

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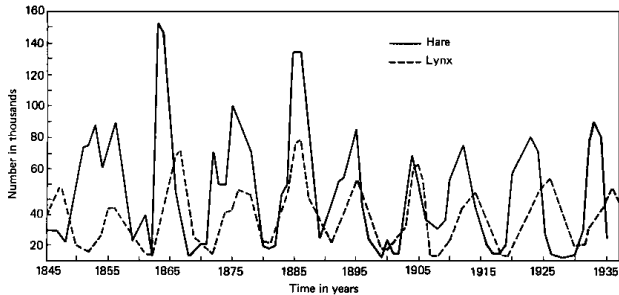
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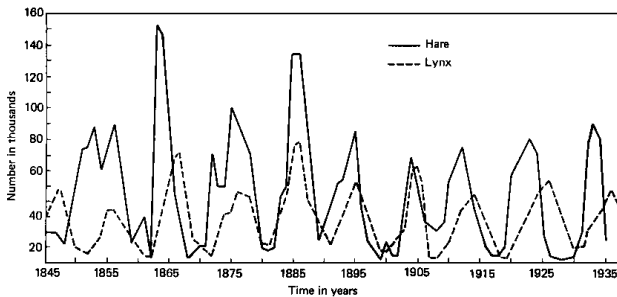
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source: <https://www.cds.caltech.edu/~murray/amwiki/images/8/8f/LHgraph.gif>



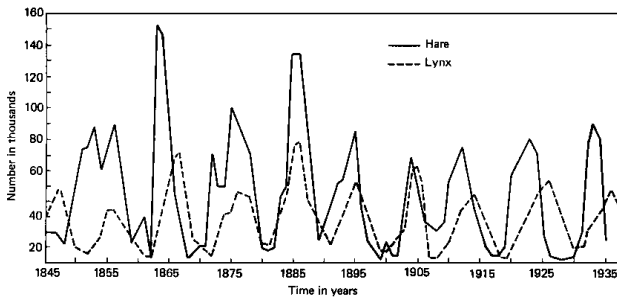
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- **Phenomenological model:** *The Lynx and Hare Cycles have a significant asynchrony (period shift) of  $x$  years*

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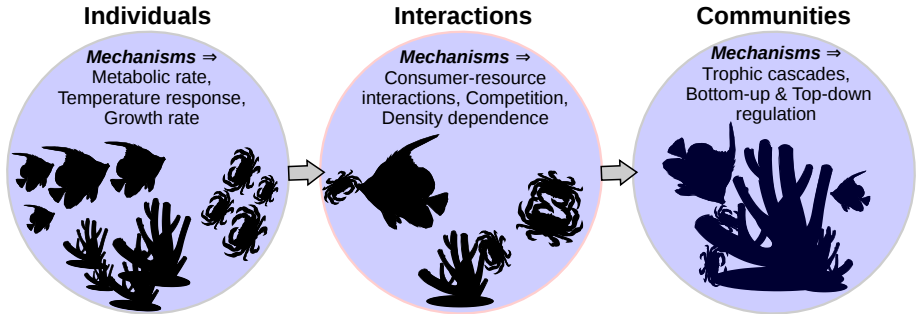
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- *Ultimately, successful, EMPIRICALLY-GROUNDED mechanistic models are the best path towards a THEORY in any scientific discipline (including ecology and evolution)*

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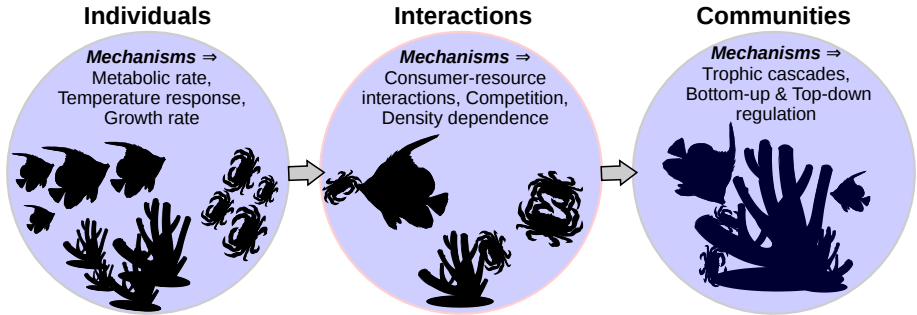
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- But is this REALLY mechanistic? What are  $r$  and  $k$  really?



# 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

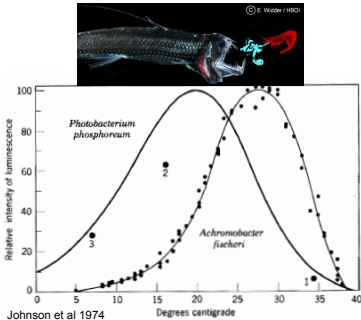


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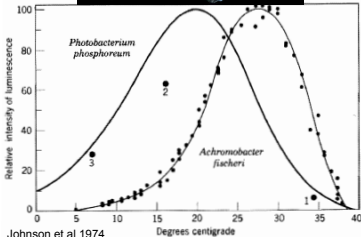
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$E$  = Activation energy (eV)

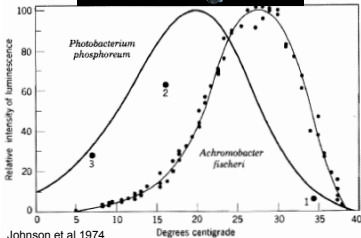
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- Surely there is more to thermal responses?
- *What about alternative models?*

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

# 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

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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 ( $\theta$ ) 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):  $-2 \ln[\mathcal{L}(\theta|x)] + p \ln(n)$   
(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)`
- Then, AIC is  $n * \log((2 * \pi) / n) + n + 2 + n * \log(rss) + 2 * p$   
(note  $n$  and  $p$ !)
- 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 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