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

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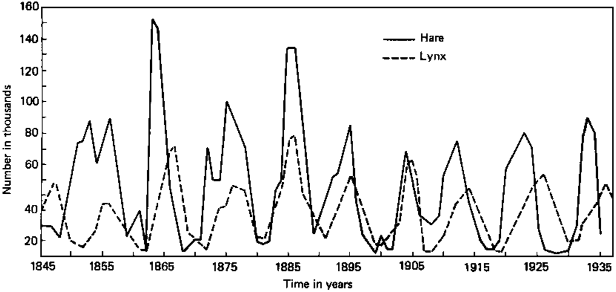
Mechanistic vs. Phenomenological model fitting



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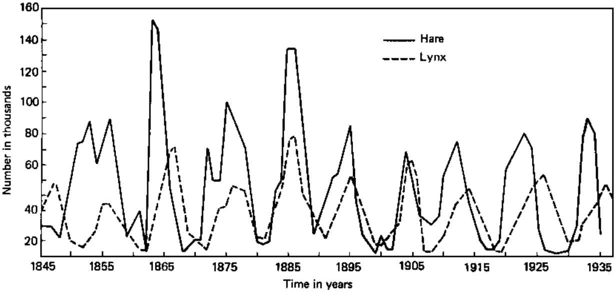

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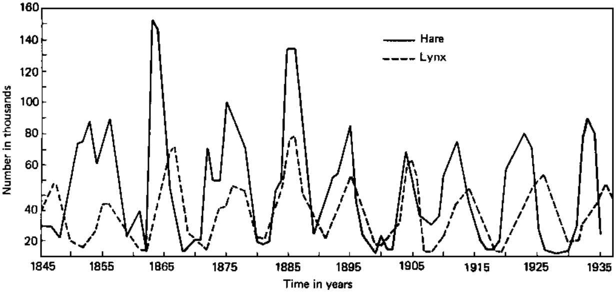

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- **Phenomenological model**: The Lynx and Hare Cycles have a significant asynchrony (period shift) of xx years

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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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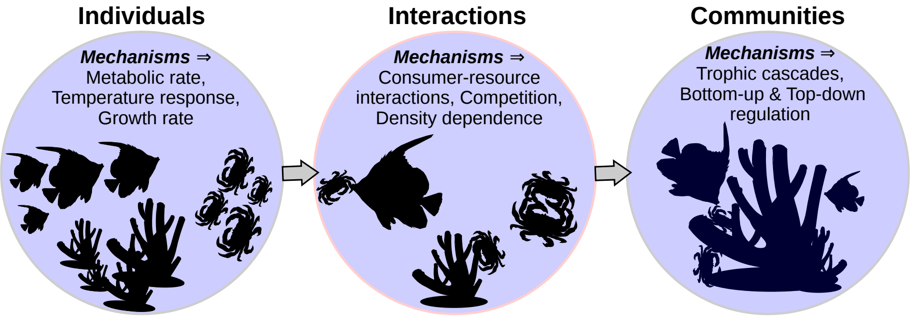

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  - For example, disease outbreaks: Do we really need to care about the underlying mechanisms if we can predict a future event using phenomenological modelling (e.g., Machine-learning of time series patterns)?

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

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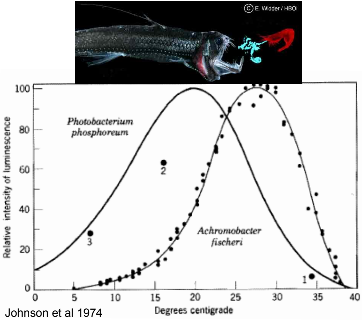

Johnson et al 1974

Example of a fundamental mechanism: metabolic rate

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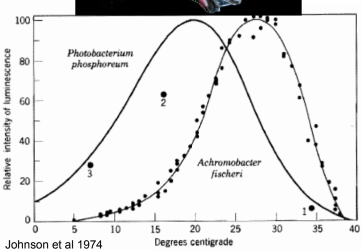

$$B = B_0 \boxed{e^{-\frac{E}{kT}}} f(T, T_{pk}, E_D)$$

T = temperature (K)
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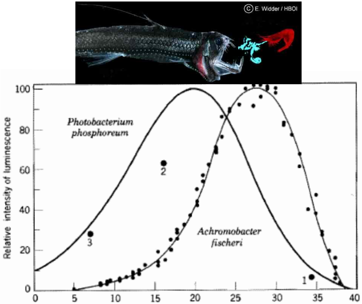

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- Surely there is more to thermal responses?
- *What about alternative models?*

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- Phenomenological/statistical models often perform better than mechanistic ones. *Why? — because they have lest restrictive assumptions*

Models: How to build them?

- It's an art, takes practice
- 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 (the thermal performance curves example: Sharpe-Schoolfield, Briere, or Polynomial?)!
- For example, the Boltzmann-Arrhenius model is a good first try describe and uncover mechanisms underlying individual level rates (e.g., vector 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 in the Miniproject

- 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 — you will learn this in Term 2, so not recommended

- AI/machine Learning: most versatile for large amounts of noisy data — you will be introduced to these at the end of term 2, so definitely not recommended

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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 likelihoods of a model*:
  AIC: $-2\ln[\mathcal{L}(\theta|x)] + 2p$
  Small sample AIC (AICc): $-2\ln[\mathcal{L}(\theta|x)] + 2p$
  BIC (Schwartz criterion): $-2ln[\mathcal{L}(\theta|x)] + p\ln(n)$
  (where $n =$ sample size, p number of free parameters)
- The lower the AIC or BIC, the better.

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- rss = sum(residuals ** 2)
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- And BIC is n + n * log(2 * pi) + n * log(rss / n) + (log(n)) * (p + 1)
- That is, $\mathcal{L}(\theta|x) = -\frac{n}{2/ln(RSS/n)}$
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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 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 .
- Some illustrative examples of (non-linear) model fitting to ecological/evolutionary data `https://groups.nceas.ucsb.edu/non-linear-modeling/projects`
- Additional readings in the git repository