Fitting Models to Data in Ecology and Evolution

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MECHANISTIC VS. PHENOMENOLOGICAL MODELS

What does "modelling data" mean to you?

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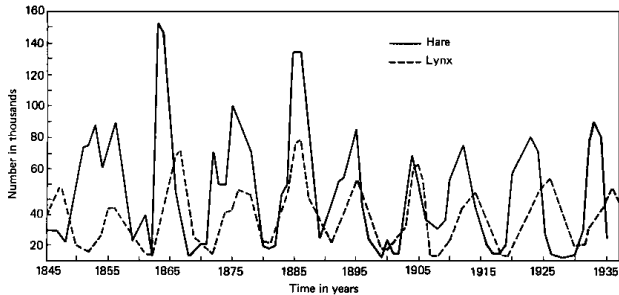
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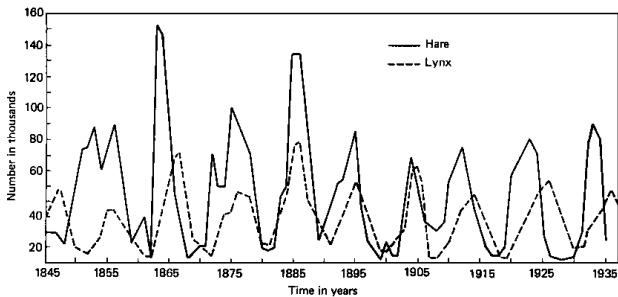
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source: https://www.cds.caltech.edu/~murray/amwiki/images/8/8f/LHgraph.gif

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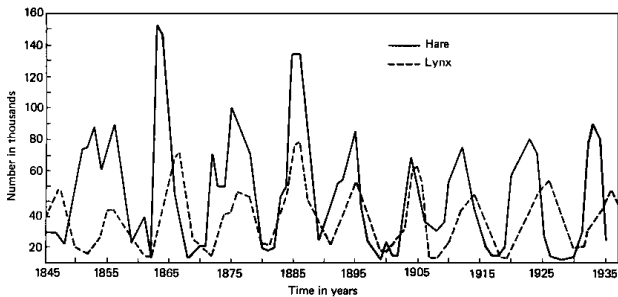
- **Mechanistic model**: *The Lynx-Hare Cycle is driven by density-dependent population growth in hares*
- **Phenomenological model**: *The Lynx and Hare Cycles have a significant asynchrony (period shift) of x years*

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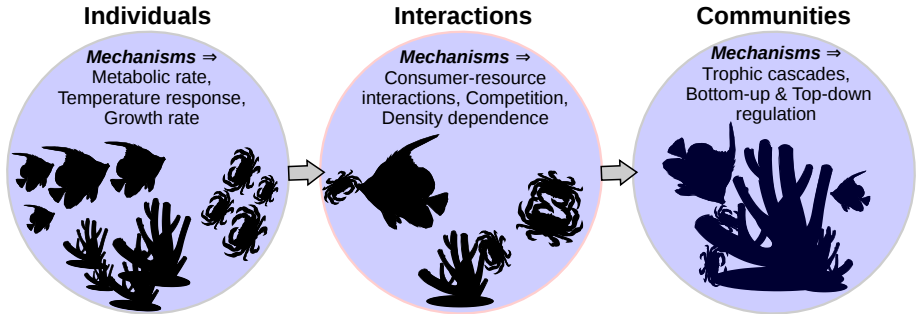 - Example: *How* climatic temperature *drives* the Lynx-Hare cycle

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- *Ultimately, successful, EMPIRICALLY-GROUNDED mechanistic models are the best path towards a THEORY in any scientific discipline (including ecology and evolution)*

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Individuals

Mechanisms ⇒ Metabolic rate, Temperature response, Growth rate

Interactions

Mechanisms ⇒ Consumer-resource interactions, Competition, Density dependence

Communities

Mechanisms ⇒ Trophic cascades, Bottom-up & Top-down regulation

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  - 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)?

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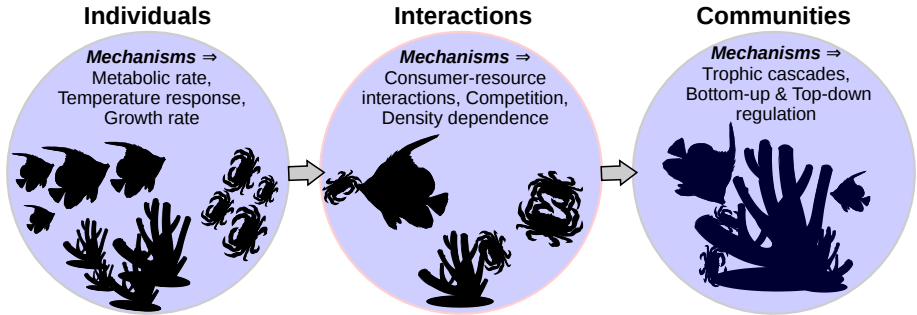
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- But is this REALLY mechanistic? What are *r* and *k* really?

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


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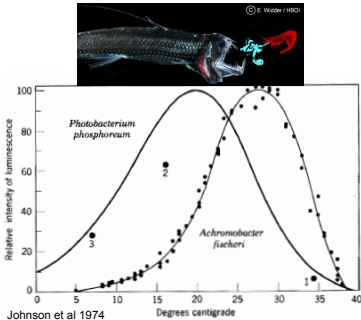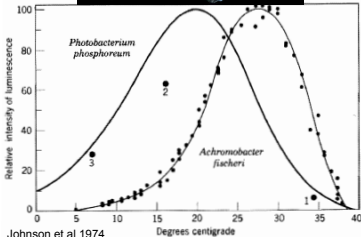
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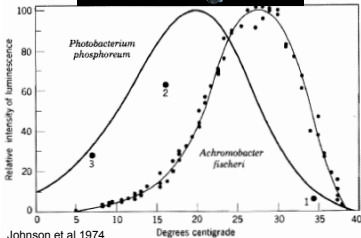E = Activation energy (eV)
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- Surely there is more to thermal responses?
- *What about alternative models?*

- *If possible*, use biological knowledge to construct models

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MODELS: HOW TO BUILD THEM?

- 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

Multiple ways to do it:

- Least Squares methods
    - Linear
    - Non-linear

- Likelihood-based methods
    - Maximum Likelihood Estimation (MLE)
    - Bayesian

- Artificial intelligence and Machine learning
    - Focus in on maximizing ability to discover pattern and predict at the cost of mechanistic insights

METHODS YOU CAN USE

- Least squares: along with Linear Model fitting, Non-linear Least Squares (NLLS) fitting is a particularly versatile and powerful approach because many mechanisms in biology and inherently non-linear

- MLE/Bayesian methods: more robust if you are able to calculate the likelihood function analytically or numerically.

- AI/machine Learning: most versatile for large amounts of noisy data

- Ideally, several competing (meaningful, not just null) hypotheses (mathematical models) should be fitted to data and compared using statistical theory

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- Necessary for developing 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)*

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- 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)

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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 will end up doing model simplification, especially in *for linear least squares model fitting* — starting with a complex model and then dropping terms till you have found a the most parsimonious version of the original model. There are 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