Mathematical Modelling, Theory, and Model Fitting in Ecology & Evolution

A MulQuaBio Lecture

January 13, 2026

OUTLINE

- Modelling: what and why
- Types of Models
- How to build 'em
- How to test 'em (AKA Fitting Models to Data)
- Summary and readings

MODELS AND MODELLING

What does "modelling" mean to you?

Caricature of a phenomenon that captures its essence
(the model's output reproduces/emulates the phenomenon)

WHY USE (MATHEMATICAL) MODELS?

- To understand/explain an observed phenomenon
- To develop accurate predictions of an observed phenomenon in the future
- To find out what is important to know in an otherwise complex system (cannot measure and monitor everything!)

HOW TO BUILD 'EM?

Essentially, all models are wrong, but some are useful
— George Box (1987) (British mathematician)

- "*All models are wrong*" — every model is a simplification of reality (e.g., the frictionless pendulum!)
- "*But some are useful*" — the appropriately simplistic ones can (*sufficiently*) explain and predict phenomena

MODELS AND MODELLING

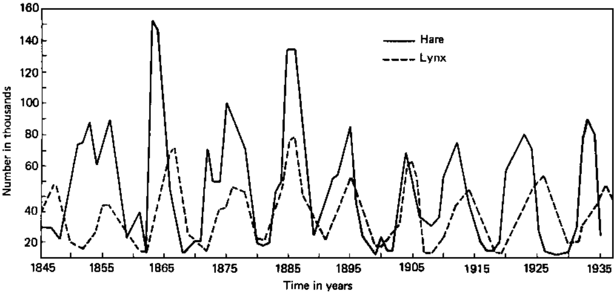
What is more important to you when it come's to a Model's capabilities - Accuracy or Precision?

Accuracy is a more fundamental property

Two Types of Models

- *Mechanistic models* aim to explain the **processes** or **mechanisms** underlying **patterns** or **phenomena** in empirical data
  - These models have a **theoretical basis**
- *Inferential/Empirical (AKA Phenomenological) models* establish the existence of **statistically significant, non-random patterns** or **phenomena** in empirical data
  - They make no assumptions about the processes or mechanisms that generate the patterns
  - That is, these models lack a **theoretical basis**

MECHANISTIC VS. INFERENTIAL MODEL FITTING



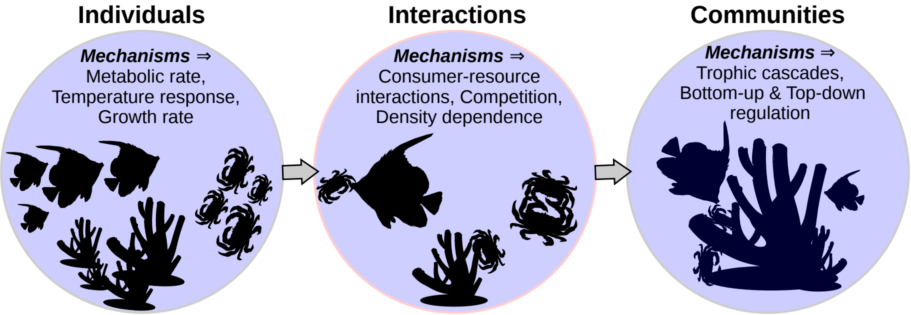
source: `https://www.cds.caltech.edu/~murray/amwiki/images/8/8f/LHgraph.gif`

- **Mechanistic model**: *The Lynx–Hare cycle is driven by density-dependent population growth in hares*
- **Inferential model**: *The Lynx and Hare cycles have a significant asynchrony (period shift) of x years*

Mechanistic vs. Inferential model fitting

- *It's not really one vs. the other*; both types of models play a role in science (and biology)
- Inferential model fitting reveals patterns in data that generate **hypotheses**
  - These can be tested using further model fitting
  - Example: *Whether* climatic temperature affects the Lynx-Hare cycle (using Generalized Linear Model-fitting)
- Mechanistic model fitting *tries* to validate a model that can *mechanistically explain* the observed pattern and generate **more accurate, mechanistic hypotheses**
  - Example: *How* climatic temperature *drives* the Lynx-Hare cycle
- *Ultimately, successful,* ***empirically grounded*** *mechanistic models are the best path towards a theory in any scientific discipline (including ecology and evolution)*

MECHANISTIC VS. INFERENTIAL MODEL FITTING



MECHANISTIC MODELS IN ECOLOGY AND EVOLUTION?

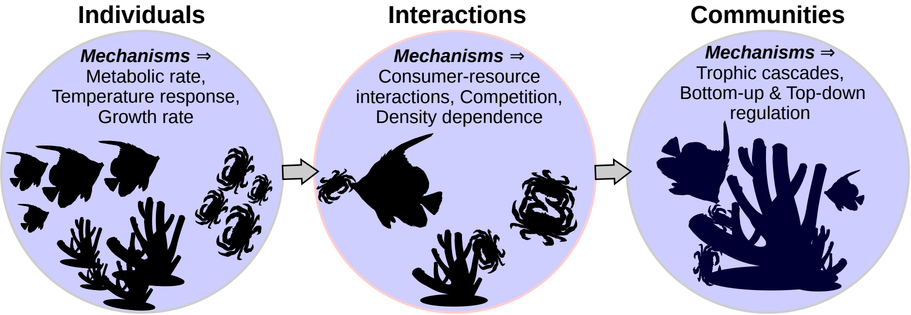
- *Do most ecological studies perform **inferential** or **mechanistic** modelling (or model fitting)?*
- The answer is mostly inferential — *why?*
  - Partly because we are still establishing the existence of **general** patterns/phenomena,
  - ... and partly because we are (or are forced to be) interested in **forecasting** rather than **explaining**.
- *So the big question is, can we forecast without explaining?*
  - For example, disease outbreaks: do we really need to care about the underlying mechanisms if we can predict a future event using inferential modelling (e.g., machine learning of time-series patterns)?

What are Mechanisms?

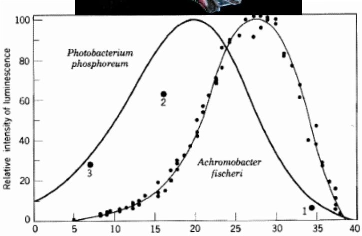
- Somewhat subjective!
- For example, the Logistic growth model can be thought of as mechanistic:
$$\frac{dN}{dt} = rN\left(1 - \frac{N}{K}\right)$$
- What is the mechanism? — Density dependence through scramble competition (Brannstrom & Sumpter 2005)
- If the logistic growth model and another model with contest competition were compared with data — some would call it mechanistic modelling because one is trying to get at the underlying mechanism — scramble vs. contest competition
- But is this really mechanistic? What are r and K, really?

Example of a fundamental mechanism: metabolic rate

- Proponents of *Metabolic Theory of Ecology* (MTE) argue that we have not progressed far enough towards mechanistic modelling because metabolism has been ignored



- The mechanistic basis of thermal performance curves (`https://youtu.be/6n8fCuDwn74`)



Johnson et al 1974

$$B = B_0 \boxed{e^{-\frac{E}{kT}}} f(T, T_{pk}, E_D)$$

T = temperature (K)
k = Boltzmann constant (eV K^{-1})
E = Activation energy (eV)
T_{pk} = Temperature of peak performance
E_D = Deactivation energy (eV)
(J H van't Hoff 1884, S Arrhenius 1889)

- Surely there is more to thermal responses?
- *What about alternative models?*

Modelling, and fitting models to data: What's the big idea?

- *If possible*, use biological knowledge to construct models
- See if the models "agree well" with data
- Whichever model "agrees best" is most likely to have the right mechanisms
- That's the one that's best for predictions (e.g., population cycles), estimating rates (e.g., population or individual growth rates), etc.
- Don't use models you already know have the wrong mechanisms just because they are popular!
- Inferential/statistical models often perform better than mechanistic ones. *Why? — because they have less restrictive assumptions*

Building Models

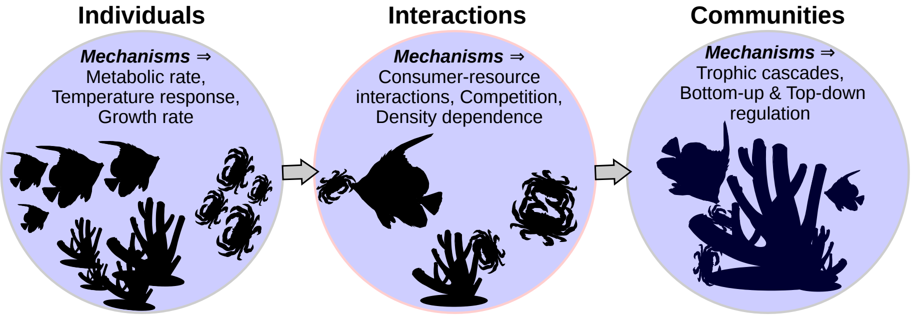
- It's an art, takes practice (Levins' paper on the strategy of model building in biology)
- Build models one mechanism at a time — in biology, it means start at the right level of organization!
- Always consider an alternative that is more parsimonious, even if it is an Inferential model!
- For example, the Boltzmann–Arrhenius model is a good first try to describe and uncover mechanisms underlying individual-level "traits" that are rates (e.g., fecundity or development rate)
- The next step would be to include species interactions with temperature-dependent individuals (or go in an evolutionary direction)

Models and Modelling?

Which modelling approach (mechanistic vs. inferential) is more likely to yield accurate predictions under global change?

Mechanisms are the key to accurate prediction!

Building EnE Models



- *You will learn about (deriving and analysing) key models (and theories) at different levels of organization in this part of the course (starting with metabolism)*

Fitting Models (to data)

- Least Squares methods
  - Linear
  - Non-linear
- Likelihood-based methods
  - Maximum Likelihood
  - Bayesian
- Machine learning and artificial intelligence

Fitting Models (to data)

- Linear and non-linear least squares model fitting: (mathematically/algorithmically simple) approaches, useful in many scenarios in biology
  - Many mechanisms in biology are inherently non-linear (i.e., data are often better explained by a non-linear mathematical model)
- Bayesian (and MLE) methods: versatile and powerful when data are limited and your (e.g., mechanistic) models are complex (many parameters). Bayesian methods can outperform MLE when you have strong prior information.
- AI/machine learning: most versatile and powerful for large amounts of noisy data, but the focus on maximizing the ability to discover patterns and predict comes at the cost of mechanistic insights

Summary: Model comparison and selection are key

- Ideally, several competing (meaningful, not just null) hypotheses (mathematical models) should be fitted to data and compared using statistical theory
- This is an advance over the traditional “null hypothesis” approach in biology
- Necessary for the advancement of biology from an observational and axiomatic discipline to one with general theories
- Necessary for understanding the mechanisms underlying biological patterns/phenomena

READINGS

- Levins, R. (1966) The strategy of model building in population biology. Am. Sci. 54, 421–431.
- Kingsland, Sharon E. (1995) Modeling Nature. University of Chicago Press. (read over the term — and beyond!)
- Otto, S.P. and Day, T. (2011) A biologist's guide to mathematical modeling in ecology and evolution. Princeton University Press. (read Chapters 1–2)
- Additional readings on the MQB Git repository (`Modelling` directory)