

# Theoretical Ecotoxicology

## Session 1: Introduction

University Duisburg-Essen SS 2025

Ralf B. Schäfer

Ecotoxicology, Faculty of Biology, UDE & RC One Health Ruhr

# Short introduction I

- Professor for Ecotoxicology at UDE and RC One Health Ruhr since April 2024
- Professor for Quantitative Landscape Ecology at RPTU Kaiserslautern-Landau and University Koblenz-Landau from 2010-2024
- Phd on effects of pesticides in small streams in Finland and France
- Postdoc in Australia on effects of salinisation and pesticides in streams

# Short introduction II

- Teaching: This course, *Ecological Modelling* and *Ecological and evolutionary concepts for Ecotoxicology*
- Research focus:
  - Understand and predict the response of communities and food webs to multiple chemicals and non-chemical stressors
  - Evaluate risks from the large-scale distribution of organic chemicals for biodiversity
  - Analyse the relationship between stressor-driven community responses and responses of ecosystem processes and services
- Research approaches: Field studies, experiments and statistical and process-based modelling

# Course organisation

- Course page on Moodle and material on github
- Check document *Course schedule* for details on dates, times and content
- Mix of seminar with practical application
- To successfully accomplish course: Work on small course-related project in small group, present outcome

# Intended learning outcomes of the course

- Knowledge of theories and tools in the area of ecotoxicology
- Knowledge of software and packages to practically implement theoretical approaches
- Ability to apply tools to model dose response curves, ecological dynamics and analyse data
- Ability to evaluate results obtained from these tools and theories

# My expectations

- Active participation in course → This includes questions!
- Self-Assessment of the learning progress based on intended learning targets using the review questions
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**What are your expectations?**

# Intended learning outcomes of today's lecture

- Understanding what a model is
- Knowledge of the of different types of models
- Ability to discriminate categories of computational models



# Intended learning outcomes of today's lecture

- Understanding what a model is
  - Discuss the main characteristics that define a model
- Knowledge of the of different types of models
  - Describe the different types of models
- Ability to discriminate categories of computational models
  - Discuss differences between (1) empirical and process-based mechanistic models, (2) classical statistical and machine learning models and (3) ODE models and IBMs.

# Course content

- Introduction, Quarto/Markdown and installation
- Ecotoxicological databases
- Complex study designs
- Dose-response and chemical mixture modelling
- Modelling of bioaccumulation and TKTD
- Ecological modelling
- Machine learning and ecotoxicity prediction
- Toxicogenomics modelling

# What is a theory?

Join at [menti.com](https://menti.com) | use code 4573 5321



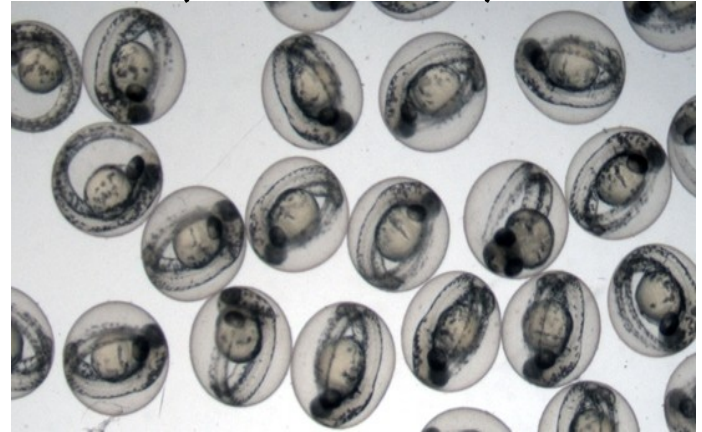
# What is a model?

Are these models and why?

Artificial streams in laboratory



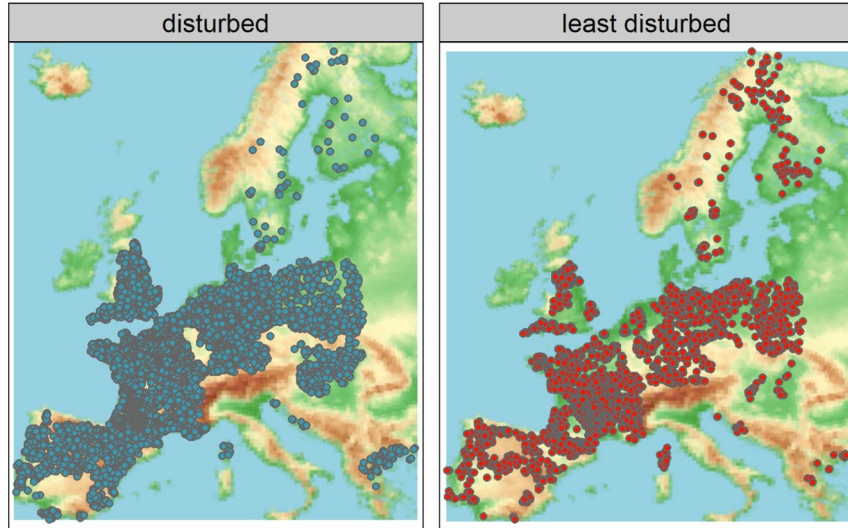
Embryos of zebrafish  
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# What is a model?

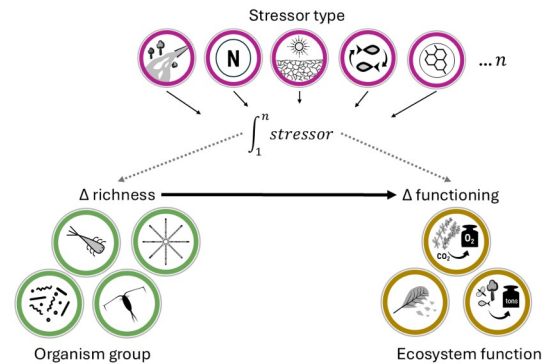
Are these models and why?

Map of Europe with sampling sites



Jupke et al. 2024 *Environ. Sci. Europ.* 36

Conceptual figure



Equation

$$\frac{dC_{org}}{dt} = k_w C_{aq} - k_e C_{org}$$

# What is a model?

„A model is a **simplified representation** of reality“

Smith & Smith 2007: 7

„A model is an **abstraction of reality**. This abstraction represents a complex reality in the simplest way that is adequate for the **purpose of the modelling**.“

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„A model can **generate expectations** about how the system will behave in a particular situation.

<https://undsci.berkeley.edu/glossary/model/>

# What is a model?

„Humans have always used models – defined as a **simplified** picture of reality – as **tools to solve problems**. [...] it is important that the model contains the characteristic features essential in the context of the problem to be solved or described“

Jorgensen & Fath 2011: 1

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- Simplified representation of phenomenon, process or system
- Guided by purpose
- Tool to solve problems and make predictions



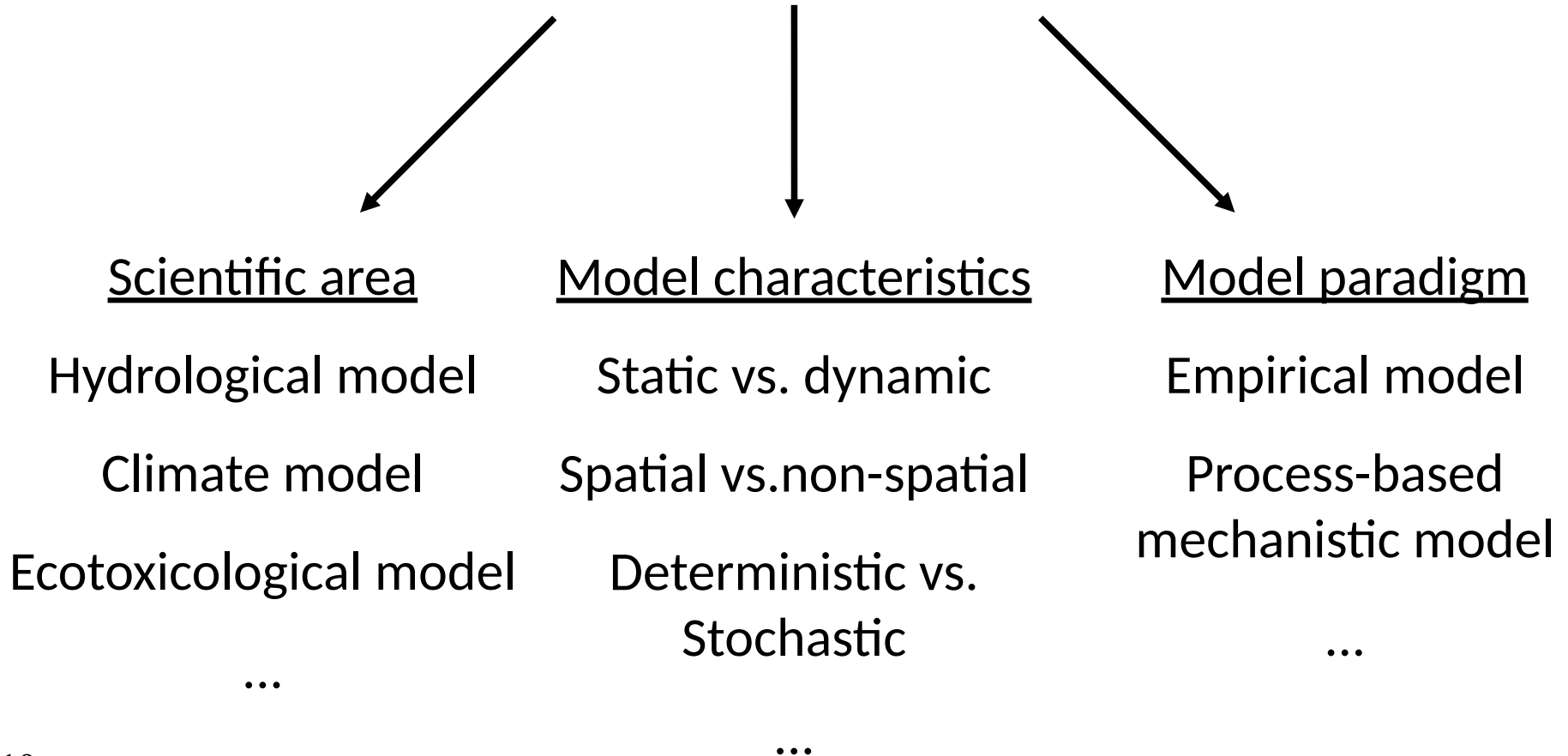
# Types of models

- Conceptual and mental model
  - e.g. Flowchart, diagram, mathematical description of nature
- Physical and material model
  - *In vivo* model
    - e.g. Test organism, mesocosm
  - *In vitro* model
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# Classification of computer models

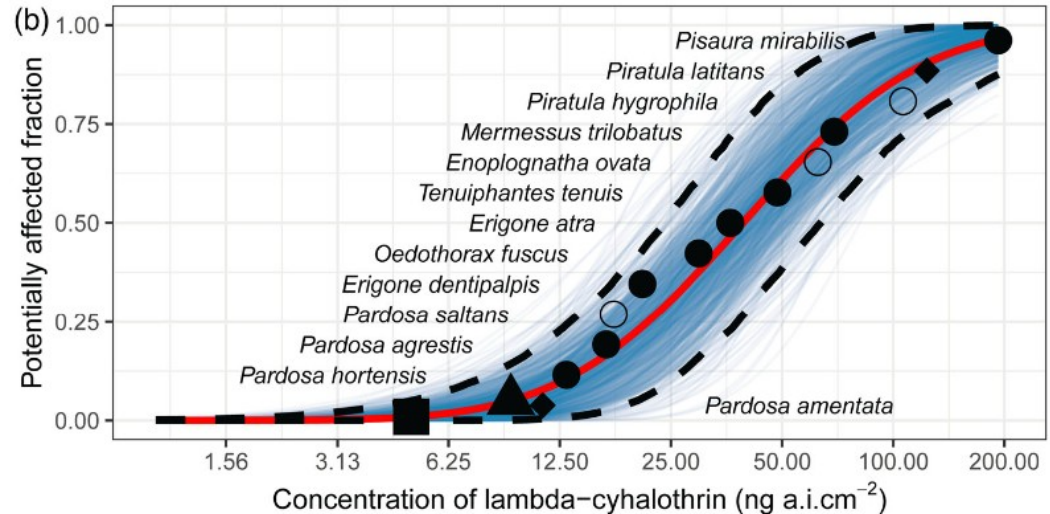


# Empirical model

- Phenomenon or system modeled based on observations
- Processes ignored
- Input and output variables linked through statistical model

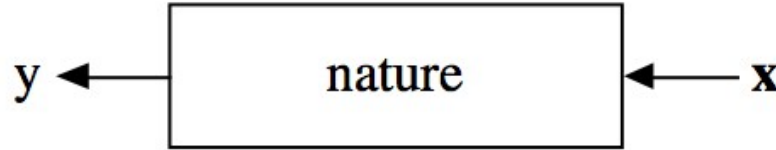
## Example: Species tolerance distribution

- Statistical relationship
- Processes related to toxicant action ignored
- Static (toxicokinetics and -dynamics ignored)

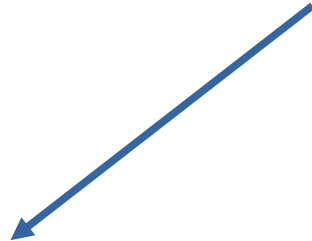


# Two cultures of empirical modelling

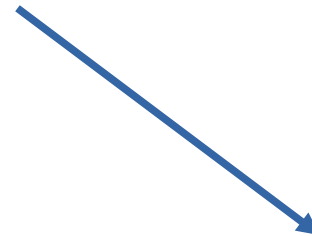
Real world: Processes lead to association between  $X$  and  $Y$



Examples for goals of statistical modelling: predict  $y$  from  $x$ , estimate relation between  $x$  and  $y$



Data modelling culture  
(classical statistics)



Algorithmic modelling culture  
(machine learning)

# Two cultures of empirical modelling

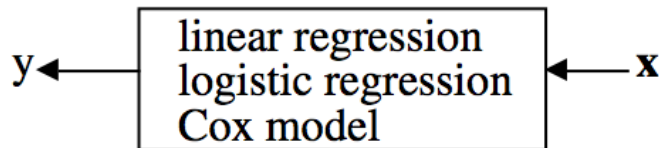
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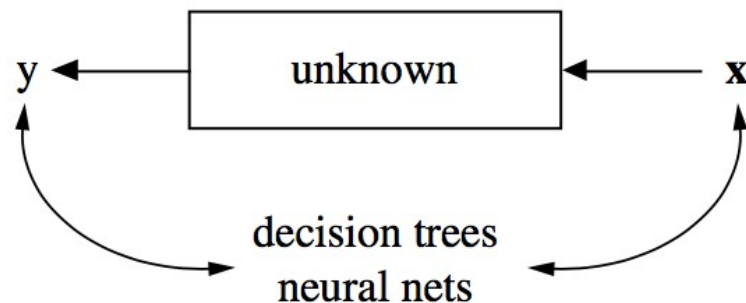
## Common data model

response variables =  $f(\text{predictor variables, random noise, parameters})$

Estimate  
parameters  
from data

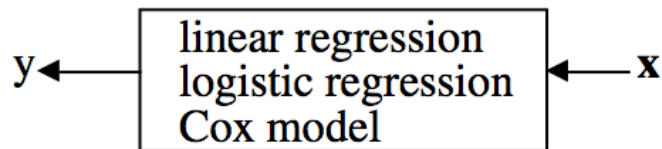


Find algorithm that operates on  $x$  to predict  $y$



# Two cultures of empirical modelling

## Data modelling culture (classical statistics)

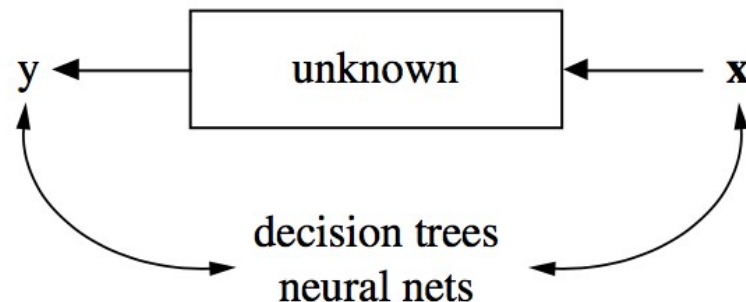


Methods appropriate for all research goals, but partly less powerful

### Bayesian vs. frequentist statistics

- Debates since decades
- Distinctions blurred in modern application
- Inclusion of prior knowledge/beliefs in models only within Bayesian framework

## Algorithmic modelling culture (machine learning)



Primarily appropriate for prediction and exploration, and partly estimation

# Process-based mechanistic models

- Describe mechanisms not just empirical correlations
  - e.g. Biomass growth depends on distribution of energy between foraging, maintenance and movement etc.
- Focuses on system behaviour including flows and interactions
  - e.g. Biomass flow in food web, feedback loops: predator-prey cycles
- Typically dynamic (simulations over time)
- Require parameters, typically measured in real systems
- Capacity to predict under different conditions



# Ordinary differential equation (ODE) model

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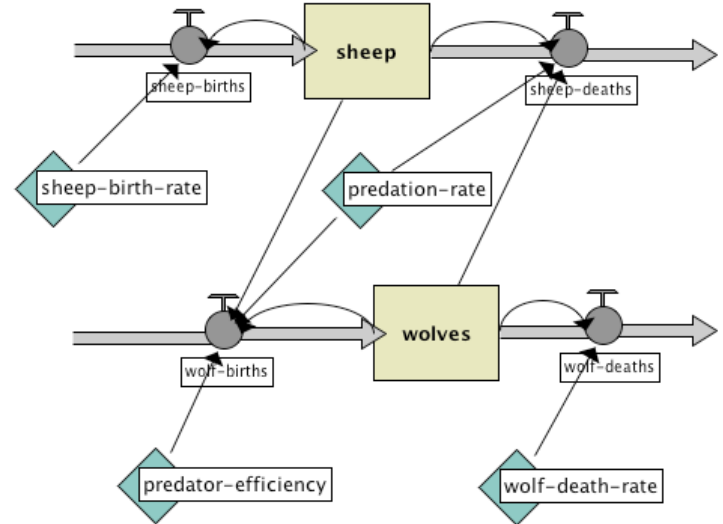
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## Example: Wolf-Sheep predation model

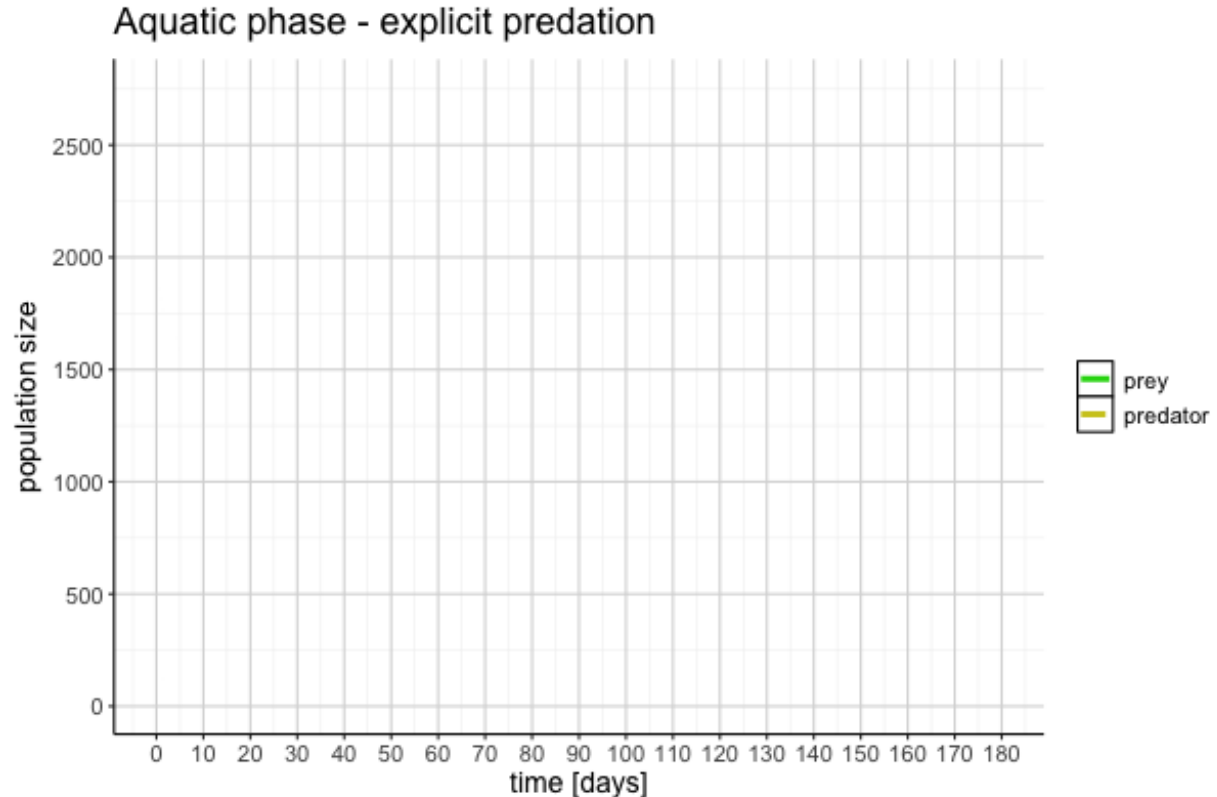
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Classical statistical  
models

Process-based models

Machine learning

# Questions?



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## Key characteristics of a theory

- Systematic and rational: Organizes ideas and principles in coherent structure to explain phenomenon/system
- Explanatory power: Provides explanations for observations.
- Predictive capability: Predicts observations.
- Testability: Scientific theories must be testable and falsifiable through empirical evidence.

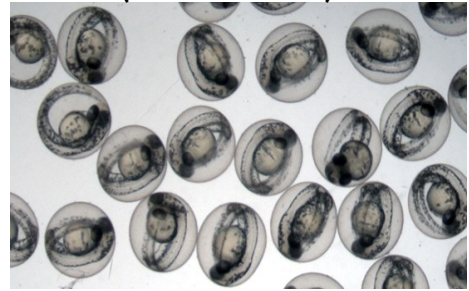
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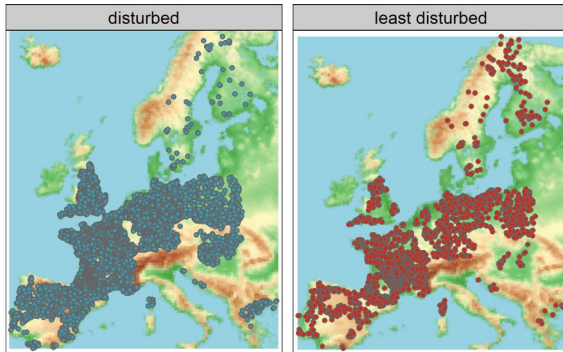


Laboratory flumes are used as models in ecotoxicology to assess the effects of pollutants on natural communities. Zebrafish embryos are used as an alternative to fish tests in ecotoxicology and toxicology.

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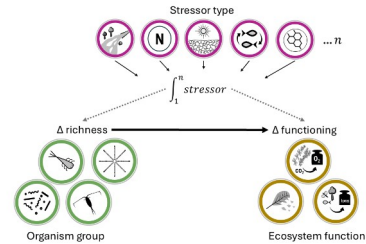
## Are these models and why?

Map of Europe with sampling sites



Jupke et al. 2024 *Environ. Sci. Europ.* 36

Conceptual figure



Equation

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Maps offer a simplified model of the world. Conceptual figures and equations provide abstract representations of relationships between entities, which may correspond to real-world phenomena or objects.

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# Types of models

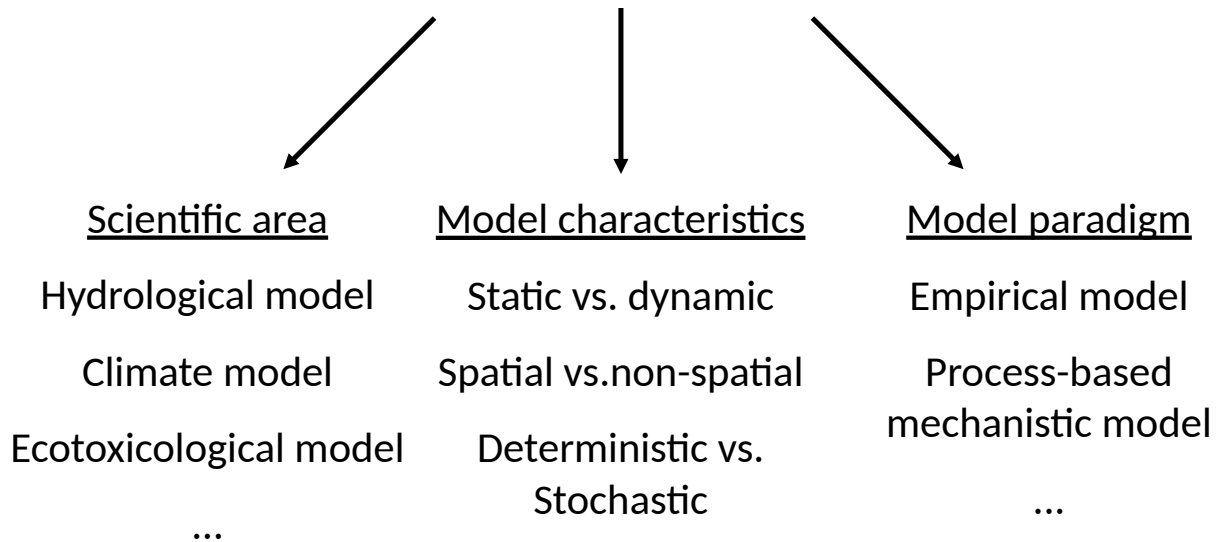
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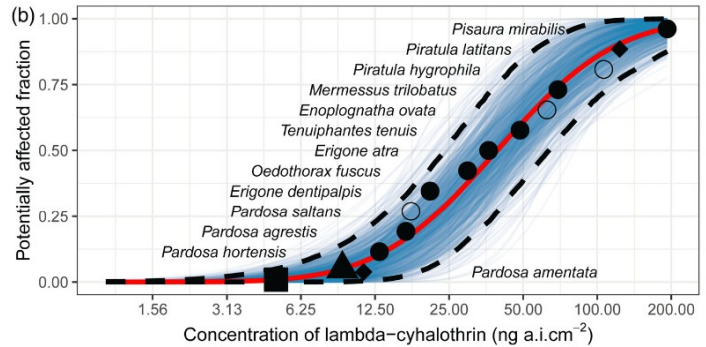


# Empirical model

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## Example: Species tolerance distribution

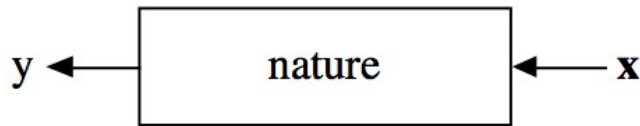
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Duque et al. 2024 *Pest Manag.Sci.* 80

# Two cultures of empirical modelling

Real world: Processes lead to association between  $X$  and  $y$



Examples for goals of statistical modelling: predict  $y$  from  $x$  or estimate relation between  $x$  and  $y$

Data modelling culture  
(classical statistics)

Algorithmic modelling culture  
(machine learning)

Breiman 2001 Sta

The very readable debate is available at:

[https://projecteuclid.org/download/pdf\\_1/euclid.ss/1009213726](https://projecteuclid.org/download/pdf_1/euclid.ss/1009213726)

For an update of the debate see: Efron, B. (2020). Prediction, estimation, and attribution. *Journal of the American Statistical Association*, 115(530), 636–655. <https://doi.org/10.1080/01621459.2020.1762613>

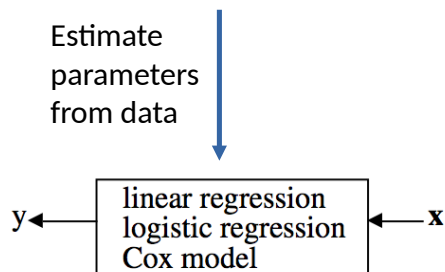
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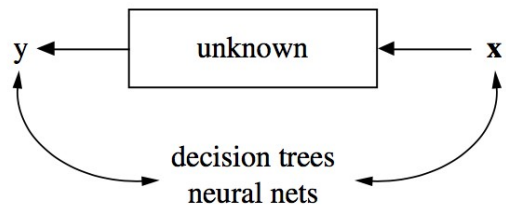
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## Common data model

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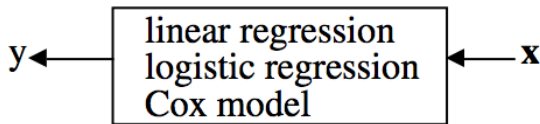


Find algorithm that operates on  $x$  to predict  $y$



# Two cultures of empirical modelling

## Data modelling culture (classical statistics)

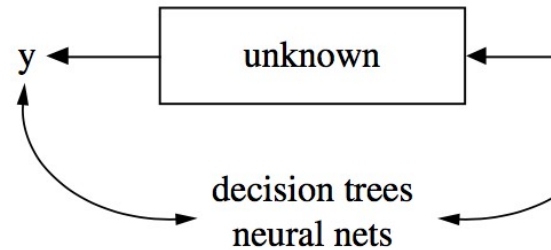


Methods appropriate for all research goals, but partly less powerful

### Bayesian vs. frequentist statistics

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- Distinctions blurred in modern application
- Inclusion of prior knowledge/beliefs in models only within Bayesian framework

## Algorithmic modelling culture (machine learning)



Primarily appropriate for prediction, exploration, and partly estimation

Breiman 2001 Sta

For how the distinctions between Bayesian and frequentist frameworks are blurred, see Efron & Hastie (2016).

Moreover, the distinction between the classical statistical and machine learning community is also becoming obsolete with the advent of many techniques that build on both statistics and machine learning. For details see Ryo & Rillig (2017).

Breiman L. (2001) Statistical modeling: The two cultures. *Statistical Science* 16, 199–215.

Efron B. & Hastie T. (2016) *Computer age statistical inference: algorithms, evidence, and data science*. Cambridge University Press, New York, NY.

Ryo M. & Rillig M.C. (2017) Statistically reinforced machine learning for nonlinear patterns and variable interactions. *Ecosphere* 8, e01976.

# Process-based mechanistic models

- Describe mechanisms not just empirical correlations
  - e.g. Biomass growth depends on distribution of energy between foraging, maintenance and movement etc.
- Focuses on system behaviour including flows and interactions
  - e.g. Biomass flow in food web, feedback loops: predator-prey cycles
- Typically dynamic (simulations over time)
- Require parameters, typically measured in real systems
- Capacity to predict under different conditions

The outcome of the simulations are typically not predictable through solving the underlying mathematical relationships analytically, though this is feasible in simple models.

# Ordinary differential equation (ODE) model

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- Mathematical equations (ODEs) define behaviour

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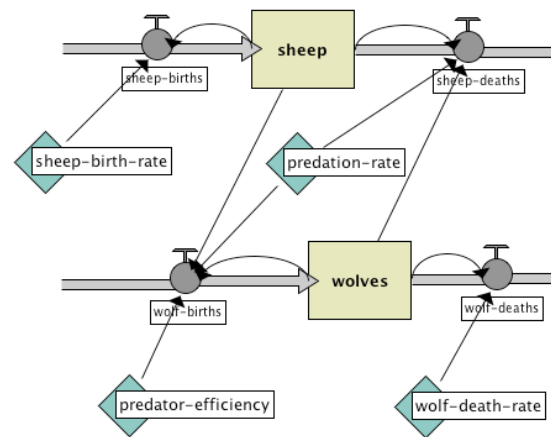
Osakpolor et al. 2024 *Theor*

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## Example: Wolf-Sheep predation model

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# Ordinary differential equation (ODE) model

## Example: Aquatic predator-prey model

- Population biomass over time
- Classical cycles:  
Prey increases  
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# Individual-based model (IBM)

- Individual is discrete, unique, and autonomous, follows rules
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<https://www.netlogoweb.org/launch#http://ccl.northwestern.edu/netlogo/models/models/Sample%20Model%20Biology/Wolf%20Sheep%20Predation.nlogo>

These models are also called Agent-based models (ABM).

Note that an individual or agent can also be a physical or chemical entity (e.g. rain drop, molecule).

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Classical statistical  
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Process-based models

Machine learning

# Questions?



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Picture taken from: <https://www.presentation-guru.com/techniques-for-handling-questions-during-a-presentation/>