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
- Revising the last lesson in preparation for the new one
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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?

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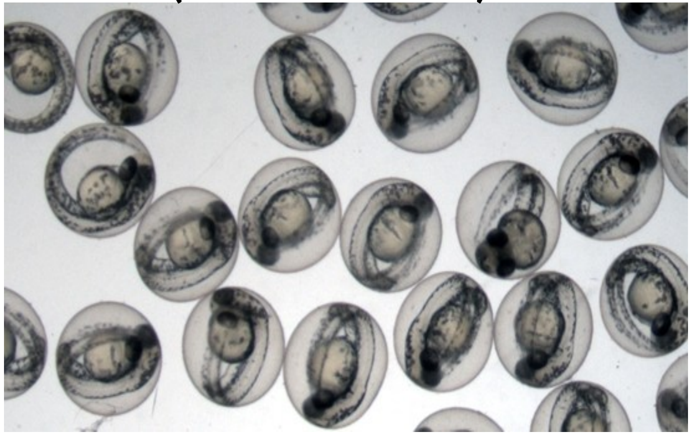
What is a model?

Are these models and why?

Artificial streams in laboratory

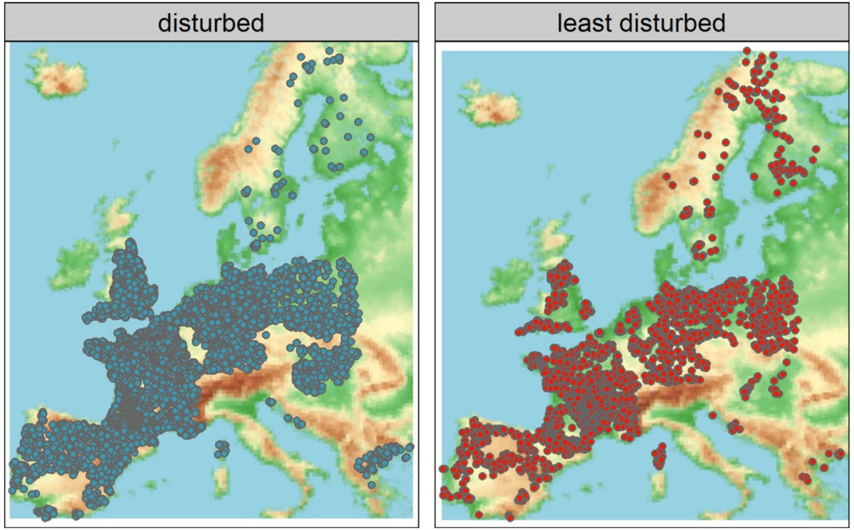
Embryos of zebrafish
(*Danio rerio*)



What is a model?

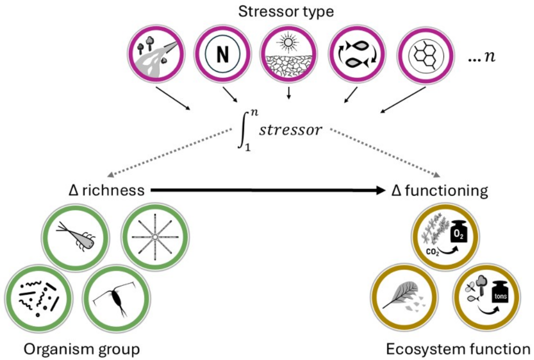
Are these models and why?

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**.“

Wainwrigt & Mulligan 2004: 8

„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
  - e.g. Zebrafish embryo bioassay, cell tests for genotoxicity
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  - e.g. Computer models

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Classification of computer models

<u>Scientific area</u>

Hydrological model

Climate model

Ecotoxicological model

…

<u>Model characteristics</u>

Static vs. dynamic

Spatial vs.non-spatial

Deterministic vs. Stochastic

…

<u>Model paradigm</u>

Empirical model

Process-based mechanistic model

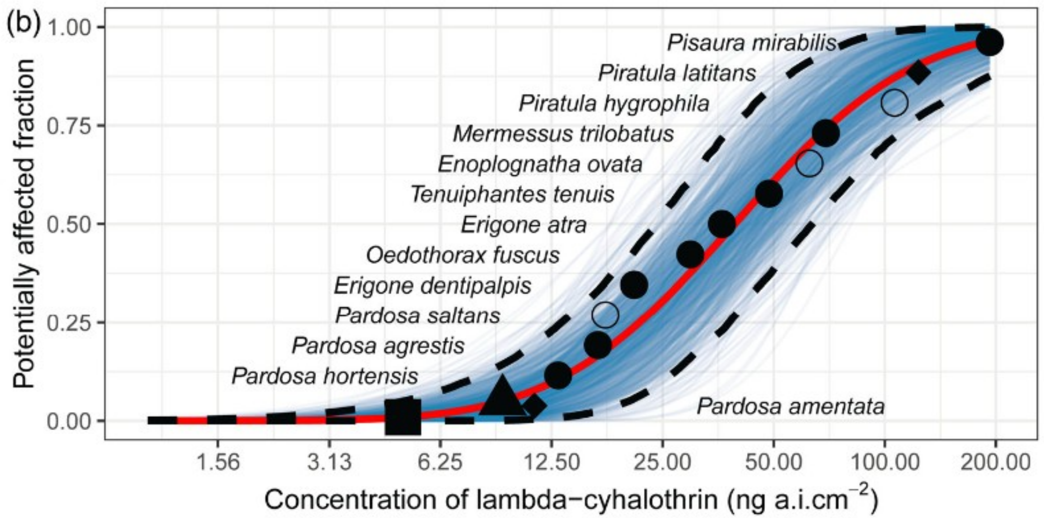
…

Empirical model

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

<u>Example: Species tolerance distribution</u>

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



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*, estimate relation between *x* and *y*

Data modelling culture
(classical statistics)

Algorithmic modelling culture
(machine learning)

Breiman 2001 *Stat. Sci.* 16

Two cultures of empirical modelling

Data modelling culture (classical statistics)

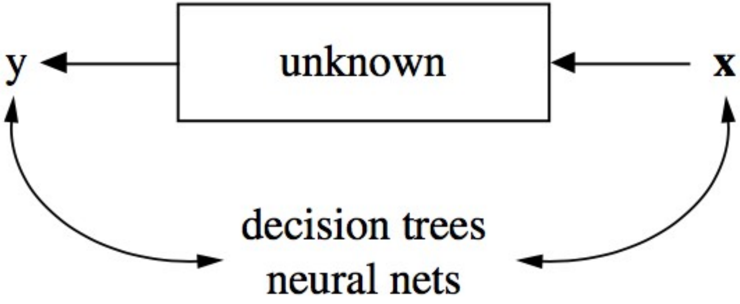
Common data model

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

Estimate parameters from data

Algorithmic modelling culture (machine learning)

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



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Two cultures of empirical modelling

Data modelling culture (classical statistics)

Methods appropriate for all research goals, but partly less powerful

<u>Bayesian vs. frequentist statistics</u>

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

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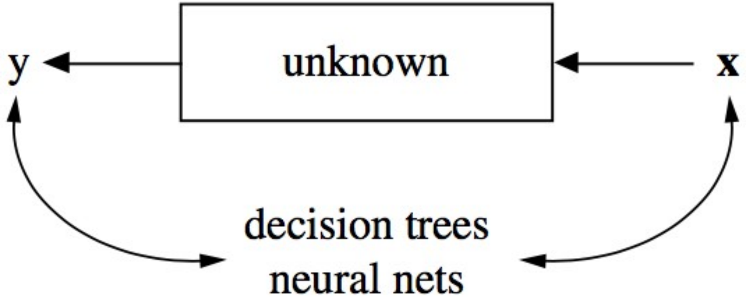

Primarily appropriate for prediction and exploration, and partly estimation

Breiman 2001 *Stat. Sci.* 16

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
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Ordinary differential equation (ODE) model

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Osakpolor et al. 2024 *Theor. Ecol.* 17

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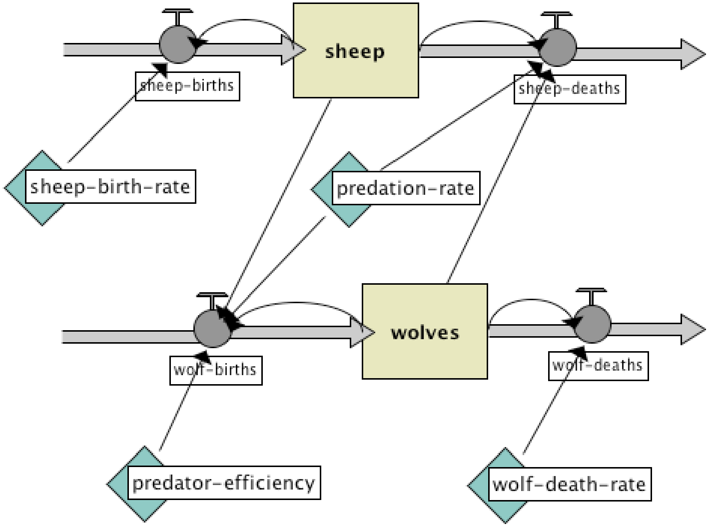

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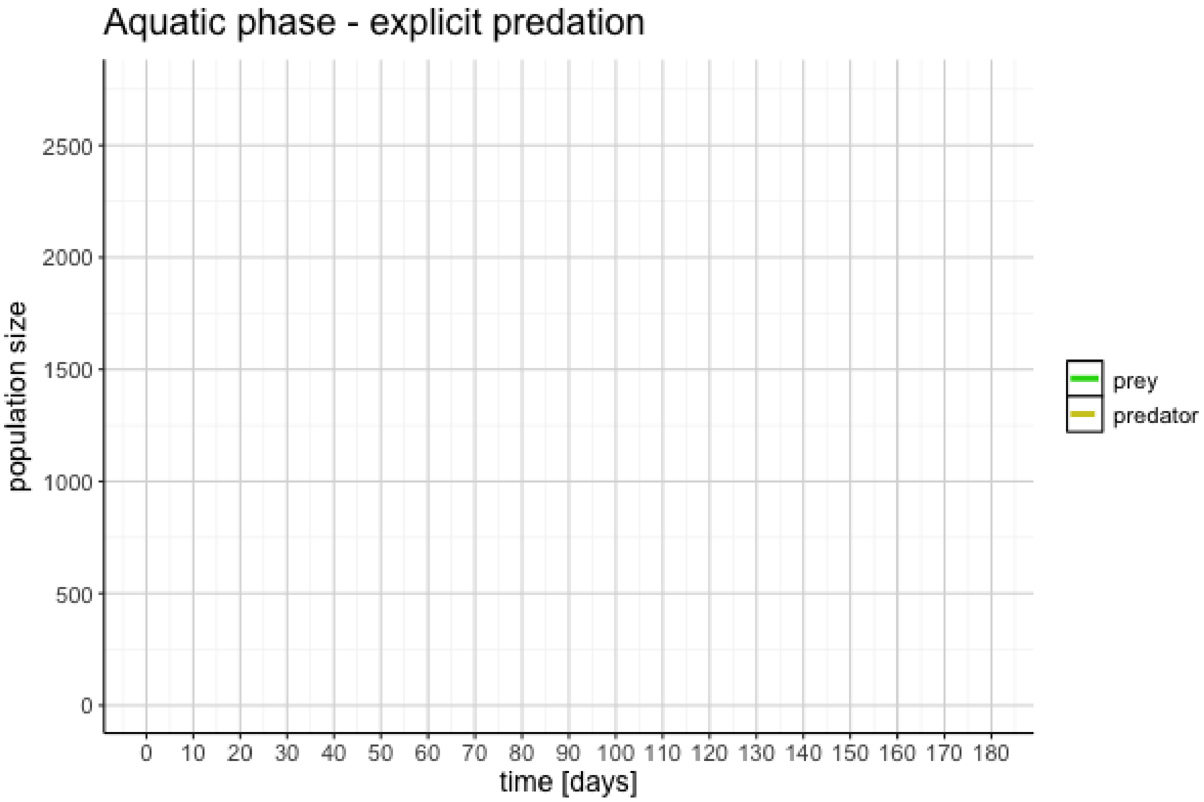

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Machine learning

Process-based models

Classical statistical models

Questions?

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What is a theory?

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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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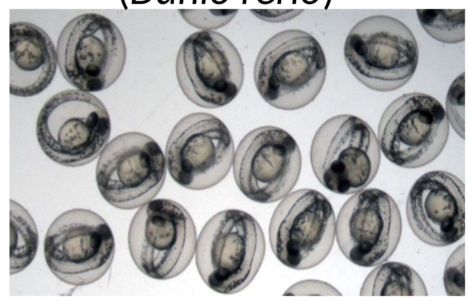

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Laboratory flumes are used as models in ecotoxicology to assess the effects of pollutants on natural communities. Zebrafish embryos are used as an alternative to fish tests in ecotoxicology and toxicology.

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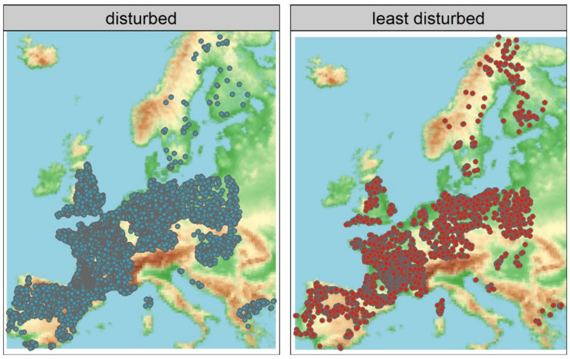

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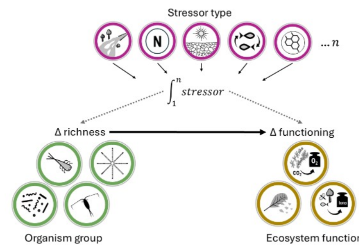
Conceptual figure



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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Classification of computer models

Scientific area	Model characteristics	Model paradigm
Hydrological model	Static vs. dynamic	Empirical model
Climate model	Spatial vs.non-spatial	Process-based mechanistic model
Ecotoxicological model	Deterministic vs. Stochastic	…
…	…	

Empirical model

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<u>Example: Species tolerance distribution</u>

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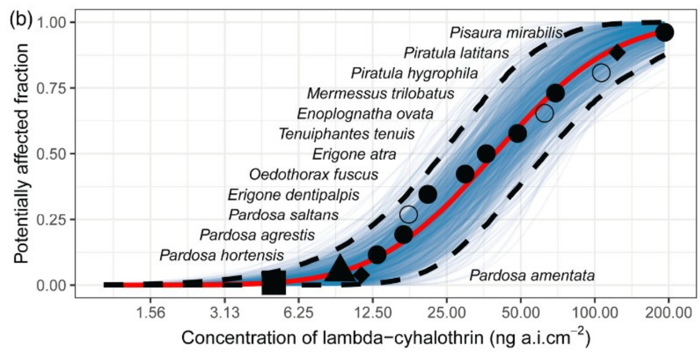

Duque et al. 2024 *Pest Manag.Sci.* 80

Two cultures of empirical modelling

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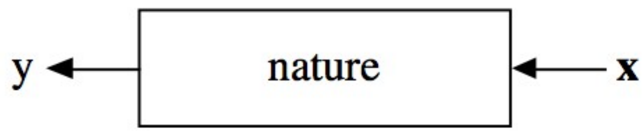

Examples for goals of statistical modelling: predict *y* from
estimate relation between *x* and *y*

Data modelling culture
(classical statistics)

Algorithmic modelling cultur
(machine learning)

Breiman 2001 *St*

The very readable debate is available at:
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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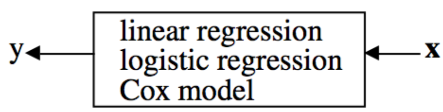
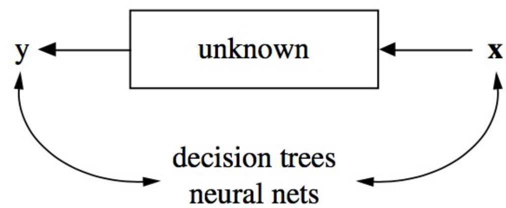


Algorithmic modelling culture (machine learning)

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



Breiman 2001 *Stat. Sci.* 16

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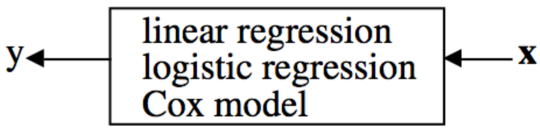

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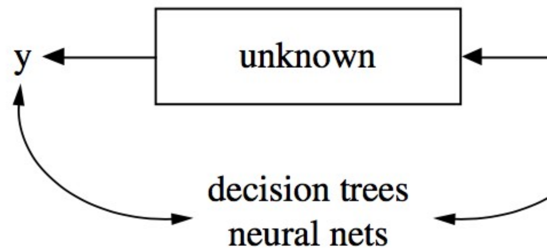

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Breiman 2001 *Sta*

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
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- Focuses on system behaviour including flows and interaction
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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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Osakpolor et al. 2024 *Theo*

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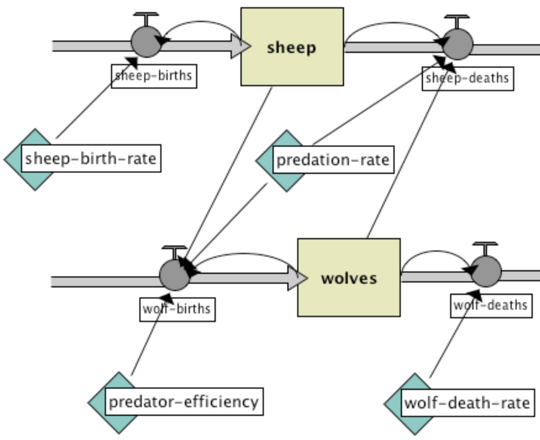

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<u>Example: Aquatic predator-prey model</u>

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https://www.netlogoweb.org/launch#http://ccl.northwestern.edu/netlogo/models/models/Sample%20Mode Biology/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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Machine learning

Process-based models

Classical statistical models

Questions?

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