Model evaluation and comparison

DAIDD 2017

Goals

- Discuss model types and model goals
- Explain the value of simulation for validating models
- Discuss metrics for evaluating fit
- Put the Goodness of fit test in its place

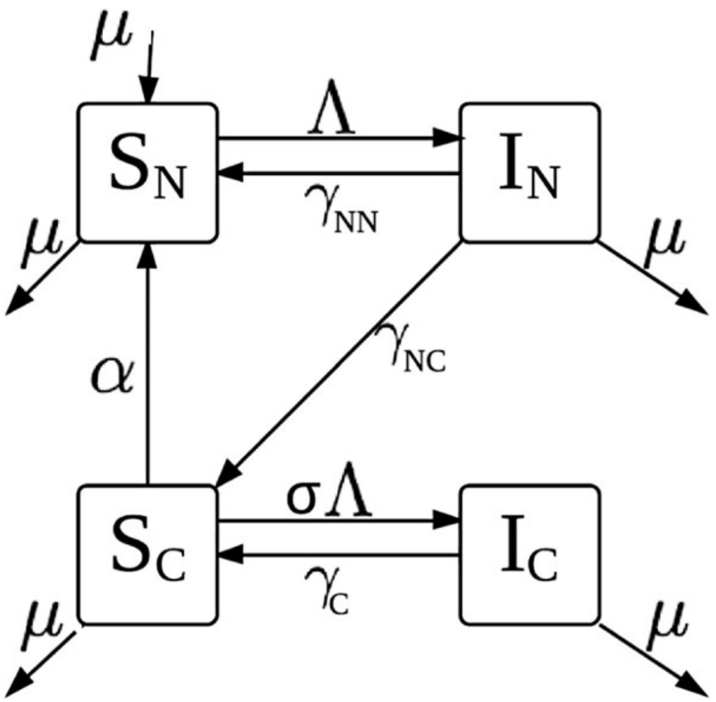
Do I have a good model?

- What is my model trying to accomplish?
  - Generating hypotheses
  - Evaluating plausibility
  - Prediction
  - Extrapolation
  - Mechanistic understanding

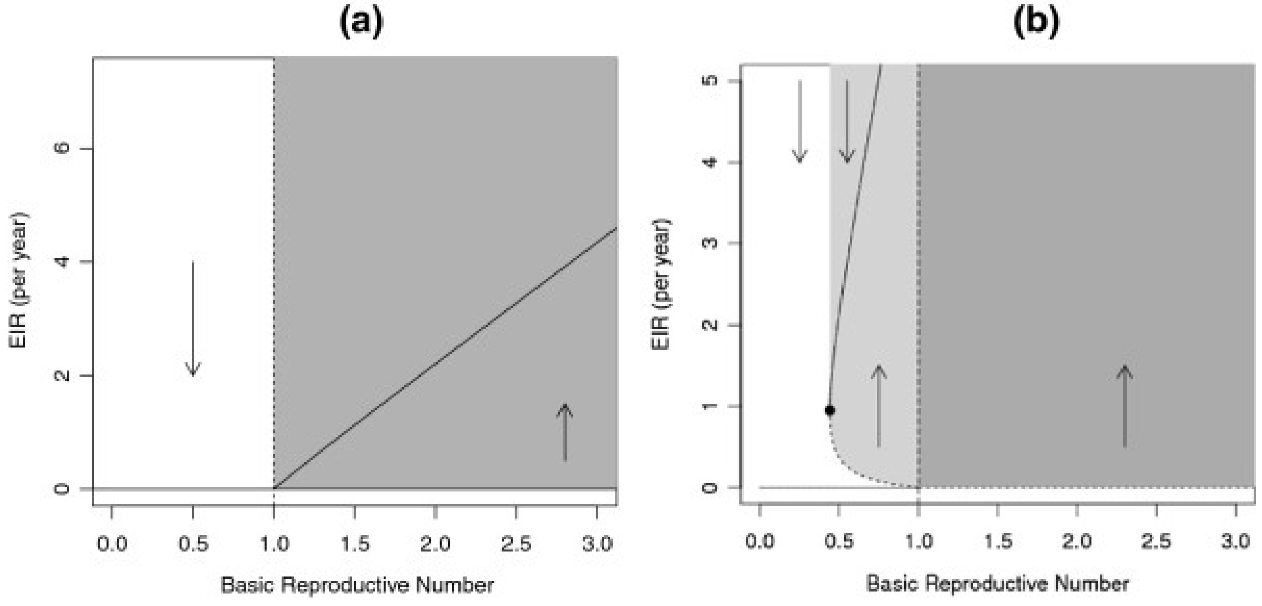
1 Conceptual models

Disease thresholds

Effects of clinical immunity



Bistability



2 Prediction

Ptolemy v. Copernicus
Where will we see cholera cases?

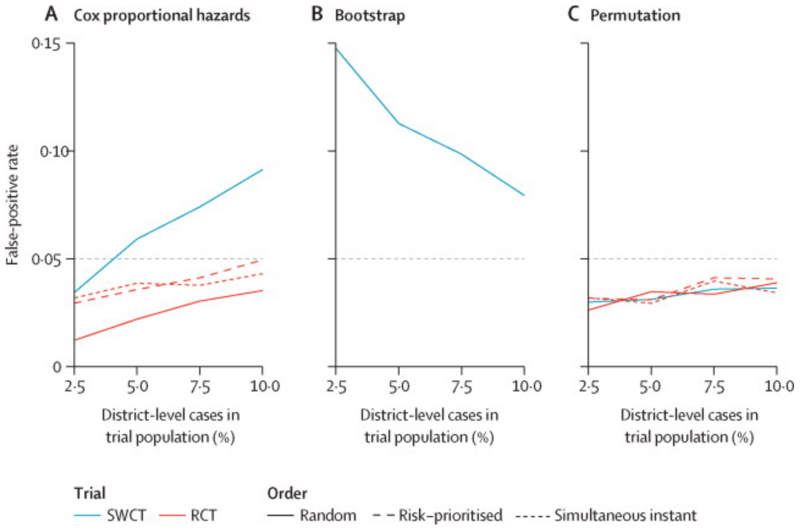
3 Model Validation

- Does your fitting algorithm match your *model world*?
- If you use your fitting algorithm on simulations from your model world, then you *know the right answer*!

Validation measures

- Coverage
- Precision
- Bias?
- Accuracy?

Coverage



- The right answer should be inside your 95% confidence interval 95% of the time
  - If more, your model is *too conservative*
  - If less, your model is *invalid*
- In many cases it's good to look at the two tails separately:
  - How often do you overestimate? Underestimate?

Precision

- You should aim to make your confidence intervals as narrow as possible
  - Provide as much information as possible
- As data increases, your precision should increase
  - CIs should approach zero width

Bias?

- Nobody wants to be biased
- You *need* to be *asymptotically* unbiased
  - Good coverage and good precision assure this
- Not so clear you need to be *absolutely* unbiased
  - Bias is the difference between the *mean* expected prediction and the true value
  - Scale dependent: an unbiased estimate of γ is automatically a biased estimate of D (but not asymptotically biased)
- It may be better to evaluate using medians (instead of means)

Accuracy?

- Nobody wants to be inaccurate
- Good coverage and good precision should guarantee good accuracy

4 Model Evaluation

- Does your model match the *real world*?

4.1 Goodness of fit

- Goodness of fit *statistics* describe how well a model prediction matches observed data
- Goodness of fit *tests* attempt to determine whehter the observed difference between model and data is statistically significant

Your model is false!

- A goodness of fit test won't make it true
- You can "pass" a goodness of fit test by:
  - having a good model
  - making very broad predictions
  - having bad data
  - choosing an inappropriate way to compare
- So why do we use P values at all in biology?

What does the P value mean?

- Low: you are seeing something clearly
- High: you are seeing something unclearly

Goodness of fit test

- Your model is *not* reality (null hypothesis is false)
- Can we see the difference clearly?
  - If no, model may be good or bad.
    - We probably can't add any more complexity based on current data
  - If yes, model may be good or bad. We *may* be able to add more complexity based on current data
    - But we may not need to

4.2 Capturing patterns

- You can ask:
  - Does your model do a reasonable job of capturing the data?
    - You can use a goodness of fit *statistic* for this, and not worry about the P value
  - Does your model capture patterns and relationships that you (or other experts) think are important?

4.3 Going beyond

Out-of-sample validation

- Does your model make predictions *outside* the range on which you calibrated it?
  - Predicting gravitational shifts in star positions from measurements in Earth laboratories
  - Predicting cholera outbreaks in Bangladesh from a model calibrated to Haiti
  - Predicting influenza patterns in 2010 from a model calibrated from 2000–2009

Test sets

- What is **test set** spelled backwards?
- Hold some data out while fitting your model
- Or just *pretend* to do this as an evaluation method
  - In other words, test what would happen under various withholding scenarios

Other model worlds

- The model you're *fitting* is probably pretty simple
- But you can *simulate* very complicated models, indeed
- How well can you do? Which details are important?

Generating hypotheses

For example:

- Safe burial is key to interrupting Ebola transmission
- Vaccinating domestic dogs can eliminate transmission of canine rabies

Testing hypotheses

- Both the Farr model and the Snow model made testable predictions about cholera
- Snow tested his hypotheses by removing the pump handle

Hard questions

Answers are not always easy

5 Conclusion

Summary

Dynamic models can help:

- Think clearly
- Understand outcomes
- Predict outcomes
- Find new mechanisms

Summary

Evaluation

- Validation (inside your model world)
- Inspection (compare patterns)
- Prediction (and other out-of-sample comparison)
- Generate and test mechanistic hypotheses

Conclusion

Saturn's shepherd moons were predicted before they were seen!
Essentially, all models are wrong, but some are useful.
– Box and Draper (1987), *Empirical Model Building . . .*