Model evaluation and comparison

DAIDD 2020

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
  - Take a long digression about statistical philosophy

Do I have a good model?

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

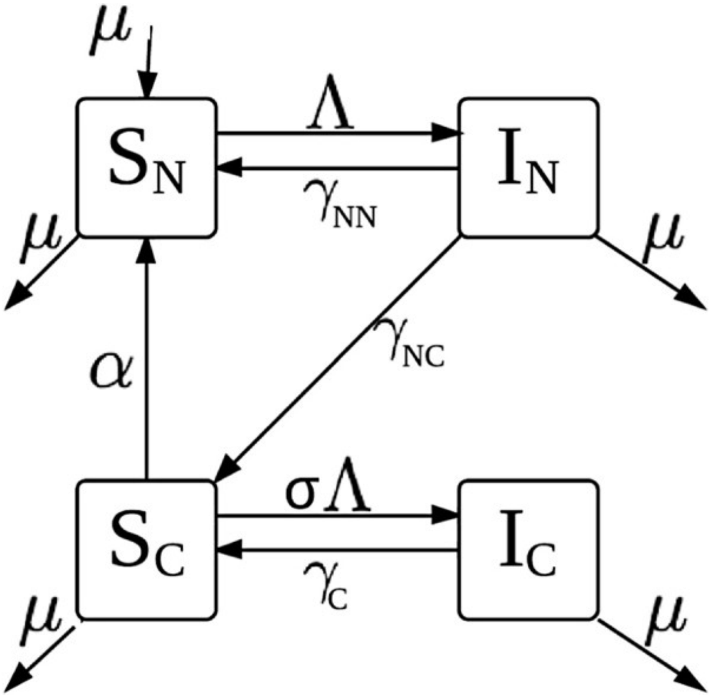
Statistical philosophy

You should develop your own statistical philosophy

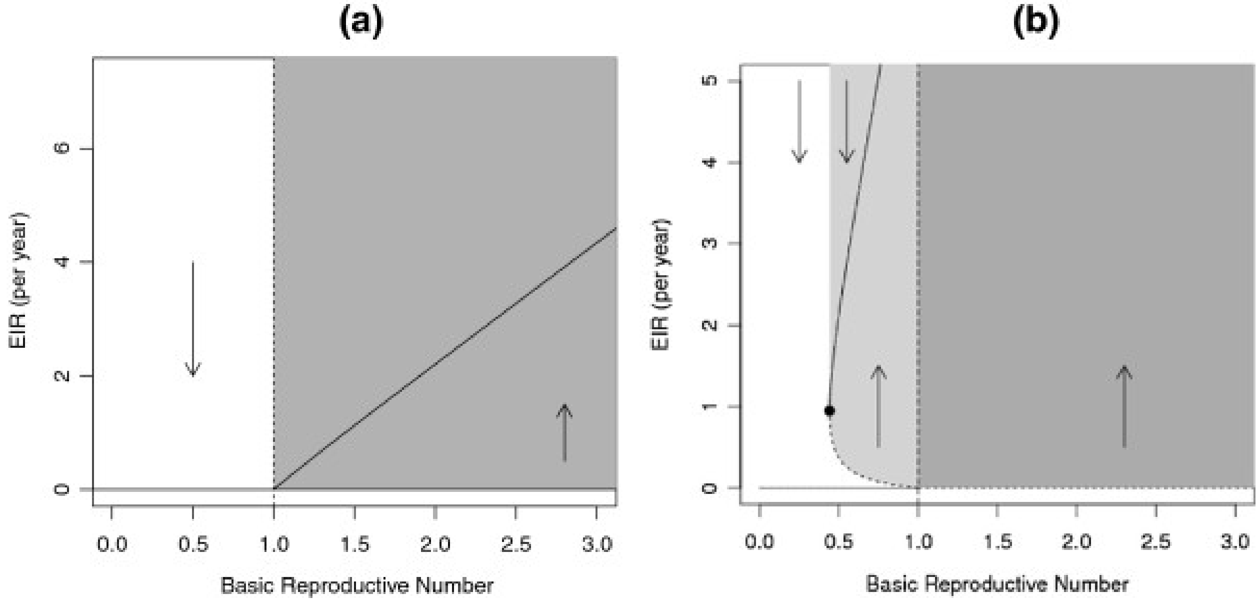
1 Conceptual models

Disease thresholds

Effects of clinical immunity



Bistability



2 Prediction

Ptolemy v. Copernicus
Where will we see cholera cases?

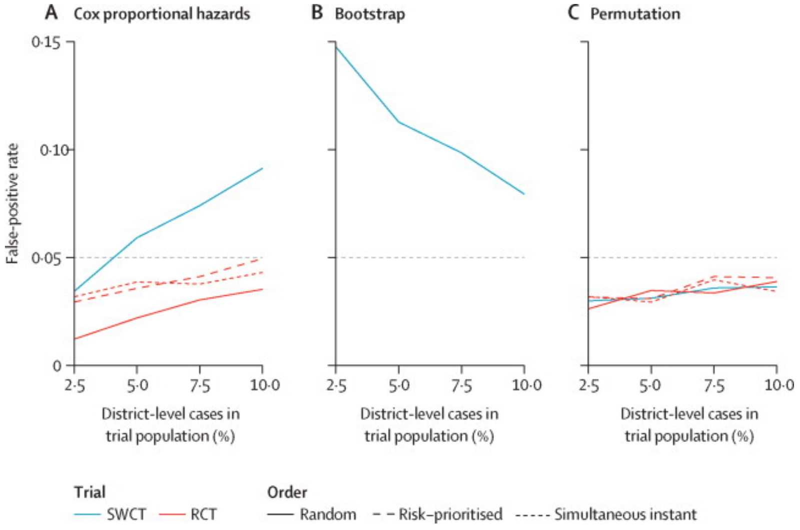
3 Model Validation

- 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

- A good model tries to provide a precise answer
  - Confidence intervals should be narrow, if possible
  - But not at the price of overconfidence (invalidity)
- As data increases, your precision should increase

  - CIs should approach zero width
  - …as long as you have data about *everything*

- Conversely, CIs should reflect a variety of sources of uncertainty

Bias and accuracy

- Good coverage and high precision should ensure high accuracy and low bias

- Don't worry about "unbiased estimators"

  - Your estimator doesn't need to be absolutely unbiased
  - Your reasonable estimator will be asymptotically unbiased

4 Model Evaluation

- Does your model match the *real world*?

  -

- How well 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 whether the observed difference between model and data is statistically significant

Your model is false!
…or at least, incomplete

- 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 would we do this?

- For that matter, why do we use P values at all in biology?

4.2 Digression

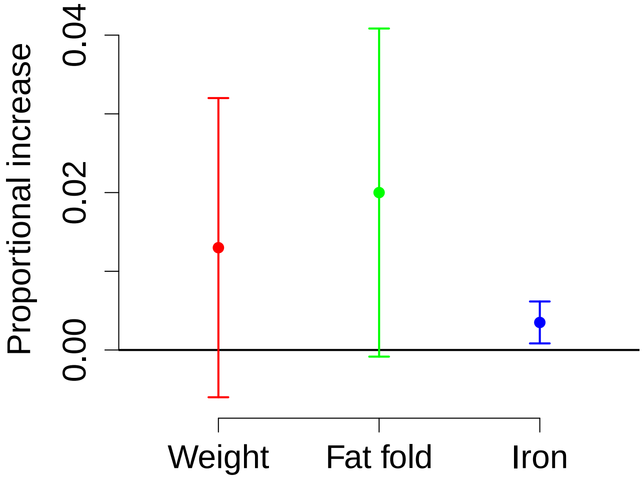
Passing goodness of fit tests

- I can make any model pass a goodness of fit test by broadening the uncertainty
- That doesn't make it a good model

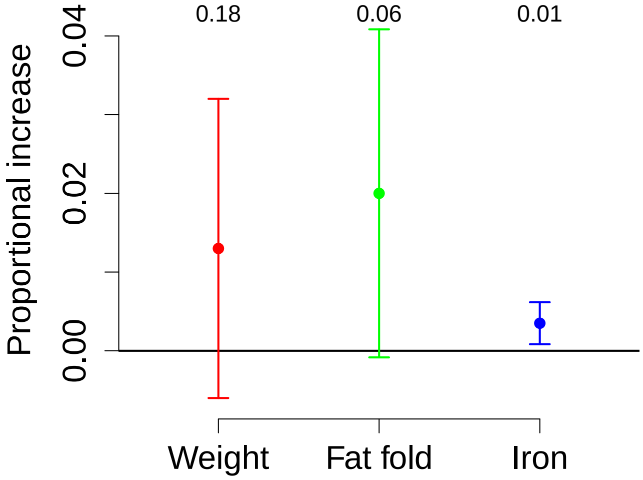
Vitamin A example

- We want to know if vitamin A supplements improve the health of village children
  - Outcome: height growth in 6 months
- What does it mean if I find a "significant P value" for some effect in this experiment?
  -
  - So what! I already know vitamin A has strong effects on metabolism
- If I'm certain that the true answer isn't exactly zero, why do I want the P value anyway?

Vitamin study



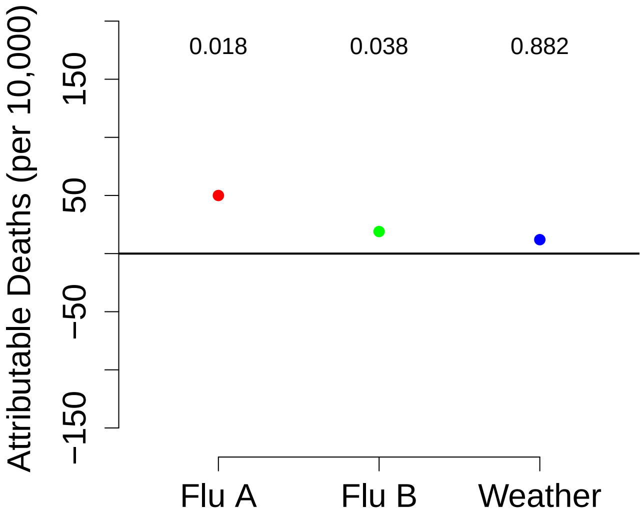
Vitamin study



Discussion

- Do you agree that in biology we should assume that the answer to our sensible question is not exactly zero?
  - Or at least have a philosophy consistent with that assumption?
    - Can we ever *prove* that an effect is zero?
- If we make that assumption (null hypothesis is false), why might we want a P value anyway?

Annualized flu deaths



- Why is weather not causing deaths at this time scale?

Low P values

High P values

Low P values

- If I have a low P value I can see something clearly
- But it's usually better to focus on what I see than the P value

High P values

- If I have a high P value, there is something I *don't* see clearly
- It *may be* because this effect is small
- High P values should *not* be used to advance your conclusion

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

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

Predicting way out of sample

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 . . .*

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
    - This can get very elaborate, and we should probably do it more

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

- Clarify thinking
  - What are our assumptions, what else do we need to know?
- Understand outcomes
  - Can heterogeneity explain the time course of HIV epidemics?
  - Is it possible that MDA could break the cycle of malaria transmission in some areas?
- Predict outcomes
  - What is the potential for a hepatitis A outbreak in Cape Town?
  - What might happen if I improve testing-and-treatment outreach in Jamaica?
- Find new mechanisms
  - Why can't I explain my data? What haven't I thought of?

Summary

Evaluation

- Validation (inside your model world)
  - Does my fitting method work (assuming my model is right)?
- Inspection (compare patterns)
- Prediction (and other out-of-sample comparison)
  - Can my model predict things I haven't told it yet?
- Generate and test mechanistic hypotheses