Ulysses’ Compass: Regularization

EES 5891-03

Bayesian Statistical Methods

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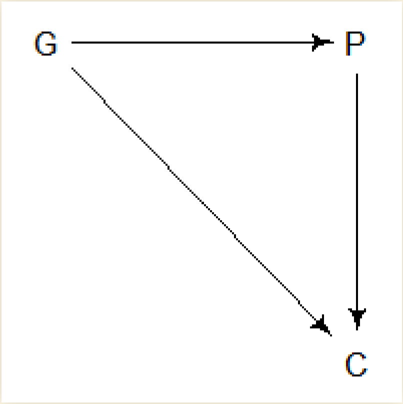
Class #9: Thursday, September 22 2022

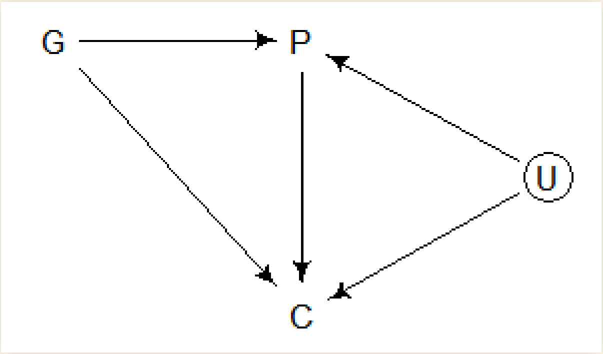
Examples of confounders

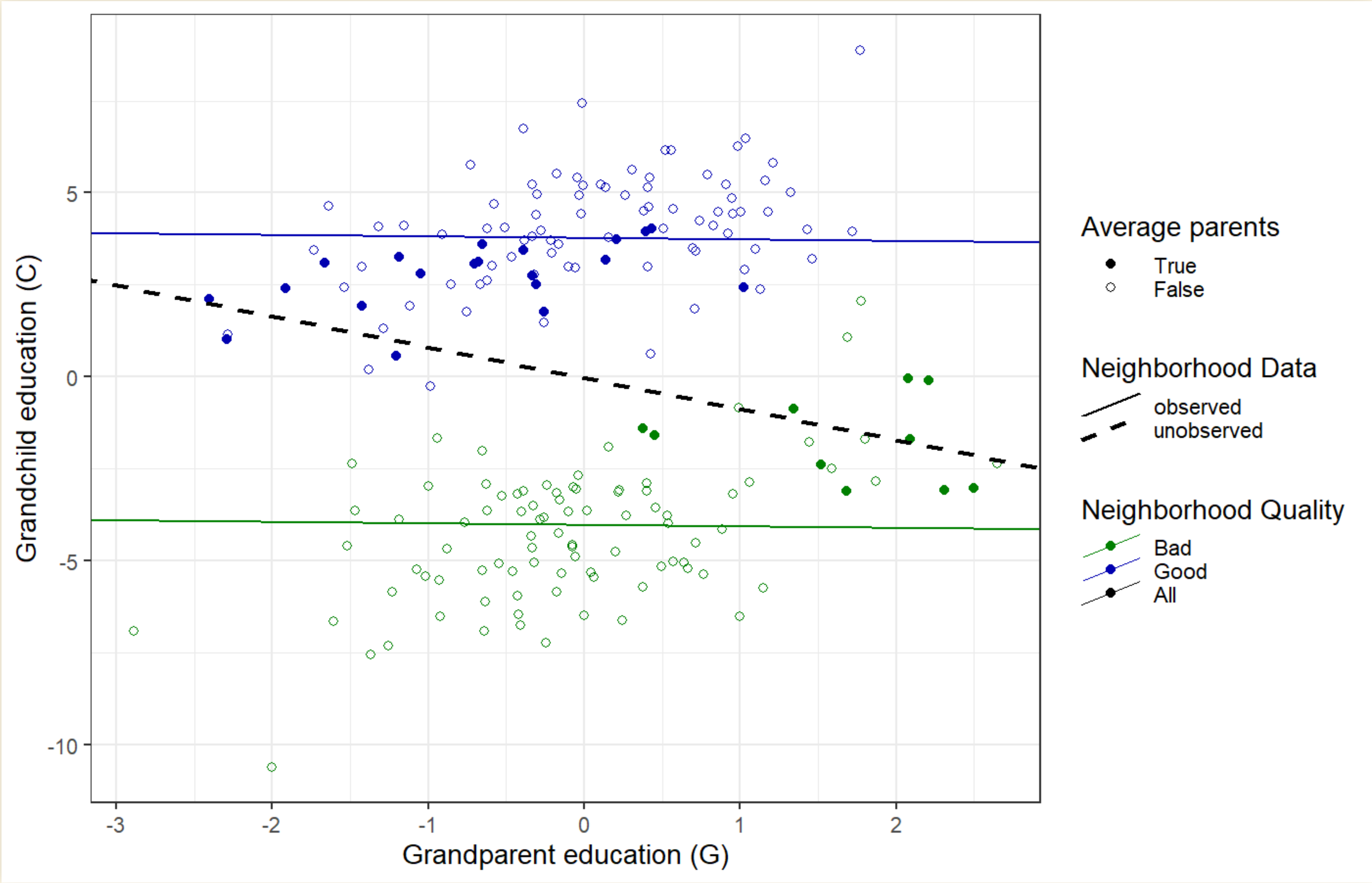
Example: Haunted DAG

- How do parents' *P* and grandparents' *G* educational attainment influence educational attainment of children *C*?



- But there are unmeasured effects here, such as the character of the neighborhood.
  - Grandparents moved into the neighborhood after they finished school,
  - Parents and children grew up in the neighborhood and are affected by it.

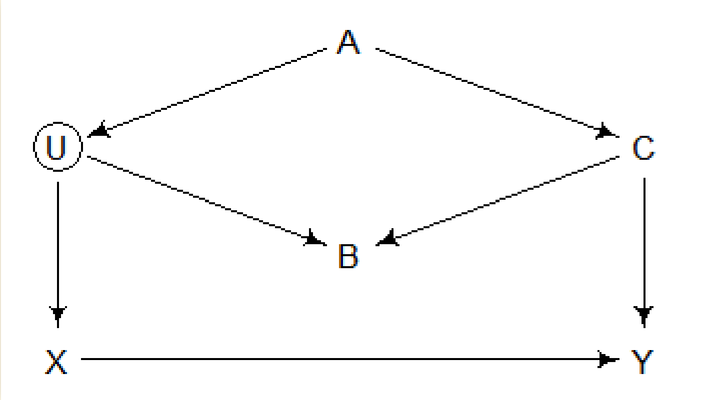




- There is a no correlation between *G* and *C* in each neighborhood
  - This is the correct answer.
- But when we don't account for the neighborhood effect, the collider bias makes it look like there's a negative correlation
  - more educated grandparents have less educated grandchildren

Backdoor Effects

- In the age and happiness example, conditioning on the marriage variable created bias,
- But in the grandparent, parent, and children example, we needed to condition on the neighborhood to avoid bias.
  - How can we tell when to condition on a variable?
- Consider this DAG:



- How does X affect Y?

- Backdoor paths:
  1. $X \leftarrow U \leftarrow A \rightarrow C \rightarrow Y$
  2. $X \leftarrow U \rightarrow B \leftarrow C \rightarrow Y$
- Which backdoor path is open?
  1. This path is open because it has no internal collider
  2. This path is closed because B is a collider.
     - If we condition on B, it will open the backdoor and introduce a collider effect.
- Closing backdoors:
  - We don't observe U, so we can't condition on it.
  - To close the backdoor path #1, condition on A or C.

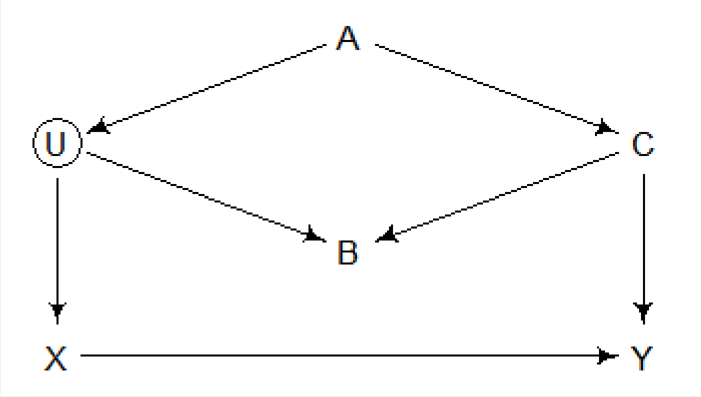
Automated Analysis

- Define the DAG

```
library(dagitty)
dag_two_roads <- dagitty("dag {
U [unobserved]
X -> Y
X <- U <- A -> C -> Y
U -> B <- C
}")
```

- Optionally, draw the DAG diagram

```
coordinates(dag_two_roads) <- list(
x = c(U = 0, X = 0, A = 1, B = 1, C = 2, Y = 2),
y = c(U = 0, X = 1, A = - 0.5, B = 0.5, C = 0, Y = 1)
)
drawdag(dag_two_roads)
```



- Analyze to identify which variables to condition on

```
adjustmentSets(dag_two_roads, exposure = "X", outcome =
        "Y")
```

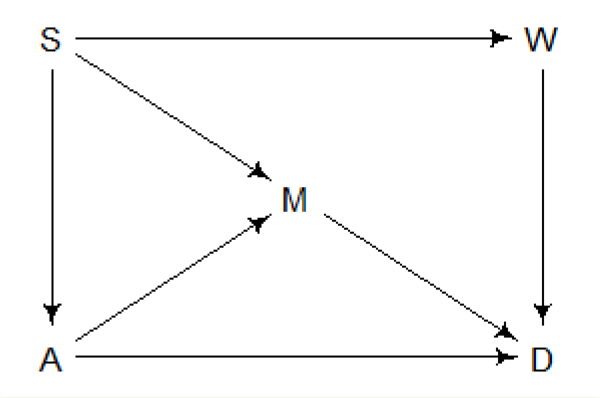
```
## { C }
## { A }
```

  - Condition on *A* or *C*

Backdoors in Waffle-House and Divorce

- Waffle-House and Divorce

```
dag_waffles <- dagitty("dag {
A -> D
A -> M -> D
A <- S -> M
S -> W -> D
}")
```



S = state, W = waffle-house restaurants,
A = median age at marriage, M = marriage rate,
and D = divorce rate.

- Identify which variables to condition on

```
adjustmentSets(dag_waffles, exposure="W", outcome="D")
```

```
## { A, M }
## { S }
```

  - What does this mean?

- Backdoors:

1. $W \leftarrow S \rightarrow M \rightarrow D$
2. $W \leftarrow S \rightarrow A \rightarrow D$
3. $W \leftarrow S \rightarrow A \rightarrow M \rightarrow D$

  - All of these pass through S.
  - To close the backdoors, either
    - Condition on S, or
    - Condition on both A and M.

- Further analysis: *conditional independencies*

```
impliedConditionalIndependencies(dag_waffles)
```

```
## A _||_ W | S
## D _||_ S | A, M, W
## M _||_ W | S
```

  - If we condition on S, then A and M should both be independent of W
  - If we simultaneously condition on A, M, and W, then D should be independent of S.

Bayes’s Theorem and Ockham’s Razor

Bayes's Theorem and Ockham's Razor

Everything should be made as simple as possible, but no simpler
— Einstein

- **Ockham's razor:** *Models with fewer hypotheses are to be preferred*
  - But we also prefer models that make better predictions
- How do we find the right balance between simplicity and completeness?
  - *Overfitting* versus *underfitting*
  - *Confounding:* Incorrect causal relationships can produce better predictions.
- Bayesian methods allow us to take a systematic formal approach to finding the best balance,
  - But we need some additional tools
- Tools for finding a good balance:
  - **Regularization:** Use a *regularizing prior* to avoid overfitting
    - Also called *penalized likelihood*.
  - **Cross-validation** and **information criteria**
    - **Cross-validation:** Fit parameters to part of your data and predict the rest.
    - **Information criteria:** Use *information theory* to measure how much value additional complexity adds.

Overfitting

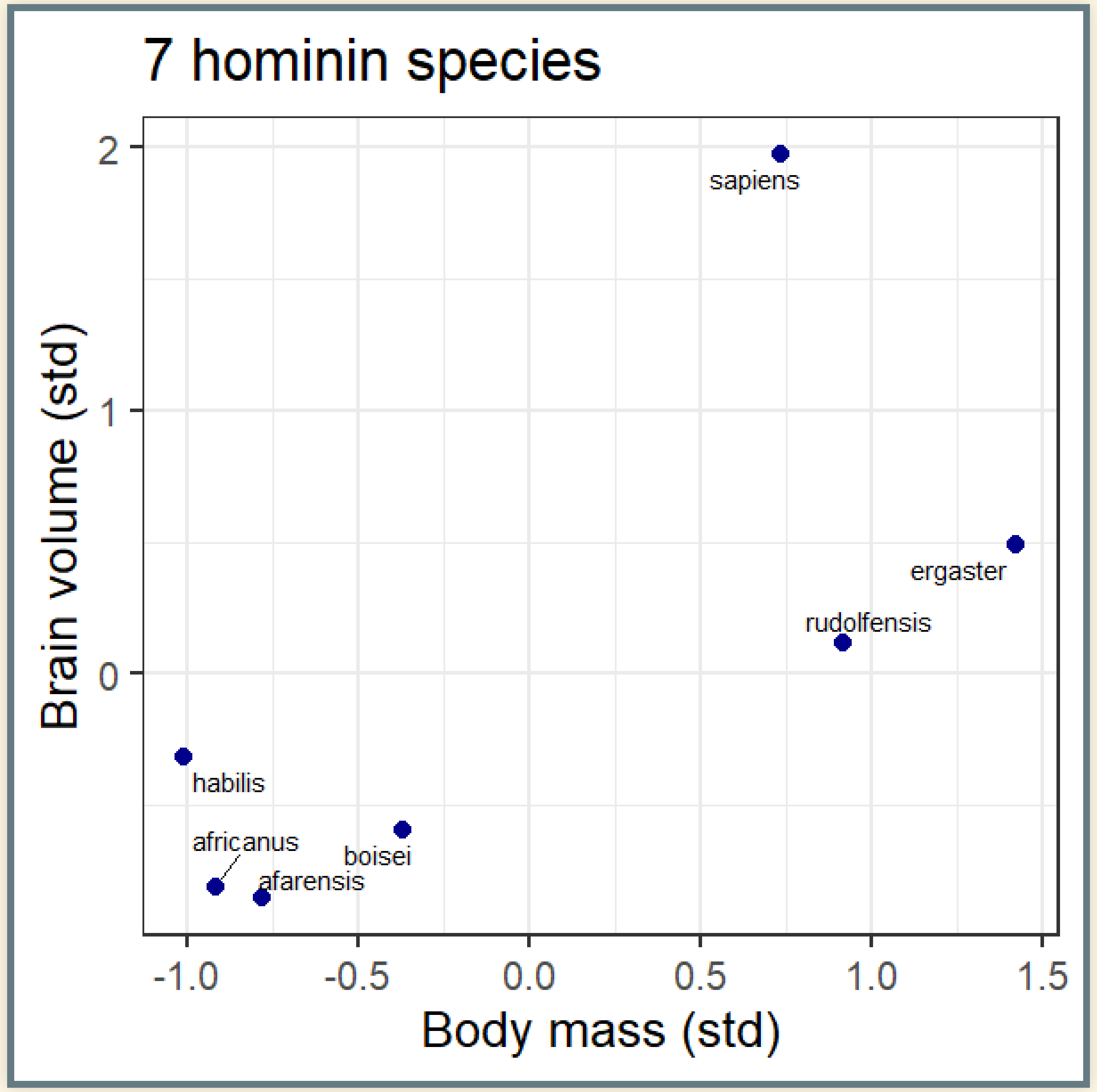
- **Correlation:** R^2

$$R^2 = \frac{\mathrm{var(data)} - \mathrm{var(residuals)}}{\mathrm{var(data)}} = 1 - \frac{\mathrm{var(residuals)}}{\mathrm{var(data)}}$$

  - R^2 increases the more parameters you add. Favors extreme overfitting.
    - Adding parameters almost always improves fit to current data
    - **Overfitting** happens when improving the fit to current data makes predictions of new data worse.

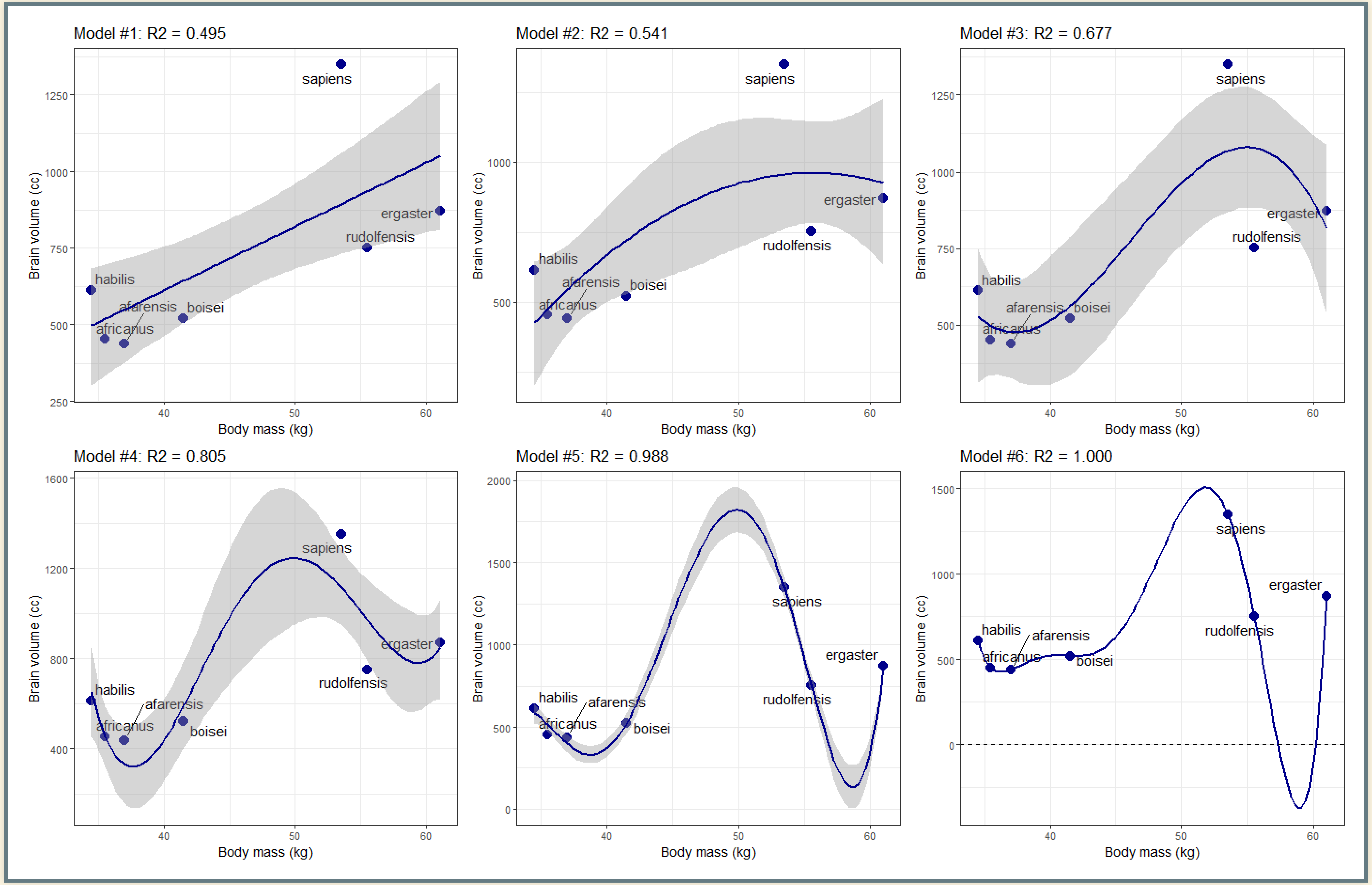
Example

- Data: relationship between brain volume and body mass for 7 hominin species.



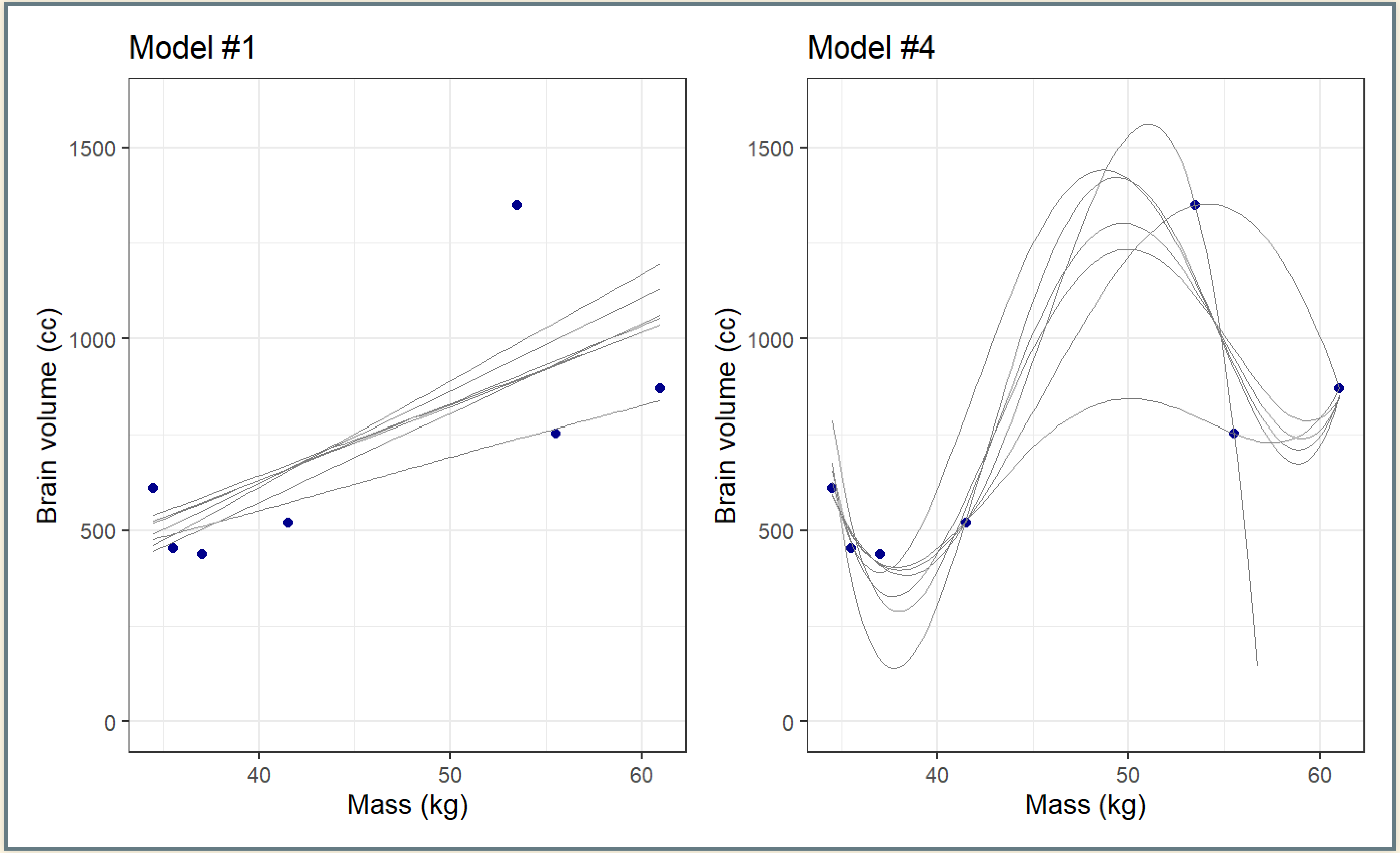
- Fit 6 models:
  1. $\mu = \alpha + \beta M$
  2. $\mu = \alpha + \beta_1 M + \beta_2 M^2$
  3. $\mu = \alpha + \beta_1 M + \beta_2 M^2 + \beta_3 M^3$
  4. $\mu = \alpha + \beta_1 M + \beta_2 M^2 + \beta_3 M^3 + \beta_4 M^4$
  5. $\mu = \alpha + \beta_1 M + \beta_2 M^2 + \cdots + \beta_5 M^5$
  6. $\mu = \alpha + \beta_1 M + \beta_2 M^2 + \cdots + \beta_6 M^6$
- Quality of fit:
  1. Model # 1 : $R^2 = 0.495$
  2. Model # 2 : $R^2 = 0.541$
  3. Model # 3 : $R^2 = 0.677$
  4. Model # 4 : $R^2 = 0.805$
  5. Model # 5 : $R^2 = 0.988$
  6. Model # 6 : $R^2 = 1.000$

Examining models



Underfitting vs. Overfitting

- Sensitivity to dropping one measurement:



Information Theory

Entropy & Accuracy

- There isn't a universal, objective standard for judging the best balance of overfitting and underfitting.
- But there are systematic procedures for arriving at the best balance
  1. Pick a **target:** what you want the model to do well at.
  2. Develop a measurement of **deviance:** How close does model come to the *target*?
- We use *information theory* to develop a systematic way of measuring *deviance*.
  - What will matter is only the *deviance* of *out-of-sample* predictions.

Assessing Accuracy

- Weather prediction:
  - On average, it rains 30% of the time and is sunny the rest of the time.
  - A naive model would predict 30% chance of rain every day
    - This model would be *well-calibrated* but fairly useless.
  - A model that says it never rains will be correct 70% of the time.
- Do we care more about some kinds of errors than others?
  - It's worse not to have an umbrella when it rains than to carry one and not need it.
- **Joint likelihood:** probability of getting day 1 right *and* day 2 right *and* day 3 right …
  - **Log scoring rule:** The log of the joint probability is the sum of the logs of the individual probabilities.
- So we use the log of the probability to score accuracy.

Infomation

- **Information** is the *reduction in uncertainty when we learn an outcome*.
  - **Information entropy:** If there are n possible events with probabilities $p_1 \ldots p_n$, then

$$H(p) = -\sum_{i=1}^{n} p_i \log(p_i)$$

    - Example: if $p_{\text{sun}} = 0.7$ and $p_{\text{rain}} = 0.3$, then $H(p) = -(0.7 \log(0.7) + 0.3 \log(0.3) = 0.61.$
    - In another place, where $p_{\text{rain}} = 0.01$ and $p_{\text{sun}} = 0.99$, $H(p) = 0.06$.
      - Because there is so much more certainty about the weather on an average day, you learn a lot less from new data.

Divergence

- *Information entropy* measures uncertainty about the world (data).
- *Divergence* compares what we know about the world from data to what our model predicts.
  - **Divergence:** is the *additional uncertainty in using probabilities from one distribution to describe another distribution*.
    - The uncertainty in using observed data to make predictions about new data
  - Kullback-Liebler divergence:

$$D_{\mathrm{KL}} = \sum_i p_i(\log(p_i) - \log(q_i)) = \sum_i \left(\frac{p_i}{q_i} \right),$$

  p_i are the true probabilities, q_i are our model's estimates of the probabilities.
    - If the model probabilities are correct, then $q_i = p_i$ and $D_{\mathrm{KL}} = 0$.

Measuring divergence

- The point of making a model is that we don't know the true probabilities p_i, and we want to estimate them with the model's q_i, so how can we measure the divergence?
- We can't measure p_i, but we can still use divergence to compare two models q and r:

$$
\begin{aligned}
D_q &= \sum_i p_i(\log(p_i) - \log(q_i)) \\
D_r &= \sum_i p_i(\log(p_i) - \log(r_i)) \\
D_q - D_r &= \sum_i p_i(\log(p_i) - \log(q_i)) - p_i(\log(p_i) - \log(r_i)) \\
&= \sum_i p_i(\log(r_i) - \log(q_i))
\end{aligned}
$$

Divergence and Entropy

- The difference in divergence between two models q and r is

$$D_q - D_r = \sum_i p_i(\log(r_i) - \log(q_i))$$

- We can approximate this as

$$S(r) - S(q),$$

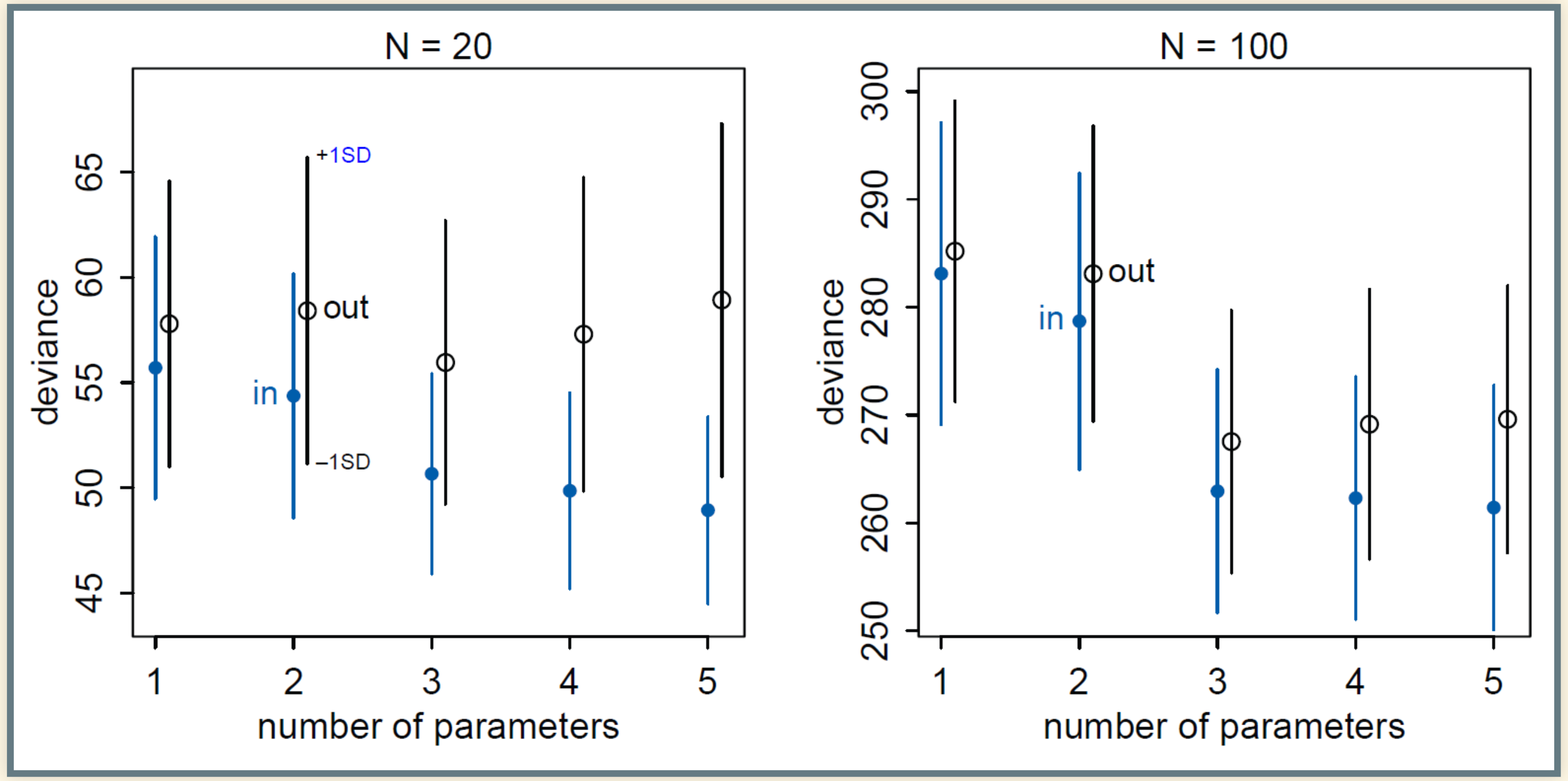
where

$$S(q) = \sum_i \log(q_i)$$

- Use the function `lppd()` from the `rethinking` package to calculate the log-point wise-predictive density from a `quap` model. `lppd(mdl, n = 1E4)` will calculate the log of the posterior probability of the model at 10,000 points. You can then use `sum()` to add these up and calculate the entropy $S(\texttt{mdl})$
- We generally define **deviance** as $-2S(q)$.
  - Larger values of deviance are worse.

Using Entropy to Test Models

- *Training data* vs. *test data*:
  - Divide your data into two parts.
    - Use the *training data* to train your models
    - Use your models to predict the *test data*
    - Compare the KL-divergence of the models using the test data predictions.
- Example:
  - Generate data using a process with 3 parameters
    - *Training* set with *N* samples
    - *Test* set with *N* examples
  - Fit models with 1 to 5 parameters, using *training* data.
  - Measure deviance:
    - *In-sample* (*training* data)
    - *Out-of-sample* (*test* data)

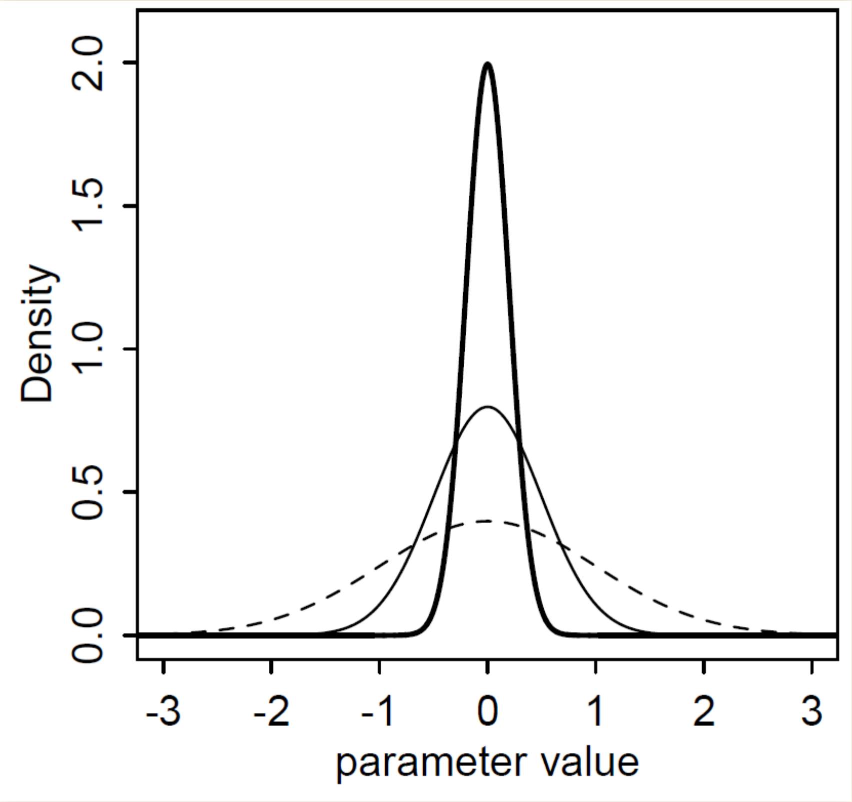


- Minimum in-sample deviance for 5 parameters
- Minimum out-of-sample deviance for 3 parameters
- Deviance estimates are more reliable for larger *N* (number of measurements)

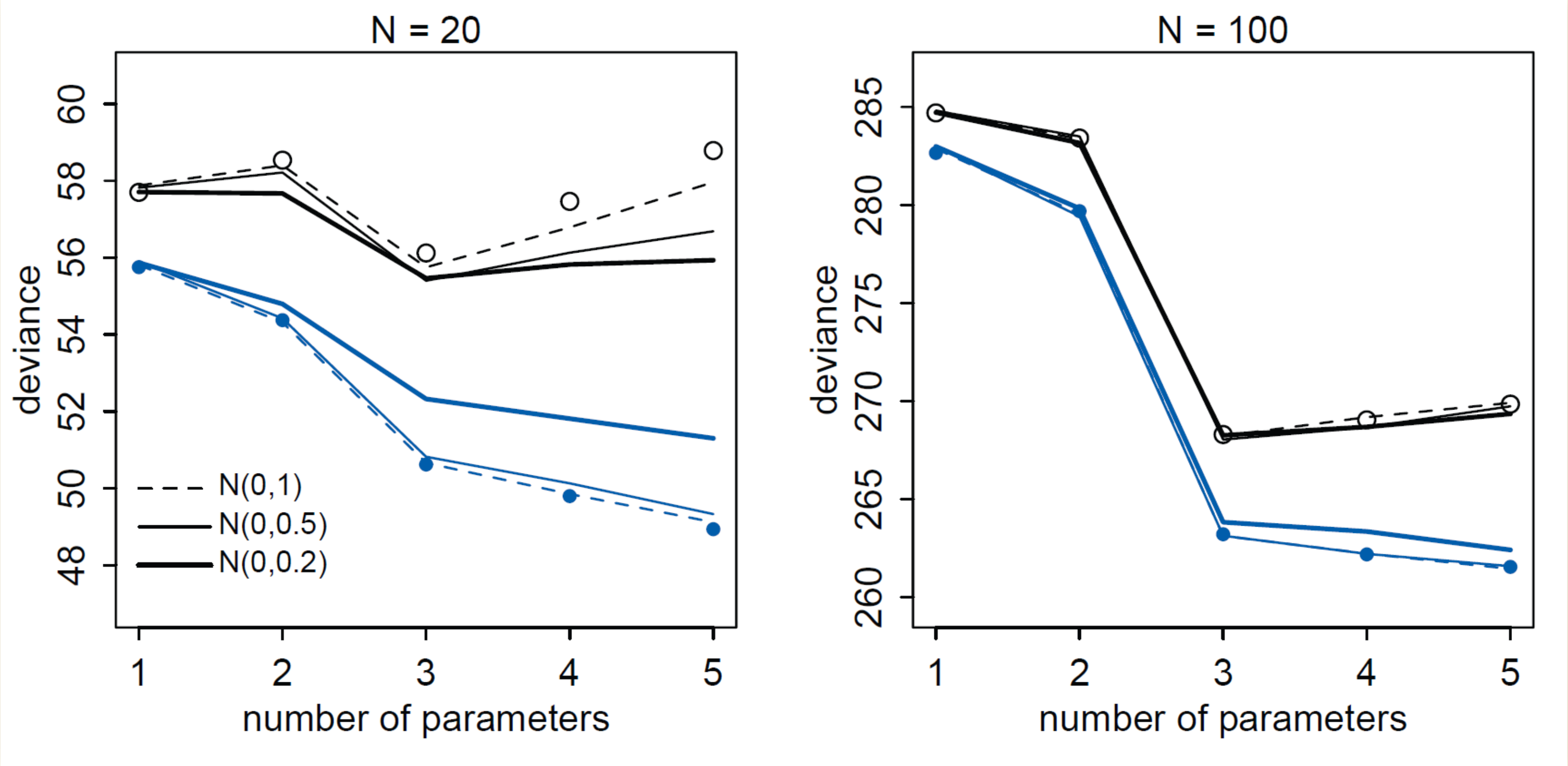
Regularization

Regularizing Priors

- Alternate approach: *regularizing priors*
  - Widely used in Machine Learning
  - Making the model worse at fitting *training data* can make it better at predicting *test data*.
  - Regularizing prior



Normal prior for β parameters:
dashed: Normal(0,1), thin: Normal(0,0.5), and thick: Normal(0,0.2).



- When there is a lot of data (*N* = 100), the regularizing priors keep the out-of-sample deviance small, even with many parameters.
- Regularizing priors tend to force unnecessary parameters to small (near-zero) values.
- Fancier regularizing priors set a threshold and push parameters to be either far from zero or else very close to zero.

Predicting Predictive Accuracy

Cross-Validation

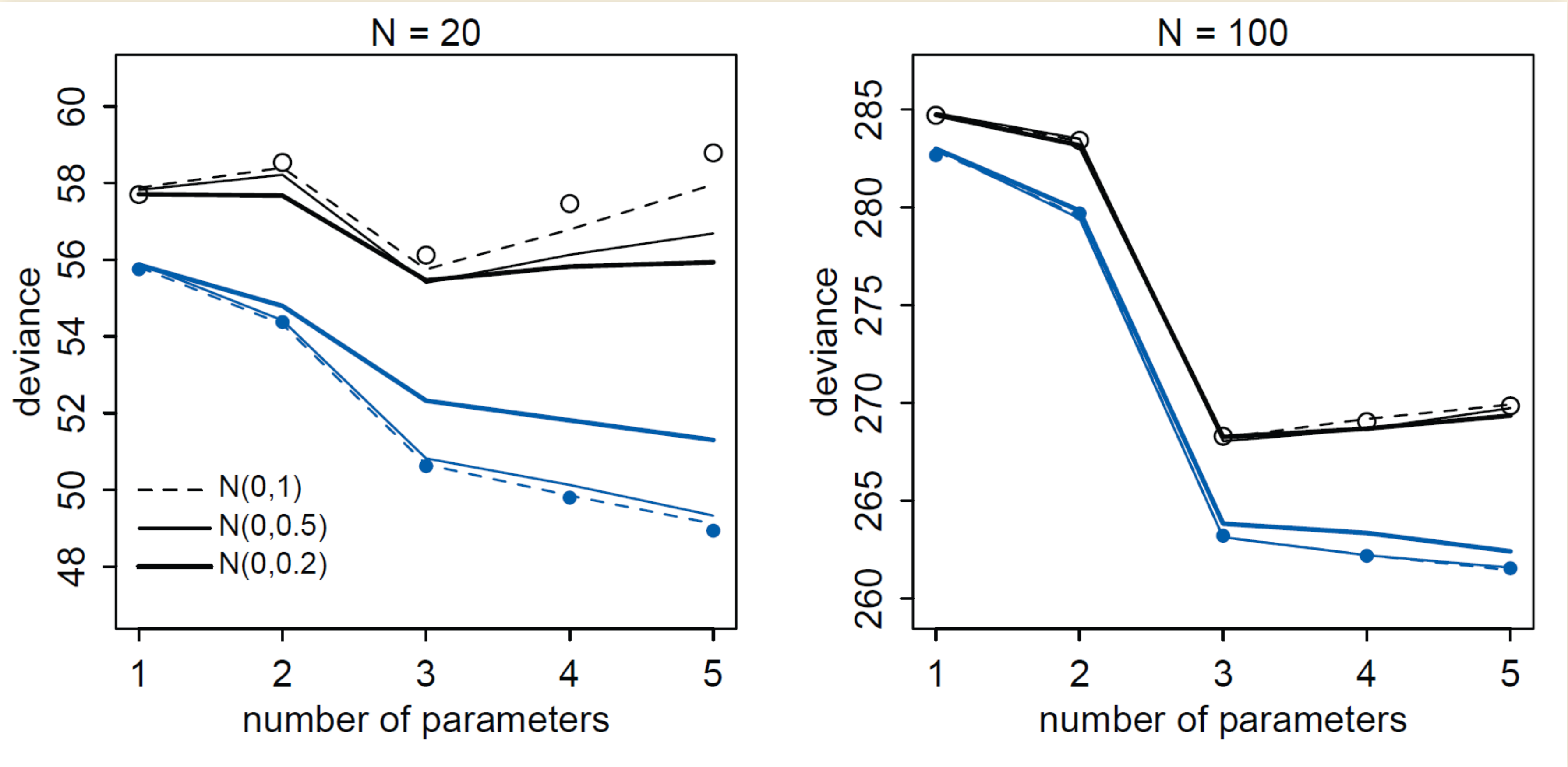
- How can we get a sense of how well our model will work with out-of-sample predictions?
- We started by splitting our data in half: *training* and *test* data.
- Sometimes it's not efficient to split our data in half.
- Can we do better?
- k-fold cross-validation:
  - Split data into k equal parts (example: k = 5)
    - For each part i (called a "fold"), fit the model to the other $k - 1$ parts and then predict part i.
    - Repeat this for all k parts.
    - Use all k folds to assess model performance
- Leave-one-out cross-validation (LOOCV):
  - An extreme form of K-fold cross-validation, where $k = N$, the size of the data.
  - For each data point, fit the model to all the others and then predict that one point.
- Problem: If you have N observations, then you have to fit your model N times. If N is large, this can be very slow.
- Pareto-Smoothed Importance Sampling (PSIS) is a fancy technique that lets us estimate LOOCV while we fit the model one time, without actually having to do real cross-validation.

Information Criteria

- As an alternative to cross-validation, use information theory to estimate the out-of-sample KL divergence.
- Examine the differences between in-sample and out-of-sample divergence in the figure
  - The difference is roughly twice the number of parameters.
    - In general, for relatively flat priors, the overfitting penalty is about twice the number of parameters.
  - Akaike Information Criterion (AIC)

$$\text{AIC} = D_{\text{train}} + 2p = -2\text{lppd} + 2p,$$

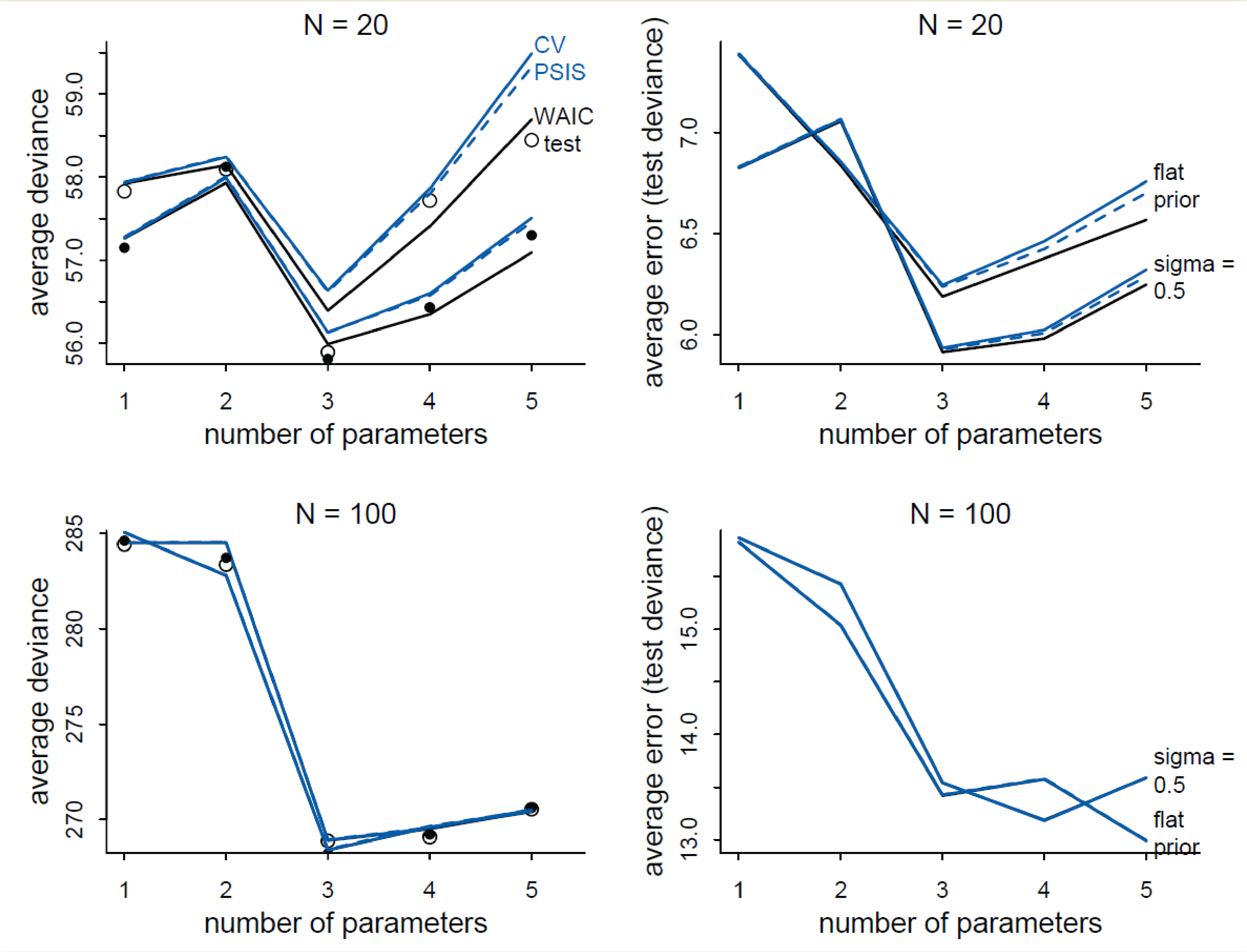
where `lppd` is the log-pointwise-predictive density (basically a sample of the posterior).



- Conditions for validity:
  - Priors are flat, or dominated by likelihood (data).
  - Posterior distribution is approximately Gaussian for each parameter.
  - The sample size N is much greater than the number of parameters k.

Other Information Criteria

- AIC is only valid under these conditions:
  - Priors are flat, or dominated by likelihood (data).
  - Posterior distribution is approximately Gaussian for each parameter.
  - The sample size *N* is much greater than the number of parameters *k*.
- Flat priors are usually not a good choice.
- DIC (Deviance Information Criteria) works with informative priors, but the other two criteria still apply.
- Watanabe-Akaike Information Criteria (WAIC, also called Widely Applicable Information Criterion) is more broadly applicable.
  - We won't go into details of calculating WAIC. The rethinking package will do it for us, and so will most other Bayesian analysis packages.
- General principle:
  - For all the information criteria we're examining, the smaller (more negative) they are, the better the model performs.



- Comparison of different measures

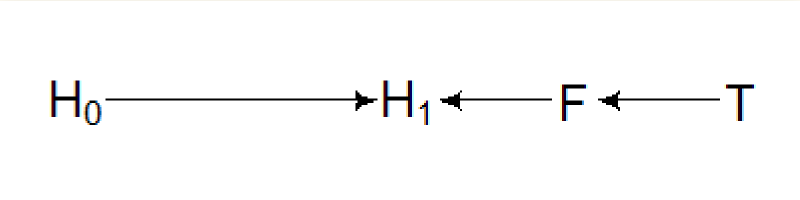
How to Compare Models

Comparison vs. Selection

- Many people use CV, PSIS, Deviance, or Information Criteria to select models
  - Use whatever model has the smallest score
- This is not wise. It only looks at what model is smallest, but doesn't consider how great the differences are between models.
  - This is like only looking at the mode (maximum) of the posterior and ignoring the rest of it.
  - The width the posterior matters too. It tells us about how uncertain the estimate is.
- When we compare models, look at how great the differences are between them.
- Remember that these criteria tell us about predictive power, but we have seen that predictive power doesn't tell us about causality.
  - Backdoor paths can have useful information, even though it's not causal.
    - But backdoor predictions only work if we don't interfere with the system.
      - In other words, if the future is just like the past.
    - In the plant-growth model, knowing about the fungus was a better predictor of plant growth than knowing about the anti-fungus treatment
      - but knowing about the fungus doesn't help us predict the effect of treating a field.

Example Using WAIC

- Plant growth experiment:
  - DAG



    H~0 = height before, H_1 = height after, T = anti-fungal treatment, F = fungus

  - Three models:

    1. μ log-Normal(0, 0.25)
    2. $\mu = \alpha + \beta_T T$
    3. $\mu = \alpha + \beta_T T + \beta_F F$

```
set.seed(11)
round(WAIC(mdl_TF), 2)
```

```
##      WAIC    lppd penalty std_err
## 1 361.45 -177.17    3.55   14.17
```

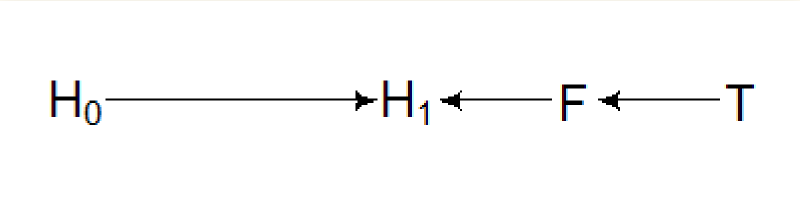
```
set.seed(77)
round(compare(mdl_0, mdl_T, mdl_TF, func = WAIC), 2)
```

```
##          WAIC    SE dWAIC   dSE pWAIC weight
## mdl_TF 361.81 14.26  0.00    NA  3.74      1
## mdl_T  402.65 11.20 40.84 10.44  2.58      0
## mdl_0  405.91 11.65 44.10 12.22  1.58      0
```

- Best predictions on top
- “d” variables are differences from the best model.
- pWAIC is prediction penalty (estimate of *out-of-sample* vs. *in-sample*)
- weight gives the relative support for each model, given the data.
  - Useful for model-averaging

Example Using WAIC

- Plant growth experiment:
  - DAG

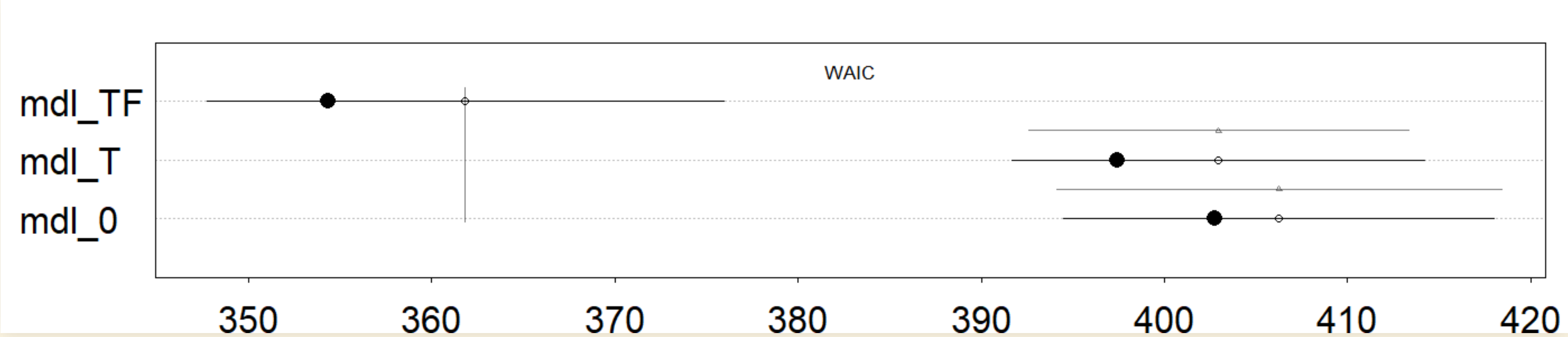


  H~0 = height before, H_1 = height after, *T* = anti-fungal treatment, *F* = fungus

  - Three models:

1. $\mu = \alpha + \beta_T T$
2. $\mu = \alpha + \beta_F F$
3. $\mu = \alpha + \beta_T T + \beta_F F$

```
plot(compare(mdl_0, mdl_T, mdl_TF, func = WAIC), cex=2,
        lwd=2)
```



- Plot:
  - Line is range of estimated out-of-sample deviance
  - Gray point is best estimate of out-of-sample deviance
  - Black point is in-sample deviance
  - Light lines over models are differences from best model
- TF model is clearly the best for predictions
  - We can't tell which of the others is better
- TF model has post-treatment confounder
  - WAIC can't tell us about causation