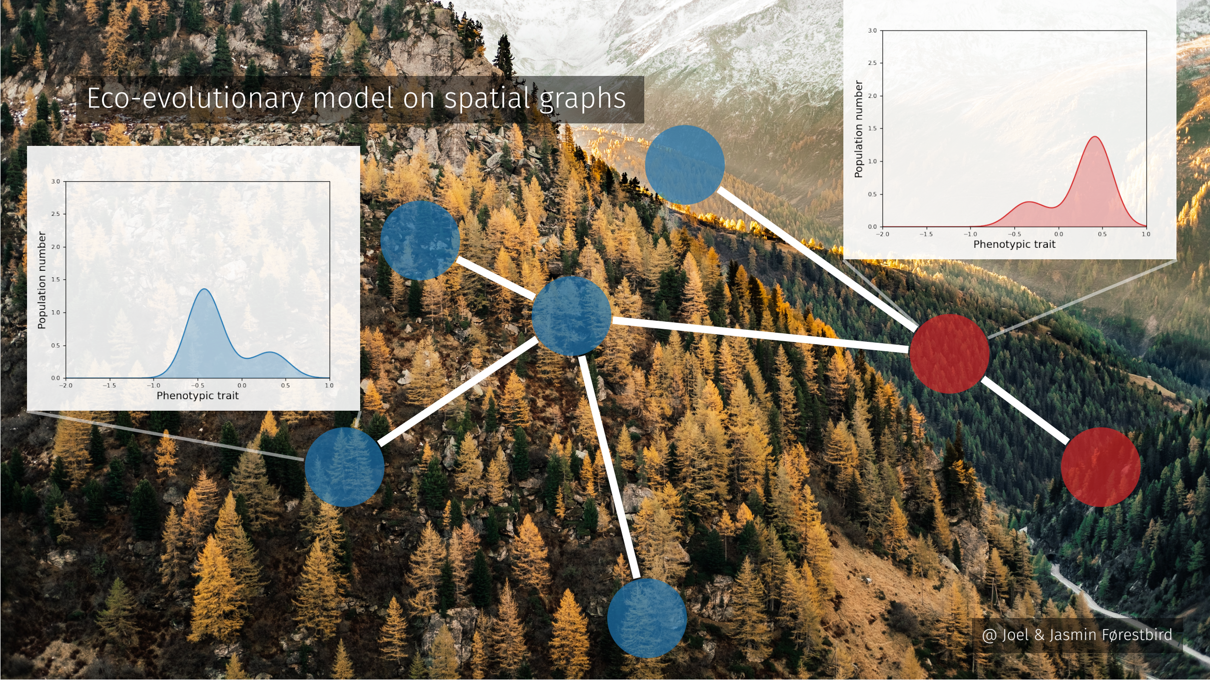
Evolutionary processes

Ecological processes


Evolutionary processes
Ecological processes

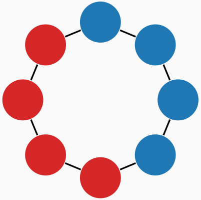

Eco-evolutionary model on spatial graphs
@ Joel & Jasmin Førestbird

Eco-evolutionary model on spatial graphs



Nonlocal PDEs

$$\partial_t n^{(i)} = n^{(i)} \left[b^{(i)}(1-m) - \frac{1}{K} \int_{\mathcal{S}} n^{(i)}(\mathbf{s}) d\mathbf{s} \right] + m \sum_{j \neq i} b_j(s) a_{i,j} n^{(j)} + \frac{1}{2} \mu \sigma_\mu^2 \Delta_s \left[b^{(i)} n^{(i)} \right]$$



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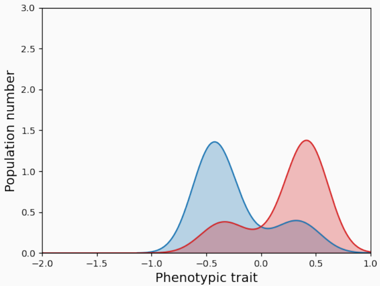

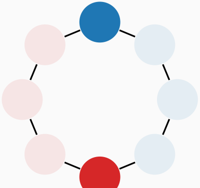

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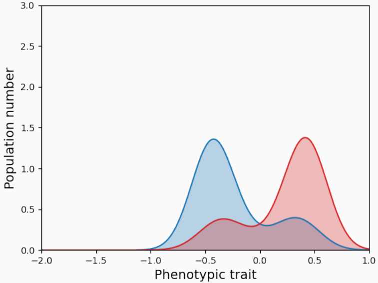

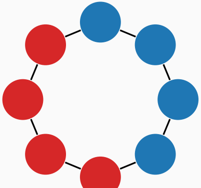

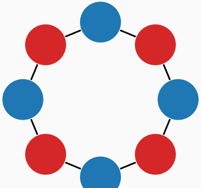

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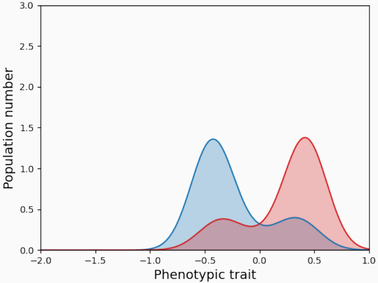

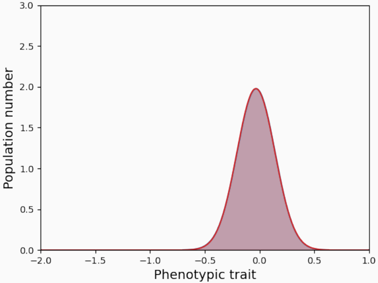

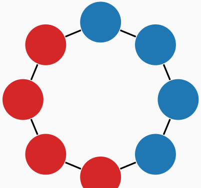

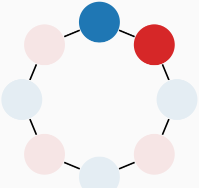

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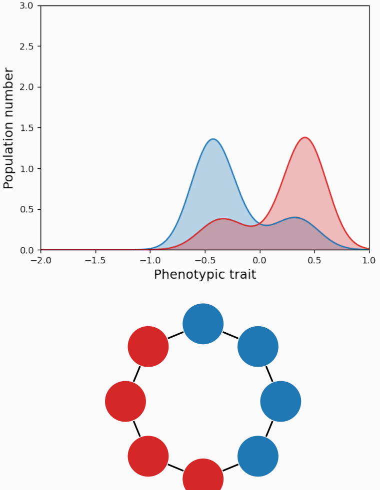

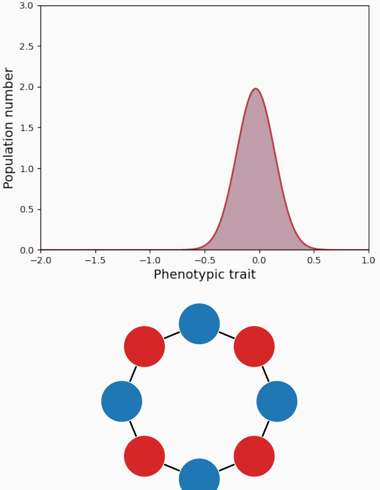

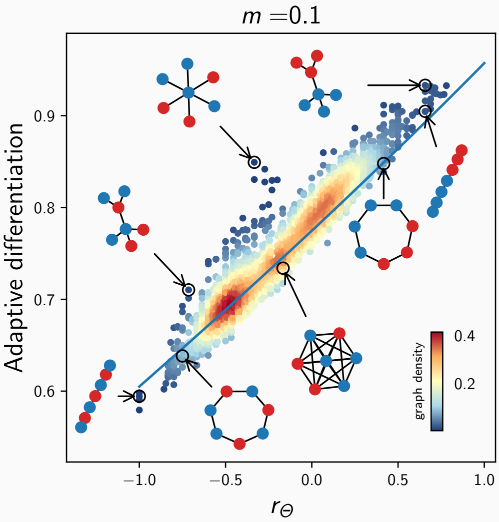

Boussange, V. & Pellissier, L., *Eco-evolutionary model on spatial graphs reveals how habitat structure affects phenotypic differentiation*. Commun Biol 5, 668 (2022).

Modelling the joint distribution of traits

@ PhyloPic

Modelling the joint distribution of traits

Numerous traits

@ PhyloPic

Modelling the joint distribution of traits

Numerous traits

- height

@ PhyloPic

Modelling the joint distribution of traits

Numerous traits

- height
- diameter

@ PhyloPic

Modelling the joint distribution of traits

Numerous traits

- height
- diameter
- surface leaf area
- ...

@ PhyloPic

Modelling the joint distribution of traits

Numerous traits

- height
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Many traits may importantly affect eco-evolutionary dynamics

@ PhyloPic

Modelling the joint distribution of traits

Numerous traits

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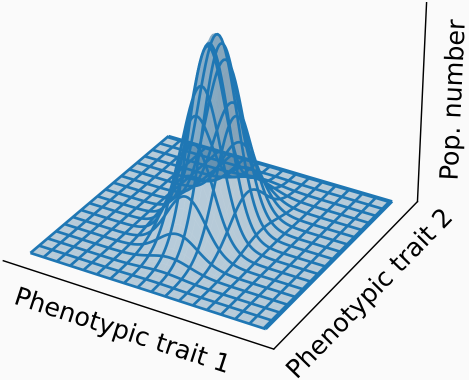
Many traits may importantly affect eco-evolutionary dynamics



Modelling the joint distribution of traits

Numerous traits

- height
- diameter
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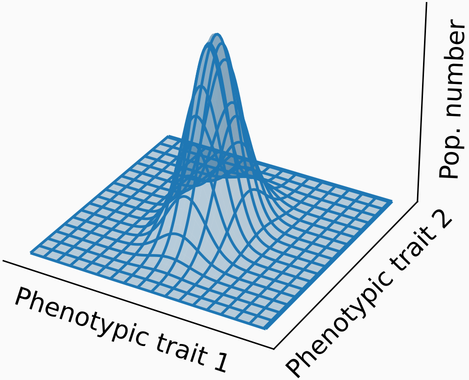
- ...

Many traits may importantly affect eco-evolutionary dynamics



Simulating **high-dimensional** phenotypic models is **not feasible with standard numerical methods**.

Curse of dimensionality

High dimensionality leads to complications for numerical simulations

Curse of dimensionality

High dimensionality leads to complications for numerical simulations

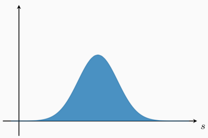
- **Computational complexity** of standard numerical schemes

Curse of dimensionality

High dimensionality leads to complications for numerical simulations

- **Computational complexity** of standard numerical schemes

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

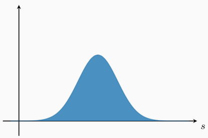


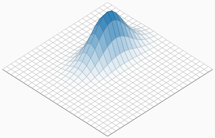
Curse of dimensionality

High dimensionality leads to complications for numerical simulations

- **Computational complexity** of standard numerical schemes

$\mathcal{O}(N)$ $\mathcal{O}(N^2)$





Curse of dimensionality

High dimensionality leads to complications for numerical simulations

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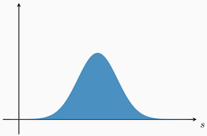
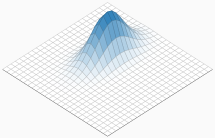
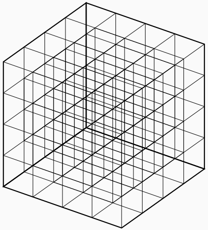




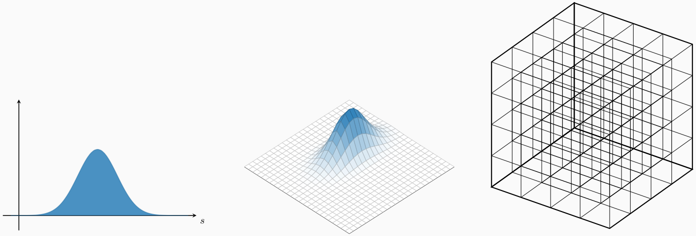


Curse of dimensionality

High dimensionality leads to complications for numerical simulations

- **Computational complexity** of standard numerical schemes

$\mathcal{O}(N)$ $\mathcal{O}(N^2)$ $\mathcal{O}(N^3)$



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

Numerical methods for simulating high-dimensional models

$\boxed{\text{Machine learning-based method}}$

Boussange, V., Becker, S., Jentzen, A., Kuckuck, B., Pellissier, L., *Deep learning approximations for non-local nonlinear PDEs with Neumann boundary conditions*. [arXiv] (2022), 59 pages. Revision requested from Partial Differential Equations and Applications.

Numerical methods for simulating high-dimensional models

Machine learning-based method

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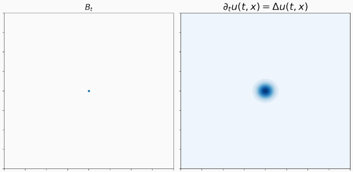
Numerical methods for simulating high-dimensional models

Machine learning-based method

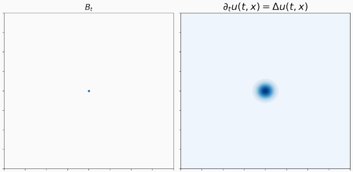
- Approximation of the solution with NNs
- NNs trained through a **stochastic reformulation** of the PDE problem (Feynman–Kac)

Boussange, V., Becker, S., Jentzen, A., Kuckuck, B., Pellissier, L., *Deep learning approximations for non-local nonlinear PDEs with Neumann boundary conditions.* [arXiv] (2022), 59 pages. Revision requested from Partial Differential Equations and Applications.

Feynman Kac formula



Feynman Kac formula



PDE Problem

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

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

Stochastic reformulation

$$u(t,x) = \int_0^t \mathbb{E}\left[f(X_{t-s}^x, u(T-s, X_{t-s}^x))ds\right] + \mathbb{E}\left[u(0, X_t^x)\right] \tag{2}$$

with

$$X_t^x = \int_0^t \mu(X_s^x)ds + \int_0^t \sigma(X_s^x)dB_s + x. \tag{3}$$

- `HighDimPDE.jl`: A new package implementing recent **solver algorithms that break down the curse of dimensionality**
- `HighDimPDE.jl` belongs to the SciML ecosystem

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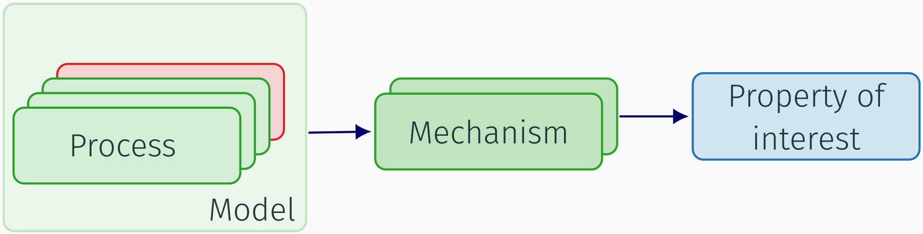
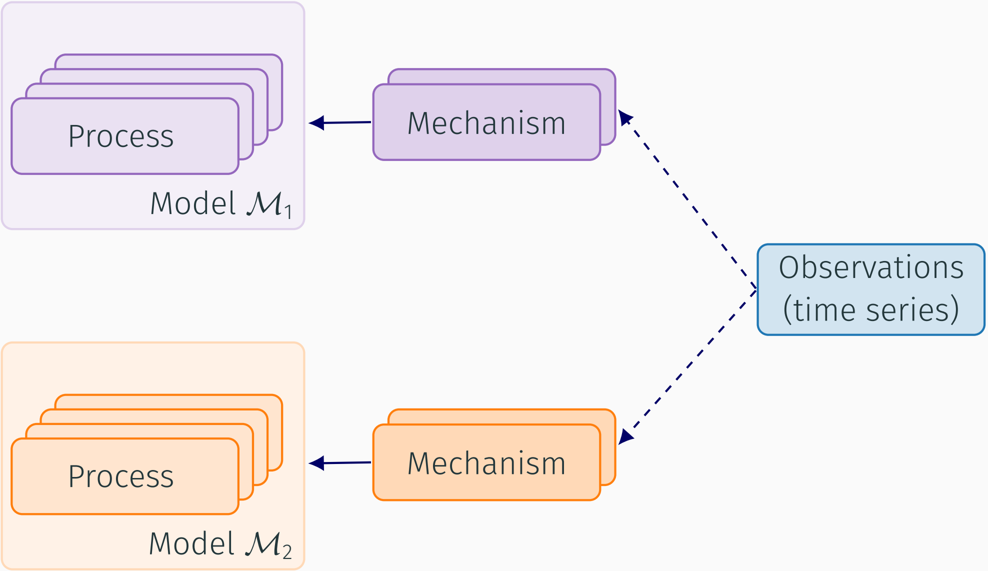
```julia
using HighDimPDE
alg = DeepSplitting(kwargs...)
prob = PIDEProblem(kwargs...)
sol = solve(prob, alg, kwargs...)
```

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

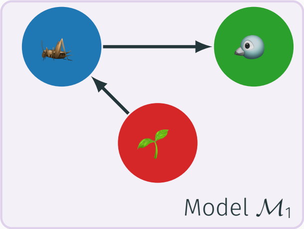
Boussange, V., Becker, S., Jentzen, A., Kuckuck, B., Pellissier, L., *Deep learning approximations for non-local nonlinear PDEs with Neumann boundary conditions*. [arXiv] (2022), 59 pages. Revision requested from Partial Differential Equations and Applications.

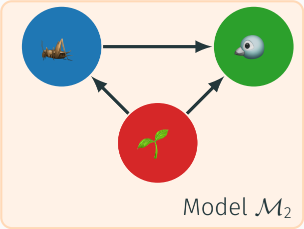
2. Machine learning for inverse modelling with ecological time series


Process
Model
Mechanism
Property of
interest

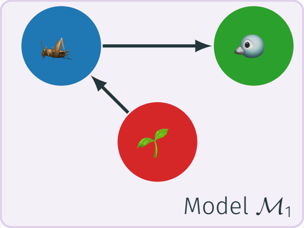

Process
Model $\mathcal{M}_1$
Mechanism
Observations (time series)
Process
Model $\mathcal{M}_2$
Mechanism

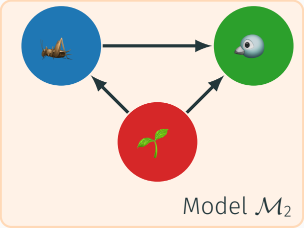
Inverse modelling

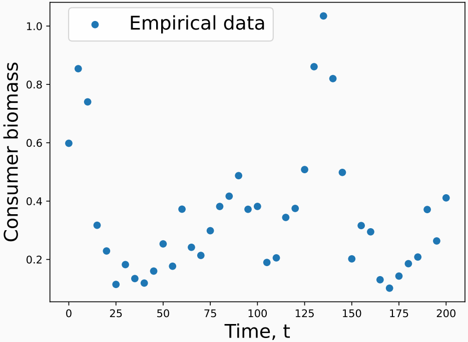




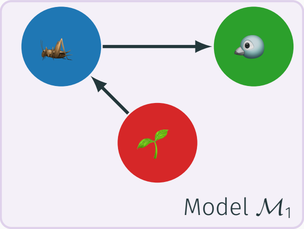
Inverse modelling

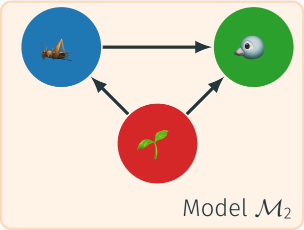


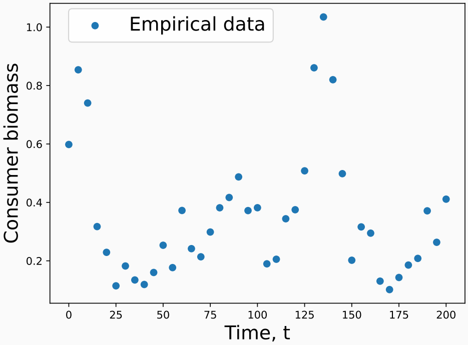




Inverse modelling



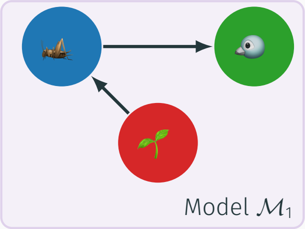


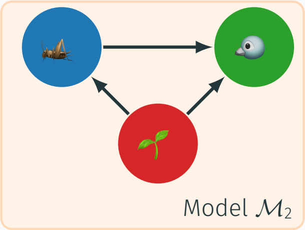


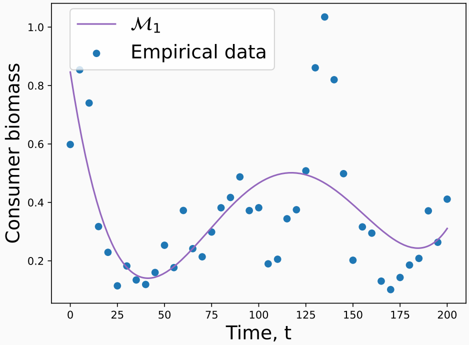
Compare model evidence

$$P(\mathcal{M}_2|\text{Data}) > P(\mathcal{M}_1|\text{Data})$$

Inverse modelling







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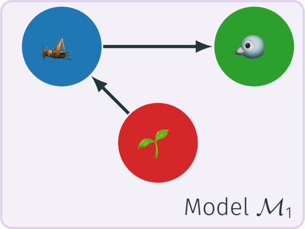
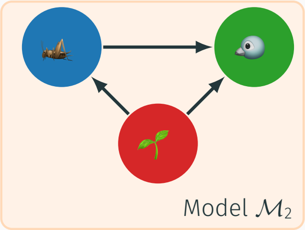
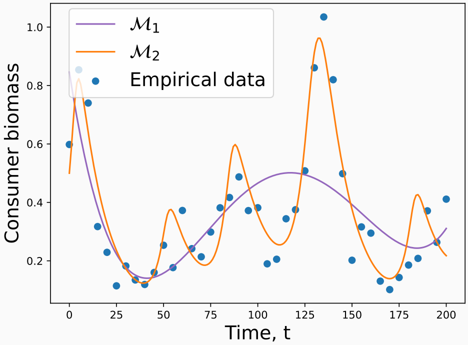






Compare model evidence

$$P(\mathcal{M}_2|\text{Data}) > P(\mathcal{M}_1|\text{Data})$$

Calculating the model evidence

$$P(\text{Data}|\mathcal{M}) = \int \underbrace{P(\theta|\mathcal{M}, \text{Data})}_{\substack{\text{Posterior distribution of} \\ \text{the model parameters}}} \, d\theta \tag{4}$$

$$\propto P(\theta^*|\mathcal{M}, \text{Data})\, \sigma(\theta^*, \mathcal{M})$$

Where θ^* is the maximum a priori estimate

Calculating the model evidence

$$
\begin{aligned}
L_{\mathcal{M}}(\theta) &= -\log P(\text{Data}|\theta, \mathcal{M})P(\theta|\mathcal{M}) \\
&= \sum_i ||\mathcal{M}(\theta, t_i) - y_{t_i}|| + ||\theta - \theta_p||
\end{aligned} \tag{5}
$$

Calculating the model evidence

$$\begin{aligned} L_{\mathcal{M}}(\theta) &= -\log P(\text{Data}|\theta, \mathcal{M})P(\theta|\mathcal{M}) \\ &= \sum_i ||\mathcal{M}(\theta, t_i) - y_{t_i}|| + ||\theta - \theta_p|| \end{aligned} \tag{5}$$

This is the bread and butter of ML practitioners!

Calculating the model evidence

$$
\begin{aligned}
L_{\mathcal{M}}(\theta) &= -\log P(\text{Data}|\theta, \mathcal{M}) P(\theta|\mathcal{M}) \\
&= \sum_i ||\mathcal{M}(\theta, t_i) - y_{t_i}|| + ||\theta - \theta_p||
\end{aligned} \tag{5}
$$

This is the bread and butter of ML practitioners!

These guys rely upon two very useful tools

Calculating the model evidence

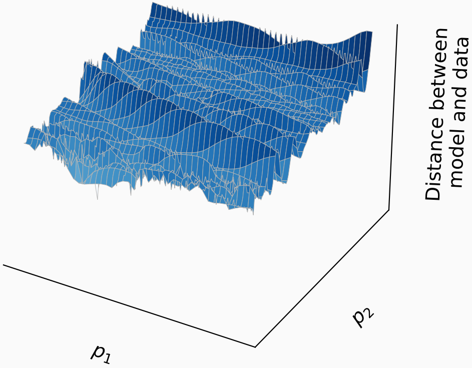
$$
\begin{aligned}
L_{\mathcal{M}}(\theta) &= -\log P(\text{Data}|\theta, \mathcal{M})P(\theta|\mathcal{M}) \\
&= \sum_i ||\mathcal{M}(\theta, t_i) - y_{t_i}|| + ||\theta - \theta_p||
\end{aligned} \tag{5}
$$

This is the bread and butter of ML practitioners!

These guys rely upon two very useful tools

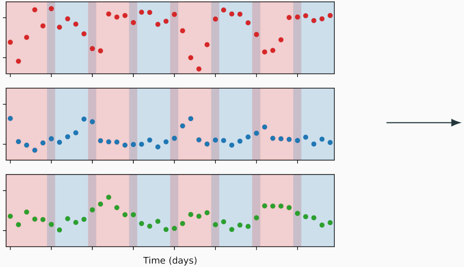
- Automatic differentiation
- Efficient optimization algorithms (e.g. Adam)

Yet another problem

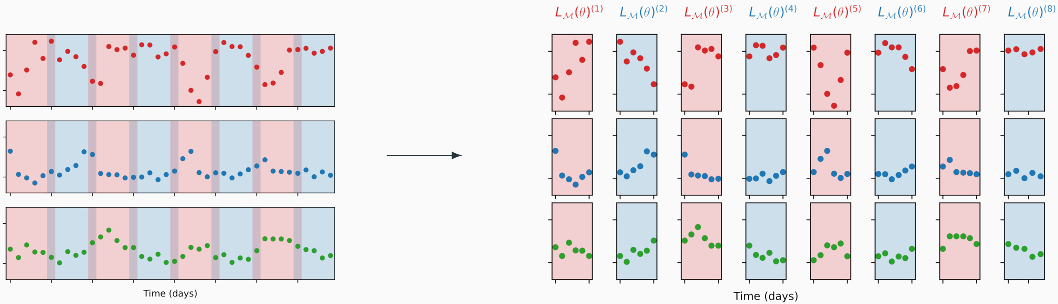


Likelihood landscape usually looks like Belledone massif

- Many local minima



Boussange, V., Vilimelis-Aceituno, P., Pellissier, L., *Mini-batching ecological data to improve ecosystem models with machine learning* [bioRxiv] (2022), 46 pages. In review.



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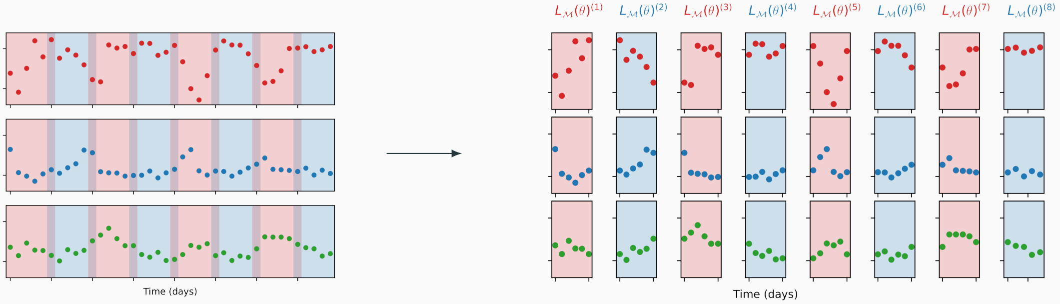
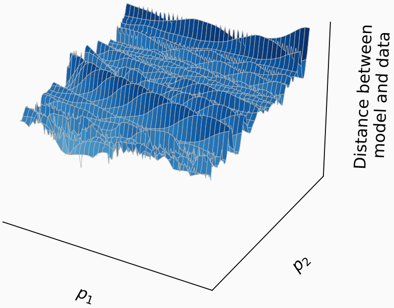
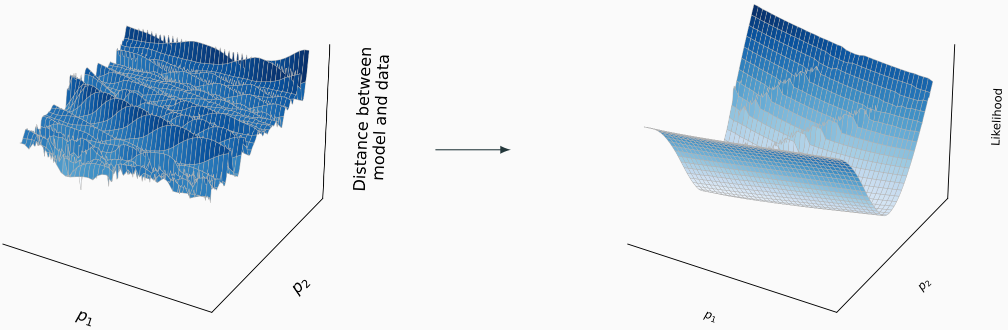


$$L_{\mathcal{M}}(\theta) = L_{\mathcal{M}}^{(1)}(\theta) + L_{\mathcal{M}}^{(2)}(\theta) + \dots \tag{6}$$

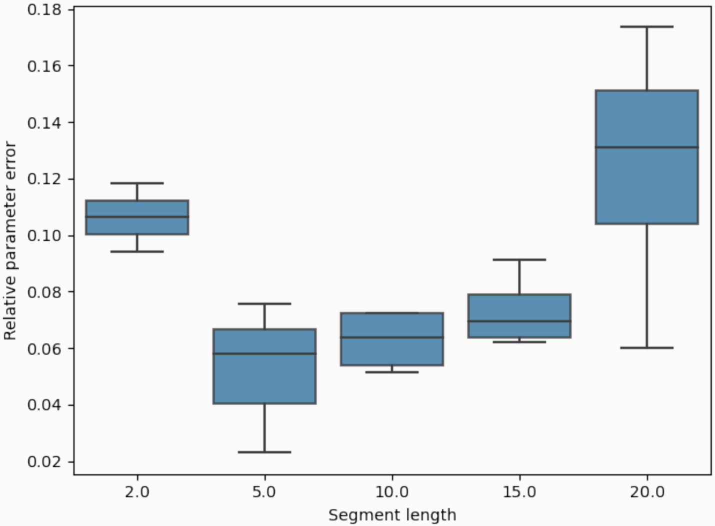
Boussange, V., Vilimelis-Aceituno, P., Pellissier, L., *Mini-batching ecological data to improve ecosystem models with machine learning* [bioRxiv] (2022), 46 pages. In review.



Distance between model and data
p_1
p_2


Distance between
model and data
p_1
p_2
Likelihood
p_1
p_2

Optimal segment length



`PiecewiseInference.jl`: a novel machine-learning framework for eco-evolutionary inverse modelling.

Boussange, V., Vilimelis-Aceituno, P., Pellissier, L., *Mini-batching ecological data to improve ecosystem models with machine learning* [bioRxiv] (2022), 46 pages. In review.

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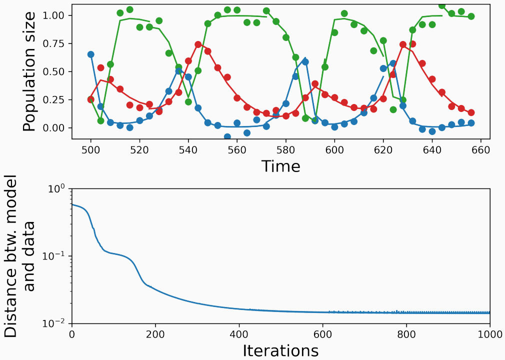
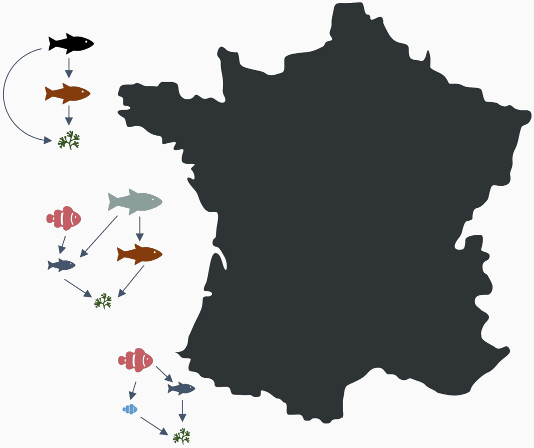


Boussange, V., Vilimelis-Aceituno, P., Pellissier, L., *Mini-batching ecological data to improve ecosystem models with machine learning* [bioRxiv] (2022), 46 pages. In review.

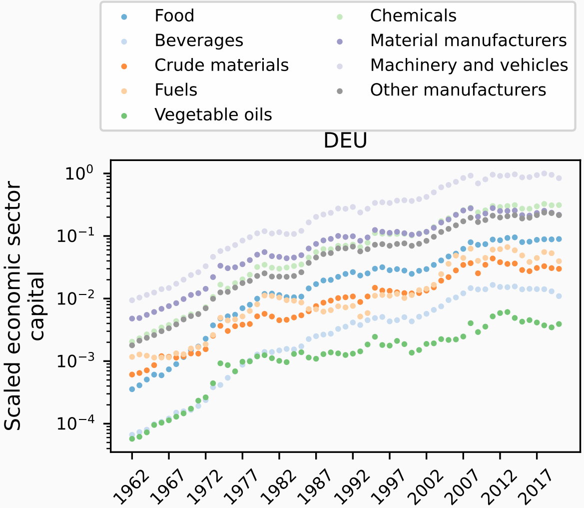
2. Applications: Reconstruction of fish food webs dynamic in the Bay of Biscay

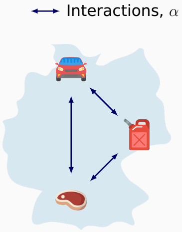
Dynamic model to forecast future changes



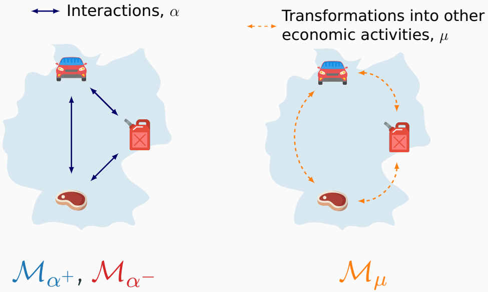
Courtesy of Romane Rozanski

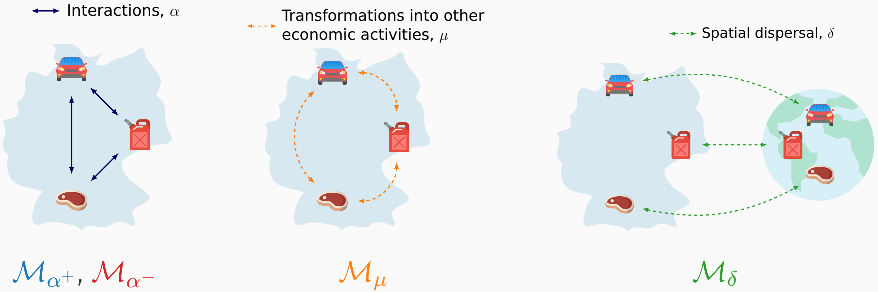
2. Applications: can eco-evolutionary processes explain long-term economic change?

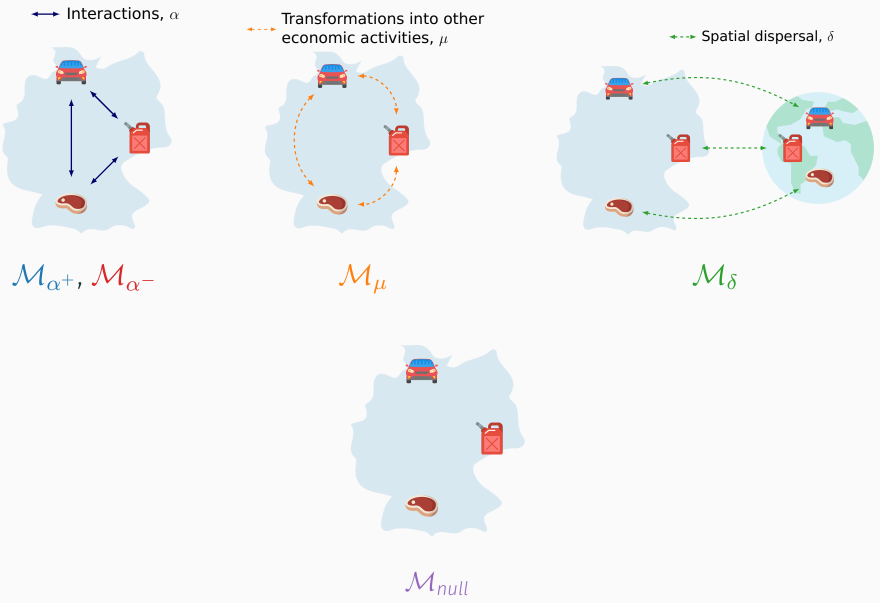

Food
Beverages
Crude materials
Fuels
Vegetable oils
Chemicals
Material manufacturers
Machinery and vehicles
Other manufacturers
DEU
Scaled economic sector capital
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
1962
1967
1972
1977
1982
1987
1992
1997
2002
2007
2012
2017

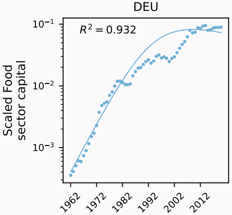


$\mathcal{M}_{\alpha^+}$, $\mathcal{M}_{\alpha^-}$

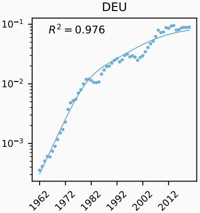

Interactions, α
Transformations into other economic activities, μ
$\mathcal{M}_{\alpha^+}$, $\mathcal{M}_{\alpha^-}$
$\mathcal{M}_{\mu}$


Interactions, α
Transformations into other economic activities, μ
Spatial dispersal, δ
$\mathcal{M}_{\alpha^+}$, $\mathcal{M}_{\alpha^-}$
$\mathcal{M}_{\mu}$
$\mathcal{M}_{\delta}$

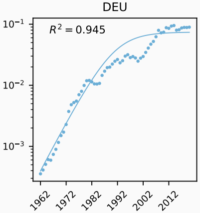

Interactions, α
Transformations into other economic activities, μ
Spatial dispersal, δ
$\mathcal{M}_{\alpha^+}$, $\mathcal{M}_{\alpha^-}$
$\mathcal{M}_{\mu}$
$\mathcal{M}_{\delta}$
$\mathcal{M}_{null}$



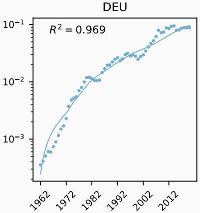
$\mathcal{M}_{\alpha^-}$



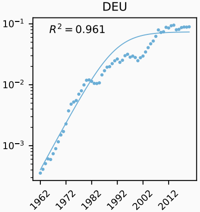
$\mathcal{M}_{\alpha^+}$



$\mathcal{M}_{\mu}$

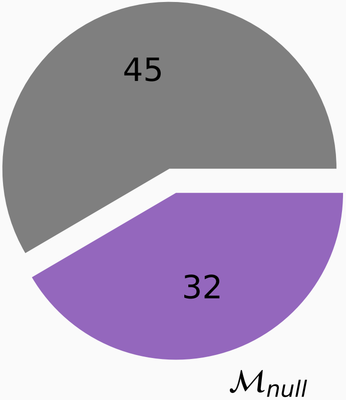


$\mathcal{M}_{\delta}$



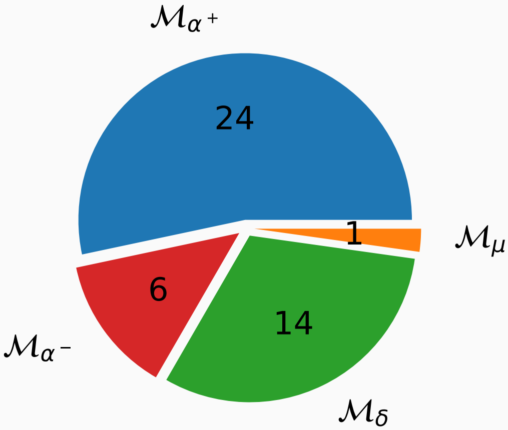
$\mathcal{M}_{null}$

Eco-evolutionary models



Nb. of countries where $\mathcal{M}_i$ is the best model

Boussange, V., Sornette, D., Lischke, H., Pellissier, L., *Analogous processes to ecological interactions and dispersal shape the dynamics of economic activities*. In preparation.



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3. Ongoing project: Machine learning to attribute changes in biodiversity to global change

natural climate variations 🌦️

anthropogenic climate change ✈️

changes in land use and land cover 🚜

natural climate variations 🌦️

anthropogenic climate change ✈️

changes in land use and land cover 🚜

🦋 biodiversity change

?

natural climate variations 🌦️

anthropogenic climate change ✈️

changes in land use and land cover 🚜

🦋 biodiversity change

?

natural climate variations 🌦️

anthropogenic climate change ✈️ — 🦋 biodiversity change

changes in land use and land cover 🚜

⇒ **Build a biodiversity model**

Building a biodiversity model from scratch

Building a biodiversity model from scratch

$$\text{Nb.}🦋 = \mathcal{M}(🌐, 🌦)$$

Ecological data is scarce!

Building a biodiversity model from scratch

$$\text{Nb.🦋} = \text{NN}_\theta(\text{🌐}, \text{🌦})$$

Ecological data is scarce!

We need to constrain the model, other than with data

Ecology-informed ML

Ecology-informed ML

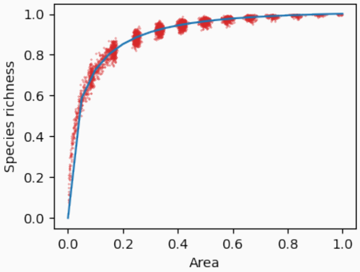
Combination of ecological theory

Ecology-informed ML

Combination of ecological theory

Species area relationships

$$y = c\,\text{Area}^z$$



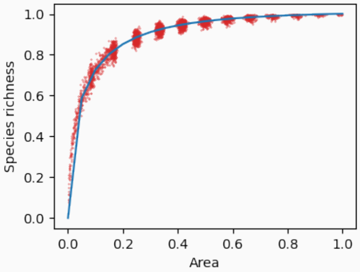
Ecology-informed ML

Combination of ecological theory

and machine learning

Species area relationships

$$y = c\,\mathrm{Area}^z$$

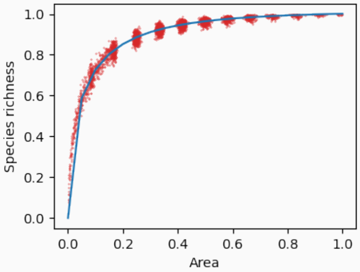


Ecology-informed ML

Combination of ecological theory

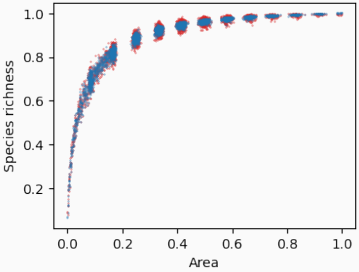
Species area relationships

$$y = c\,\mathrm{Area}^{z}$$



and machine learning

$$y = c\,\mathrm{Area}^{\mathrm{NN(env.\ vars)}}$$



Summary

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