Fitting Models to Data in Ecology and Evolution CMEE Masters

Samraat Pawar

Imperial College London

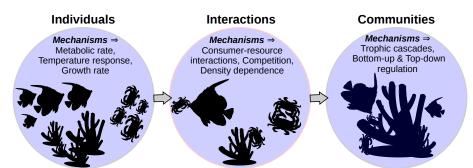
November 18, 2016

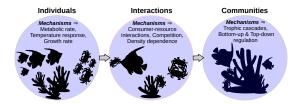
MECHANISTIC VS. PHENOMENOLOGICAL MODELS

- Mechanistic models aim to explain the PROCESSES underlying observed patterns
- Empirical or phenomenological models show relationships between observed data (e.g. population size as a function of temperature or rainfall), but provide no insights into why they are related

MECHANISTIC VS. PHENOMENOLOGICAL MODELS

- Mechanistic models aim to explain the PROCESSES underlying observed patterns
- Empirical or phenomenological models show relationships between observed data (e.g. population size as a function of temperature or rainfall), but provide no insights into why they are related



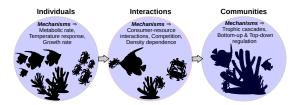


 Ecological studies often focus on explaining phenomena using somewhat phenomenological models.

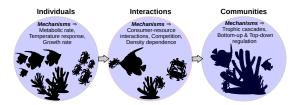


- Ecological studies often focus on explaining phenomena using somewhat phenomenological models.
- For example, insect invasions, outbreaks and spread

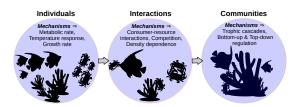
 (http://www.sandyliebhold.com/pubs/science_DC1/) papers in your Readings
 directory; (http://www.imperial.ac.uk/gmee-cdt/supervisors/)



- Ecological studies often focus on explaining phenomena using somewhat phenomenological models.
- For example, insect invasions, outbreaks and spread
 (http://www.sandyliebhold.com/pubs/science_DC1/) papers in your Readings directory;
 (http://www.imperial.ac.uk/qmee-cdt/supervisors/)
 - Why the cycles?, Why the travelling waves?



- Ecological studies often focus on explaining phenomena using somewhat phenomenological models.
- For example, insect invasions, outbreaks and spread
 (http://www.sandyliebhold.com/pubs/science_DC1/) papers in your Readings directory;
 (http://www.imperial.ac.uk/qmee-cdt/supervisors/)
 - Why the cycles?, Why the travelling waves?



- Ecological studies often focus on explaining phenomena using somewhat phenomenological models.
- For example, insect invasions, outbreaks and spread
 (http://www.sandyliebhold.com/pubs/science_DC1/) papers in your Readings directory;
 (http://www.imperial.ac.uk/gmee-cdt/supervisors/)
 - Why the cycles?, Why the travelling waves? What mechanisms operate? (budmoth/parasitoid interaction? (budmoth/food quality interaction?) Are these truly mechanisms?
- Another example, disease outbreaks (Papers in your Readings directory)

Somewhat subjective!

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

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

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

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

 What is the mechanism? — Density dependence through scramble competition (Brannstrom & Sumpter 2005)

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

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

- 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

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

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

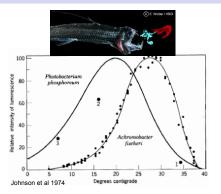
- What is the mechanism? Density dependence through scramble competition (Brannstrom & Sumpter 2005)
- If the Ricker model and another model with contest competition were compared with data — some would call it mechanistic modelling because one is trying to get at the underlying mechanism, scramble or contest competition
- But is this REALLY mechanistic? What are r and k really?

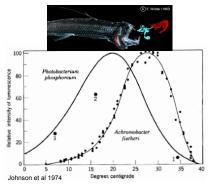
- Somewhat subjective!
- For example, the Ricker model can be thought of as mechanistic:

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

- 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?
- Many (including yours truly!) now argue that we have not progressed far enough because the first level has been ignored!







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

T = temperature (K)

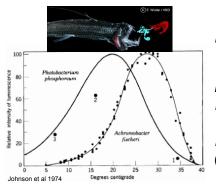
 $k = \text{Boltzmann constant (eV K}^{-1})$

E = Activation energy (eV)

 T_{pk} = Temperature of peak performance

 E_D = Deactivation energy (eV)

(J H van't Hoff 1884, S Arrhenius 1889)



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

T = temperature (K)

 $k = \text{Boltzmann constant (eV K}^{-1})$

E = Activation energy (eV)

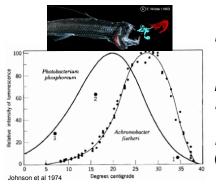
 T_{pk} = Temperature of peak performance

 E_D = Deactivation energy (eV)

(J H van't Hoff 1884, S Arrhenius 1889)

- Surely there is more to thermal responses?
 - Oxygen limitation
 - Complexity of metabolic network
 - Hormonal regulation





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

T = temperature (K)

 $k = \text{Boltzmann constant (eV K}^{-1})$

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?
 - Oxygen limitation
 - Complexity of metabolic network
 - Hormonal regulation
- What about alternative models?

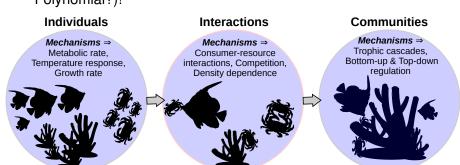


MODELLING, AND FITTING MODELS TO DATA: WHAT'S THE BIG IDEA?

- 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. growth rates), etc.
- Don't use models you already know have the wrong mechanisms!
- Phenomenological models often perform better than mechanistic ones

MODELS: HOW TO BUILD THEM?

- It's an art, take practice (look at 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 a alternative that is more parsimonous, even if it is phenomenological (the TPC example: Sharpe-Schoolfield, or Polynomial?)!



MODELS: HOW TO BUILD THEM?

- For example, the Boltzmann-Arrhenius model is a good first try describe and uncover mechanisms underlying individual level rates
- The next step would be to include high-temperature effects (e.g., the Schoolfield model)
- The next step would be to include species interactions with temperature dependence of individuals (or go in an evolutionary direction!)

Next: A primer on mechanistic model fitting

Next: A primer on mechanistic model fitting

But first: A preview of the Miniproject (back to Notes)

FITTING MODELS TO DATA

Two common ways to do it:

- One-step forecasting (appropriate for discrete models)
- Ensemble fitting (appropriate for full time series or responses) this is what you will be doing in NLLS

There include maximum likelihood, bayesian methods, and Non-linear least squares (NLLS) optimization or fitting. Many of you will use NLLS. Basically, this is how it works:

Start with an initial value for each parameter in the model

- Start with an initial value for each parameter in the model
- @ Generate the curve defined by the initial values

- Start with an initial value for each parameter in the model
- @ Generate the curve defined by the initial values
- Oalculate the residual sum-of-squares (rss)

- Start with an initial value for each parameter in the model
- @ Generate the curve defined by the initial values
- Oalculate the residual sum-of-squares (rss)
- Adjust the parameters to make the curve come closer to the data points. This the tricky part — you will use the Levenberg-Marquardt algorithm in the lmfit package in python

- Start with an initial value for each parameter in the model
- @ Generate the curve defined by the initial values
- Oalculate the residual sum-of-squares (rss)
- Adjust the parameters to make the curve come closer to the data points. This the tricky part — you will use the Levenberg-Marquardt algorithm in the lmfit package in python
- Adjust the parameters again so that the curve comes even closer to the points (rss decreases)

- Start with an initial value for each parameter in the model
- @ Generate the curve defined by the initial values
- Calculate the residual sum-of-squares (rss)
- Adjust the parameters to make the curve come closer to the data points. This the tricky part — you will use the Levenberg-Marquardt algorithm in the lmfit package in python
- Adjust the parameters again so that the curve comes even closer to the points (rss decreases)
- Repeat 4–5

- Start with an initial value for each parameter in the model
- @ Generate the curve defined by the initial values
- Calculate the residual sum-of-squares (rss)
- Adjust the parameters to make the curve come closer to the data points. This the tricky part — you will use the Levenberg-Marquardt algorithm in the lmfit package in python
- Adjust the parameters again so that the curve comes even closer to the points (rss decreases)
- Repeat 4–5
- Stop simulations when the adjustments make virtually no difference to the rss



Once the algorithm as converged (hopefully – but you may be surprised how well it usually works),

 Report the best-fit results, including sums of deviations of the data from the final model fit

Once the algorithm as converged (hopefully – but you may be surprised how well it usually works),

- Report the best-fit results, including sums of deviations of the data from the final model fit
- Then compare multiple models (e.g., Schoolfield vs. cubic)

Once the algorithm as converged (hopefully – but you may be surprised how well it usually works),

- Report the best-fit results, including sums of deviations of the data from the final model fit
- Then compare multiple models (e.g., Schoolfield vs. cubic)

Once the algorithm as converged (hopefully – but you may be surprised how well it usually works),

- Report the best-fit results, including sums of deviations of the data from the final model fit
- Then compare multiple models (e.g., Schoolfield vs. cubic)

The precise parameter values you obtain will depend in part on the initial values chosen and the stopping criteria –

Once the algorithm as converged (hopefully – but you may be surprised how well it usually works),

- Report the best-fit results, including sums of deviations of the data from the final model fit
- Then compare multiple models (e.g., Schoolfield vs. cubic)

The precise parameter values you obtain will depend in part on the initial values chosen and the stopping criteria – so different programs will not always give exactly the same results

- It's all about the "Likelihood" of a model:
- That is, the likelihood of a set of parameter values (of a 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 use estimated likelihoods of a model

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

Both use estimated likelihoods of a model

The lower the AIC or BIC, the better. This is how you calculate them (using python syntax):

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

Both use estimated likelihoods of a model

The lower the AIC or BIC, the better. This is how you calculate them (using python syntax):

- residuals = Observations Predictions
- rss = sum(residuals ** 2)
- Then, AIC is n * log((2 * pi) / n) + n + 2 + n * log(rss) + 2 * k (what is n and k?)
- And BIC is n + n * log(2 * pi) + n * log(rss / n) + (log(n)) * (k + 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

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

Both use estimated likelihoods of a model

The lower the AIC or BIC, the better. This is how you calculate them (using python syntax):

- residuals = Observations Predictions
- rss = sum(residuals ** 2)
- Then, AIC is n * log((2 * pi) / n) + n + 2 + n * log(rss) + 2 * k (what is n and k?)
- And BIC is n + n * log(2 * pi) + n * log(rss / n) + (log(n)) * (k + 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:

 R² = 1 - (rss/tss), where tss is total sum of squares: tss = sum((Observations - mean(Predictions)) ** 2) (a useful measure of goodness of fit – you should report it)

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.
- For the suggested fitting TPCs project: Papers in the Temperature_response_papers directory, but especially Schoolfield, R. M., Sharpe, P. J. & Magnuson, C. E. 1981 Non-linear regression of biological temperature-dependent rate models based on absolute reaction-rate theory. J. Theor. Biol. 88, 719–31.