

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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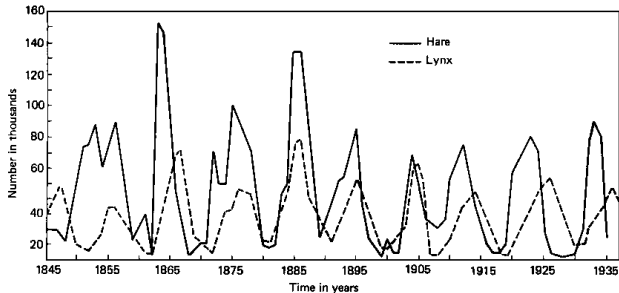
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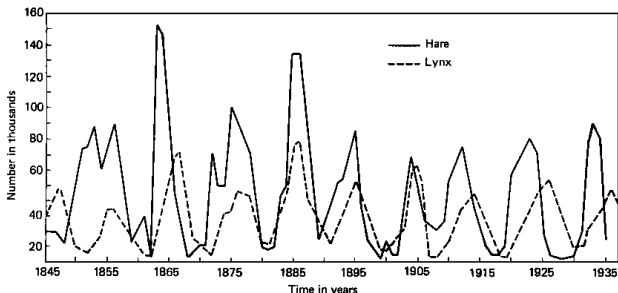
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 - That is, these models lack a THEORETICAL BASIS

MECHANISTIC VS. PHENOMENOLOGICAL MODEL FITTING



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

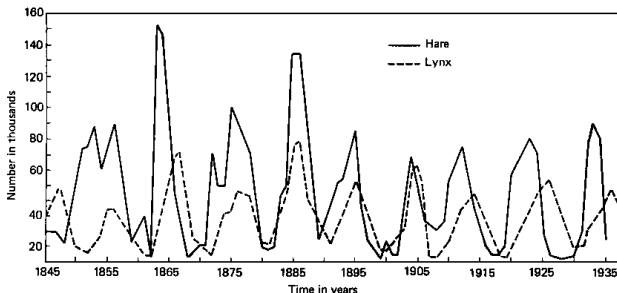
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- **Mechanistic model:** *The Lynx-Hare Cycle is driven by density-dependent population growth in hares*
- **Phenomenological model:** *The Lynx and Hare Cycles have a significant asynchrony (period shift) of x years*

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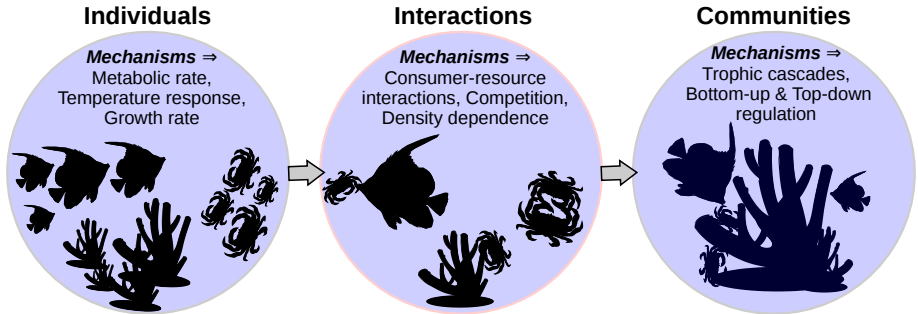
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- *Ultimately, successful, EMPIRICALLY-GROUNDED mechanistic models are the best path towards a THEORY in any scientific discipline (including ecology and evolution)*

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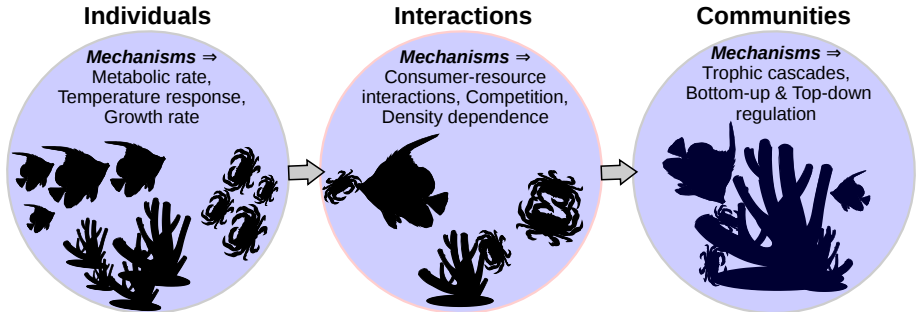
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- But is this REALLY mechanistic? What are r and k really?

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

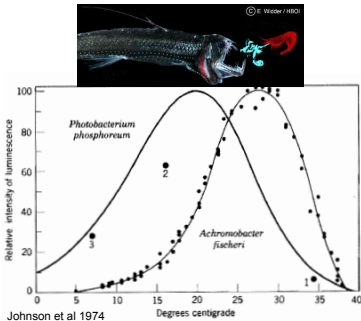


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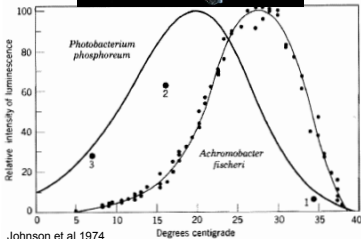
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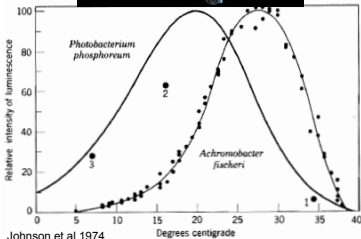
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- Surely there is more to thermal responses?
- What about alternative models?

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- Phenomenological/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 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 Artificial 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

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- 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

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): $-2 \ln[\mathcal{L}(\theta|x)] + p \ln(n)$
(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

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

- And

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- *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:

- $R^2 = 1 - (\text{rss}/\text{tss})$, where tss is total sum of squares:
 $\text{tss} = \text{sum}((\text{Observations} - \text{mean}(\text{Predictions})) ** 2)$
(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