Model evaluation and comparison

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DAIDD 2018

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

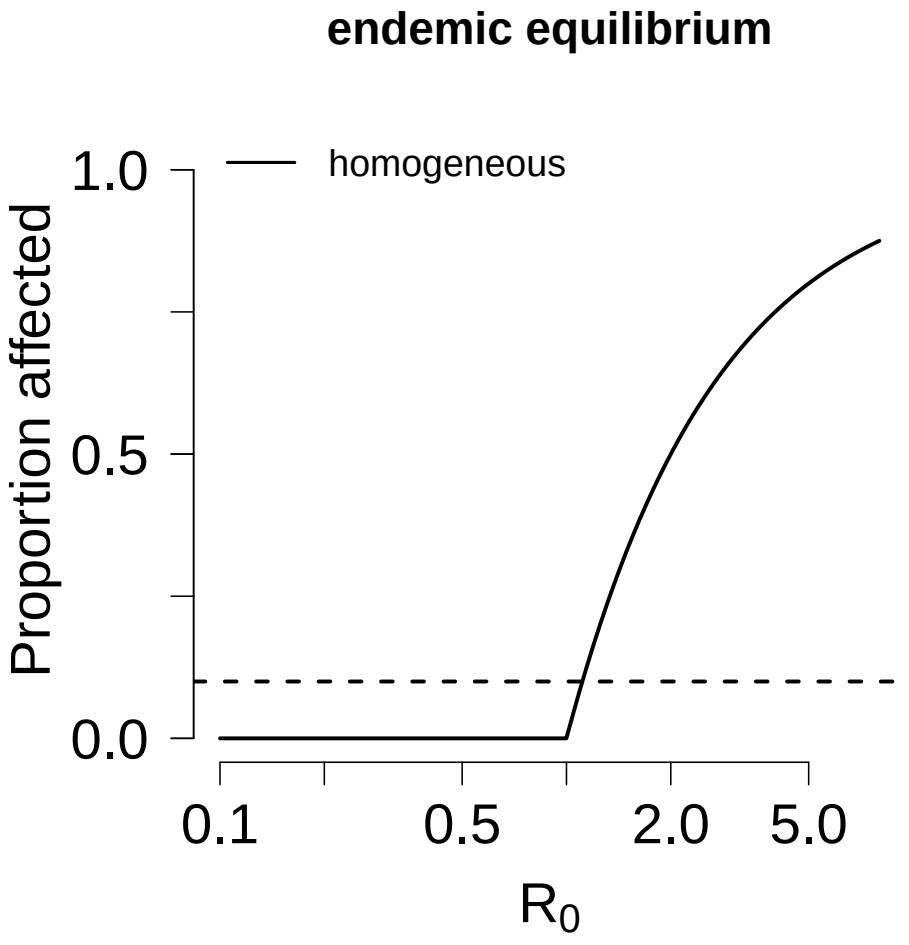
Do I have a good model?

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

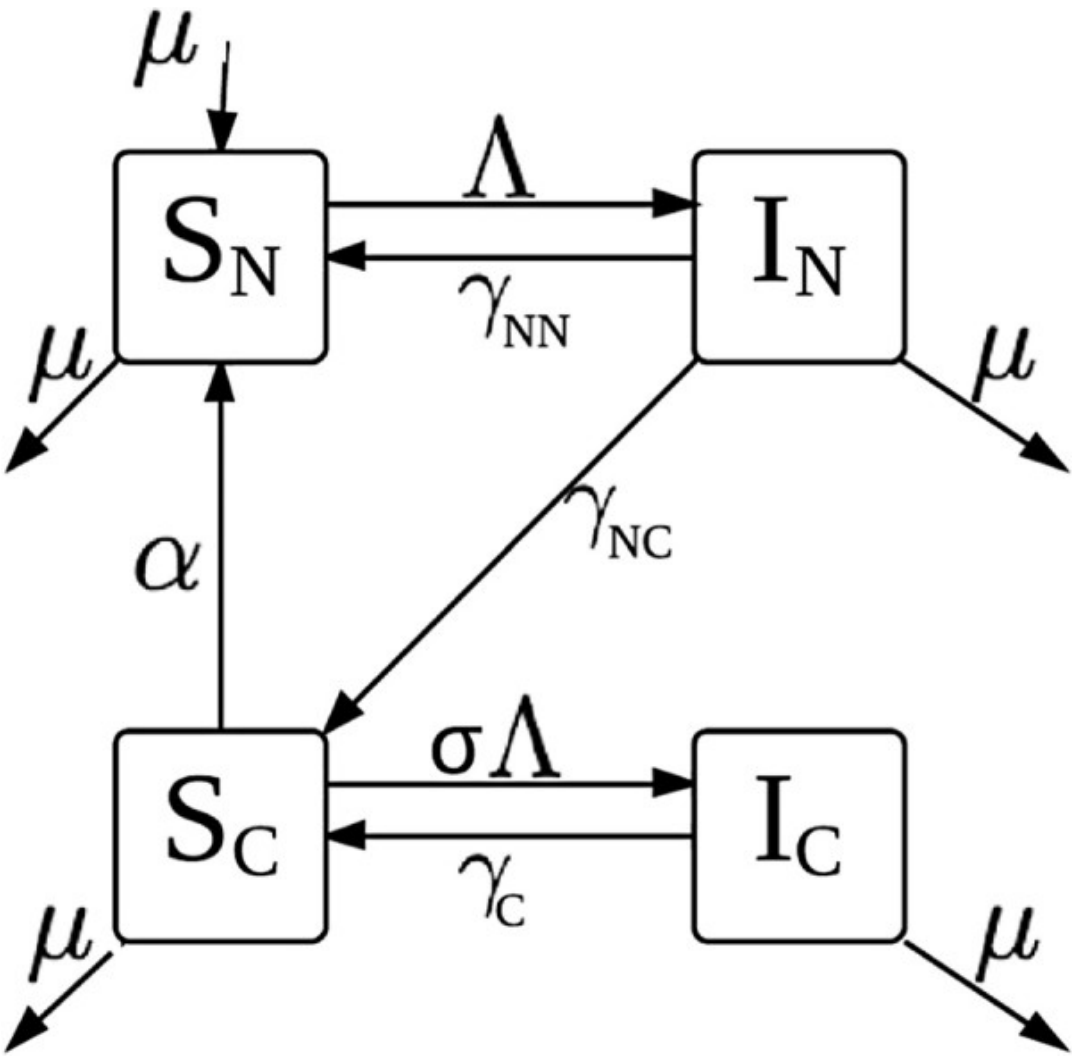
Statistical philosophy

Outline

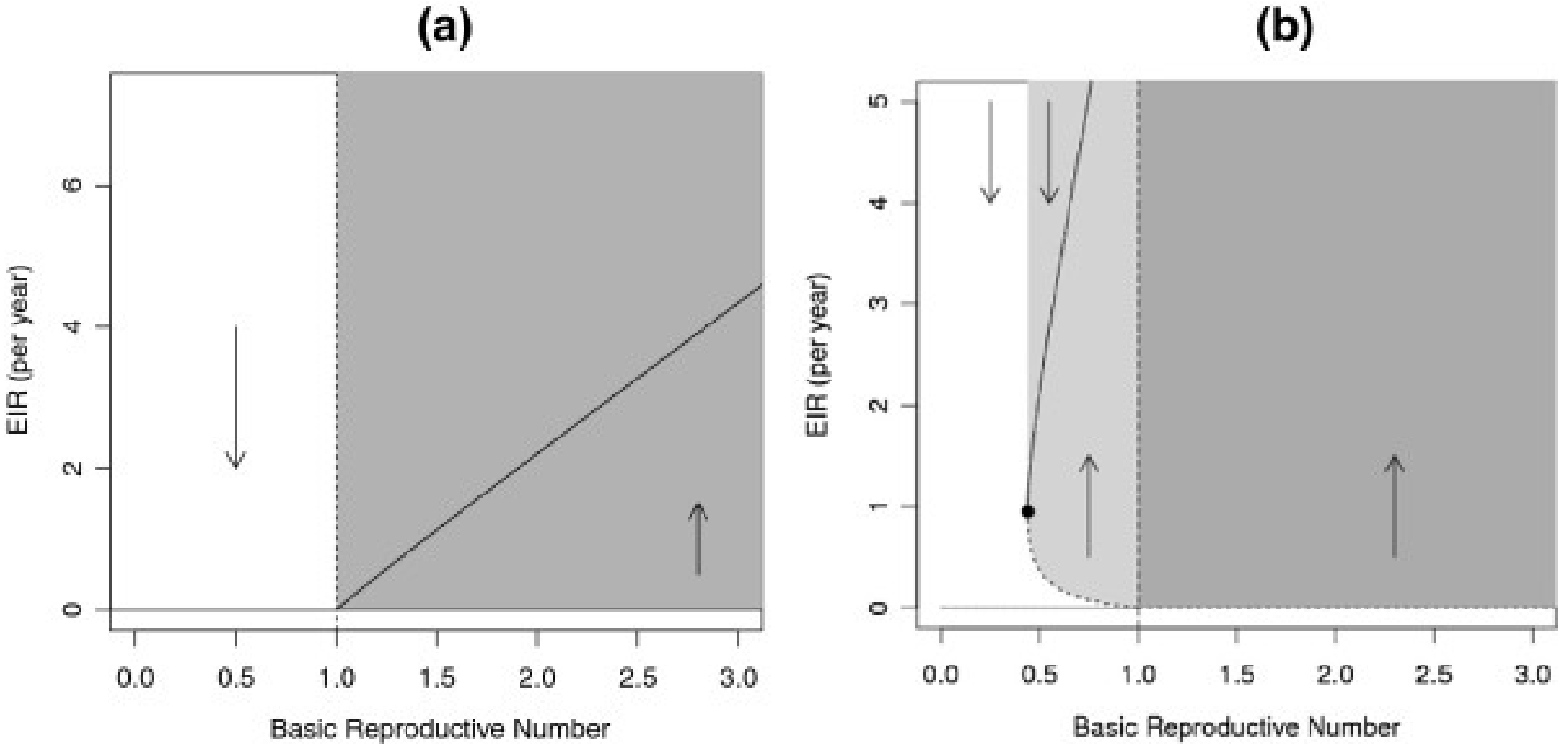
Disease thresholds



Effects of clinical immunity

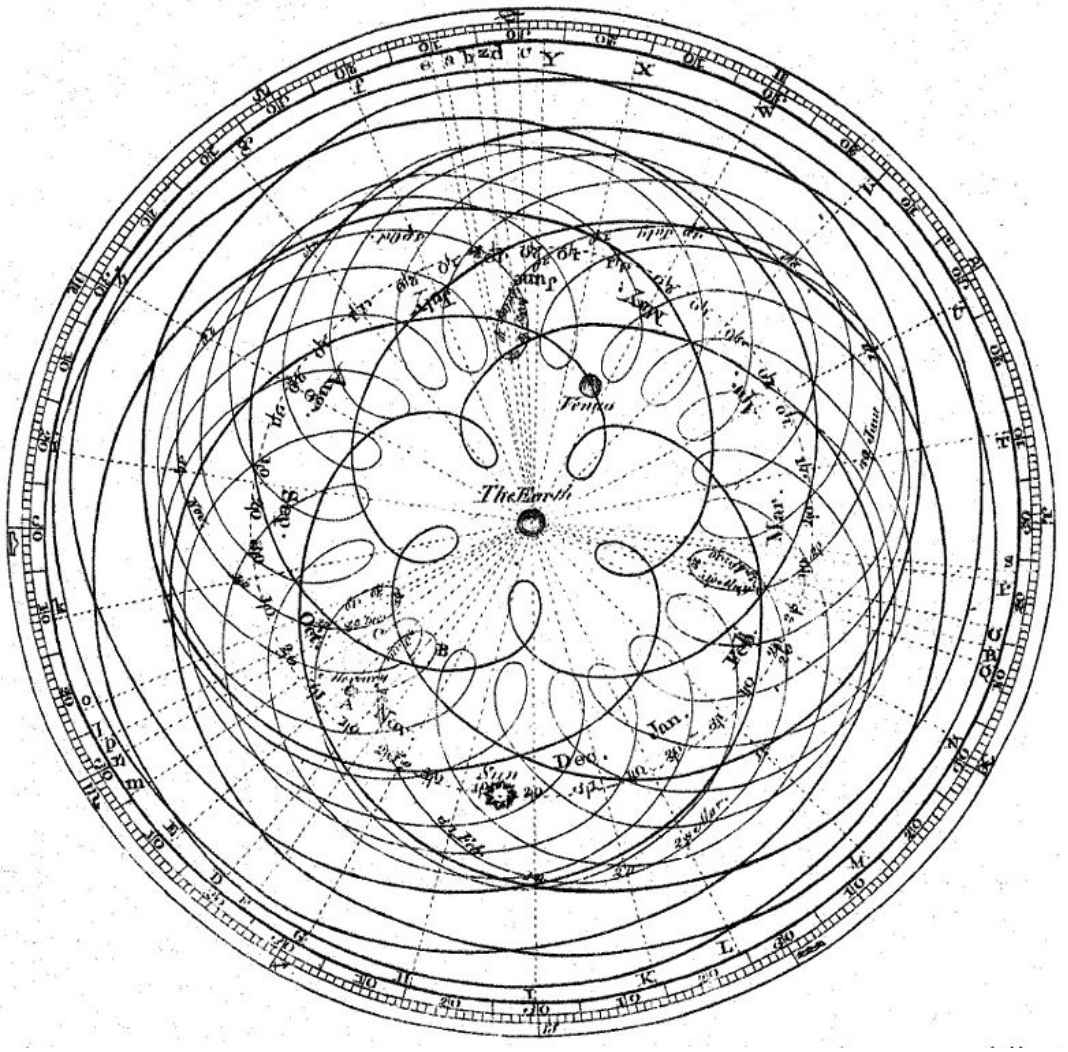


Bistability

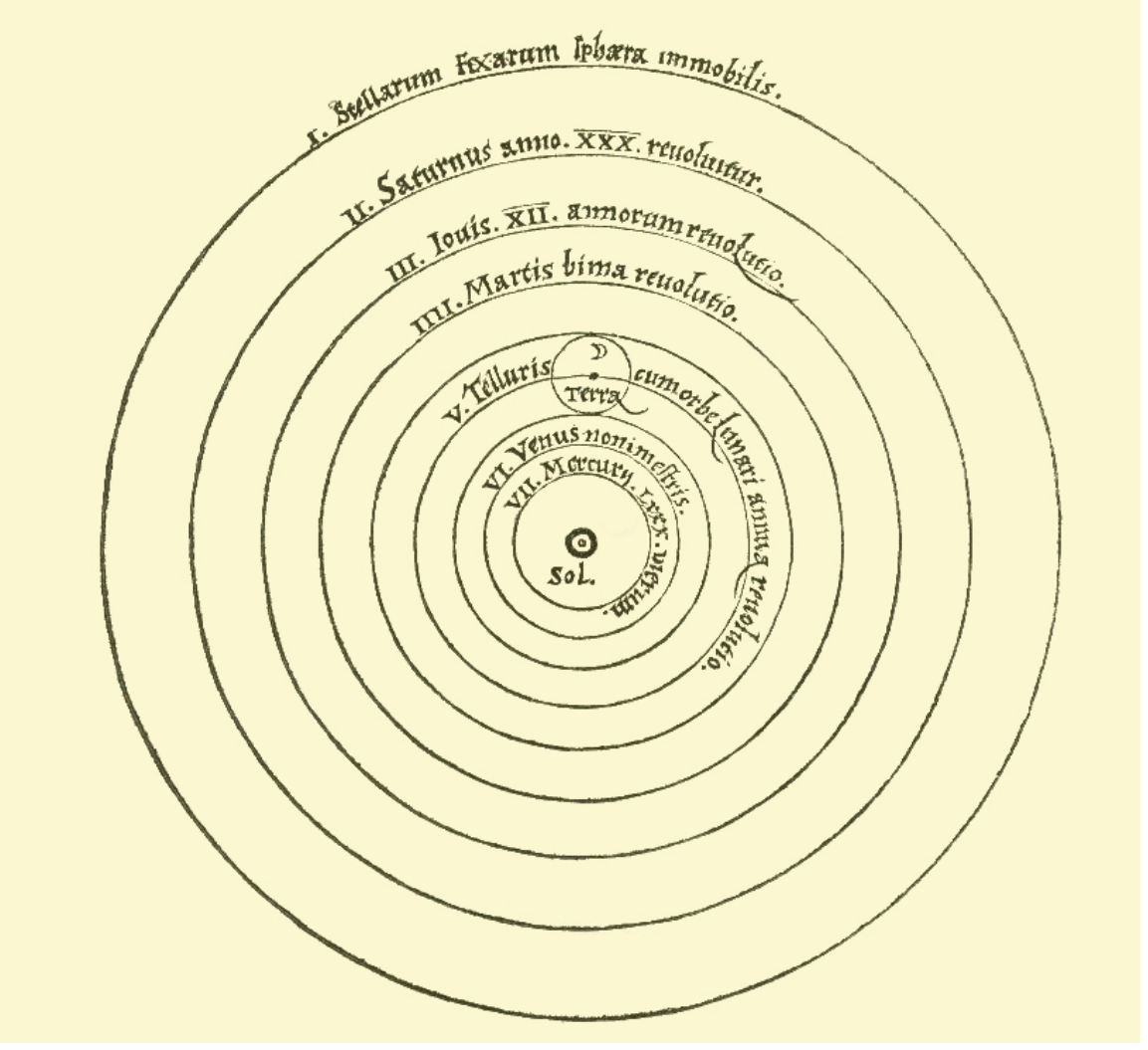


Outline

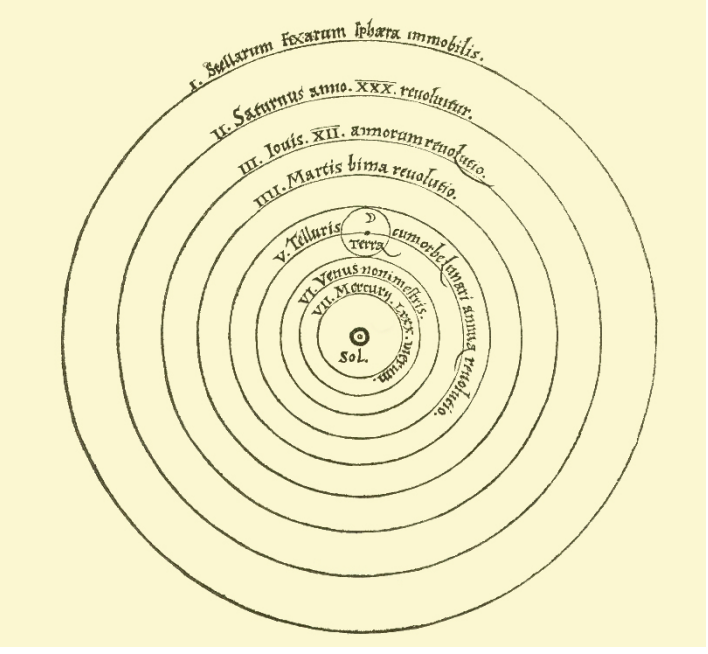
Ptolemy v. Copernicus

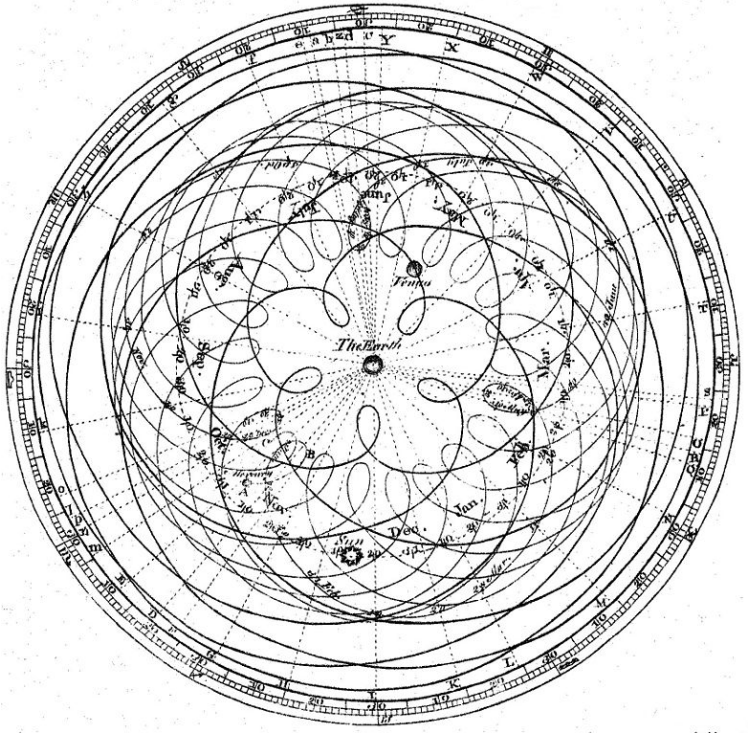


Ptolemy v. Copernicus

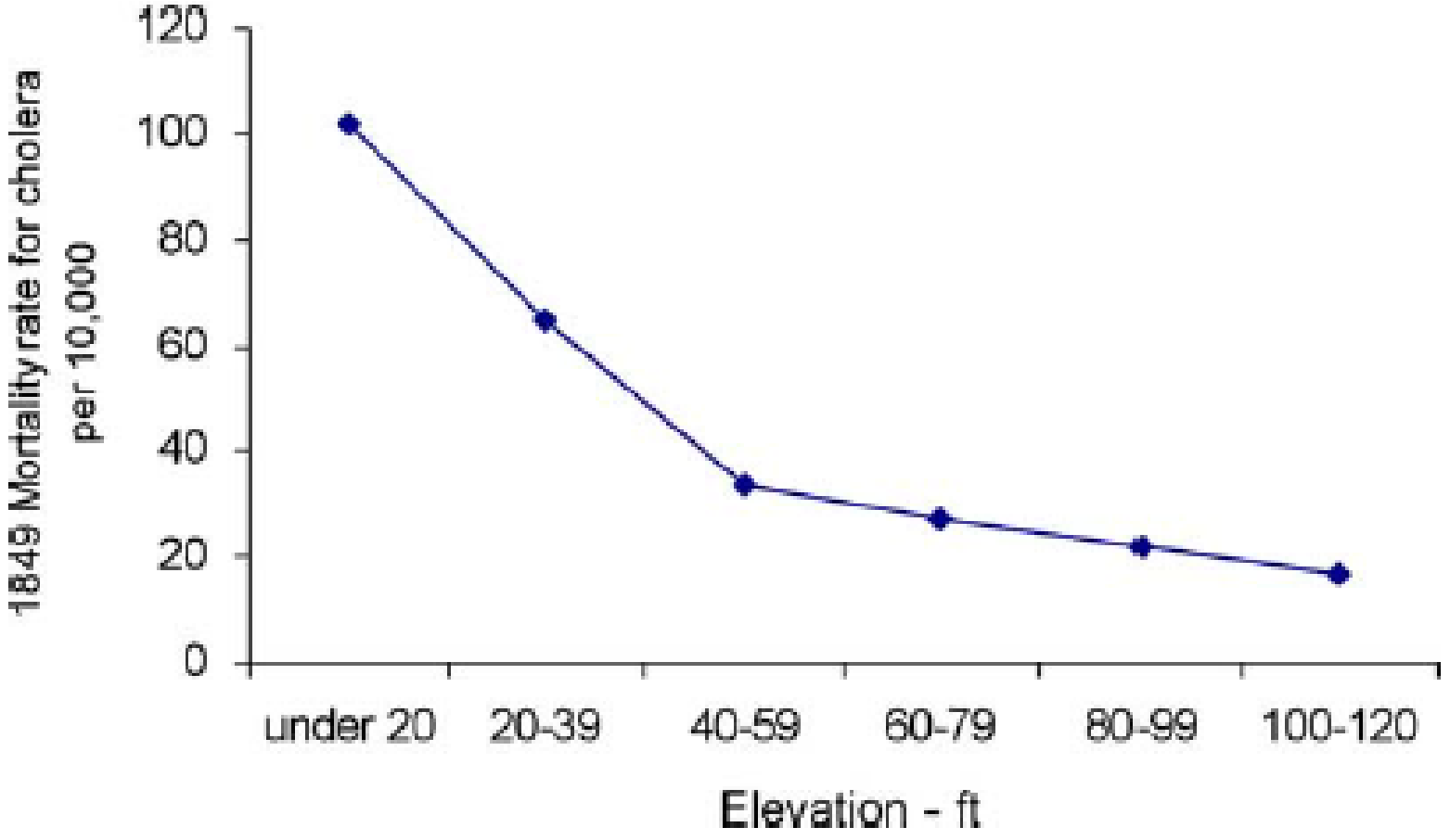


Ptolemy v. Copernicus





Where will we see cholera cases?

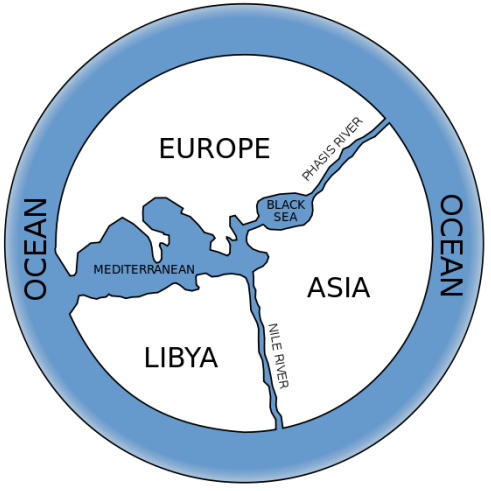


Where will we see cholera cases?

Outline

Model Validation

- Does your fitting algorithm match your *model world*?

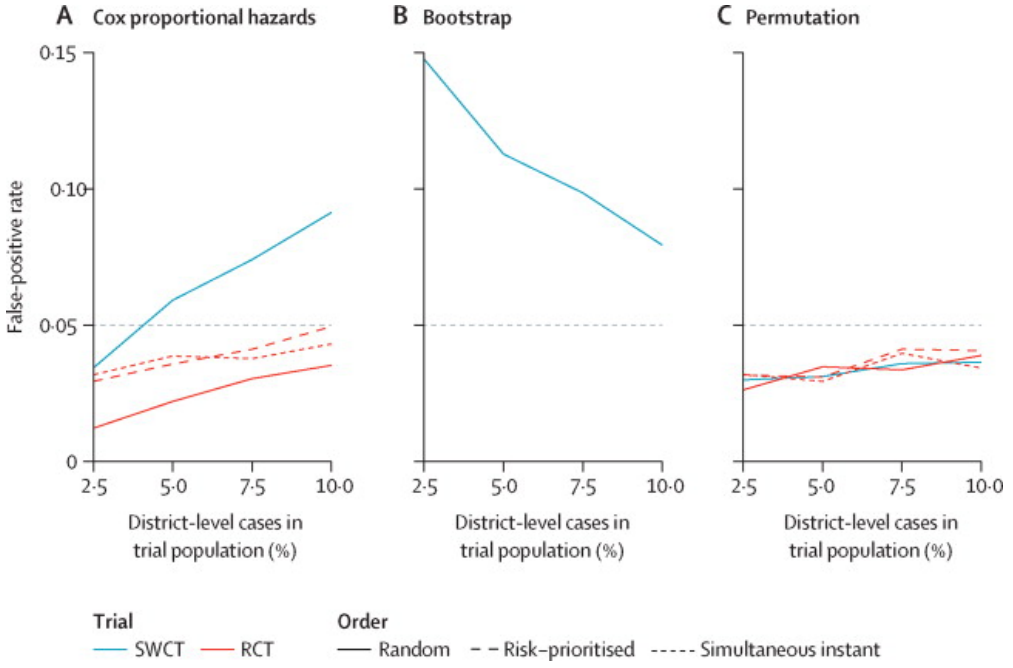


- If you use your fitting algorithm on simulations from your model world, then you *know the right answer*!

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

Outline

Model Evaluation

- Does your model match the *real world*?
  - * No!
- How well does your model match the real world?

Outline

Goodness of fit

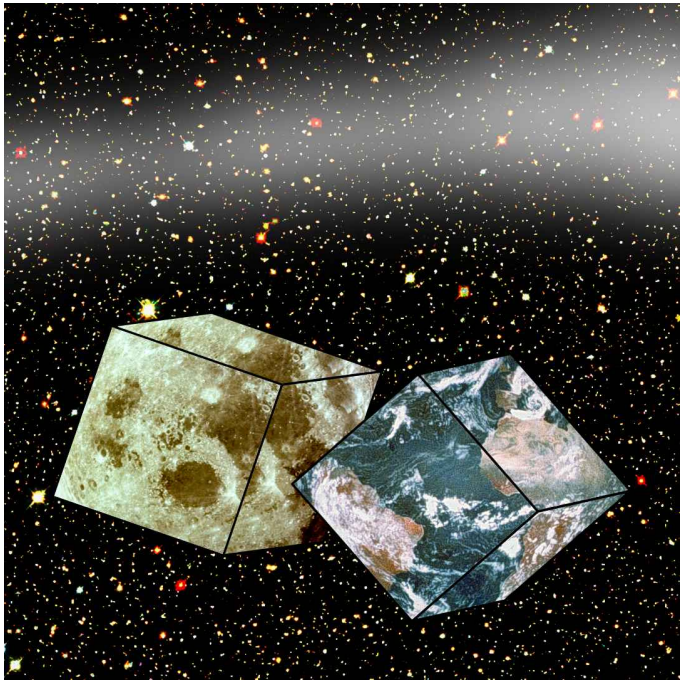
- Goodness of fit *statistics* describe how well a model prediction matches observed data
- Goodness of fit *tests* attempt to determine whether the observed difference between model and data is statistically significant

Your model is false!

- 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?

Passing goodness of fit tests

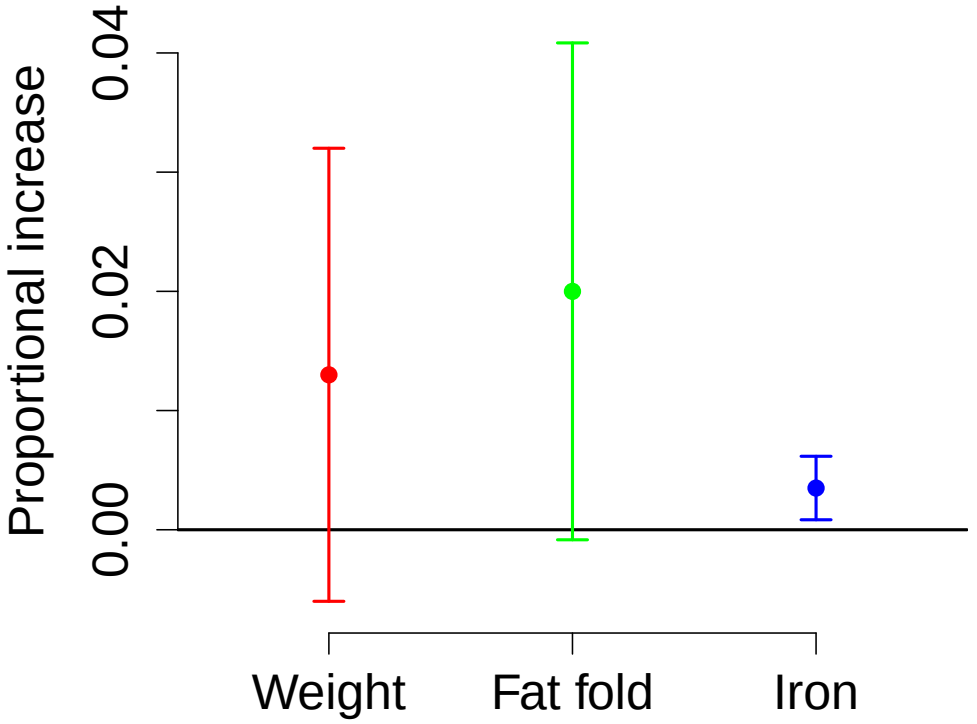
- I can make any model pass a goodness of fit test by broadening the uncertainty
- That doesn't make it a good model



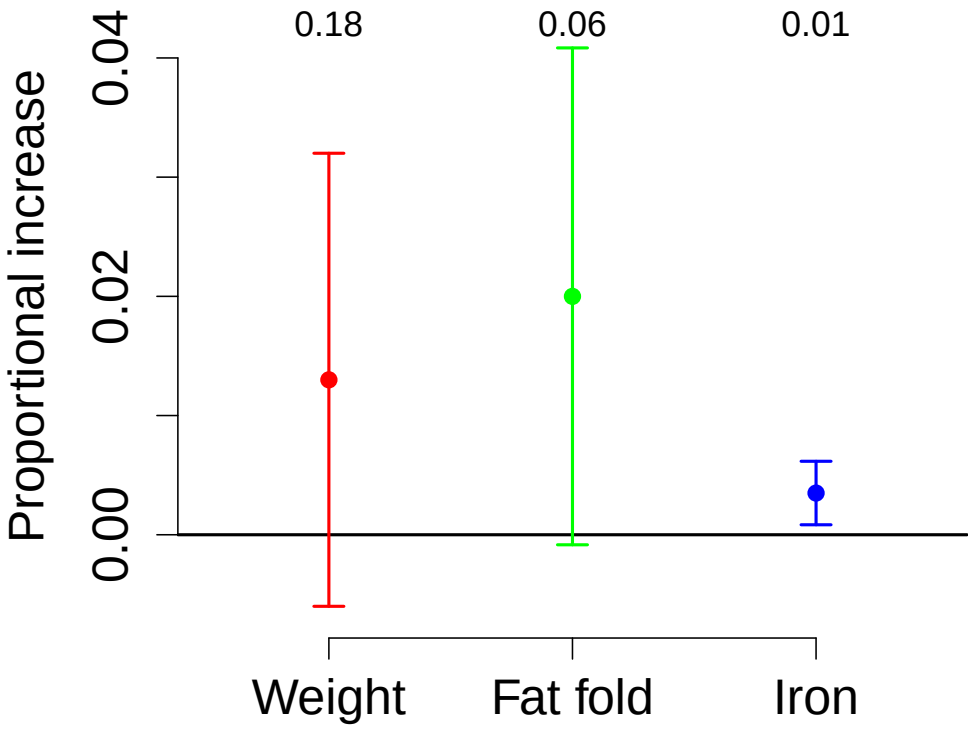
Vitamin A example

- 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?
  - * The difference is unlikely to be due to chance
  - 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



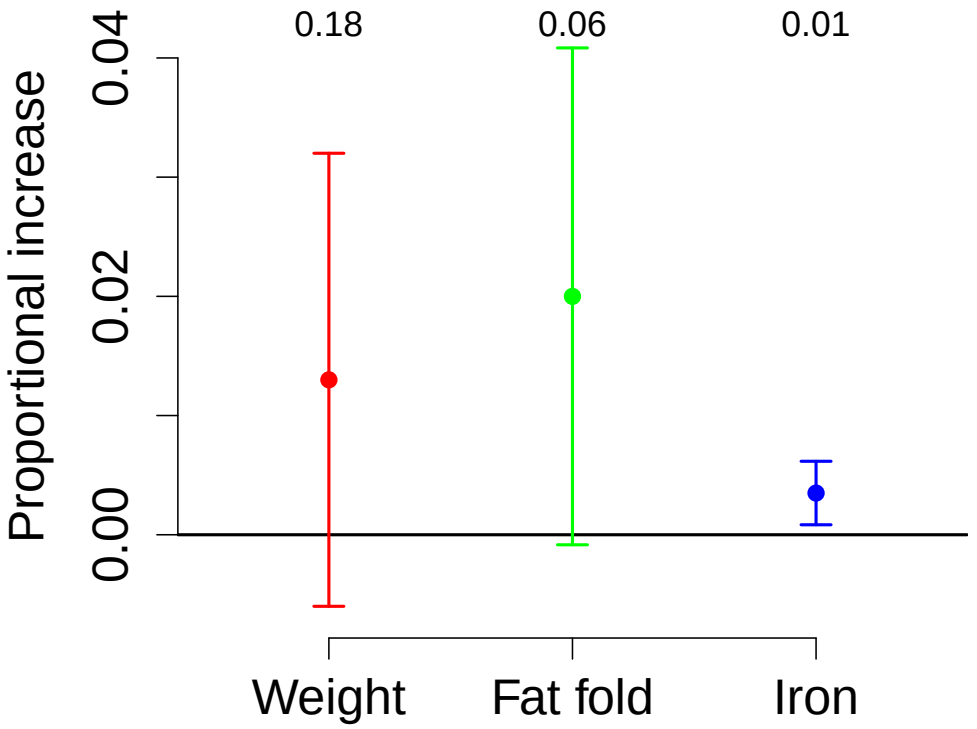
Vitamin study



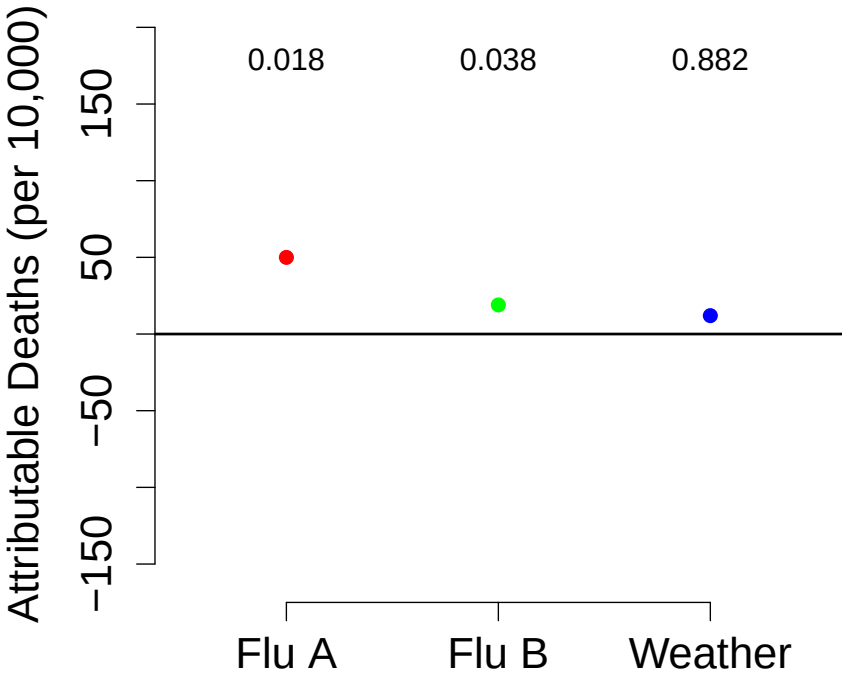
Discussion

- 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?

Vitamin study

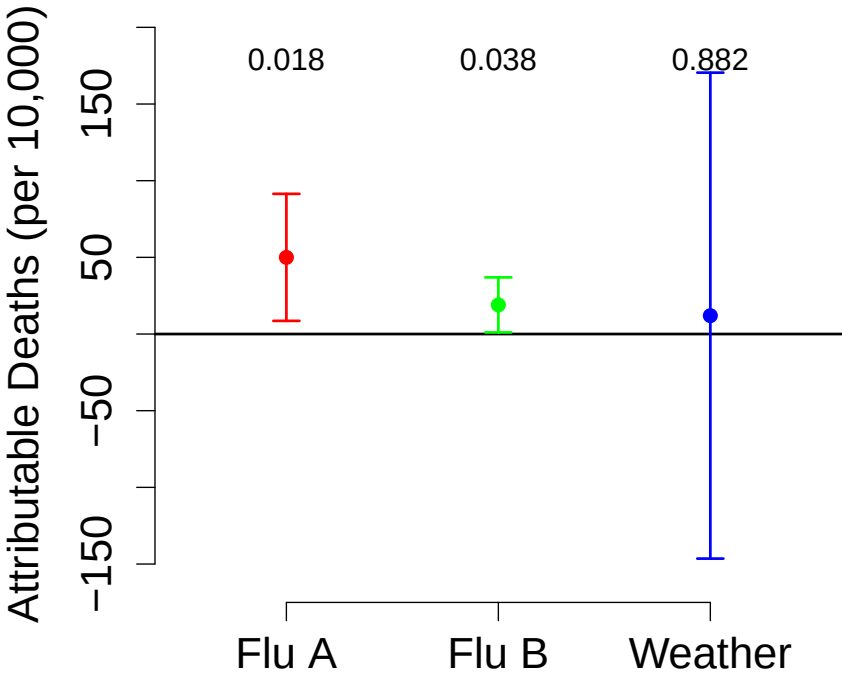


Annualized flu deaths



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

... with confidence intervals



- **Never** say: A is significant and B isn't, so $A > B$
- **Instead:** Construct a statistic for the hypothesis $A > B$
  - May be difficult

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

Outline

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?

Outline

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

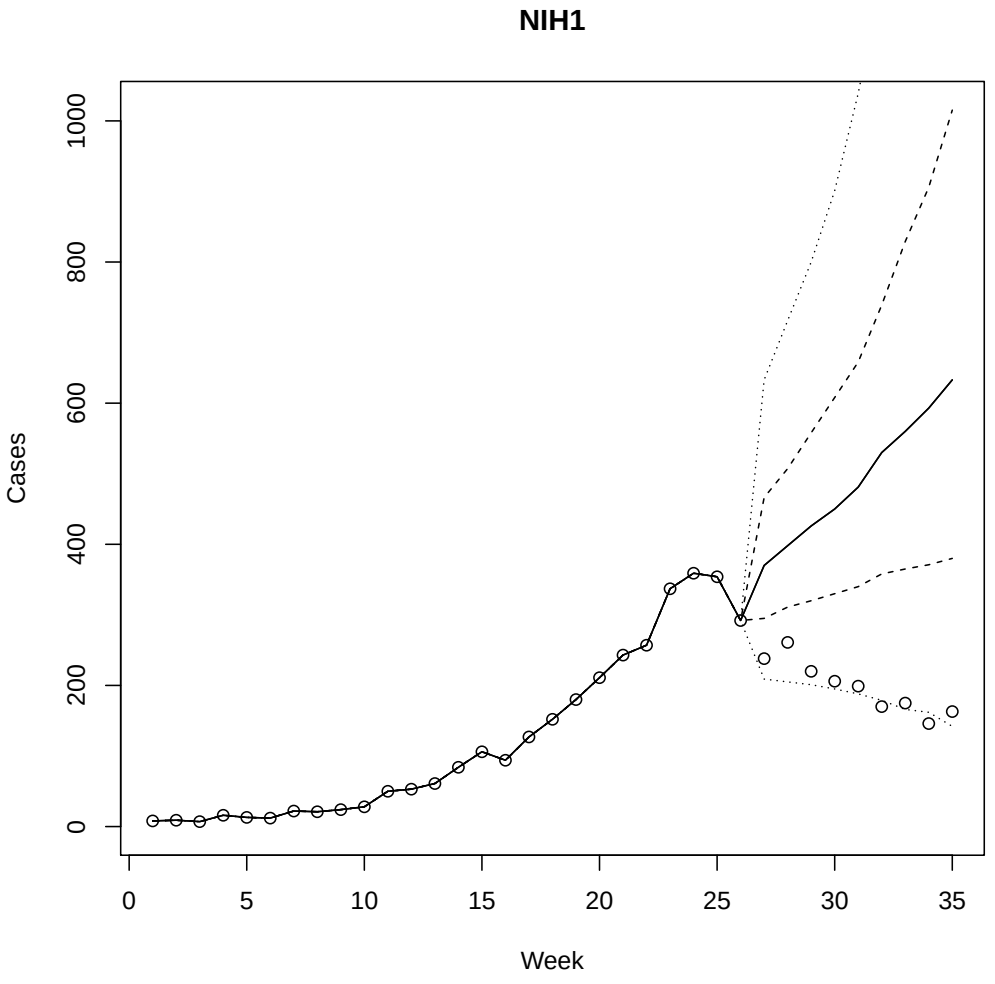
- What is **test set** spelled backwards?
- Hold some data out while fitting your model
- Or just *pretend* to do this as an evaluation method
  - In other words, test what would happen under various withholding scenarios

Other model worlds

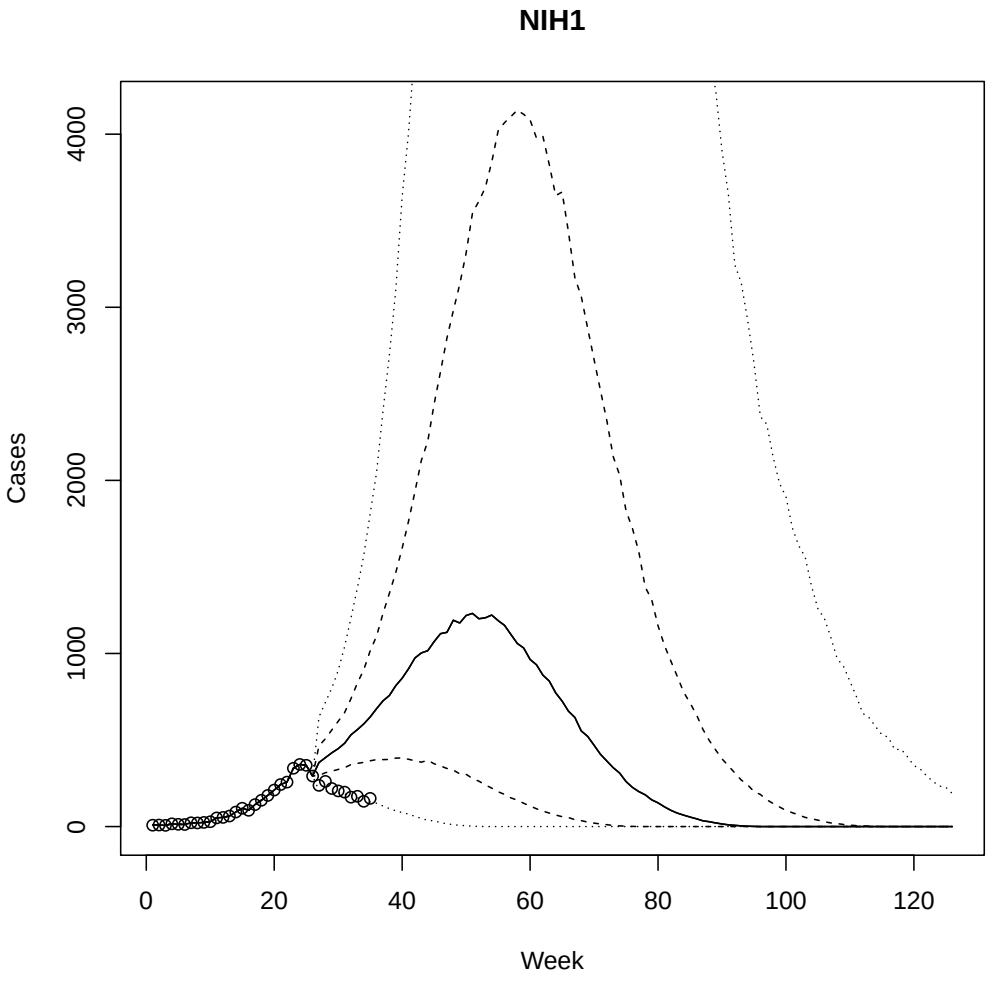
- The model you're *fitting* is probably pretty simple
- But you can *simulate* very complicated models, indeed

- How well can you do? Which details are important?

Other model worlds

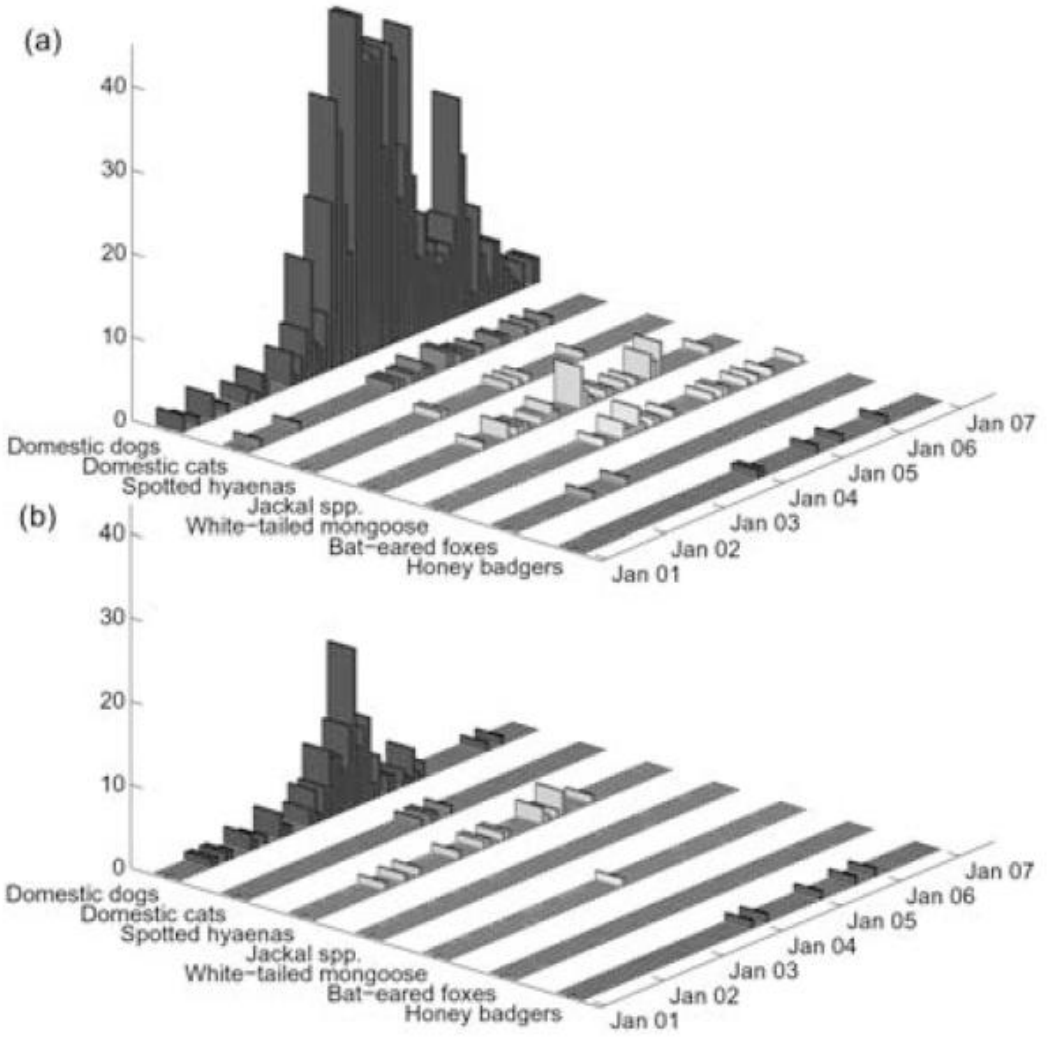


Other model worlds

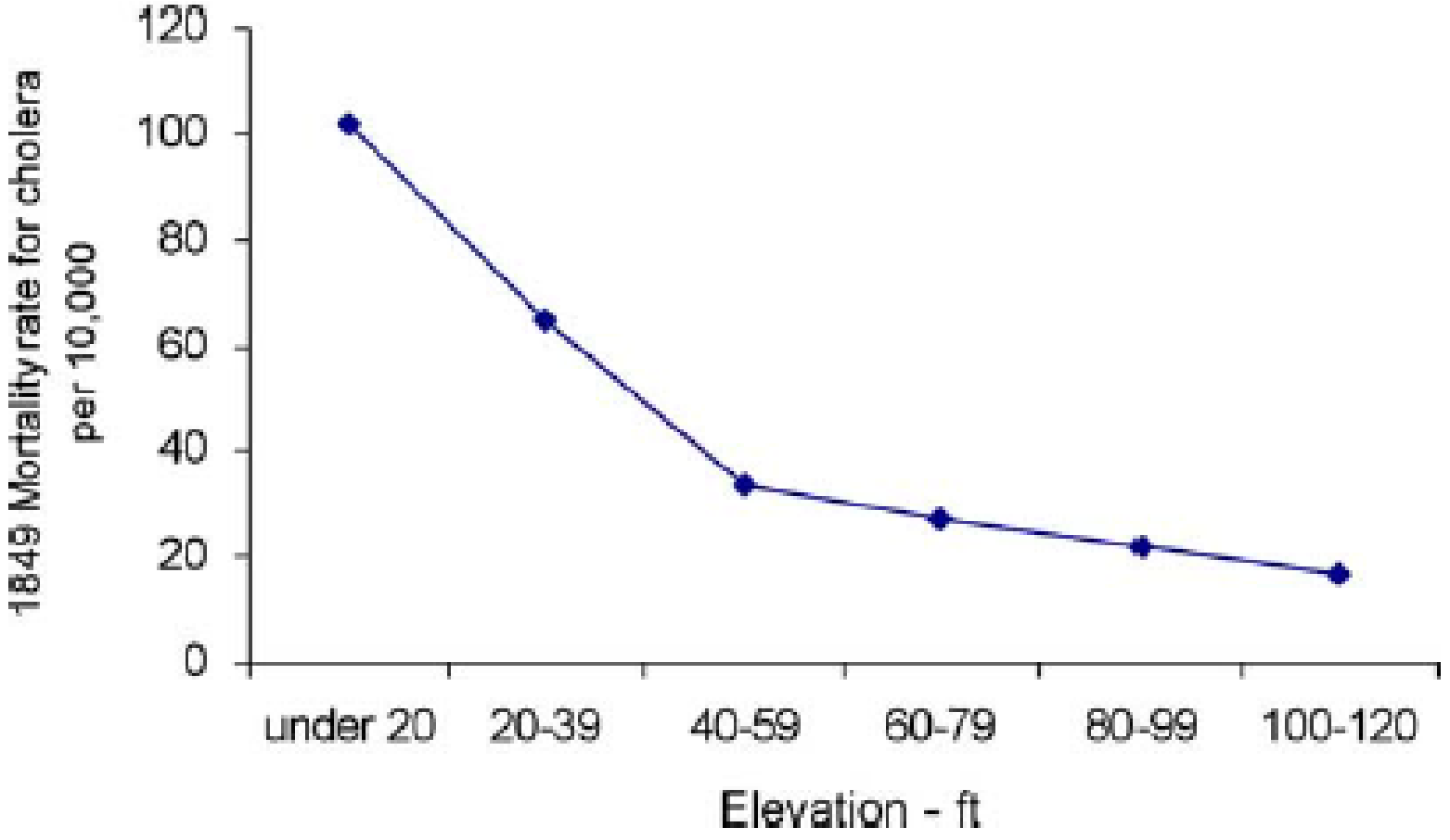


Generating hypotheses

Generating hypotheses



Testing hypotheses



Testing hypotheses

Testing hypotheses

Hard questions

Answers are not always easy

Outline

Summary

Dynamic models

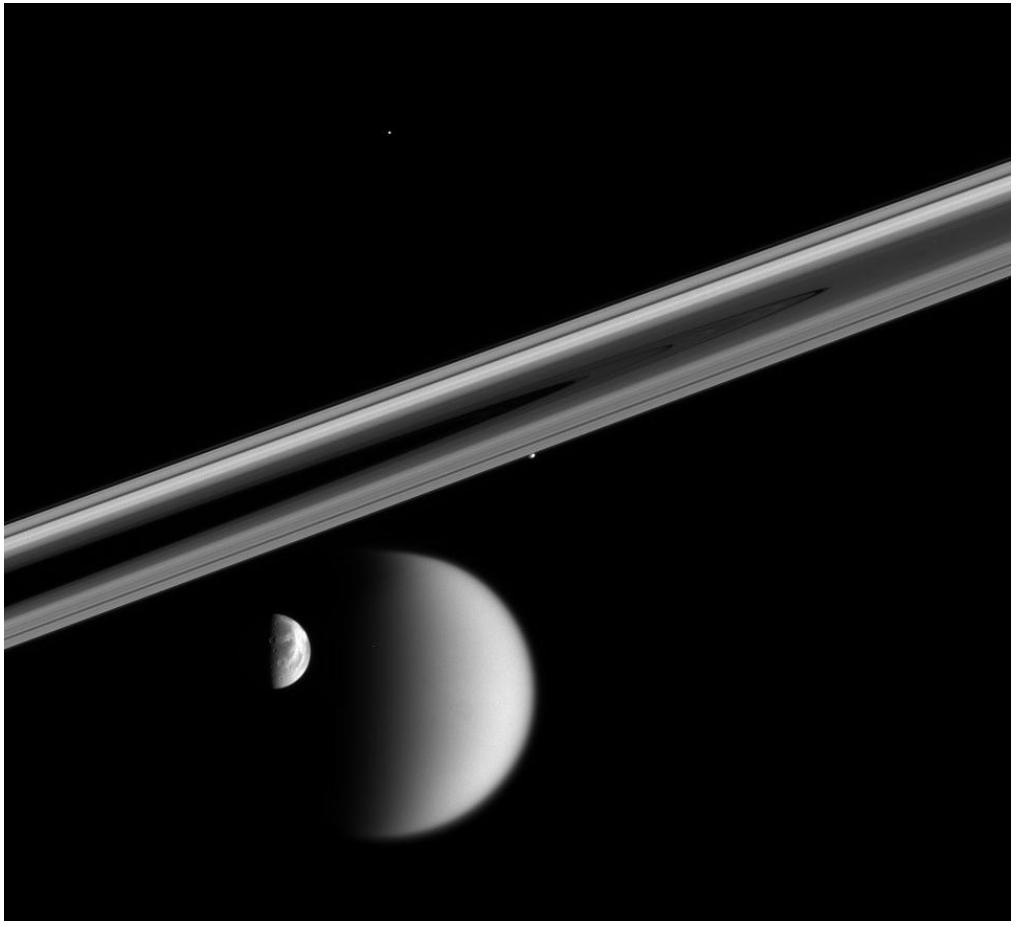
- Clarify thinking
  - What are our assumptions, what else do we need to know?
- Understand outcomes
  - Can heterogeneity explain the time course of HIV epidemics?
  - Is it possible that MDA could break the cycle of malaria transmission in some areas?
- Predict outcomes
  - What is the potential for 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

Conclusion



Essentially, all models are wrong, but some are useful.
– Box and Draper (1987), *Empirical Model Building . . .*

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