AARHUS UNIVERSITY

Methods 4 - 7

Chris Mathys

BSc Programme in Cognitive Science

Spring 2024

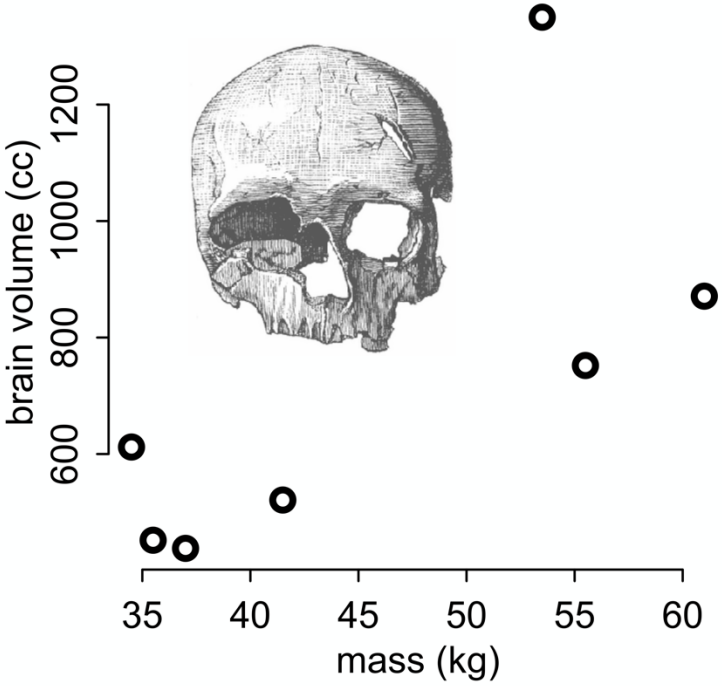
Problems of Prediction

What function describes these points? (fitting, compression)

What function explains these points? (causal inference)

What would happen if we changed a point's mass? (intervention)

What is the next observation from the same process? (prediction)



Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Leave-one-out cross-validation

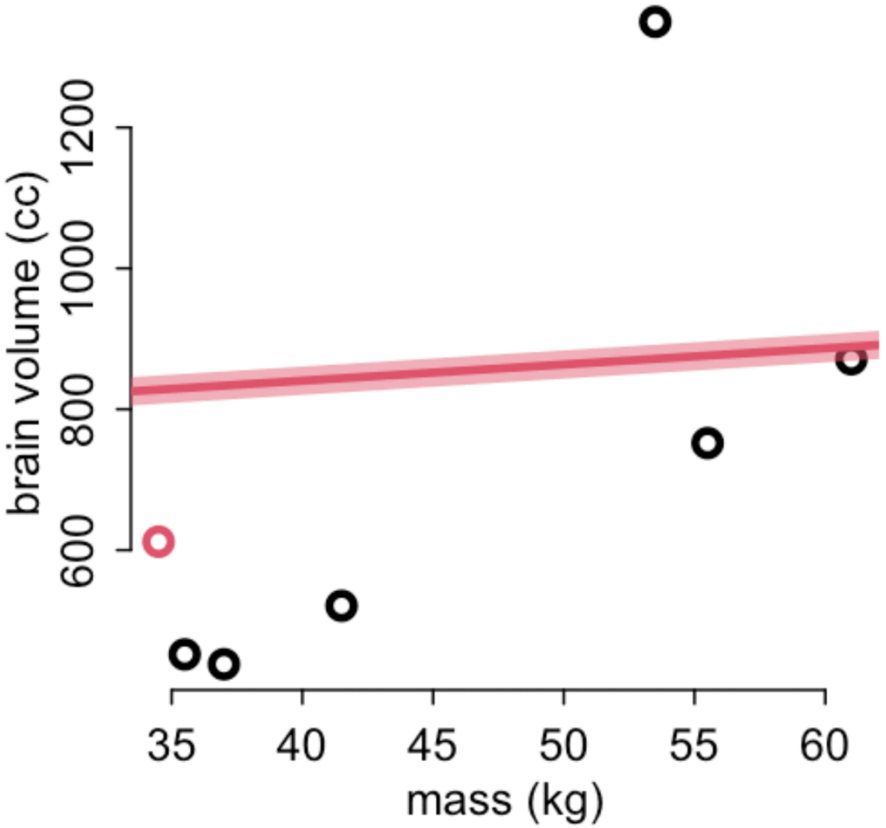
(1) Drop one point

(2) Fit line to remaining

(3) Predict dropped point

(4) Repeat (1) with next point

(5) Score is error on dropped



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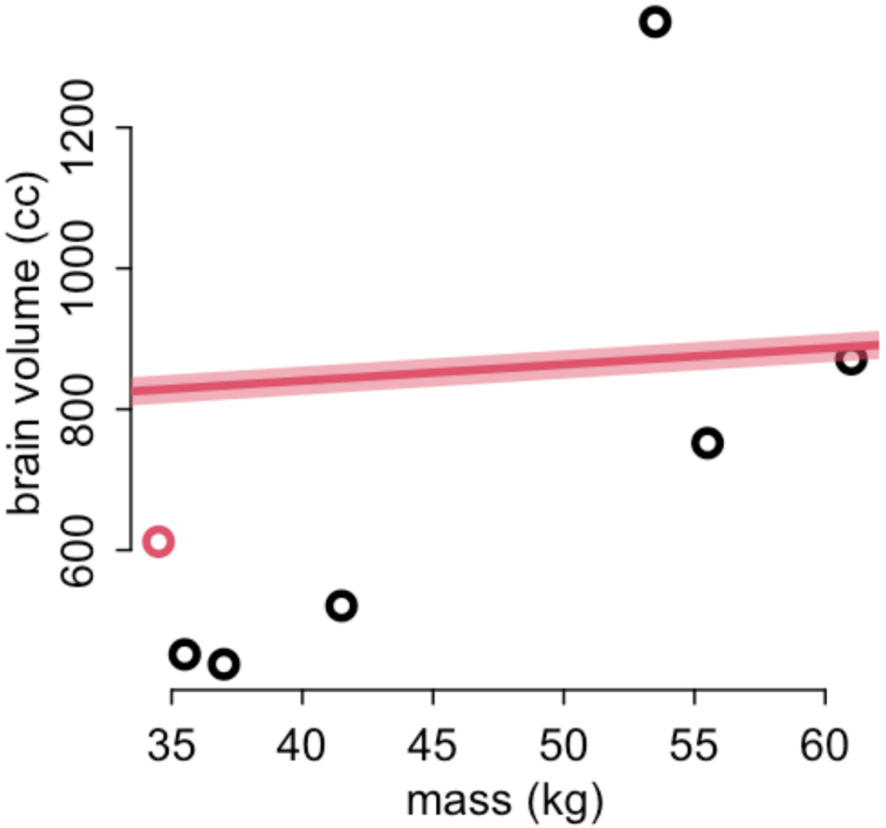

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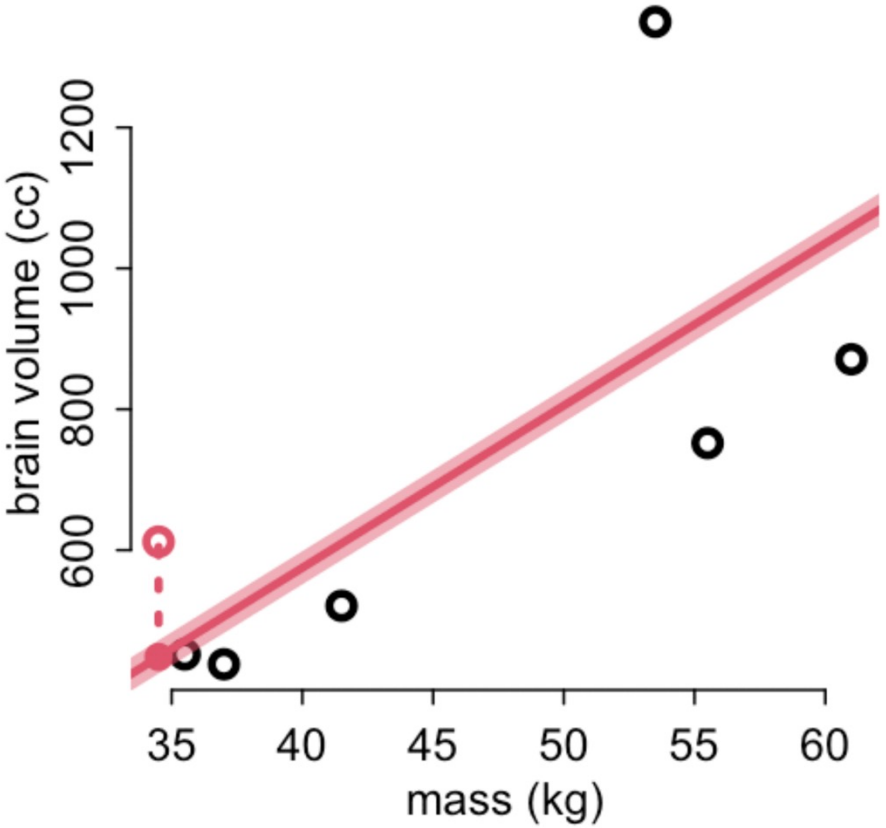

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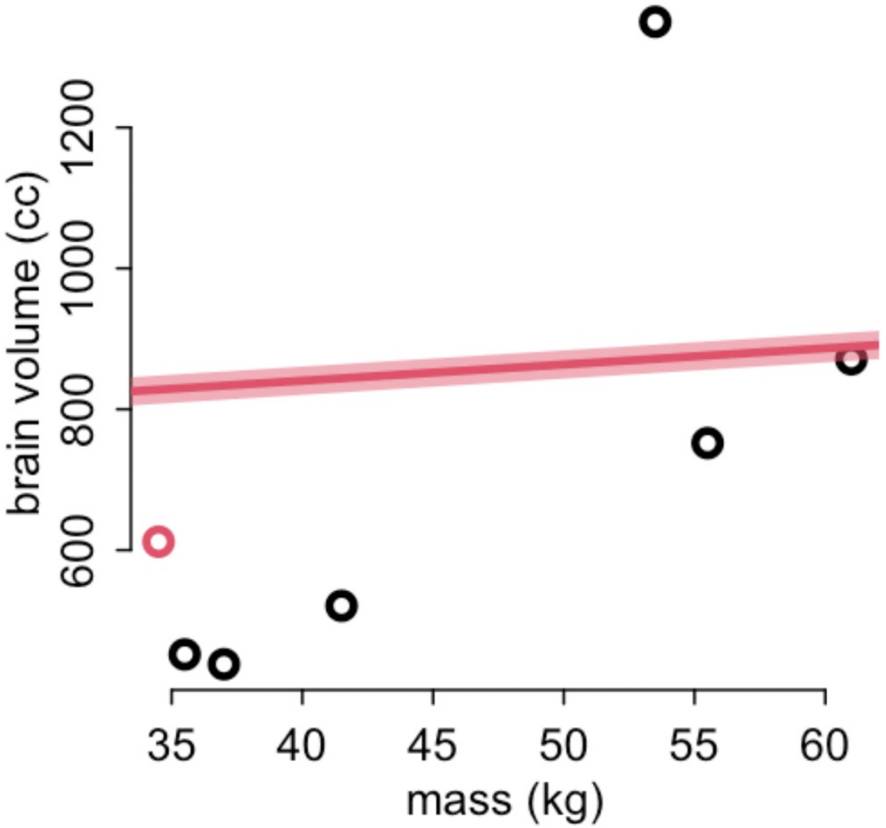

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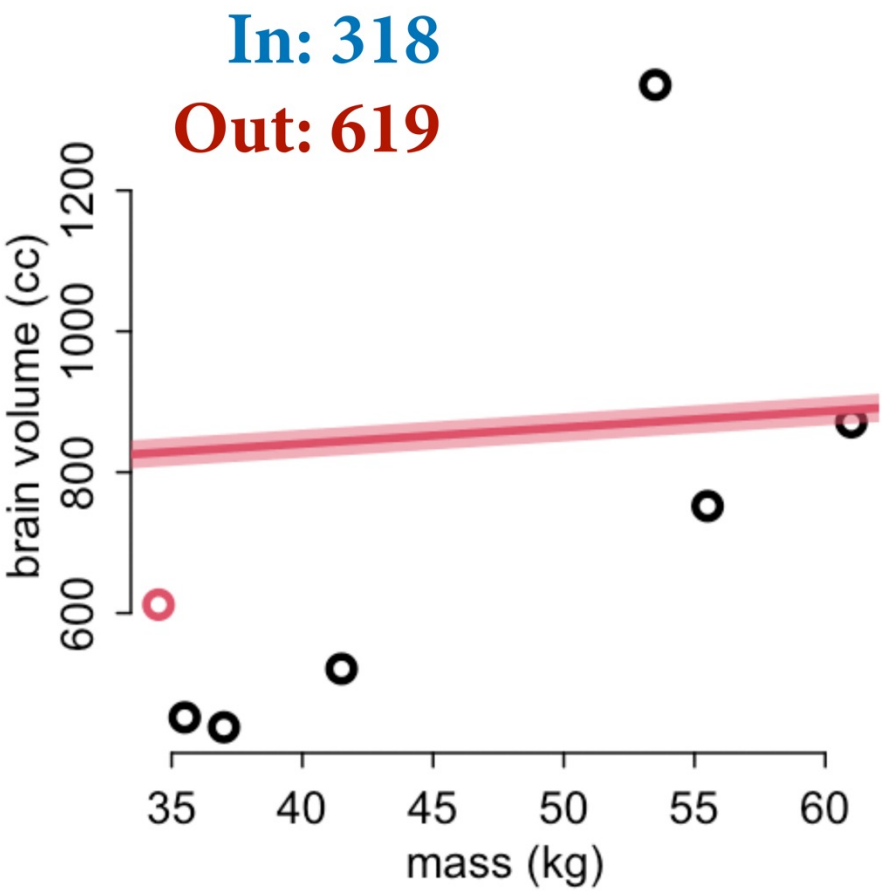

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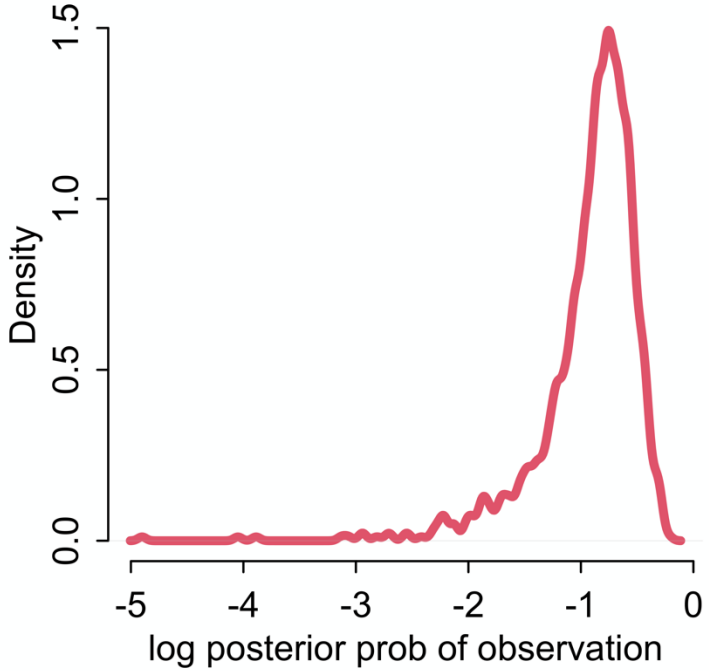
Bayesian Cross-Validation

We use the entire posterior, not just a point prediction

Cross-validation score is:

$$\text{lppd}_{\text{CV}} = \sum_{i=1}^{N} \frac{1}{S} \sum_{s=1}^{S} \log \Pr(y_i | \theta_{-i,s})$$



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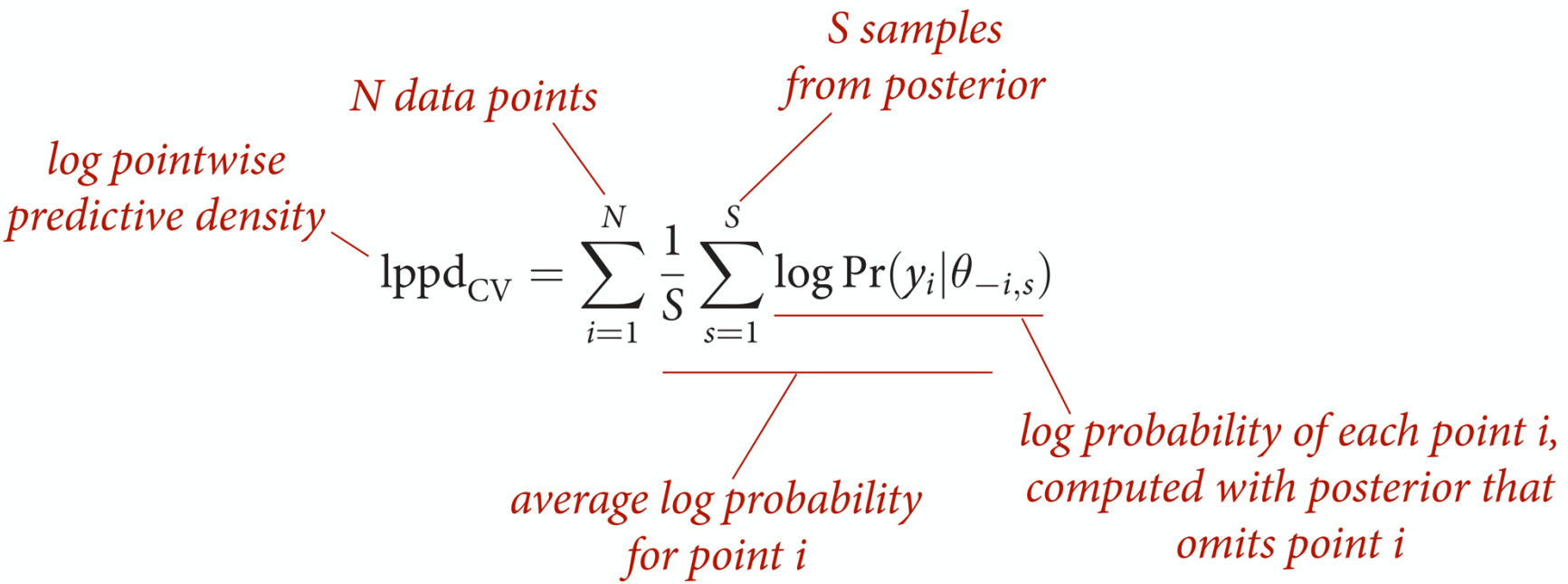
Bayesian Cross-Validation



Pages 210 and 218

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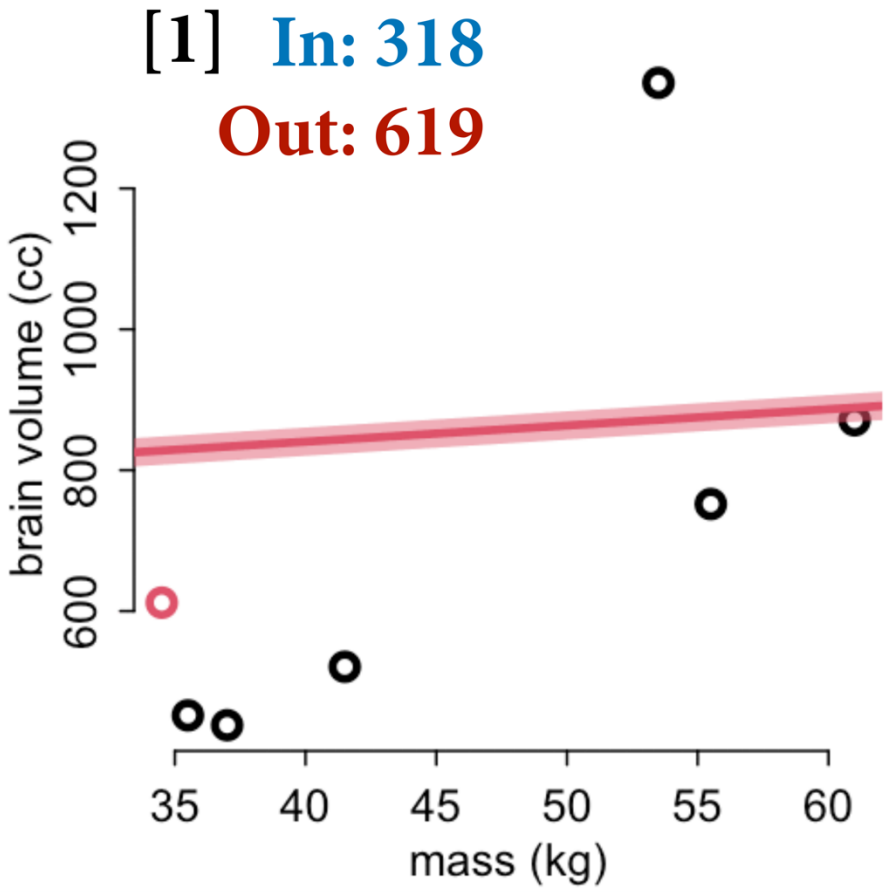

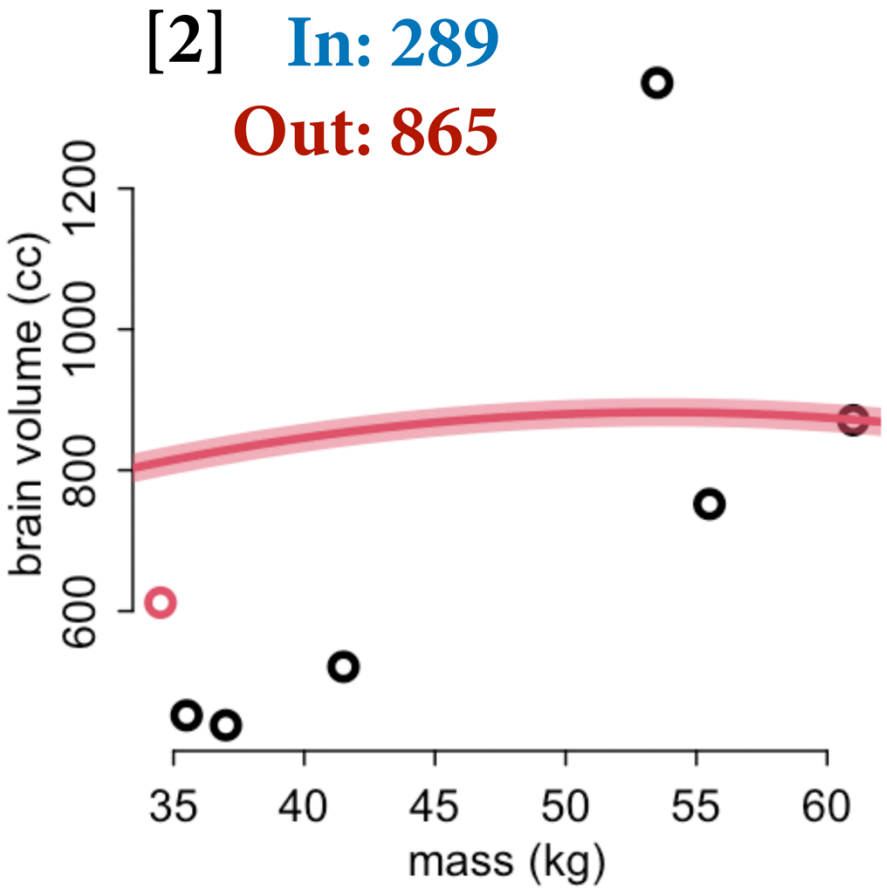

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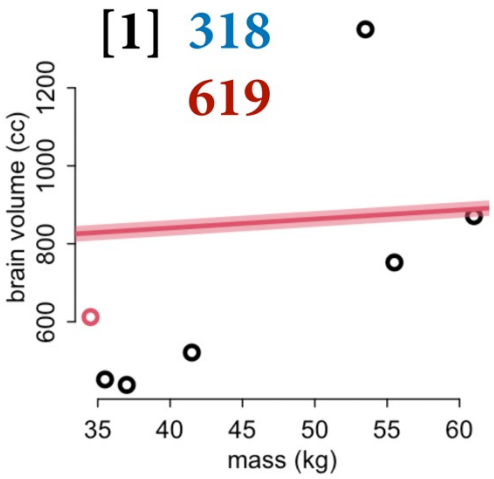

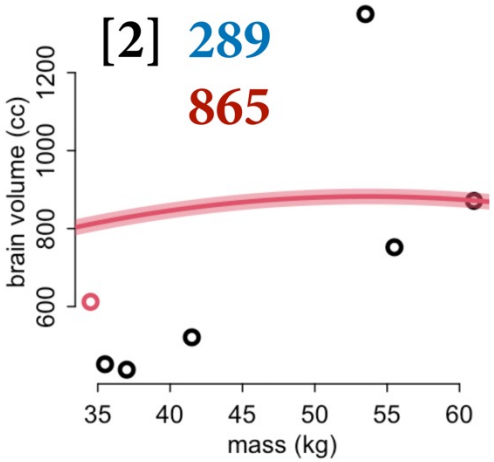

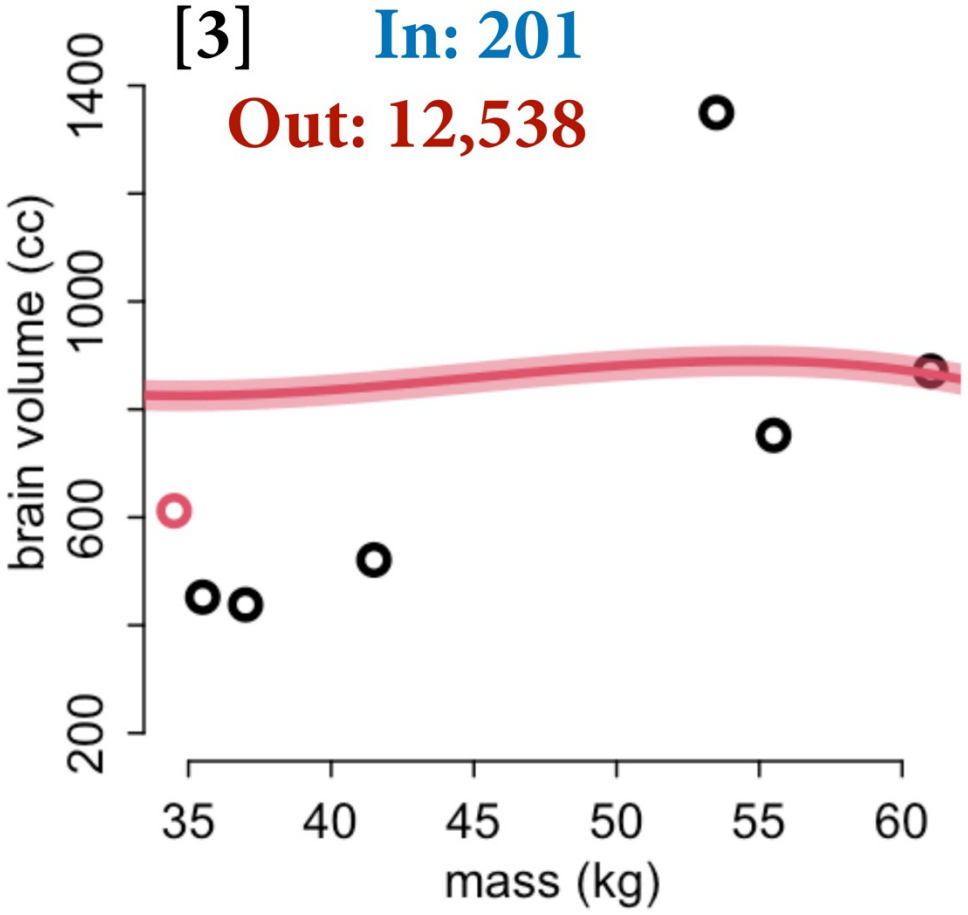

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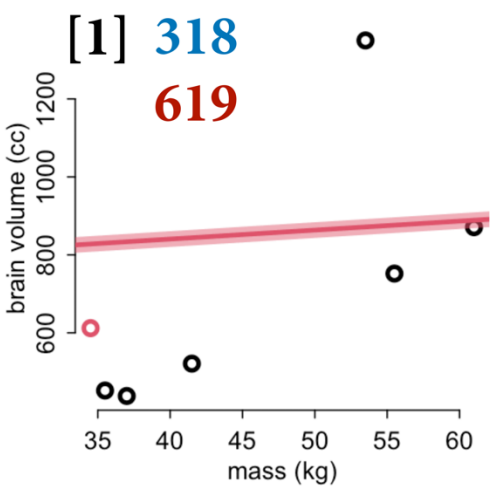

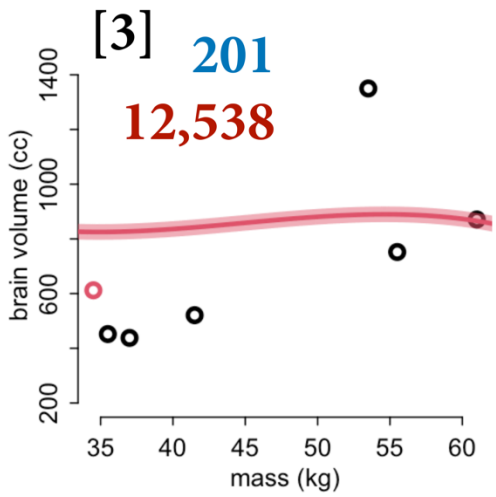

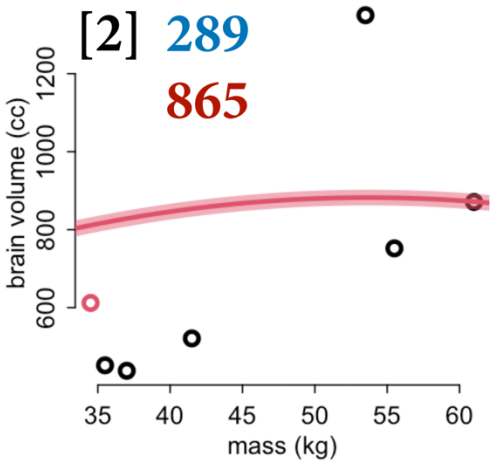

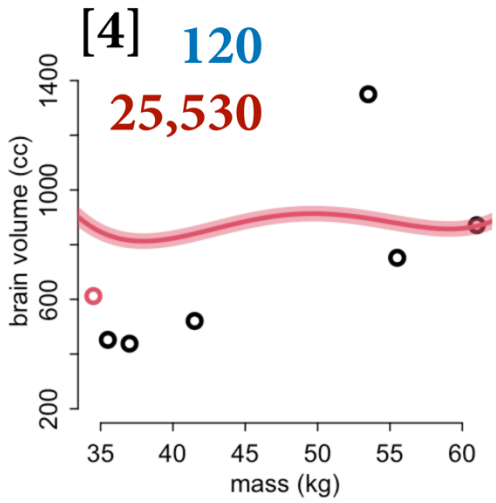

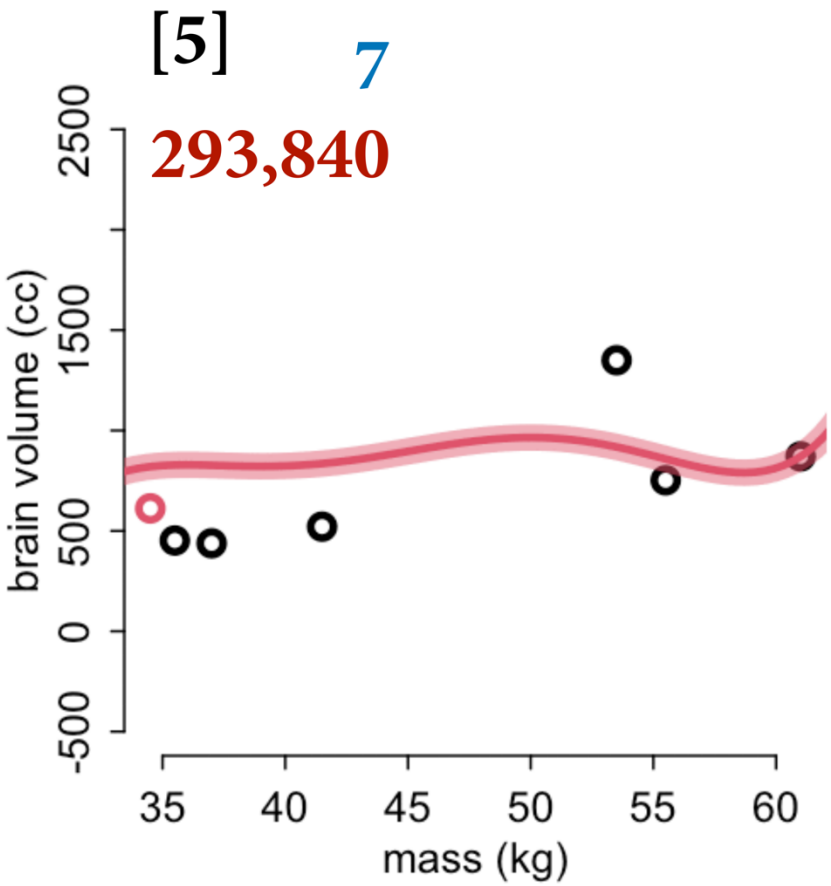

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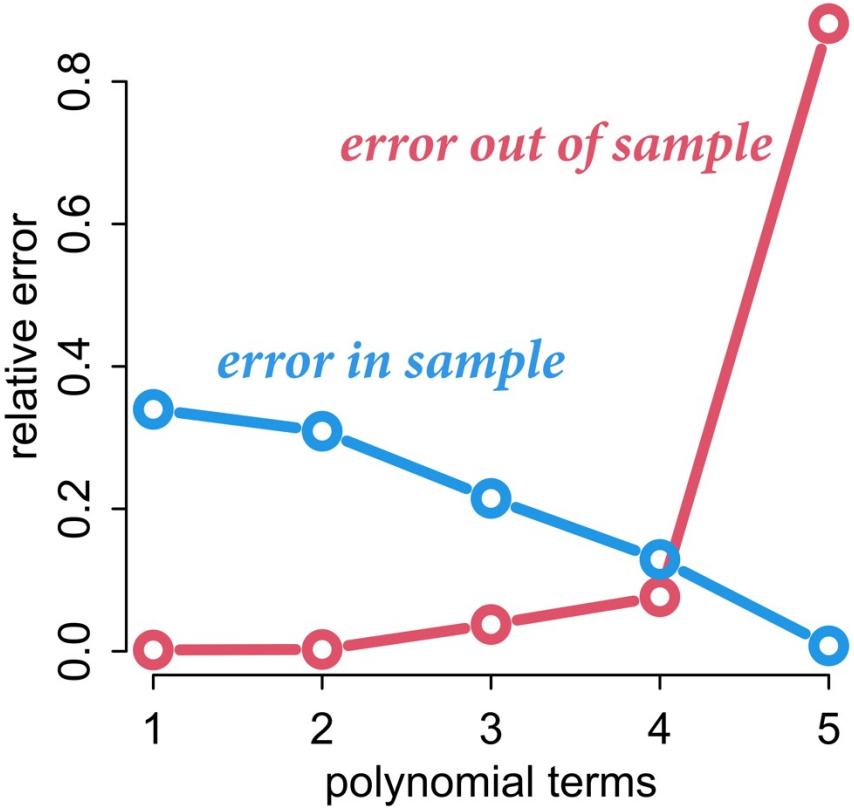
Cross-validation

For simple models, increasing parameters improves fit to sample

But may reduce accuracy of predictions out of sample

Most accurate model trades off flexibility with overfitting



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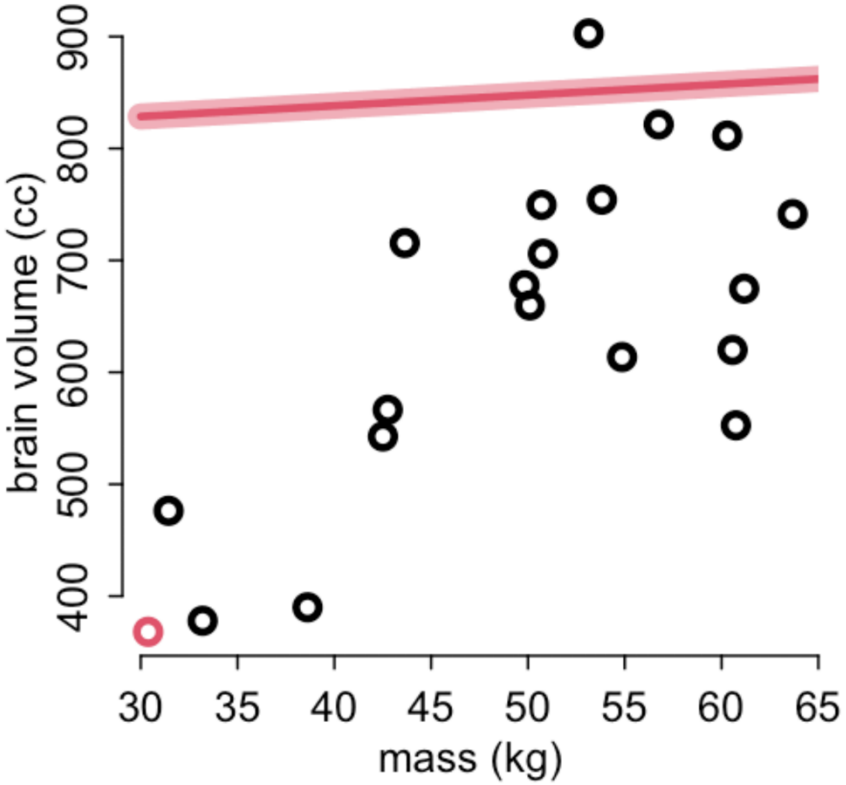
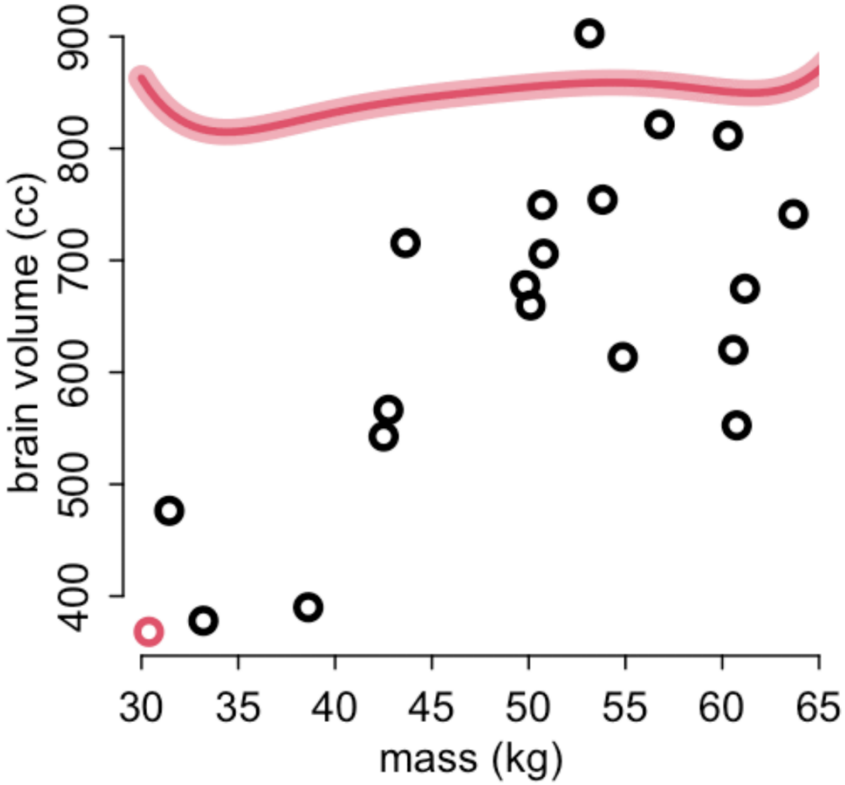
1st degree polynomial



6th degree polynomial



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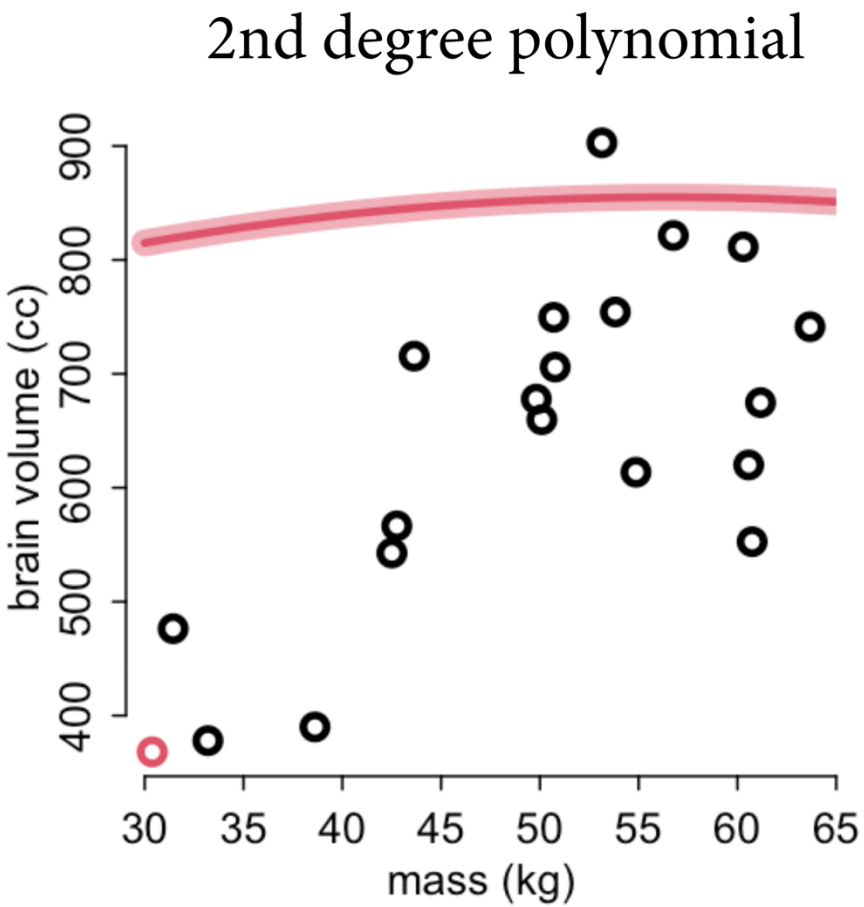

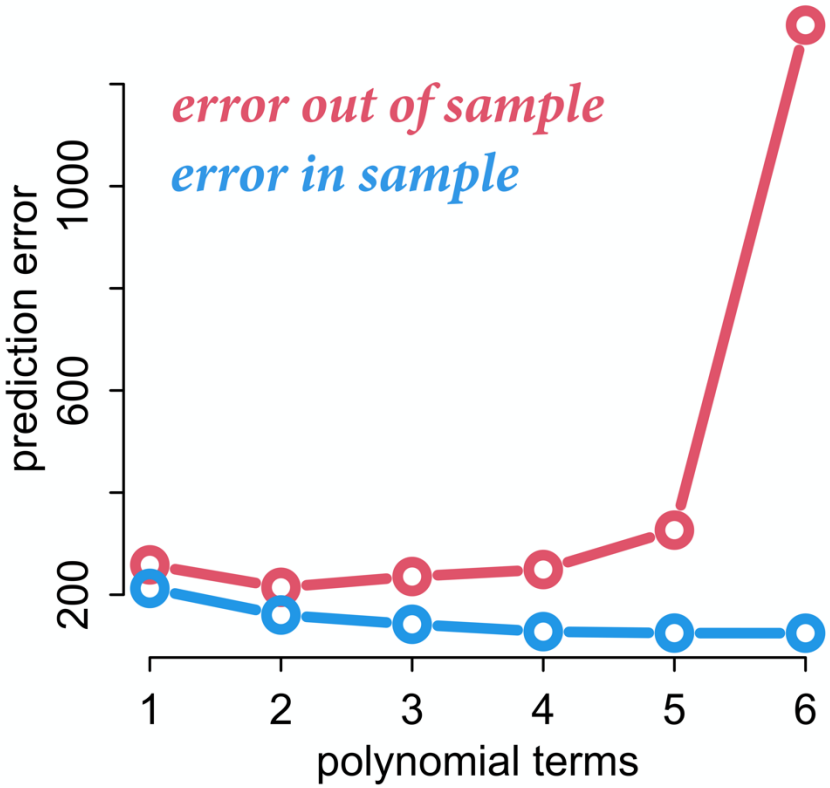

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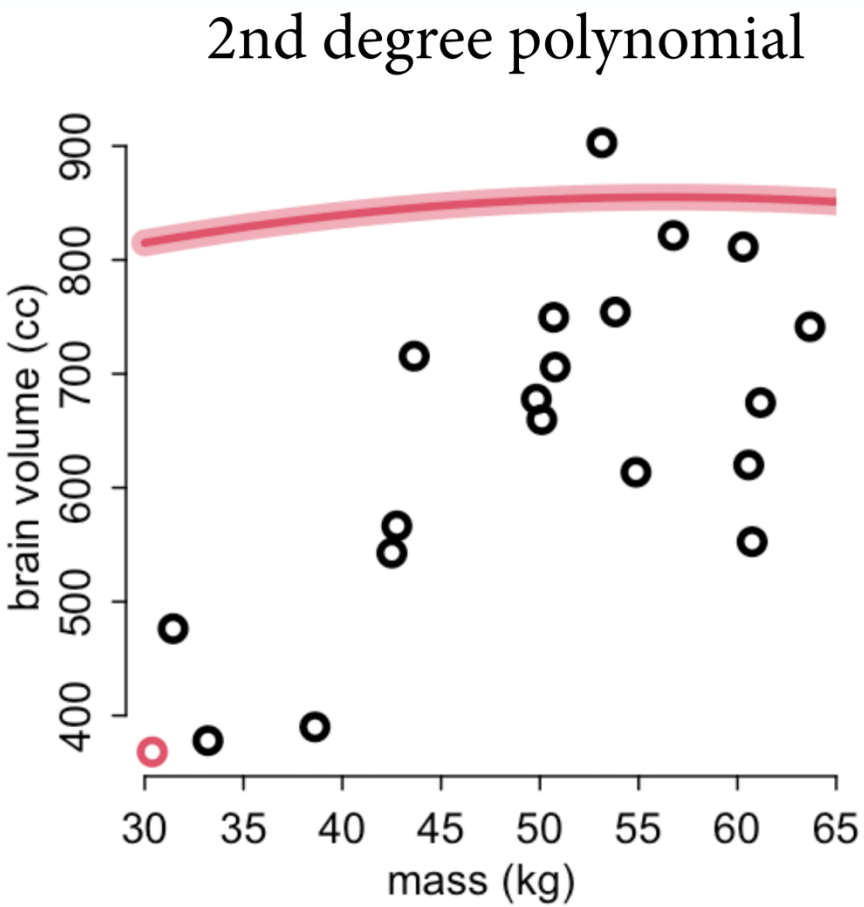
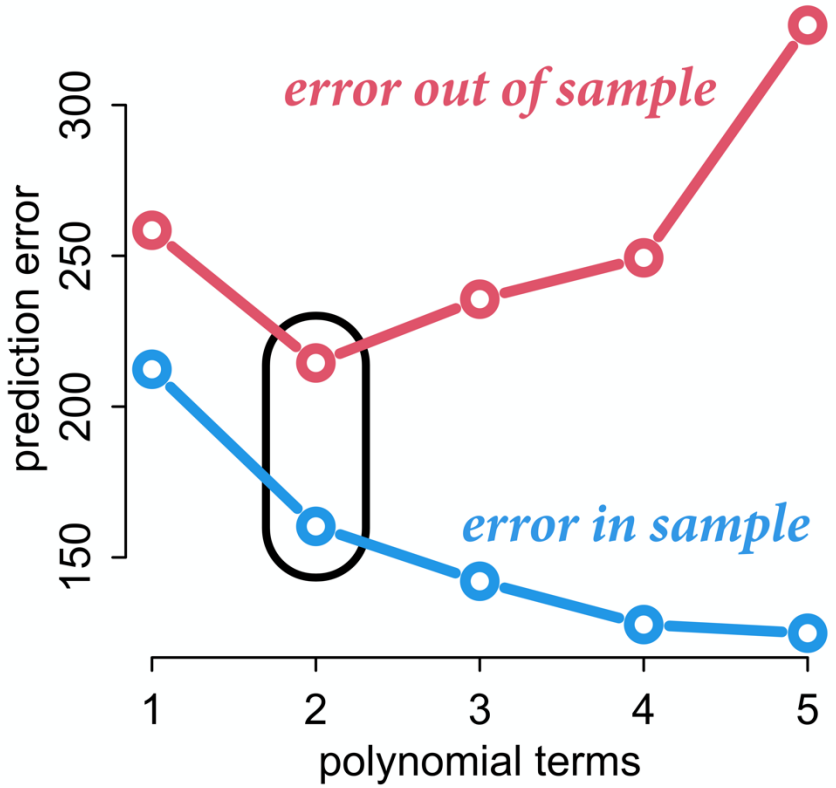




Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Regularization

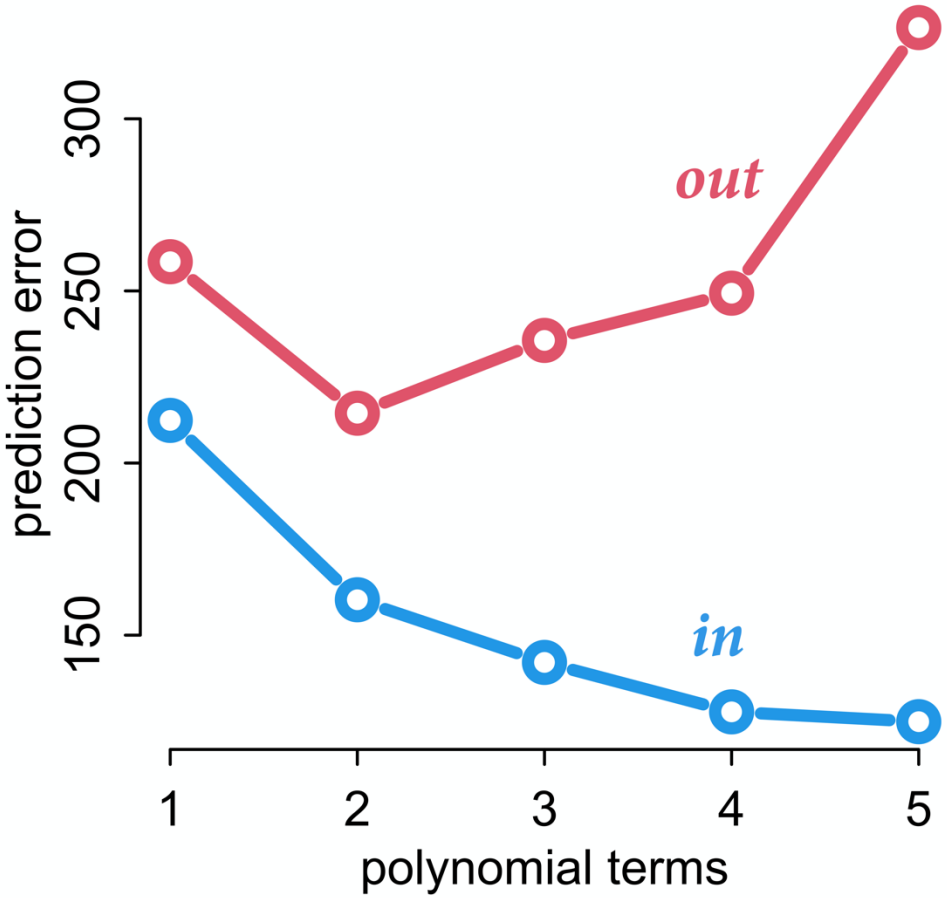
Overfitting depends upon the priors

Skeptical priors have tighter variance, reduce flexibility

Regularization: Function finds regular features of process

Good priors are often tighter than you think!

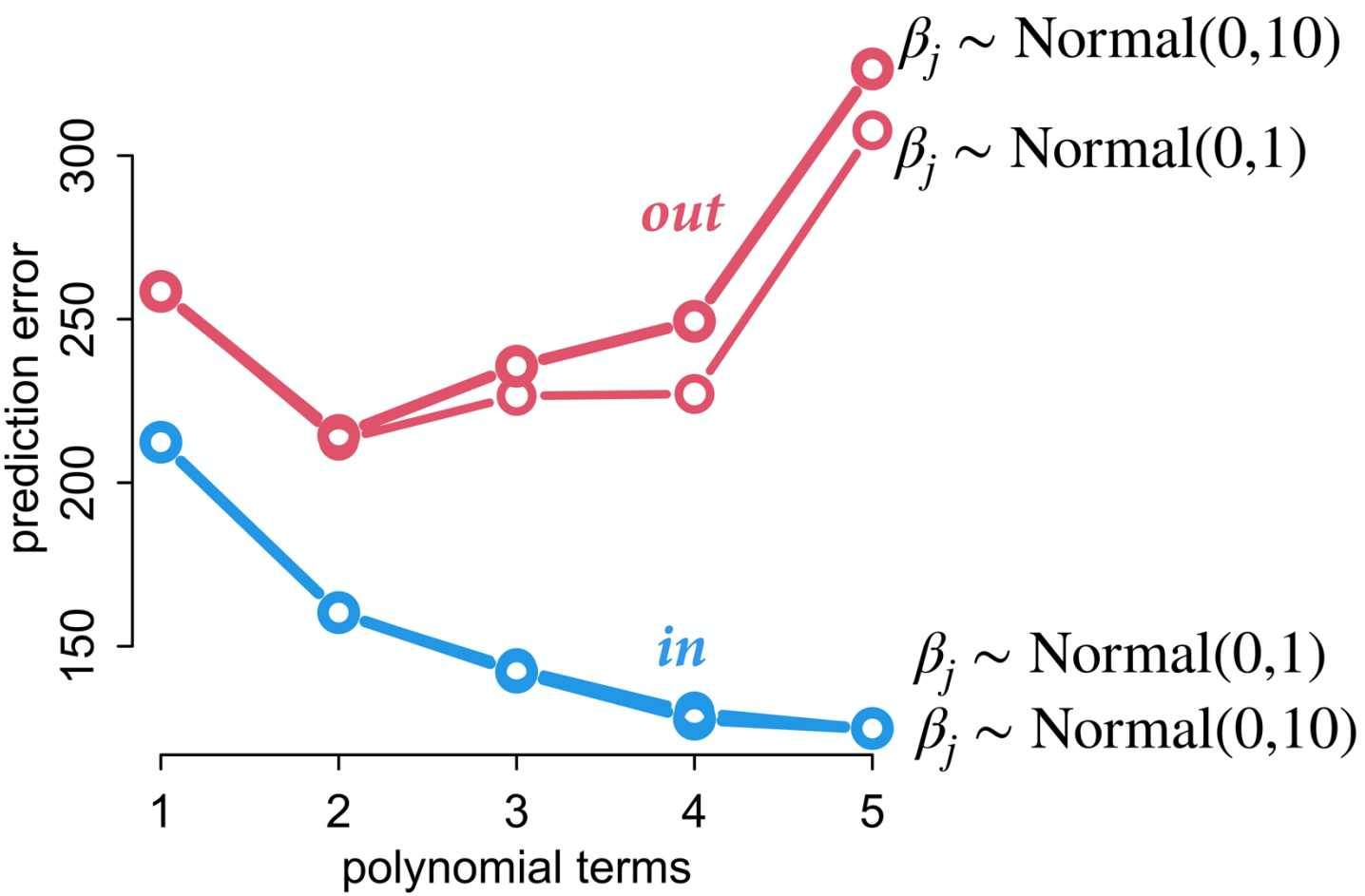
Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022



$$\mu_i = \alpha + \sum_{j=1}^{m} \beta_j x_i^j$$

$$\beta_j \sim \text{Normal}(0,10)$$

Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022



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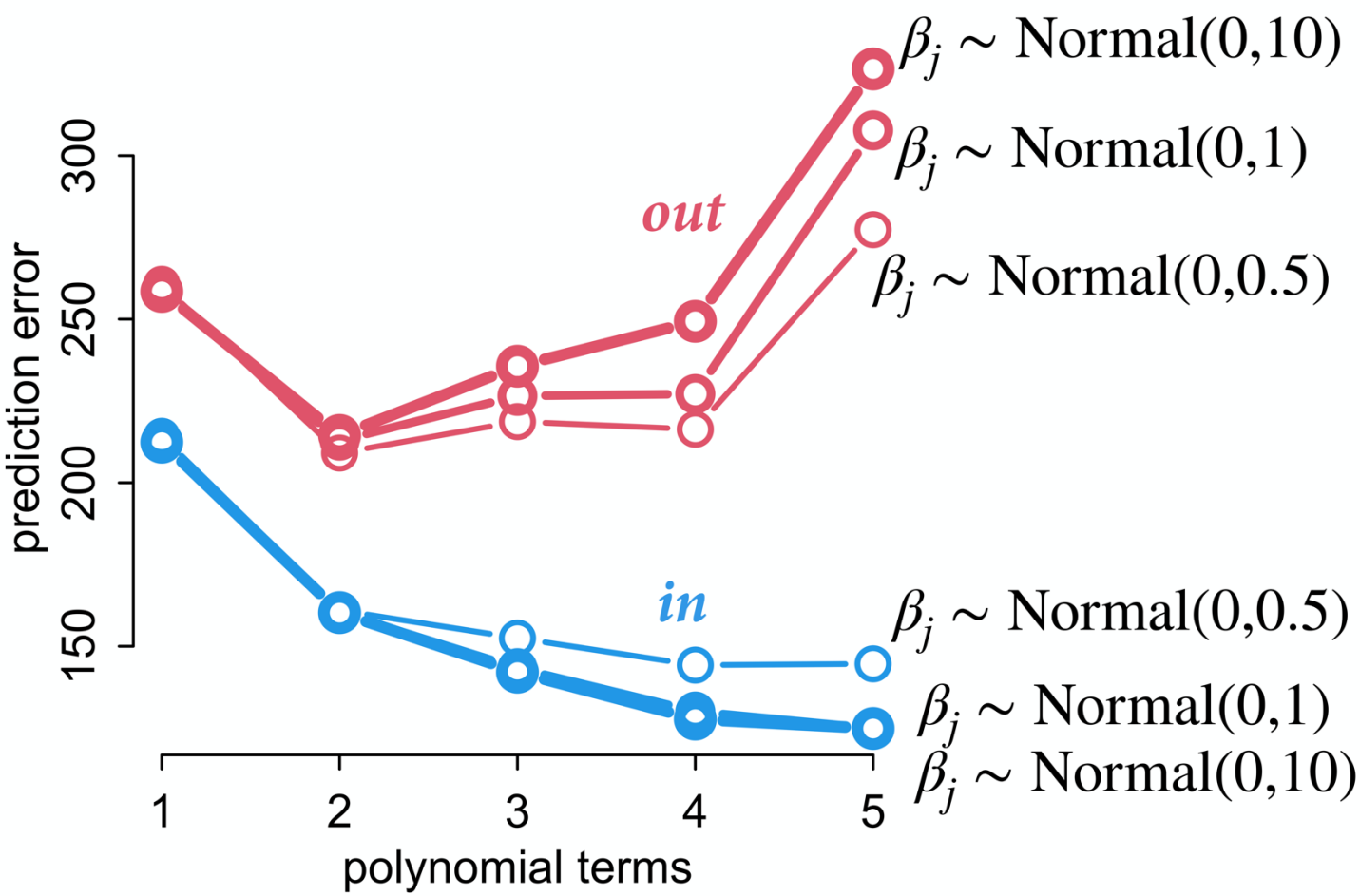

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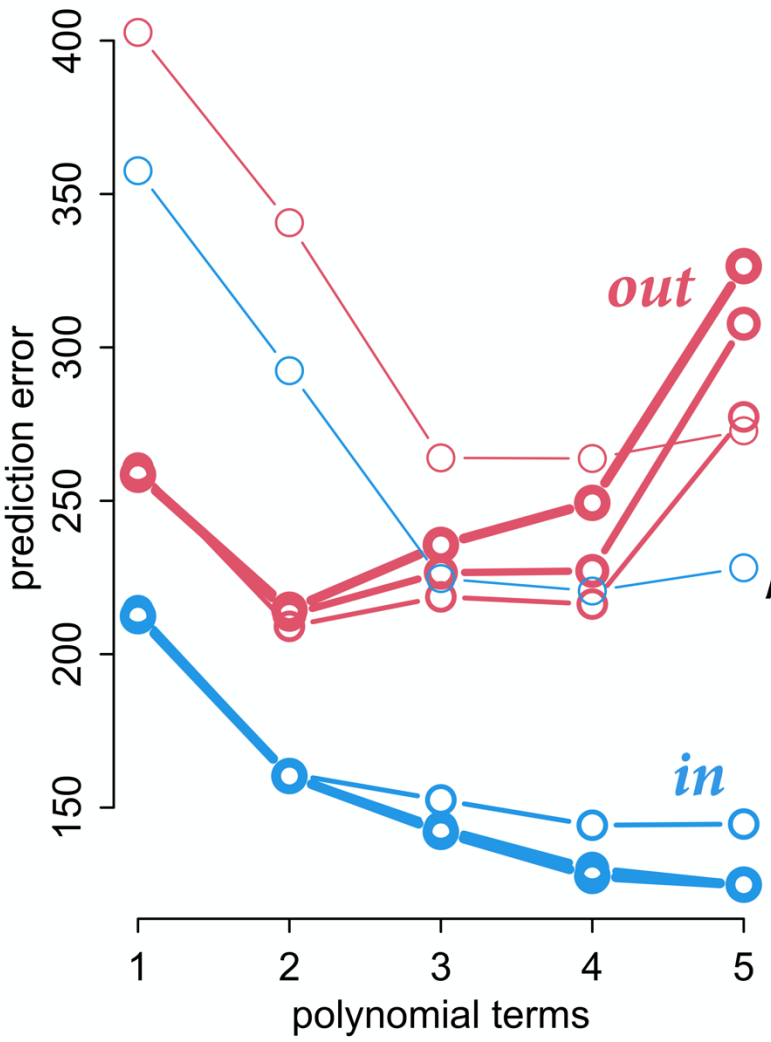


$$\beta_j \sim \text{Normal}(0,0.1)$$

Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Regularizing priors

How to choose width of prior?

For causal inference, use science

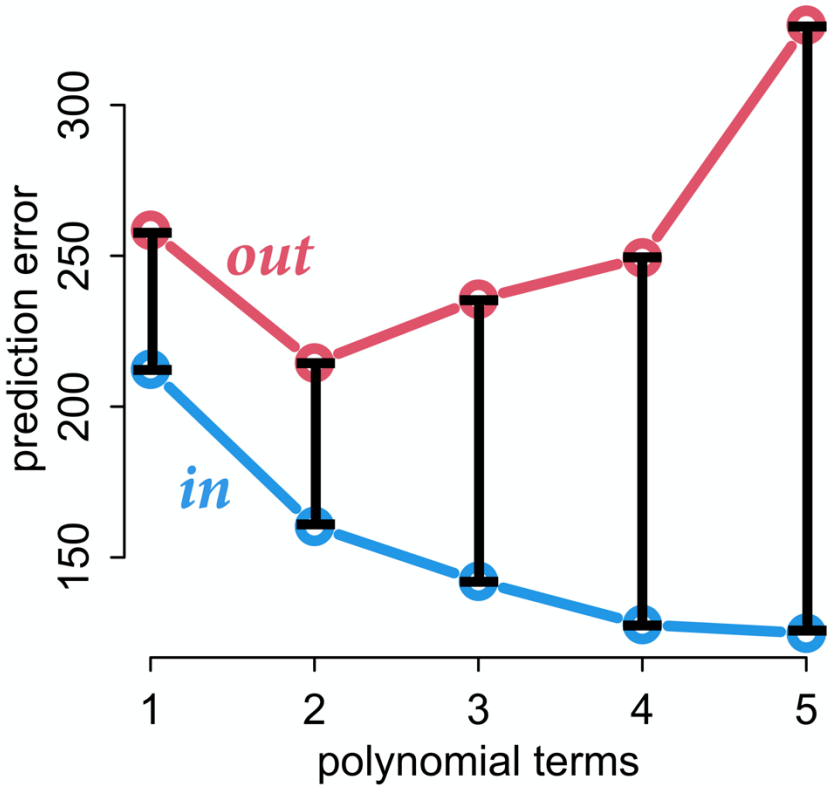
For pure prediction, can tune the prior using cross-validation

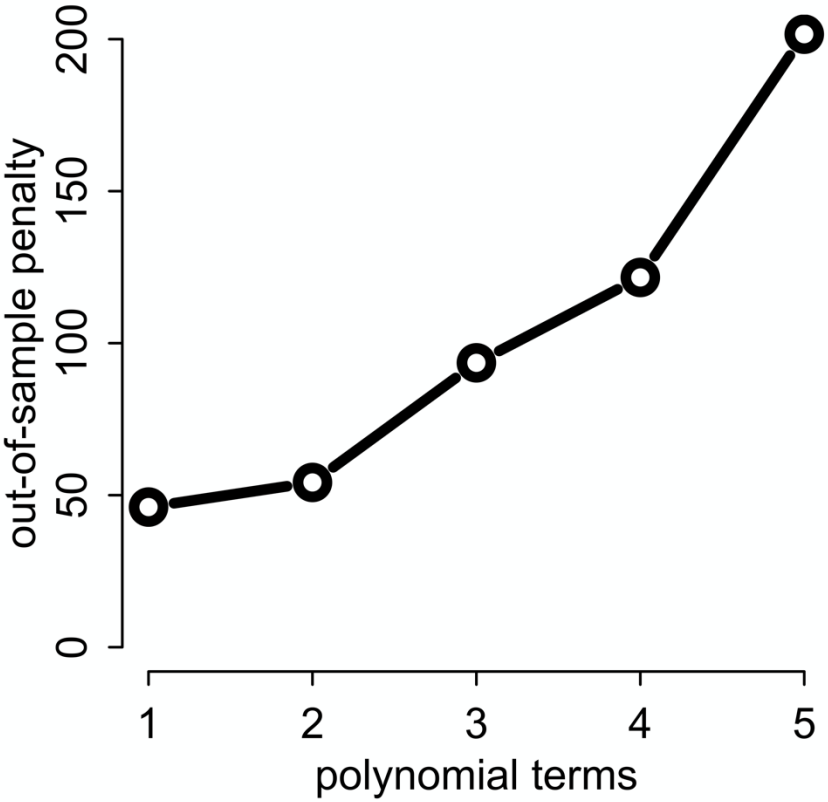
Many tasks are a mix of inference and prediction

No need to be perfect, just better

Source: Richard McElreath, https://github.com/rmcelreath/stat_rethinking_2022

Prediction penalty





Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Penalty prediction

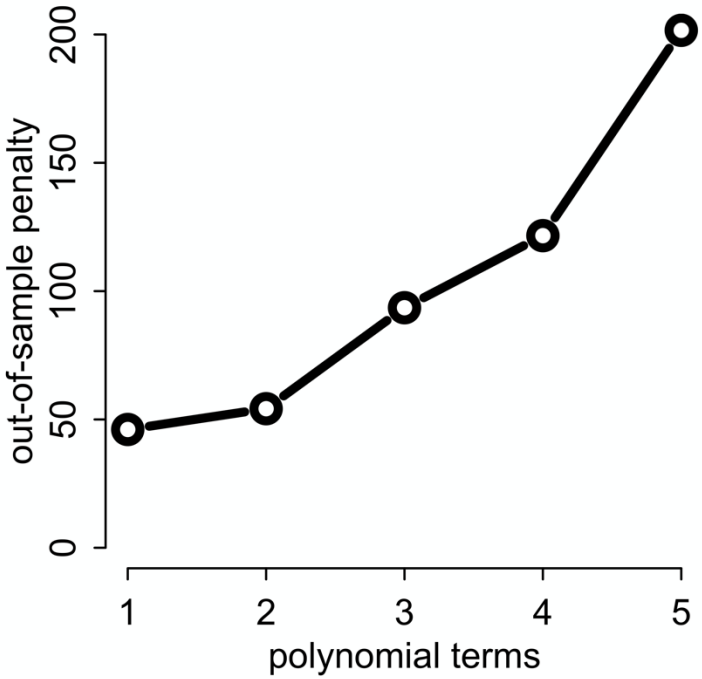
For N points, cross-validation requires fitting N models

What if you could compute the penalty from a single model fit?

Good news! You can:

Importance sampling (PSIS)

Information criteria (WAIC)



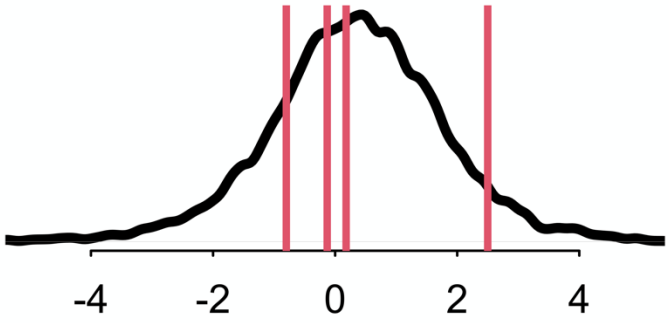
Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Importance Sampling

Importance sampling: Use a single posterior distribution for N points to sample from each posterior for $N-1$ points

Key idea: Point with **low** probability has a strong influence on posterior distribution

Can use pointwise probabilities to reweight samples from posterior



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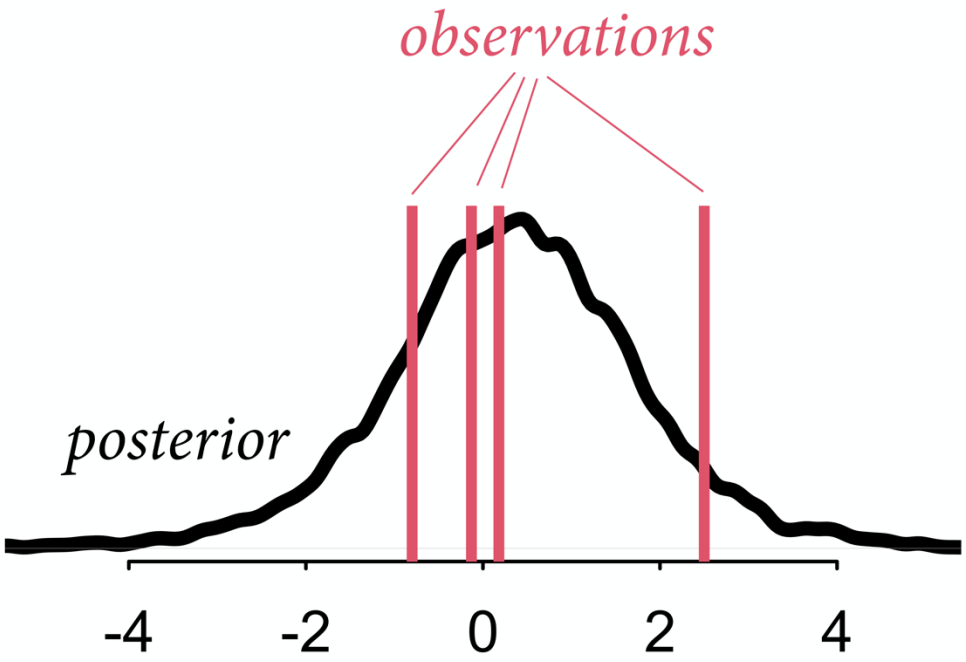

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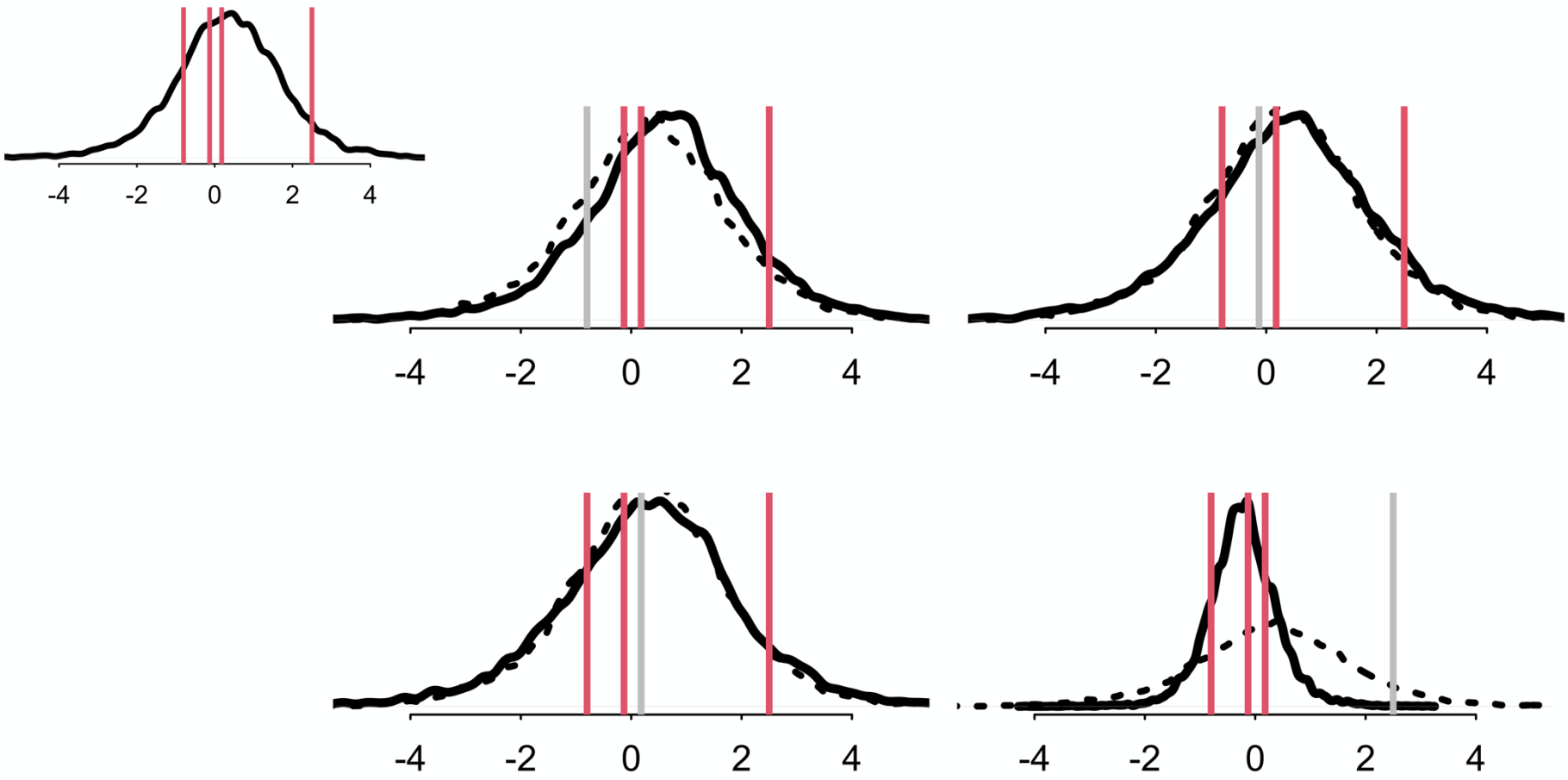


Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Smooth Importance Sampling

Importance sampling tends to be unreliable, has high variance

Pareto-smoothed importance sampling (PSIS) more stable (lower variance)

Useful diagnostics

Identifies important (high leverage) points ("outliers")

Prof Aki Vehtari (Helsinki), smooth estimator

Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Akaike information criterion

[ah–ka–ee–kay]

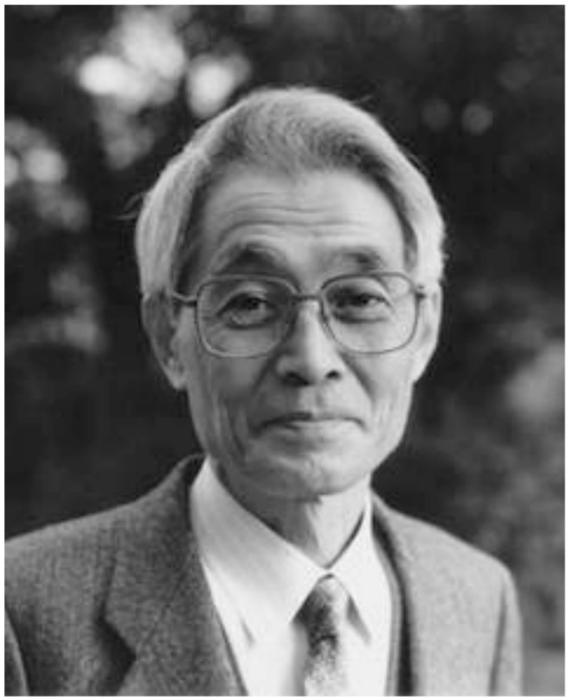
Estimate information-theoretic measure of predictive accuracy (K-L Distance)

For flat priors and large samples:

$$\text{AIC} = (-2) \times \text{lppd} + 2k$$

log pointwise predictive density

number of parameters



Hirotugu Akaike (1927–2009)

赤池弘次

Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Widely Applicable IC

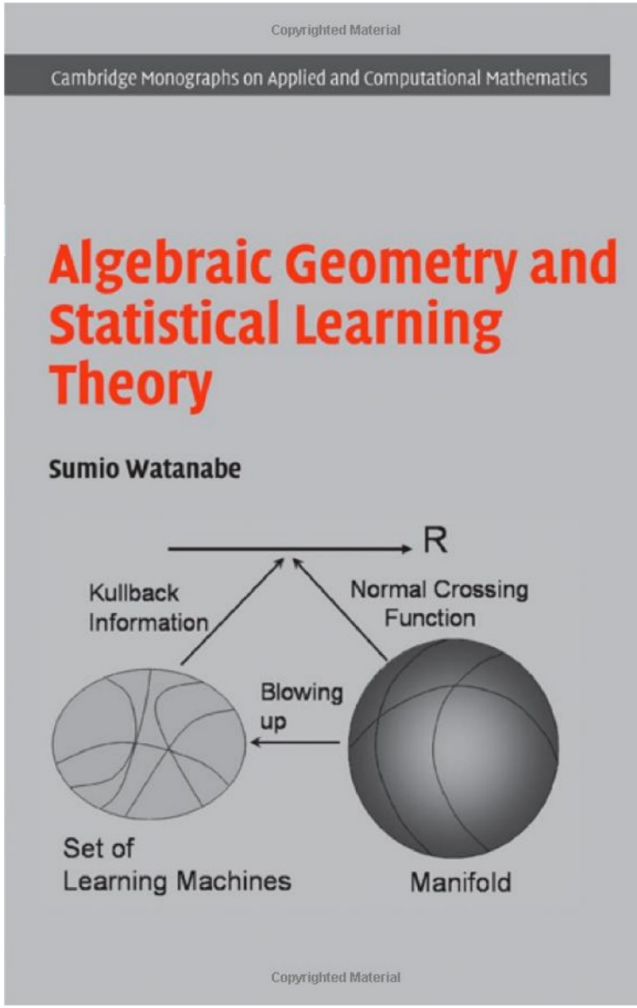
AIC of historical interest now

Widely Applicable Information Criterion (WAIC)

Sumio Watanabe (渡辺澄夫) 2010

$$\text{WAIC}(y, \Theta) = -2\Big(\text{lppd} - \underbrace{\sum_i \text{var}_\Theta \log p(y_i|\Theta)}_{\text{penalty term}}\Big)$$

Very similar to PSIS score, but no automatic diagnostics



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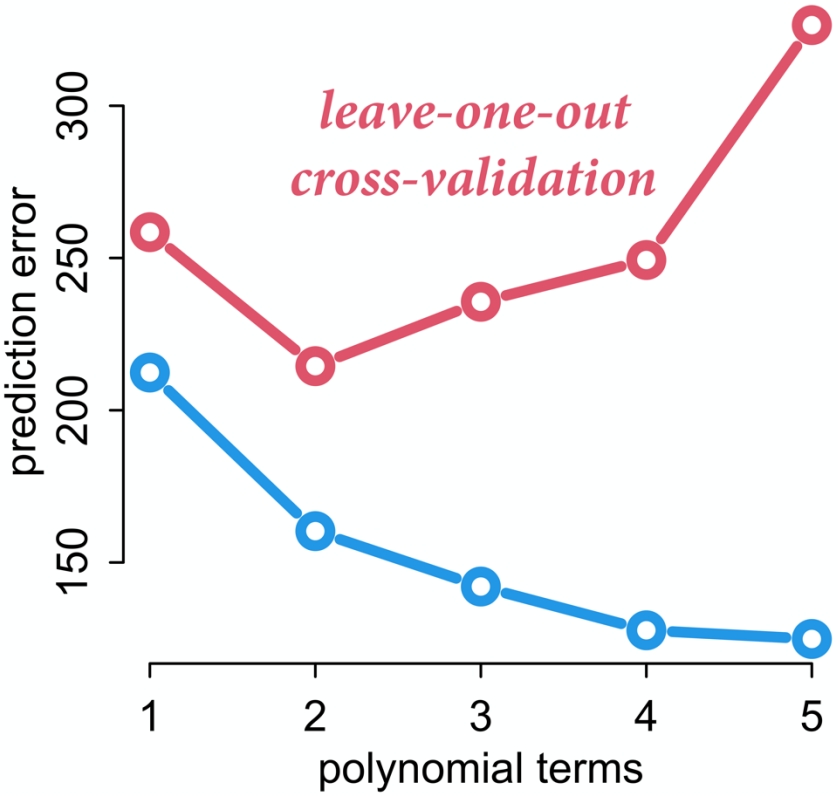
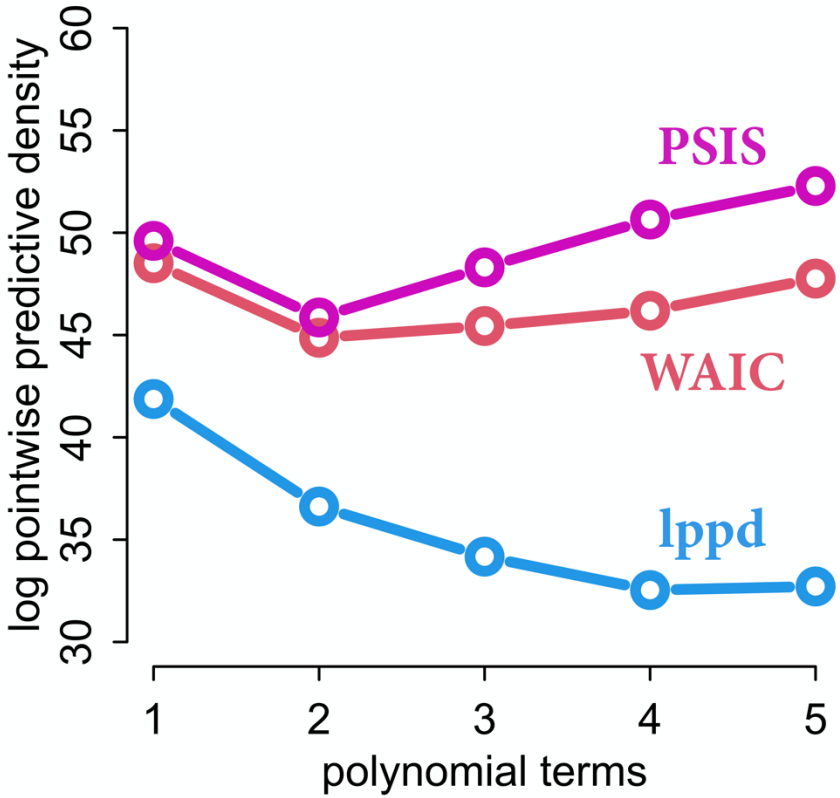




Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

WAIC,PSIS,CV measure overfitting

Regularization manages overfitting

None directly address causal inference

All important to understanding how statistical inference works

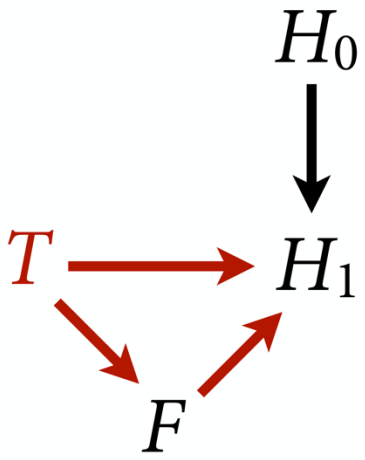
Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Model Mis-selection

Do not use predictive criteria (WAIC, PSIS, CV) to choose a causal estimate

Predictive criteria actually prefer confounds & colliders

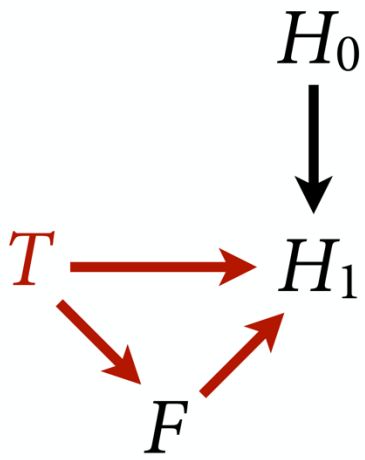
Example: Plant growth experiment



Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

$$H_1 \sim \text{Normal}(\mu_i, \sigma)$$
$$\mu_i = H_0 \times p_i$$
$$p_i = \alpha + \beta_T T_i + \beta_F F_i$$

Wrong adjustment set for total causal effect of treatment (blocks mediating path)



$$H_1 \sim \text{Normal}(\mu_i, \sigma)$$
$$\mu_i = H_0 \times p_i$$
$$p_i = \alpha + \beta_T T_i$$

Correct adjustment set for total causal effect of treatment

Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

$$H_1 \sim \text{Normal}(\mu_i, \sigma)$$

$$\mu_i = H_0 \times p_i$$

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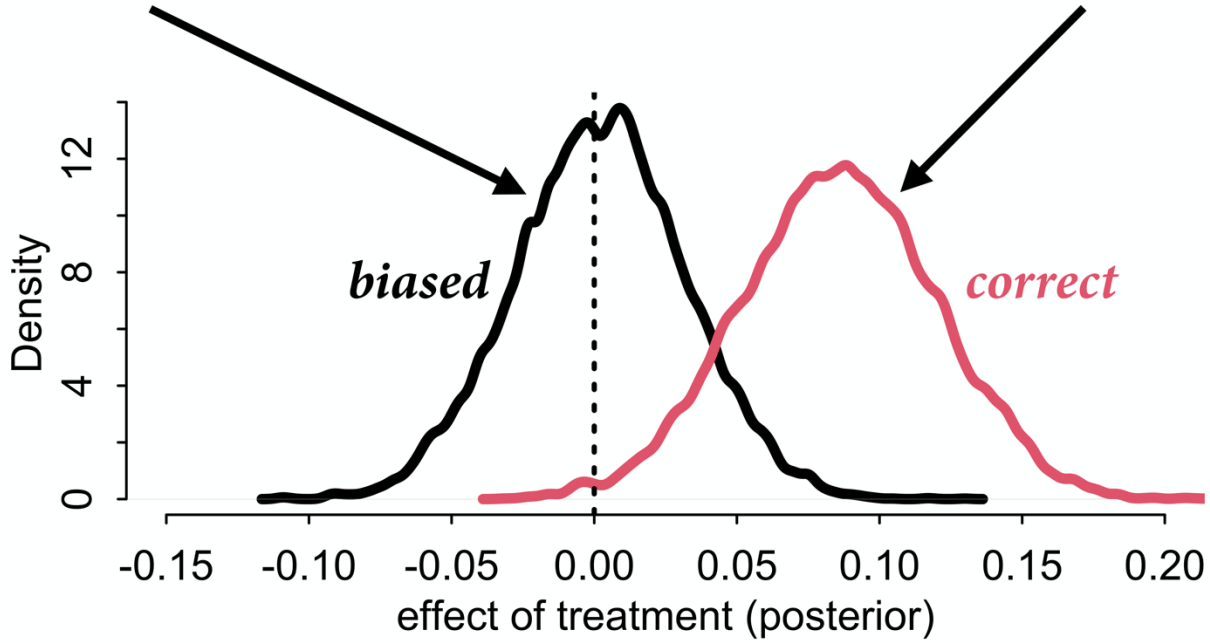

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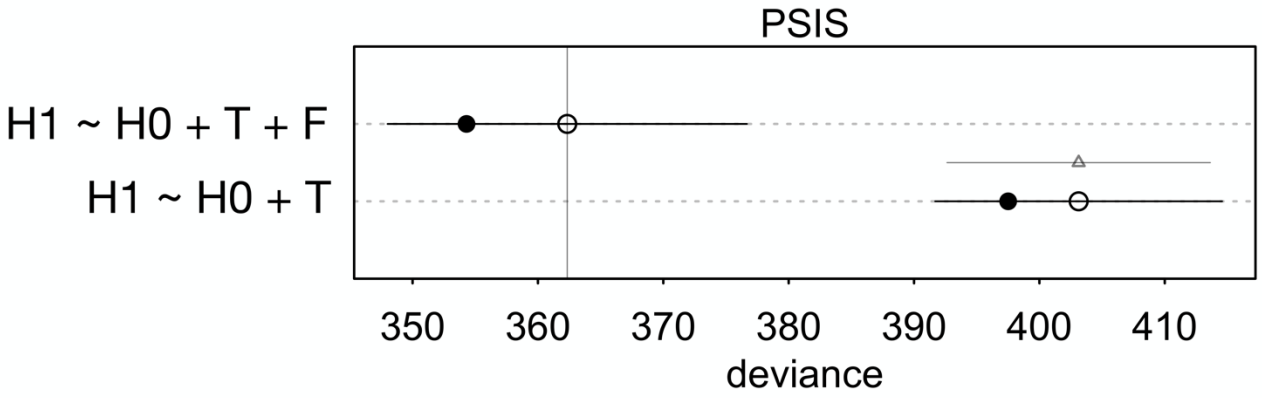
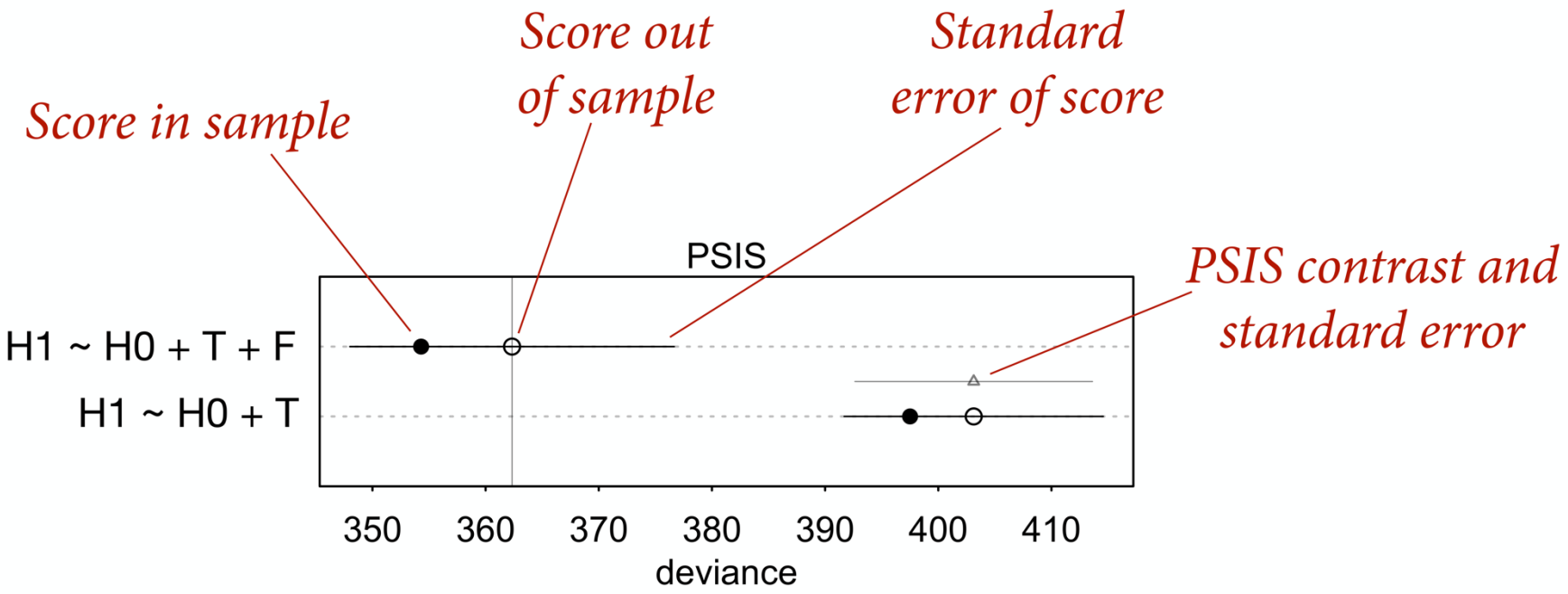


Wrong model wins at prediction

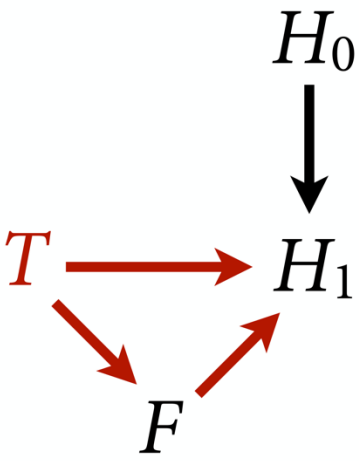
Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

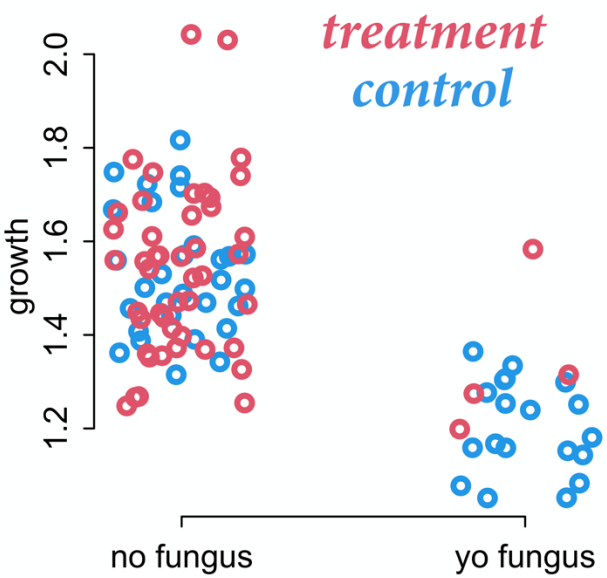


Wrong model wins at prediction

Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Why does the wrong model win at prediction?





Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

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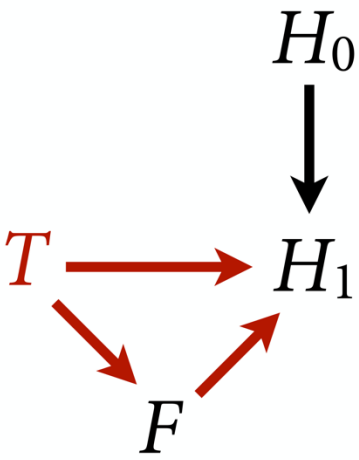
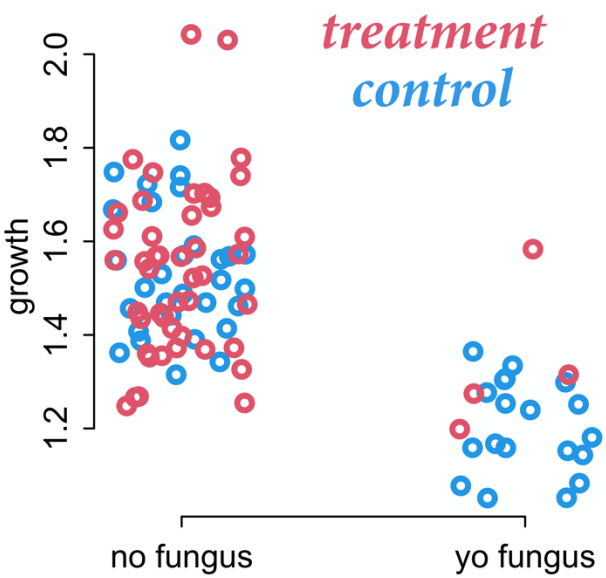
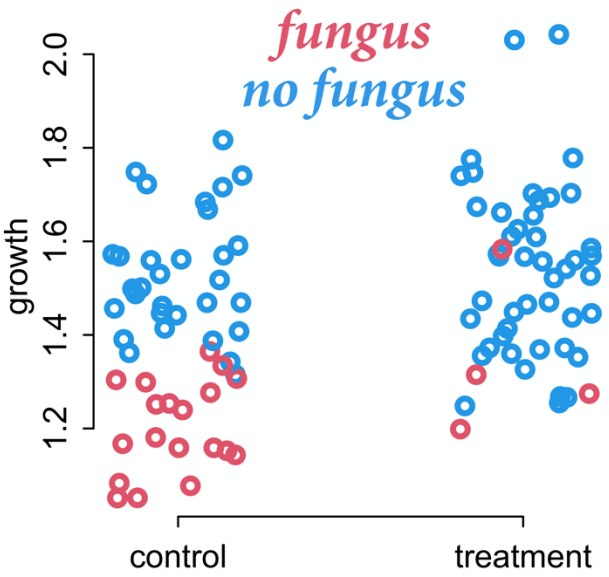






Fungus is in fact a better predictor than treatment

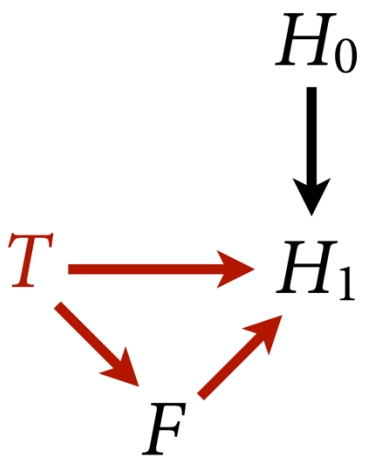
Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Model Mis-selection

Do not use predictive criteria (WAIC, PSIS, CV) to choose a causal estimate

However, many analyses are mixes of inferential and predictive chores

Still need help finding good functional descriptions while avoiding overfitting



Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

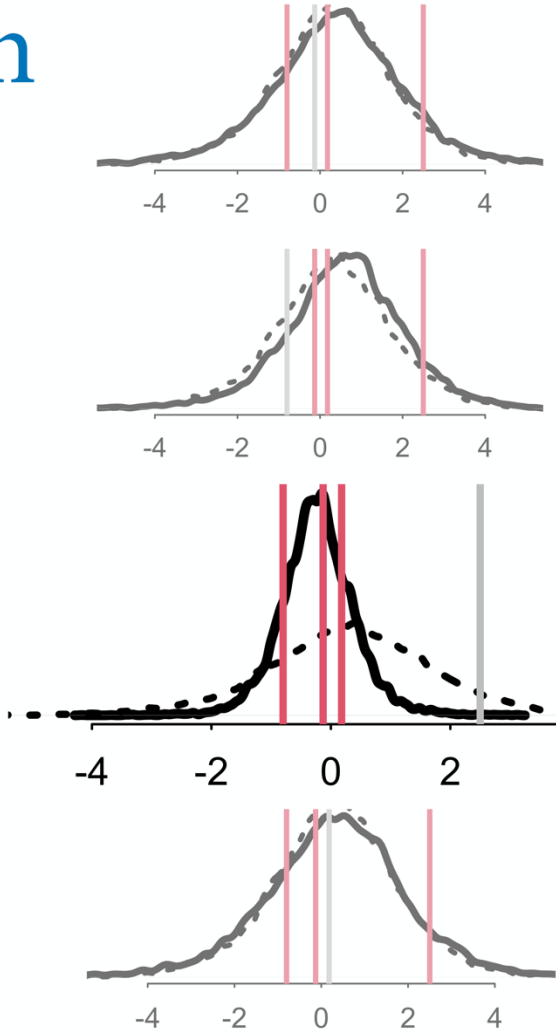
Outliers & Robust Regression

Some points are more influential than others

"Outliers": Observations in the tails of predictive distribution

Outliers indicate predictions are possibly overconfident, unreliable

The model doesn't expect enough variation



Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

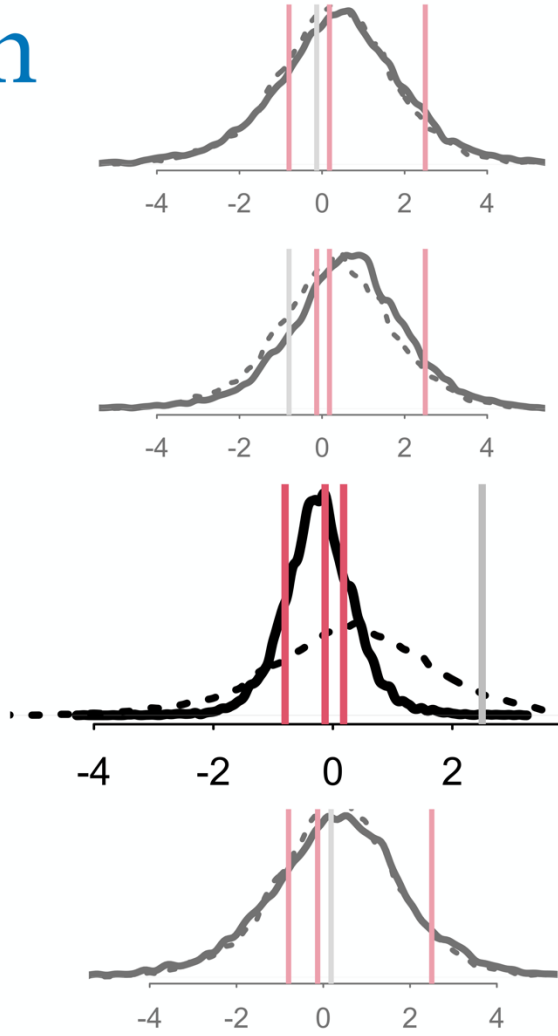
Outliers & Robust Regression

Dropping outliers is bad: Just ignores the problem; predictions are still bad!

It's the model that's wrong, not the data

First, quantify influence of each point

Second, use a mixture model (robust regression)



Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

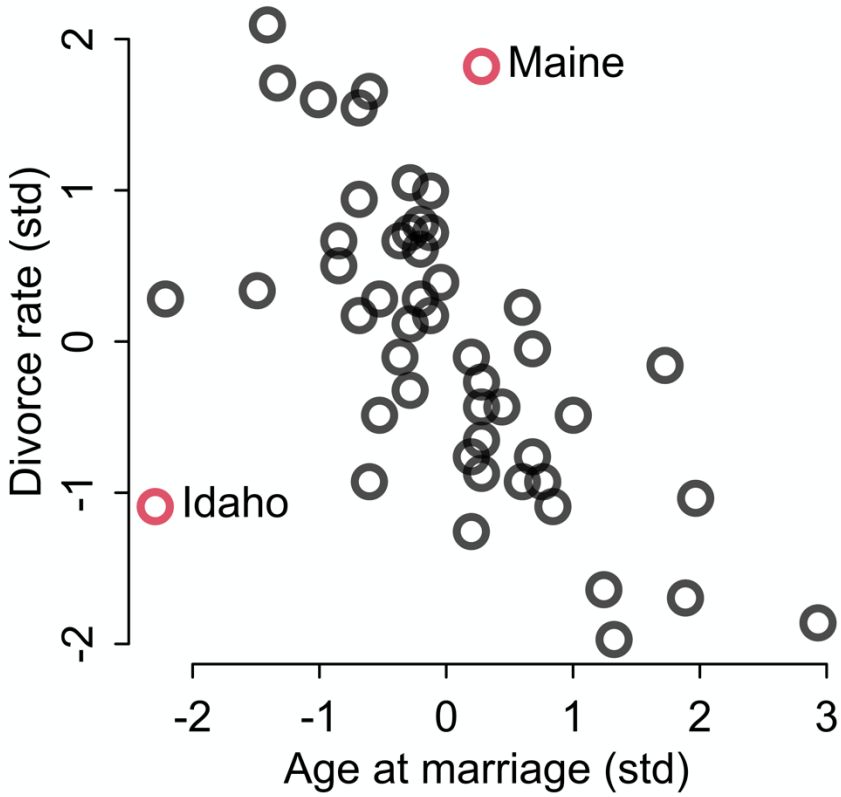
Outliers & Robust Regression

Divorce rate example

Maine and Idaho both highly unusual

Maine: high divorce for trend

Idaho: low divorce for trend



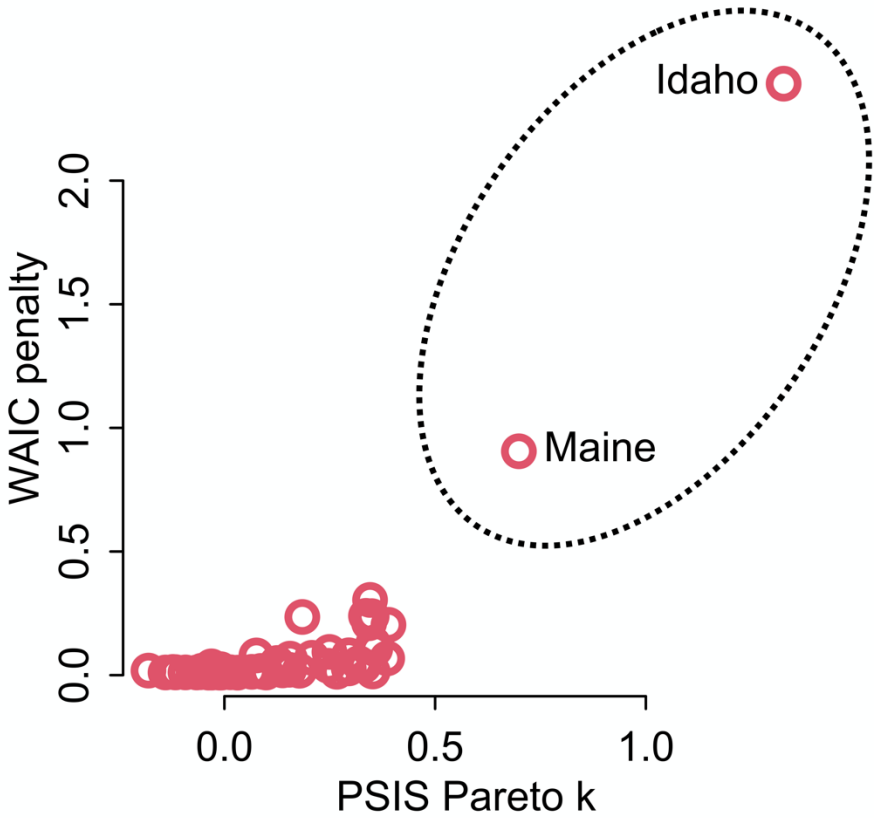
Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

Outliers & Robust Regression

Quantify influence:

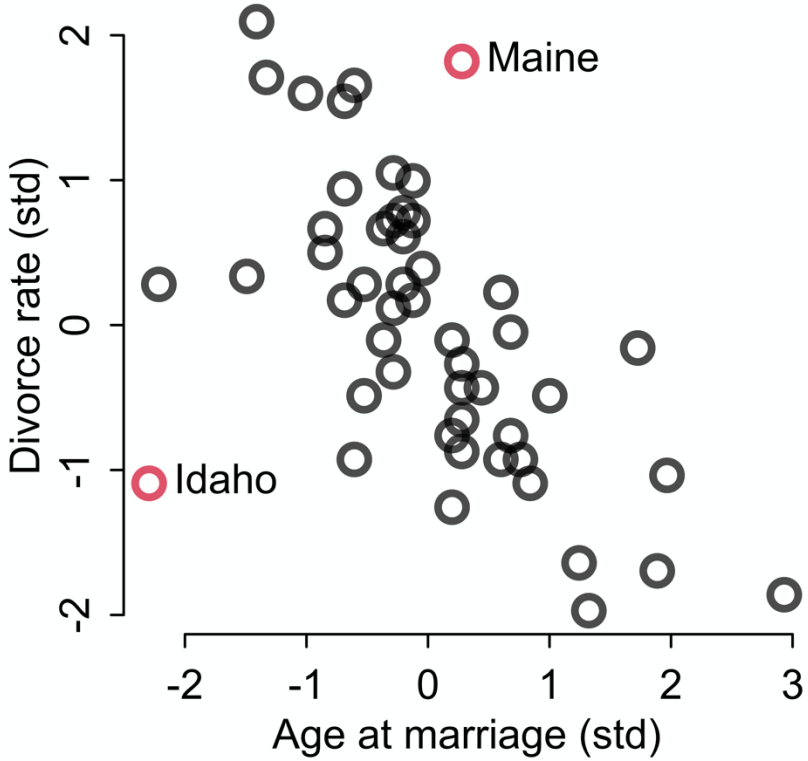
PSIS *k* statistic

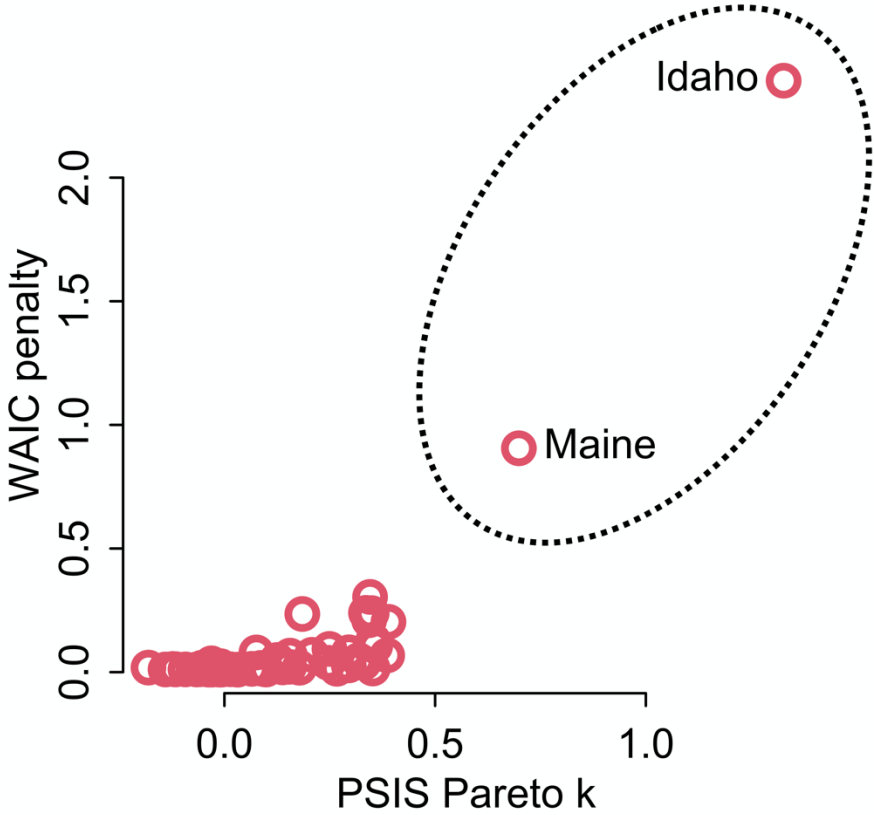
WAIC penalty term ("effective number of parameters")



Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

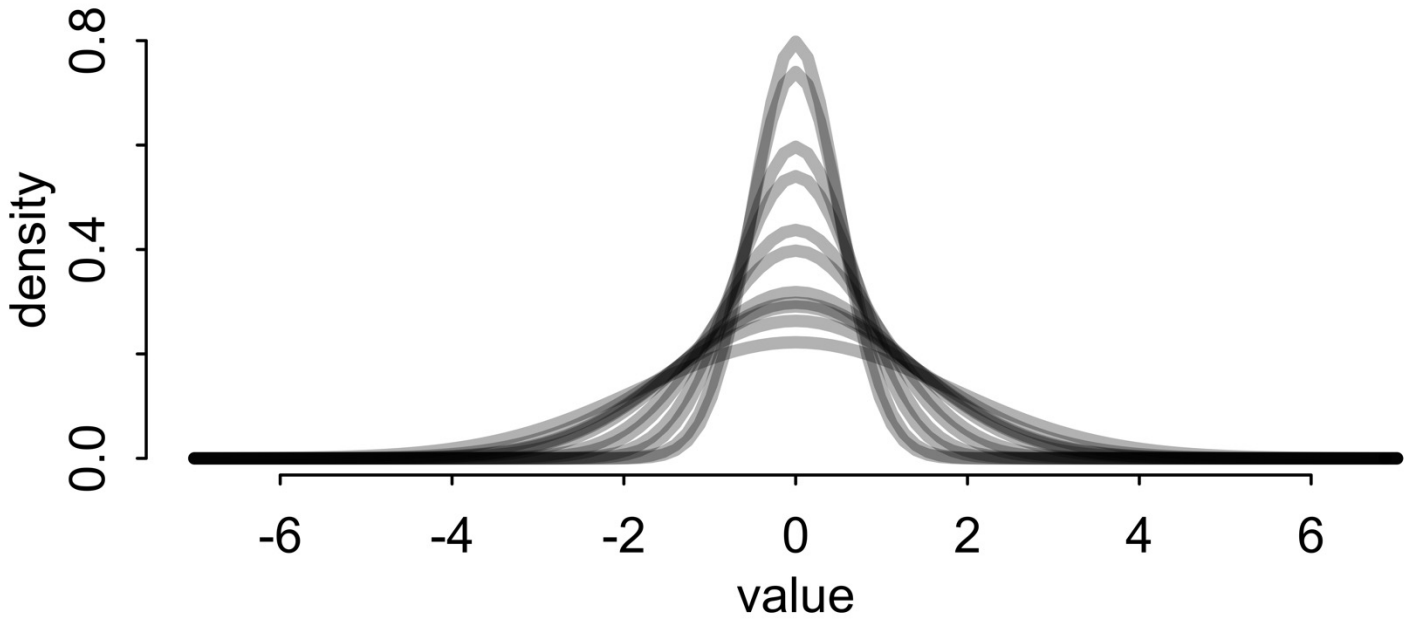
Outliers & Robust Regression





Source: Richard McElreath, https://github.com/rmcelreath/stat_rethinking_2022

Mixing Gaussians



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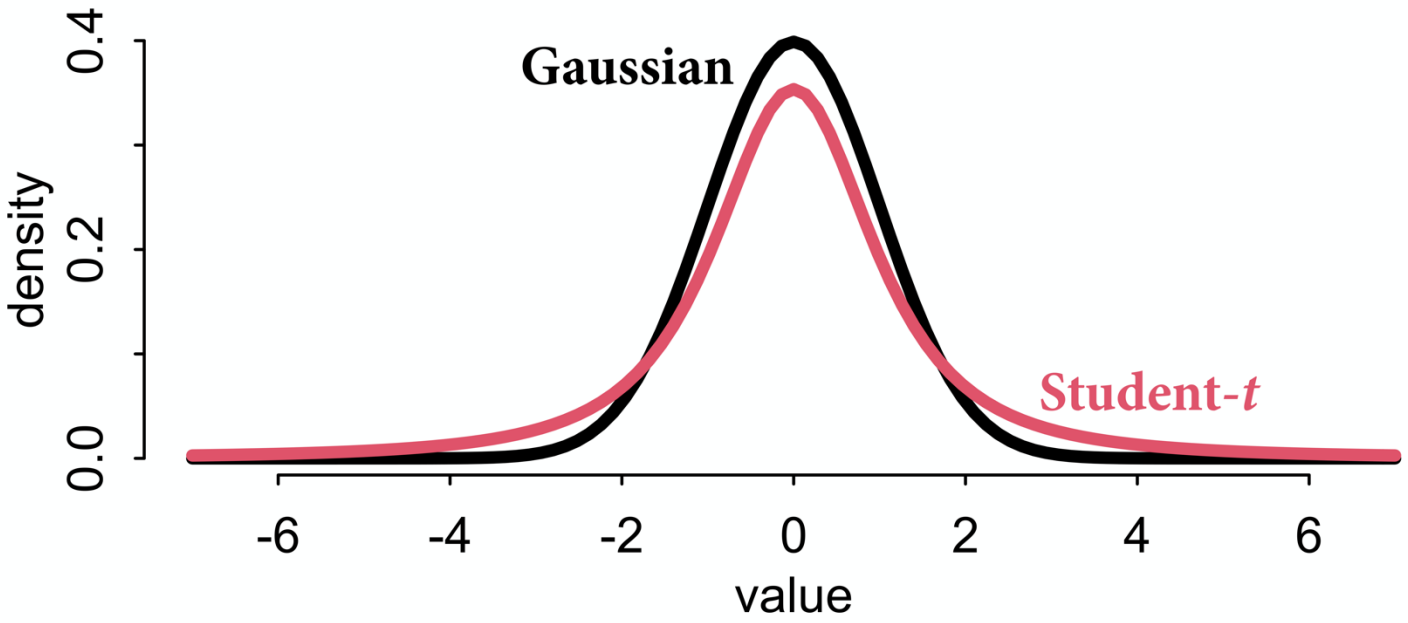
Mixing Gaussians



Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

```
m5.3 <- quap(
    alist(
        D ~ dnorm( mu , sigma ) ,
        mu <- a + bM*M + bA*A ,
        a ~ dnorm( 0 , 0.2 ) ,
        bM ~ dnorm( 0 , 0.5 ) ,
        bA ~ dnorm( 0 , 0.5 ) ,
        sigma ~ dexp( 1 )
) , data = dat )

m5.3t <- quap(
    alist(
        D ~ dstudent( 2 , mu , sigma ) ,
        mu <- a + bM*M + bA*A ,
        a ~ dnorm( 0 , 0.2 ) ,
        bM ~ dnorm( 0 , 0.5 ) ,
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    ) , data = dat )
```

Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

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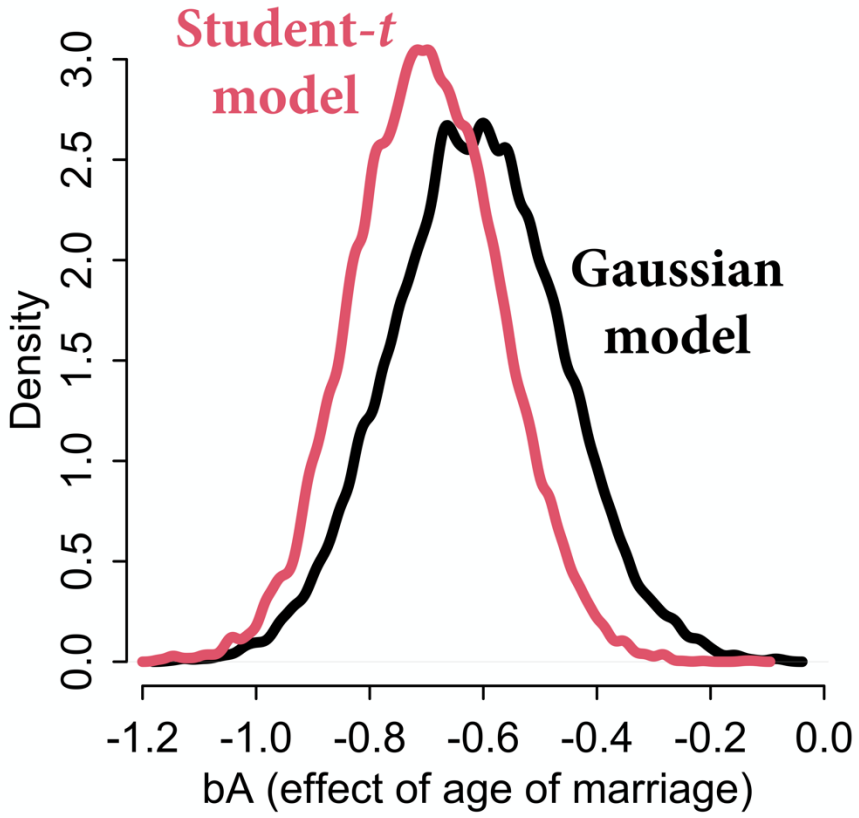


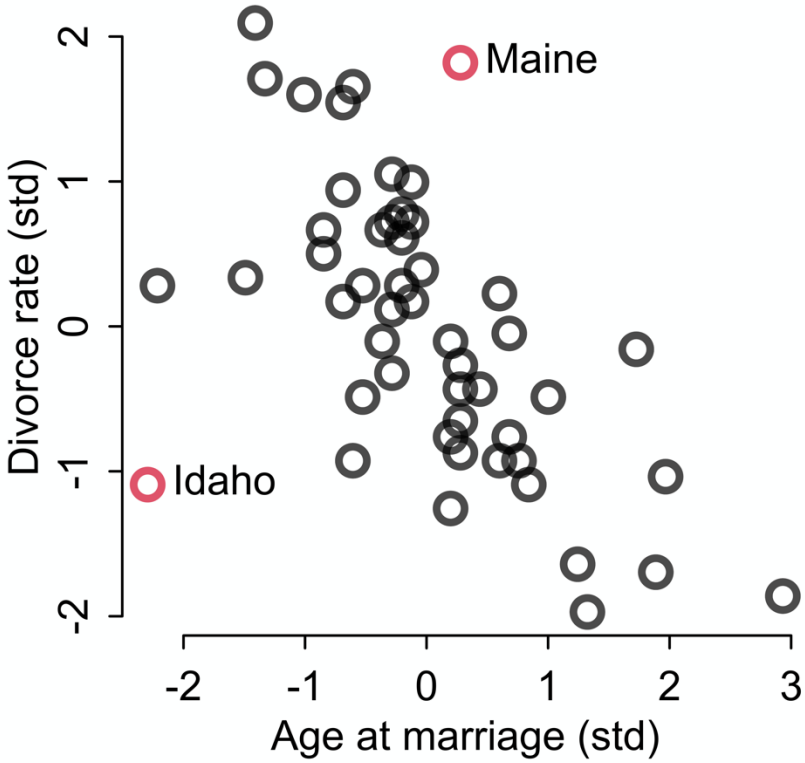
Source: Richard McElreath, https://github.com/rmcelreath/stat_rethinking_2022

Robust Regressions

Unobserved heterogeneity => mixture of Gaussians

Thick tails means model is less surprised by extreme values

Less surprise, possibly better predictions if extreme values are rare



Source: Richard McElraeth, https://github.com/rmcelreath/stat_rethinking_2022

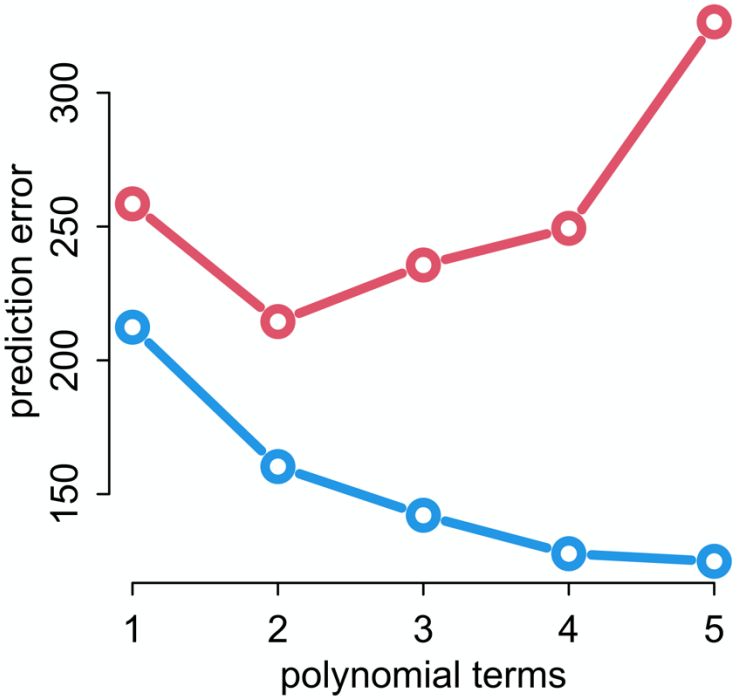
Problems of Prediction

What is the next observation from the same process? (prediction)

Possible to make very good predictions without knowing causes

Optimizing prediction does not reliably reveal causes

Powerful tools (PSIS, regularization) for measuring and managing accuracy



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