Fitting Models to Data in Ecology and Evolution

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MECHANISTIC VS. PHENOMENOLOGICAL MODELS

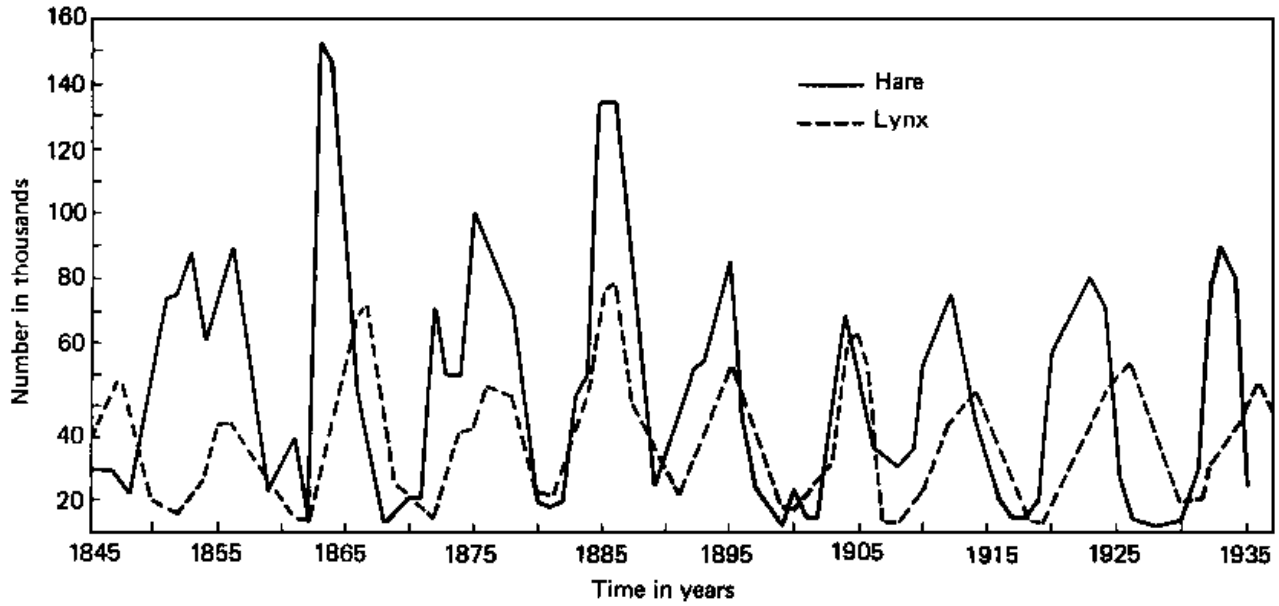
What does "modelling data" mean to you?

MECHANISTIC VS. PHENOMENOLOGICAL MODELS

- *Mechanistic models* aim to explain the PROCESSES or MECHANISMS underlying PATTERNS or PHENOMENA in empirical data
  - These models have a THEORETICAL BASIS

- *Empirical/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. PHENOMENOLOGICAL MODEL FITTING



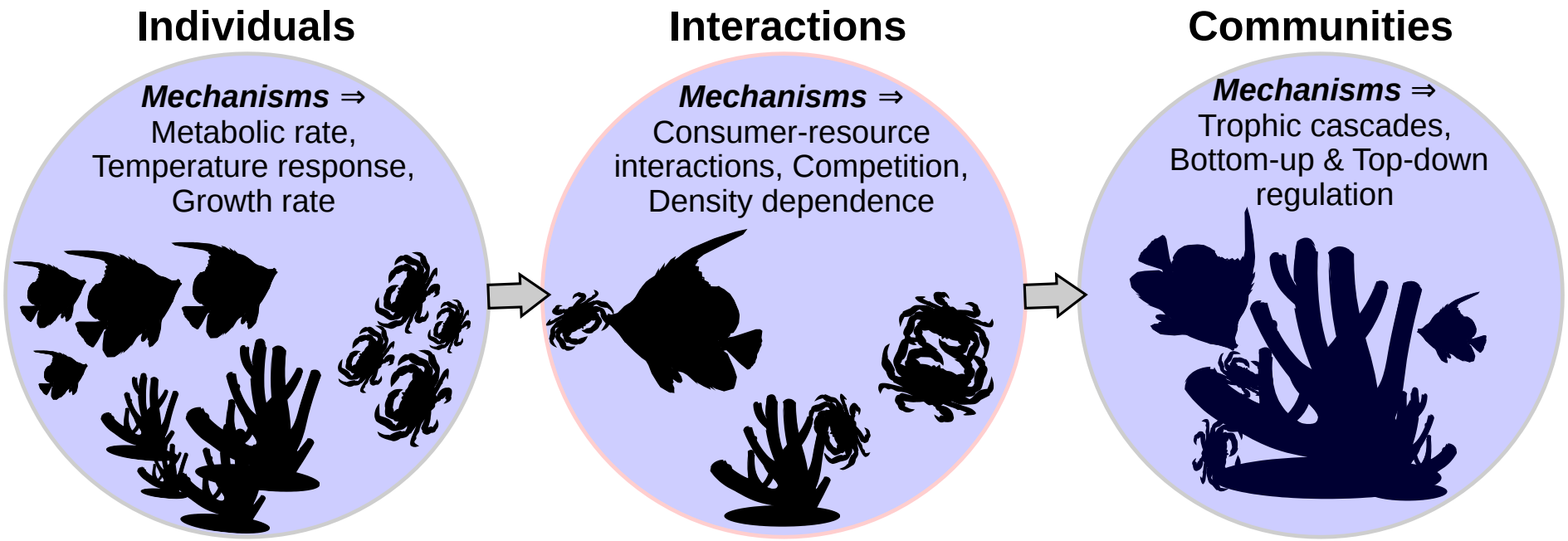
source: `https://www.cds.caltech.edu/~murray/amwiki/images/8/8f/LHgraph.gif`

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

MECHANISTIC VS. PHENOMENOLOGICAL MODEL FITTING

- *It's not really one vs. the other*; Both types of models play a role in science (and Biology)
- Phenomenological 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 mechanistic model that can explain the observed phenomenological 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. Phenomenological model fitting



MECHANISTIC MODELS IN ECOLOGY AND EVOLUTION?

- *Do most ecological studies perform phenomenological or mechanistic modelling (or model-fitting)?*
- The answer is mostly Phenomenological — *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 phenomenological modelling (e.g., Machine-learning of time series patterns)?

What are Mechanisms?

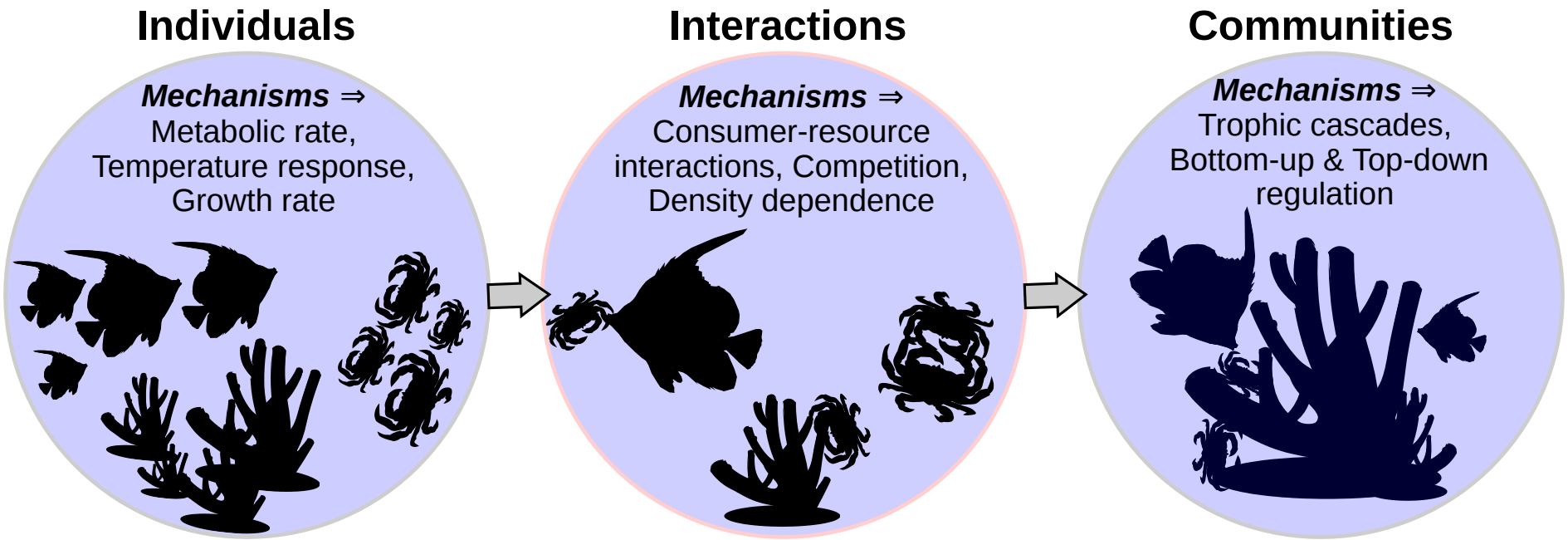
- Somewhat subjective!
- For example, the Ricker model can be thought of as mechanistic:

$$N_{t+1} = N_t e^{r\left(1-\frac{N_t}{k}\right)}$$

- What is the mechanism? — Density dependence through scramble competition (Brannstrom & Sumpter 2005)
- If the Ricker 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 or contest competition
- But is this REALLY mechanistic? What are r and k really?

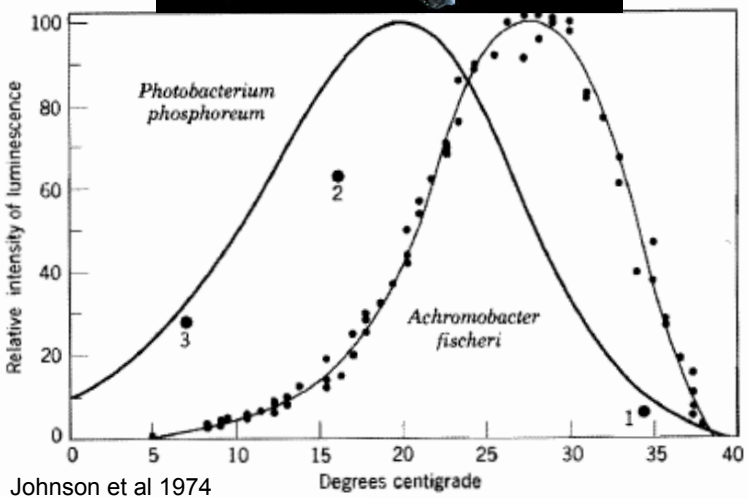
Example of a fundamental mechanism: metabolic rate

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



Example of a fundamental mechanism: metabolic rate

- 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!
- Phenomenological/statistical models often perform better than mechanistic ones. *Why? — because they have lest 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 phenomenological!
- For example, the Boltzmann-Arrhenius model is a good first try 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 dependence of individuals (or go in an evolutionary direction)

Fitting Models (to data)

- Least Squares methods
  - Linear
  - Non-linear
- Likelihood-based methods
  - Maximum Likelihood Estimation (MLE)
  - Bayesian
- Machine learning and Artifical intelligence

FITTING MODELS (TO DATA)

- Linear and non-linear least squares model fitting: (and mathematically/algorithmically simple) approaches, useful in many scenarios in biology
  - *Non-linear* Least Squares (NLLS) fitting is often necessary because many mechanisms in biology are inherently non-linear (i.e., r data are better-explained by a non-linear mathematical model)
- MLE/Bayesian methods: Versatile and powerful more robust if you are able to calculate the likelihood function analytically or numerically
- AI/machine Learning: most versatile and powerful for large amounts of noisy data, but the focus on maximizing ability to discover pattern and predict comes at the cost of mechanistic insights

SUMMARY: MODEL SELECTION IS THE 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 from an observational and axiomatic discipline to one with general theories
- Necessary for understanding the mechanisms underlying biological patterns/phenomena

COMPARING AND SELECTING MODELS

- It's all about the "Likelihood" of a model:
  the set of parameter values of the model (θ) given outcomes (x), equals the probability of those observed outcomes given those parameter values, that is,

$$\mathcal{L}(\theta|x) = P(x|\theta)$$

- The easiest thing to do for you is to use information theory (including AIC and BIC) to compare models.

- Both AIC and BIC use the *estimated (log-) likelihood of a model*:
  - AIC: $-2\ln[\mathcal{L}(\theta|x)] + 2p$
  - BIC (Schwartz criterion): $-2ln[\mathcal{L}(\theta|x)] + p\ln(n)$
    ($n =$ sample size, p = number of free parameters)

- The lower the AIC or BIC, the better

AIC AND BIC

- In models fitted with least squares and normally-distributed errors, $\ln[\mathcal{L}(\theta|x)] = -\frac{n}{2}\ln\left(\frac{RSS}{n}\right)$
- Thus

$$\begin{aligned} \text{AIC} &= -2\ln[\mathcal{L}(\theta|x)] + 2p \\ &= n + 2 + n\ln\left(\frac{2\pi}{n}\right) + n\ln(\text{RSS}) + 2p \end{aligned}$$

- And

$$\begin{aligned} \text{BIC} &= -2ln[\mathcal{L}(\theta|x)] + p\ln(n) \\ &= n + 2 + n\ln\left(\frac{2\pi}{n}\right) + n\ln(\text{RSS}) + p\ln(n) \end{aligned}$$

- *The small-sample AIC can also be calculated similarly (see Johnson & Omland 2004)*

COMPARING AND SELECTING MODELS

This is how you calculate AIC and BIC (using python syntax):

- residuals = Observations - Predictions
- rss = sum(residuals ** 2)
- Then, AIC = n + 2 + n * log((2 * pi) / n) + n * log(rss) + 2 * p
  (*note n and p!*)
- And BIC = n + 2 + n * log((2 * pi) / n) + n * log(rss) + (log(n)) * (p + 1)
- For both AIC and BIC, If model **A** has AIC lower by 2-3 or more than model **B**, it's better — Differences of less than 2-3 don't really matter

Also note that:

- R^2 = 1 - (rss/tss), where tss is total sum of squares:
  tss = sum((Observations - mean(Predictions)) ** 2)
  (a useful measure of goodness of fit)

COMPARING AND SELECTING MODELS: MORE STUFF

- You can also calculate Akaike Weights, which is very useful/important when comparing > 2 models. These weights can then be used to perform *model averaging*
- Model selection using the Likelihood-Ratio test (LRT) is another option when you are comparing 2 models
- Adjusted R^2 can be used to get a rigorous "idea" about how alternative models are performing
- Very often, you can do step-wise model simplification, especially in *for linear least squares model fitting*: Start with a complex model and drop terms till you have found a the most *parsimonious* simpler version of the original model
  - There are ready-made functions in `R` to do this (of course!)

Readings

- Levins, R. (1966) The strategy of model building in population biology. Am. Sci. 54, 421–431.
- Johnson, J. B. & Omland, K. S. (2004) Model selection in ecology and evolution. Trends Ecol. Evol. 19, 101–108.
- Bolker, B. M. et al. (2013) Strategies for fitting nonlinear ecological models in R, AD Model Builder, and BUGS. Methods Ecol. Evol. 4, 501–512 .
- Additional readings on the TheMulQuaBio git repository