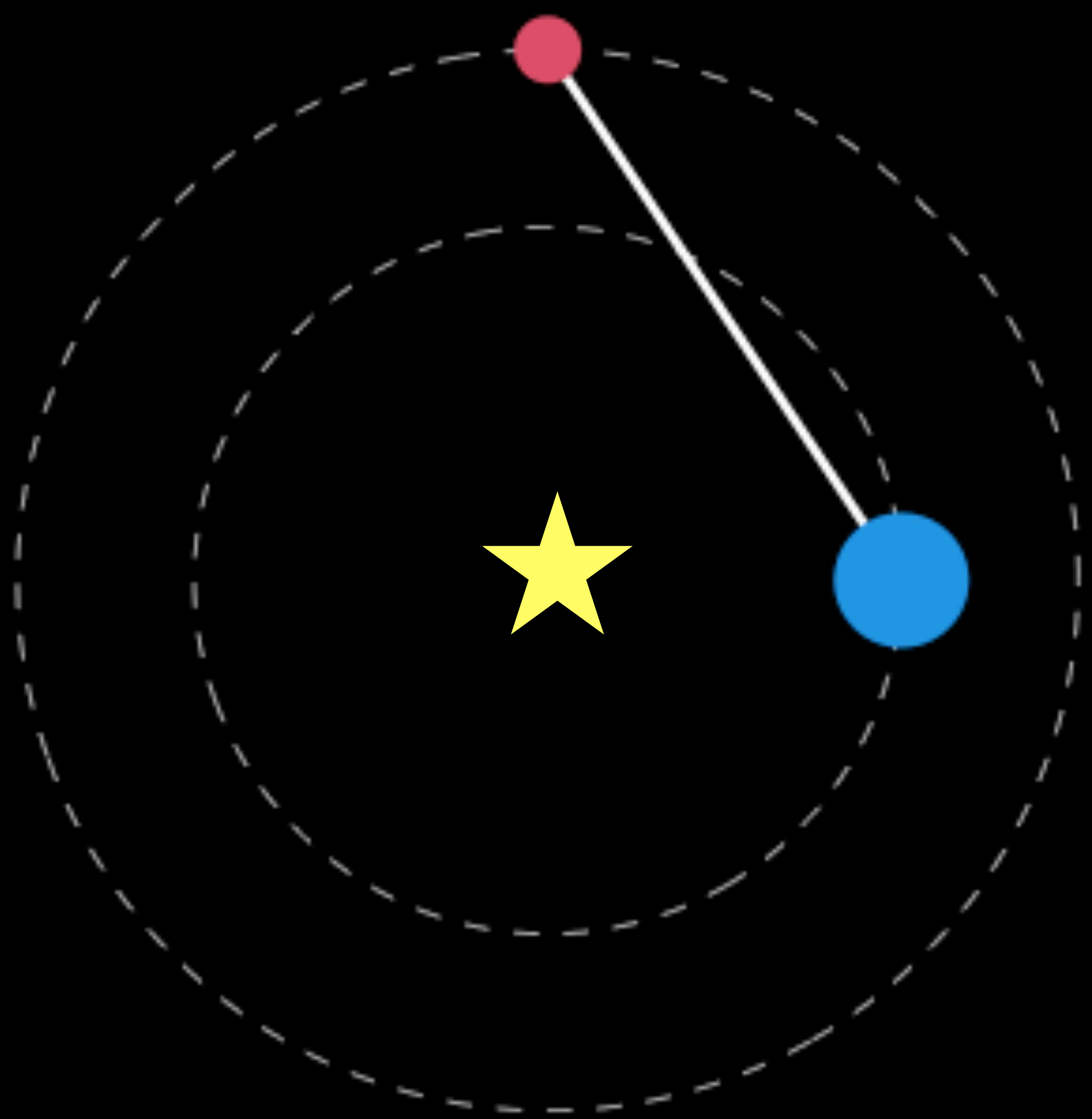
Statistical Rethinking
2023

7. Fitting Over & Under

Mikołaj Kopernik (1473–1543)

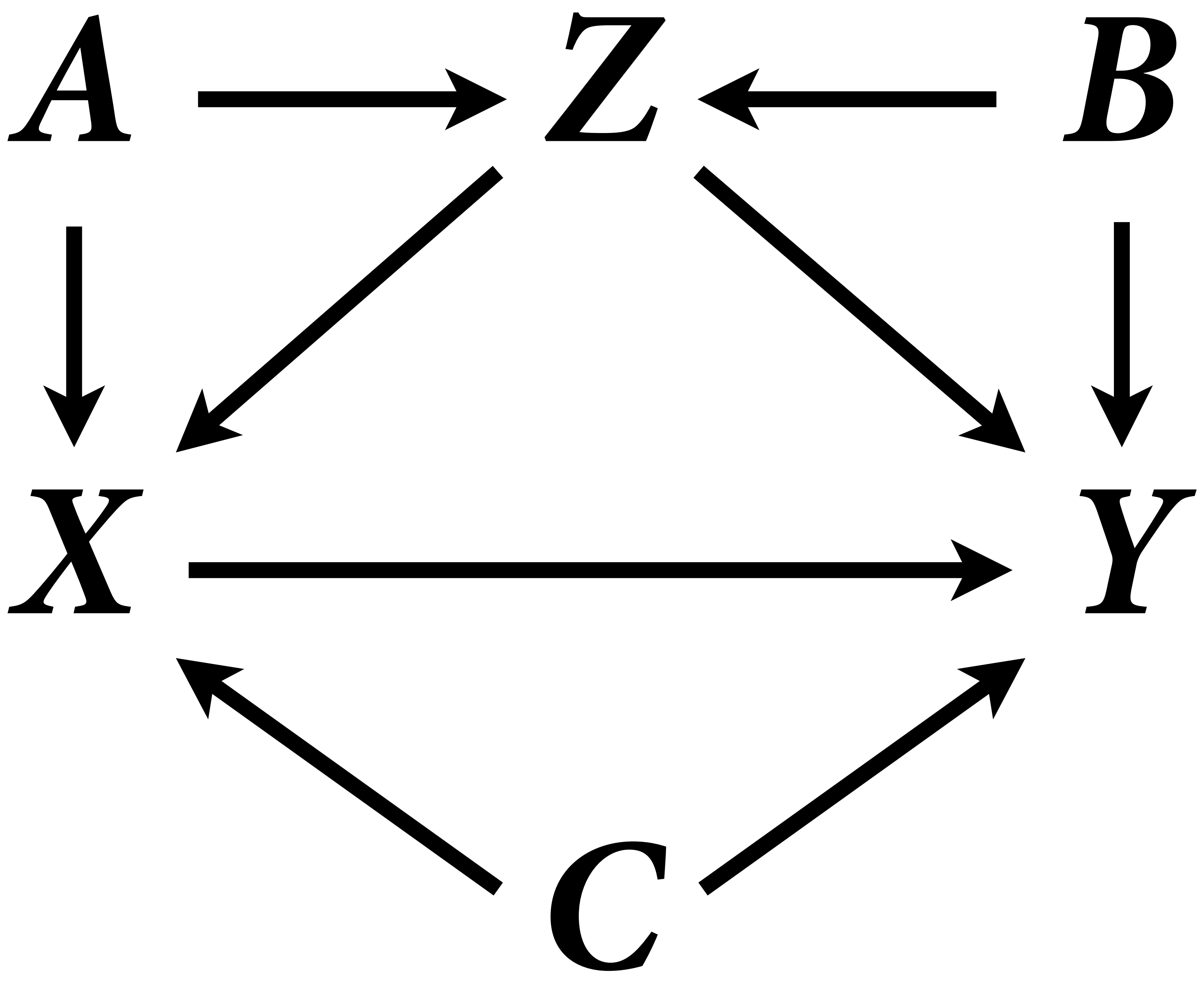


Infinite causes, finite data

Estimator might exist, but not be useful

Struggle against causation: How to use causal assumptions to design estimators, contrast alternative models

Struggle against data: How to make the estimators work



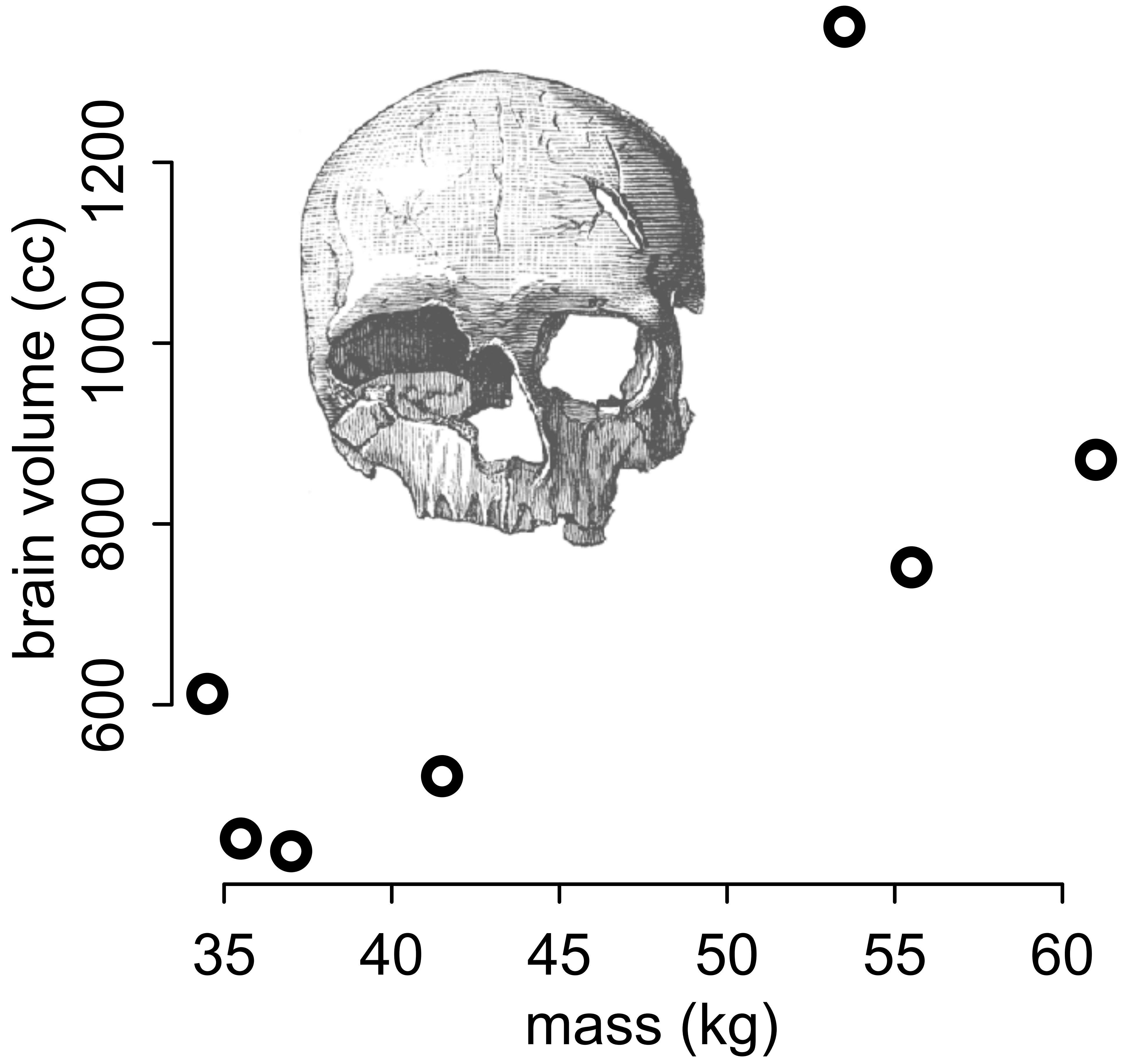
Problems of Prediction

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)



Leave-one-out cross-validation

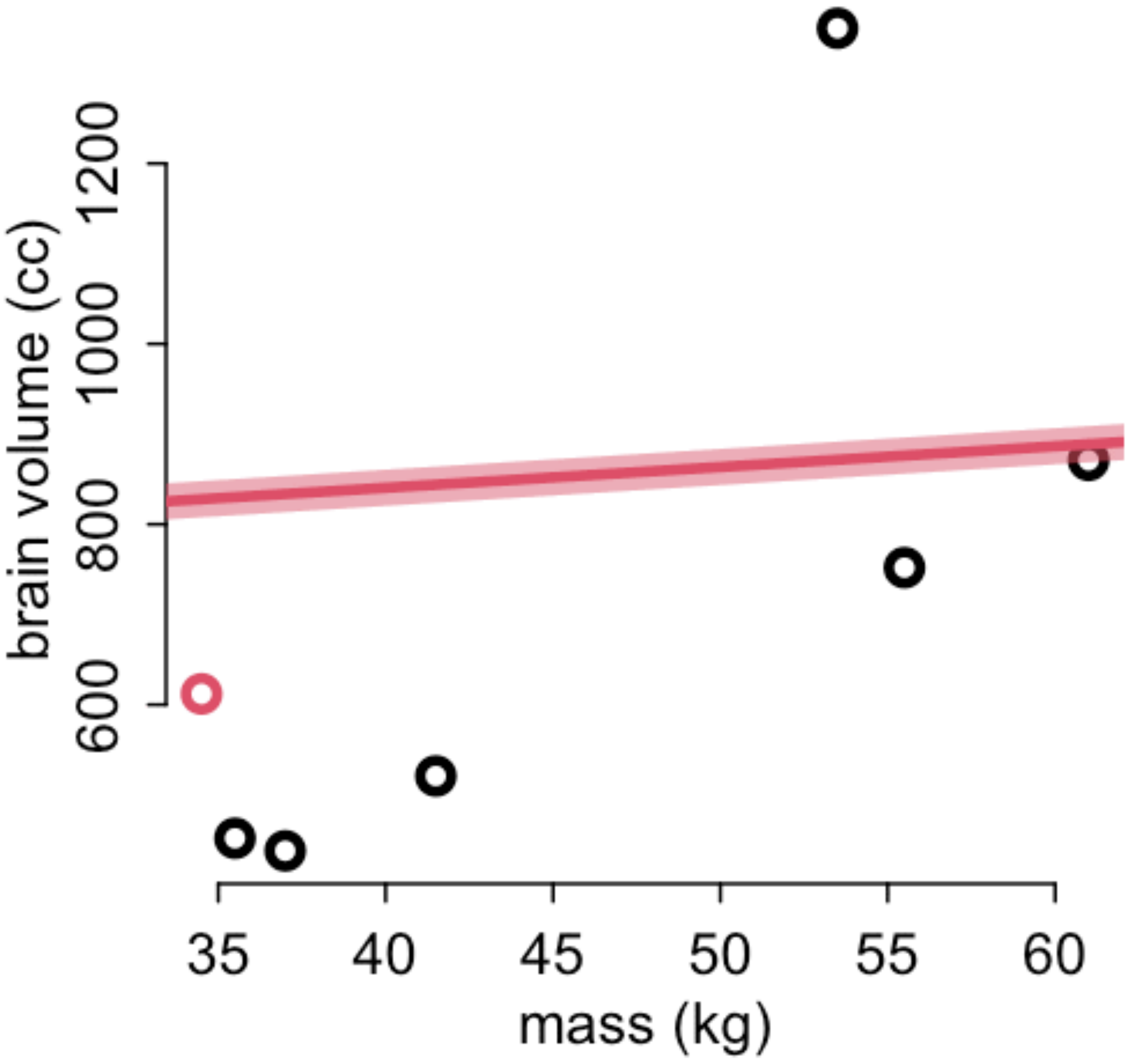
(1) Drop one point

(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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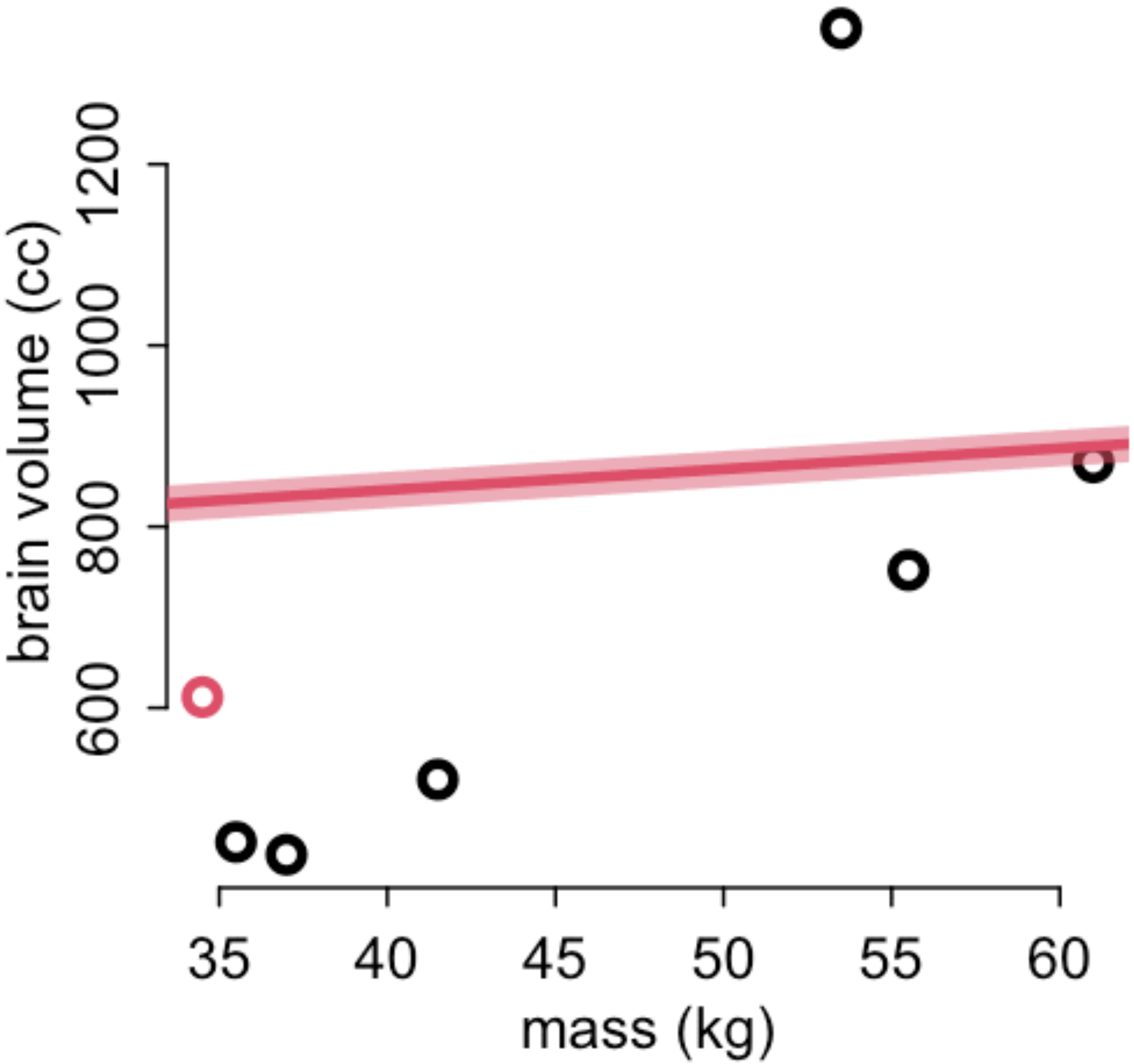

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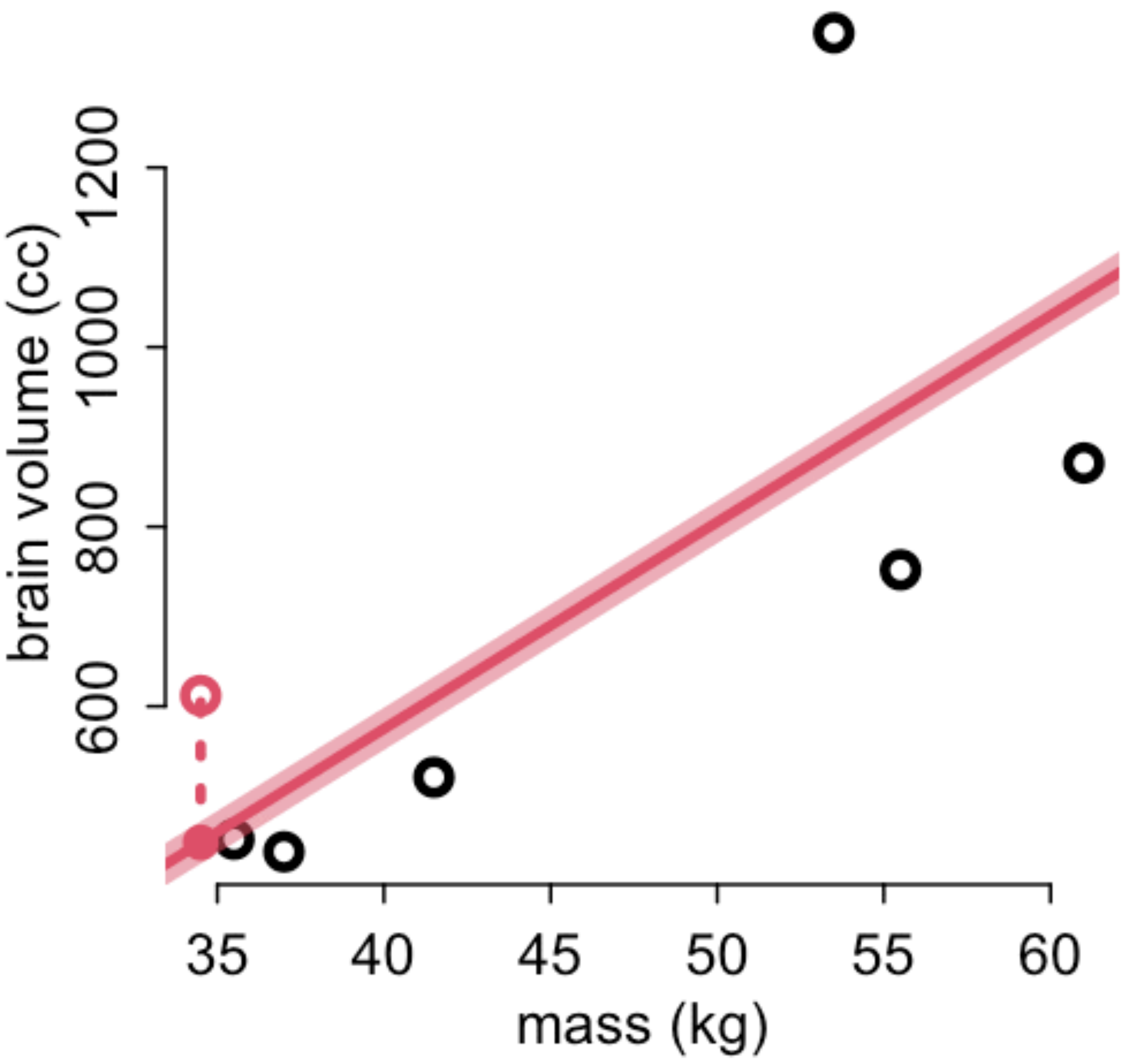

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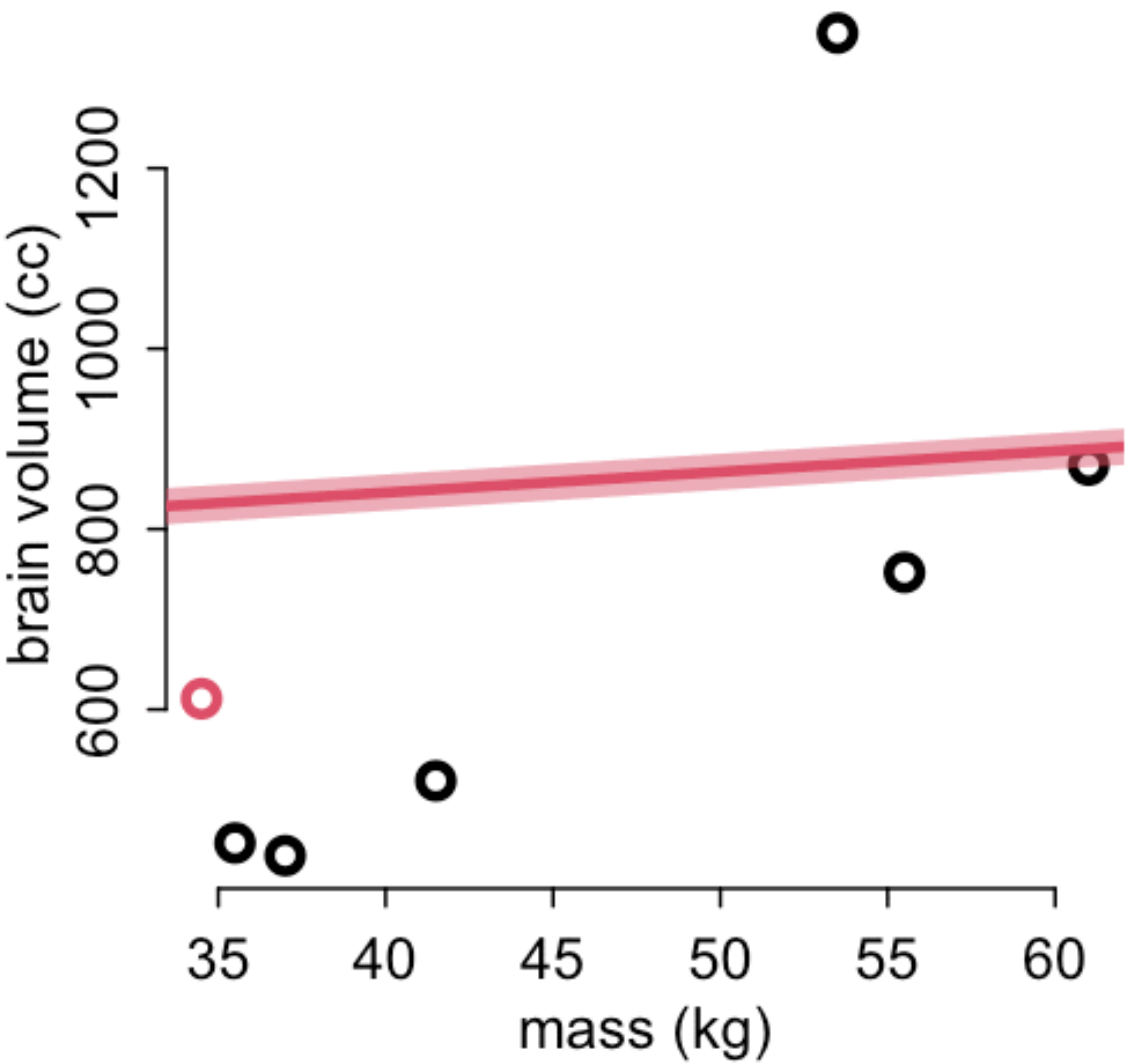

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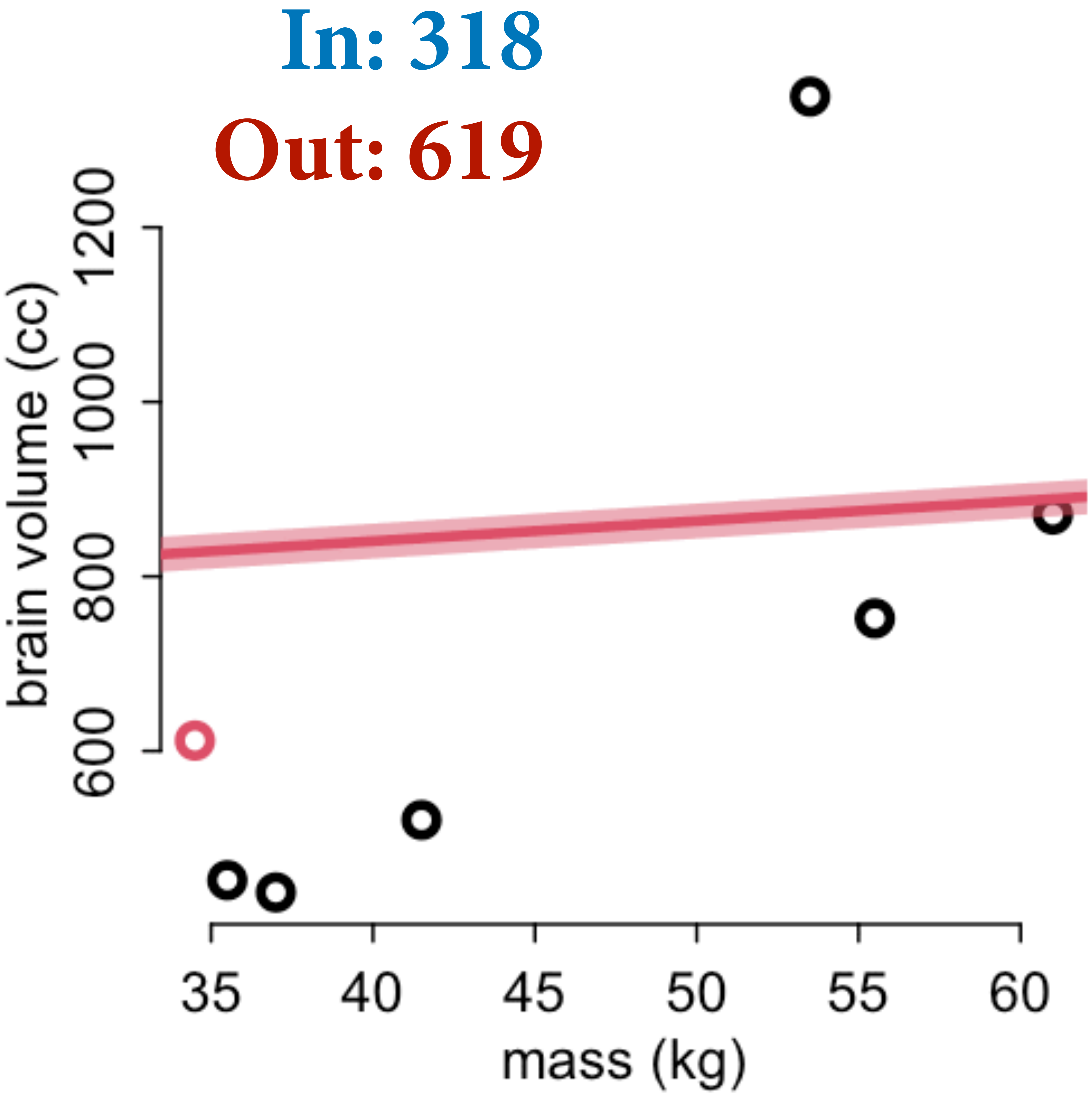
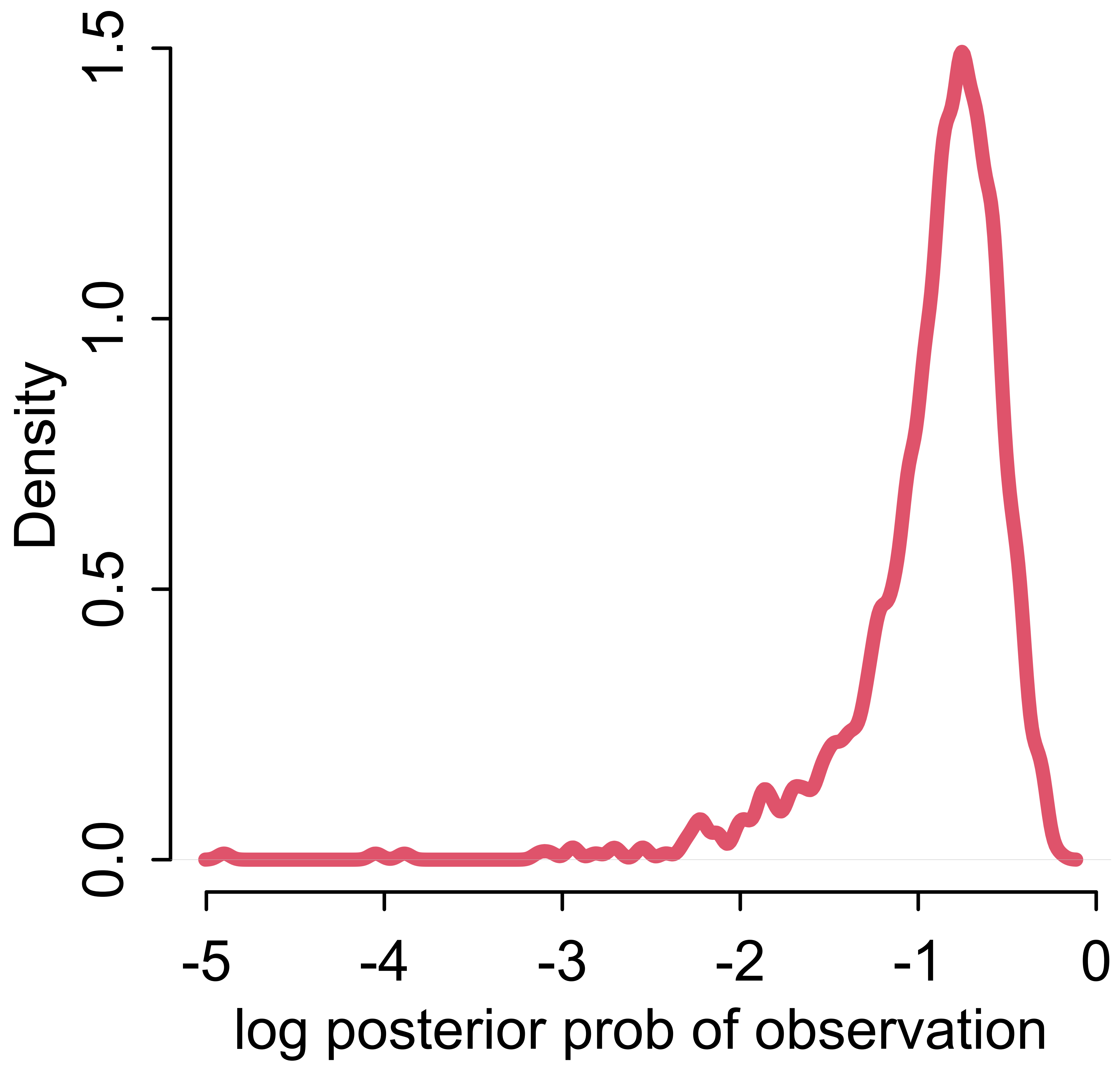


Bayesian Cross-Validation

We use the entire posterior, not just a point prediction

Cross-validation score is:

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



Bayesian Cross-Validation

S samples from posterior

N data points

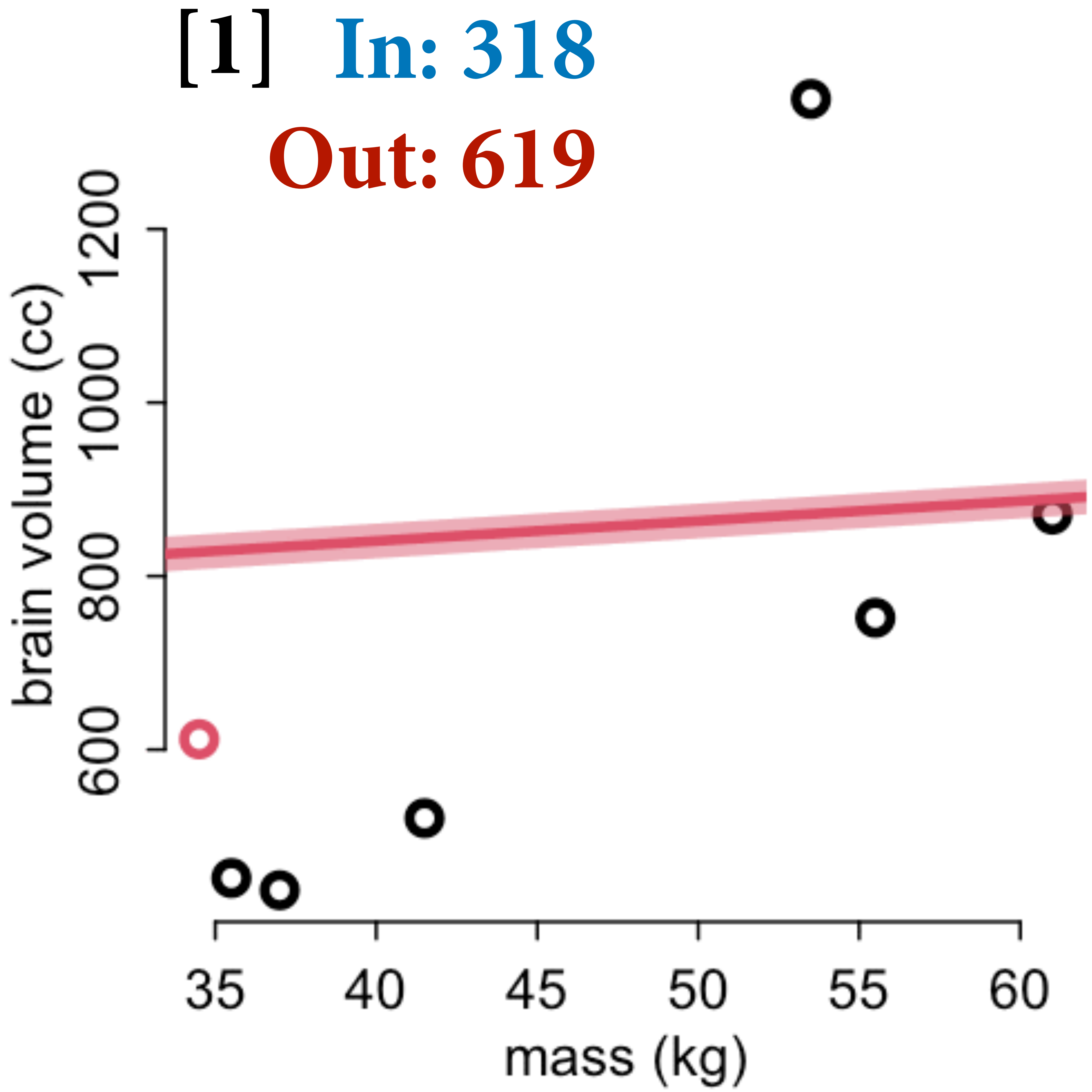
log pointwise predictive density

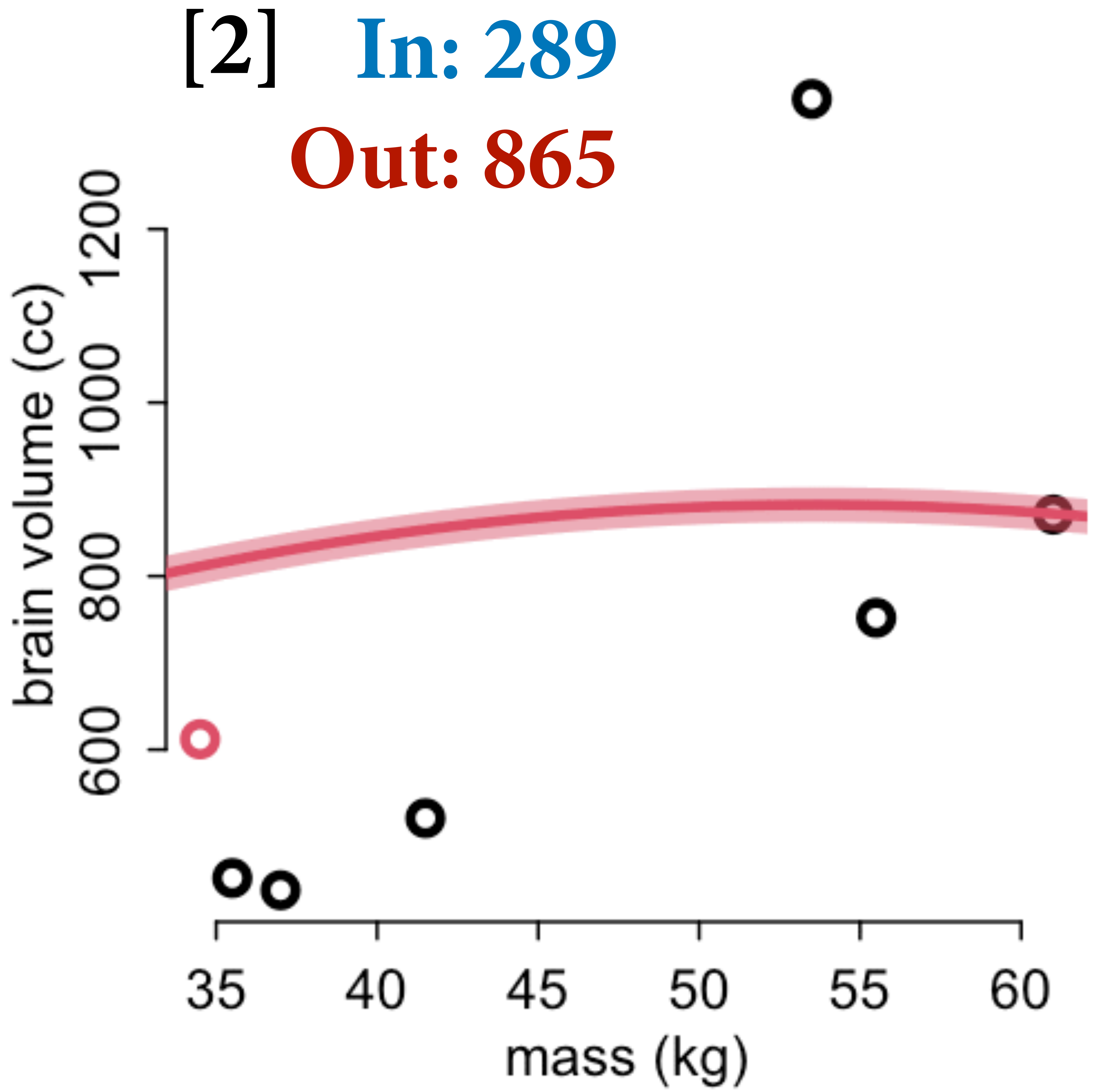
$$\text{lppd}_{\text{CV}} = \sum_{i=1}^{N} \underbrace{\frac{1}{S} \sum_{s=1}^{S} \underline{\log \Pr(y_i | \theta_{-i,s})}}$$

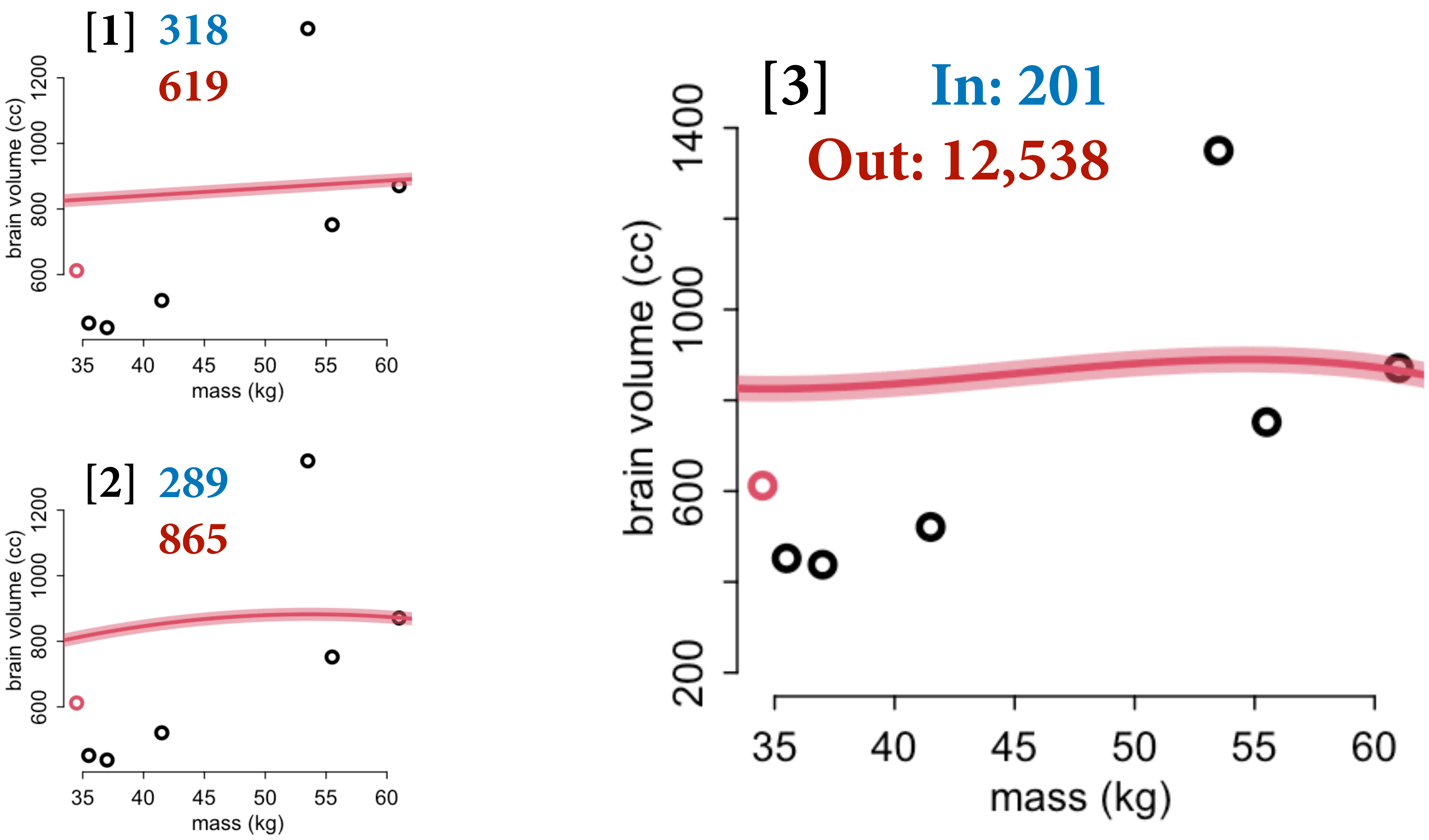
log probability of each point i, computed with posterior that omits point i

average log probability for point i

Pages 210 and 218


[1]
In: 318
Out: 619
brain volume (cc)
600
800
1000
1200
35
40
45
50
55
60
mass (kg)


[2]
In: 289
Out: 865
brain volume (cc)
600
800
1000
1200
35
40
45
50
55
60
mass (kg)


[1] 318
619
brain volume (cc)
mass (kg)
[2] 289
865
brain volume (cc)
mass (kg)
[3] In: 201
Out: 12,538
brain volume (cc)
mass (kg)

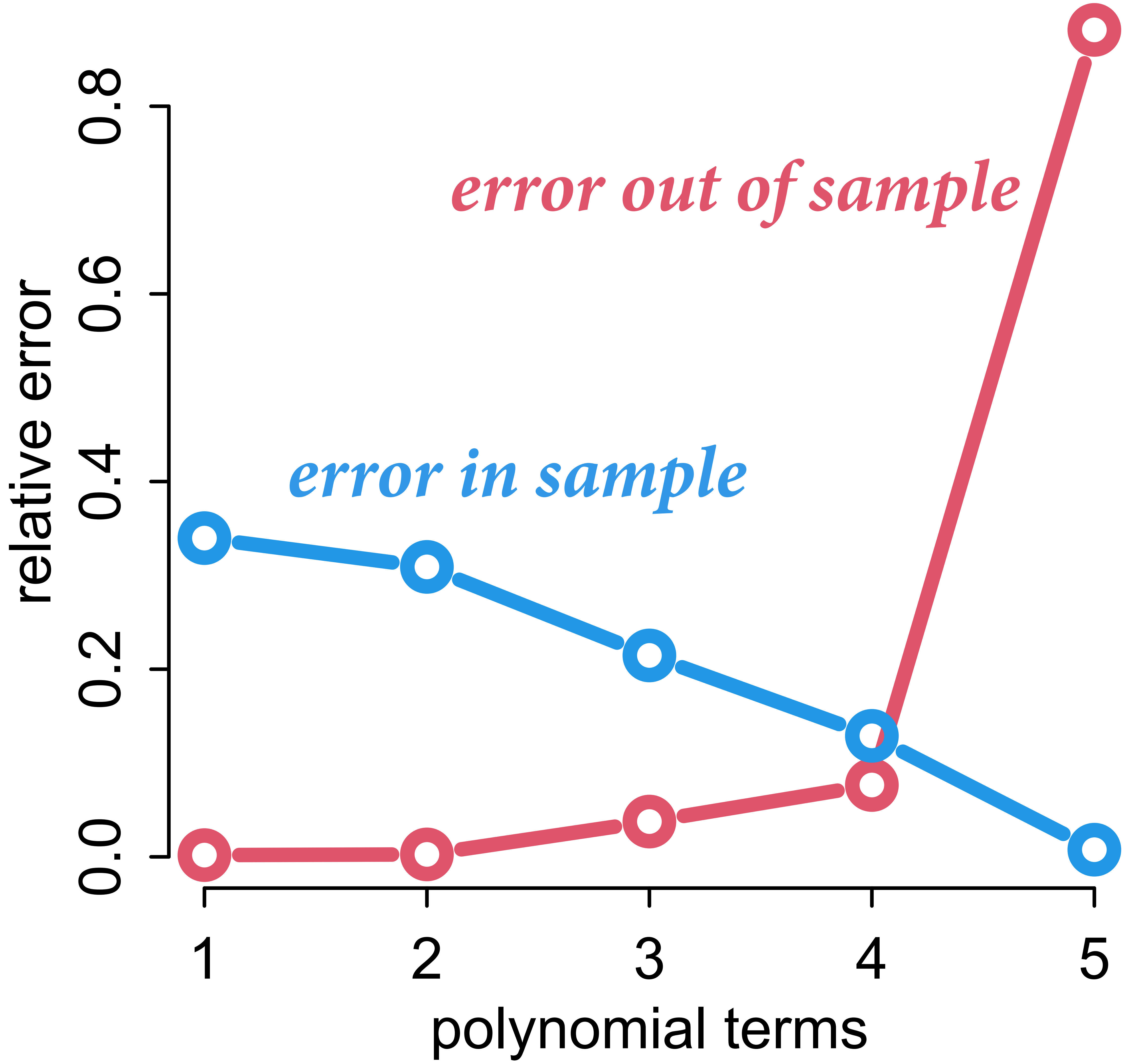
[1] 318
619
[2] 289
865
[3] 201
12,538
[4] 120
25,530
[5] 7
293,840
brain volume (cc)
mass (kg)

Cross-validation

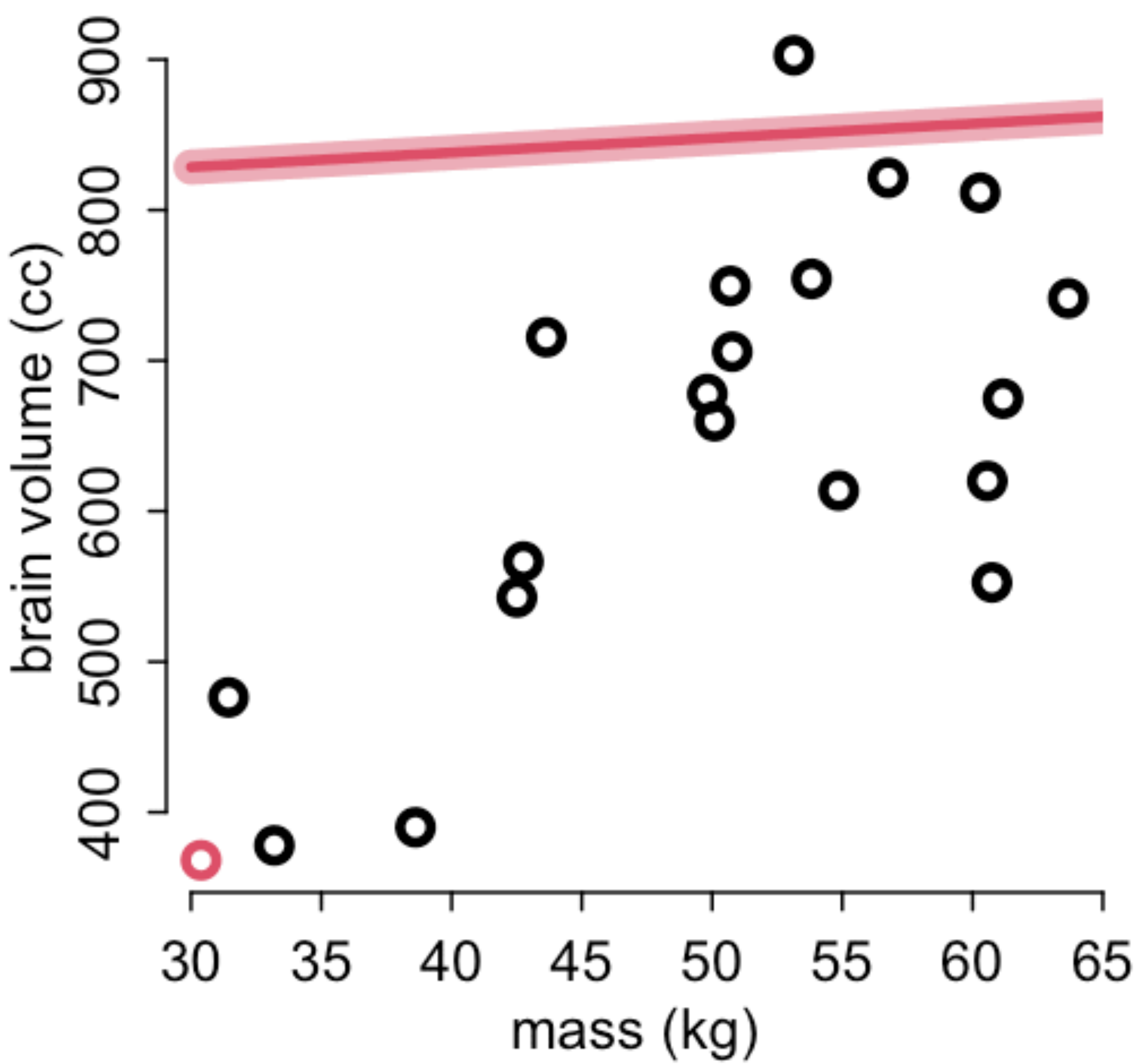
For **simple** models, more parameters improves fit to sample

But may reduce accuracy of predictions out of sample

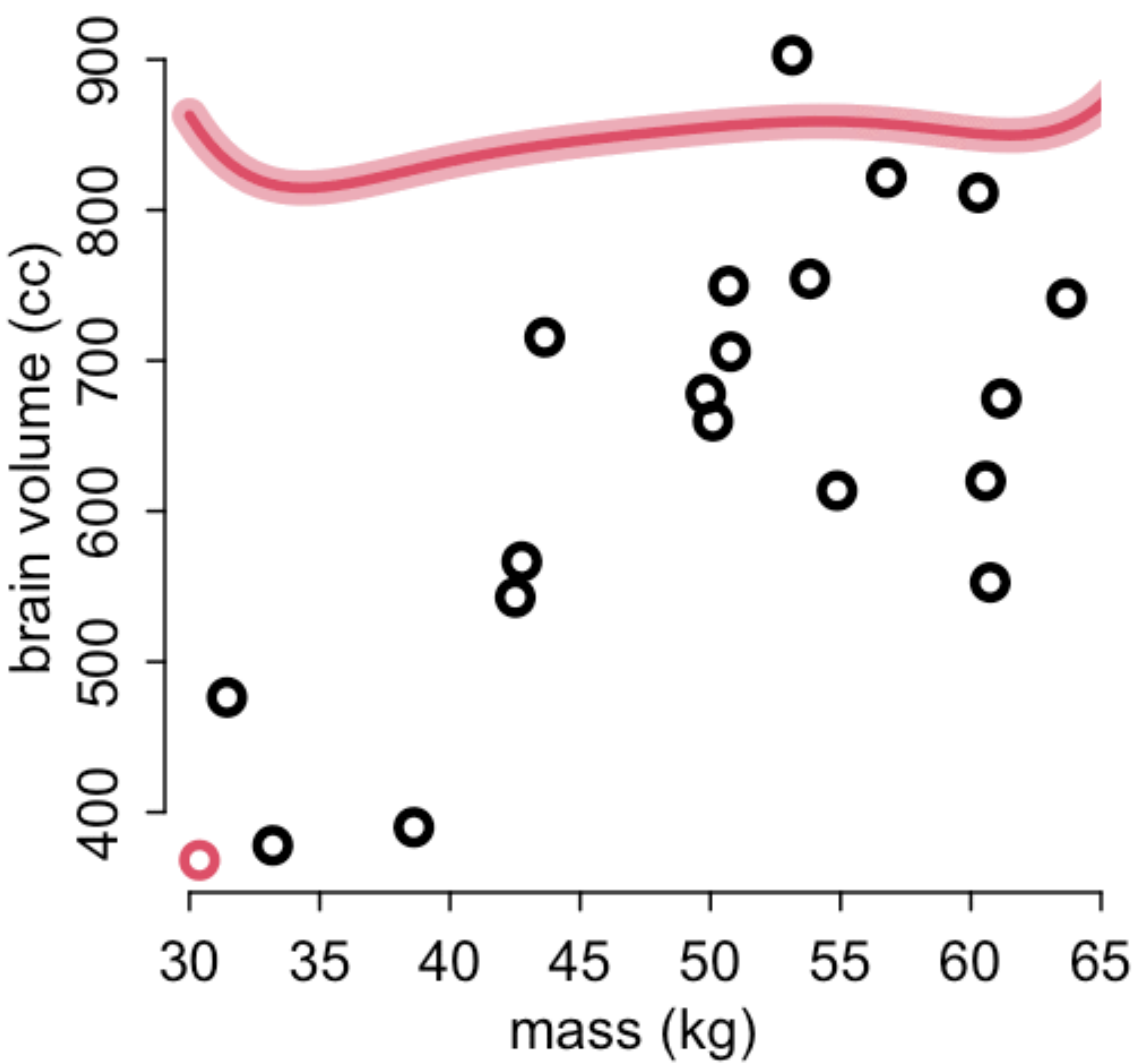
Most accurate model trades off flexibility with **overfitting**



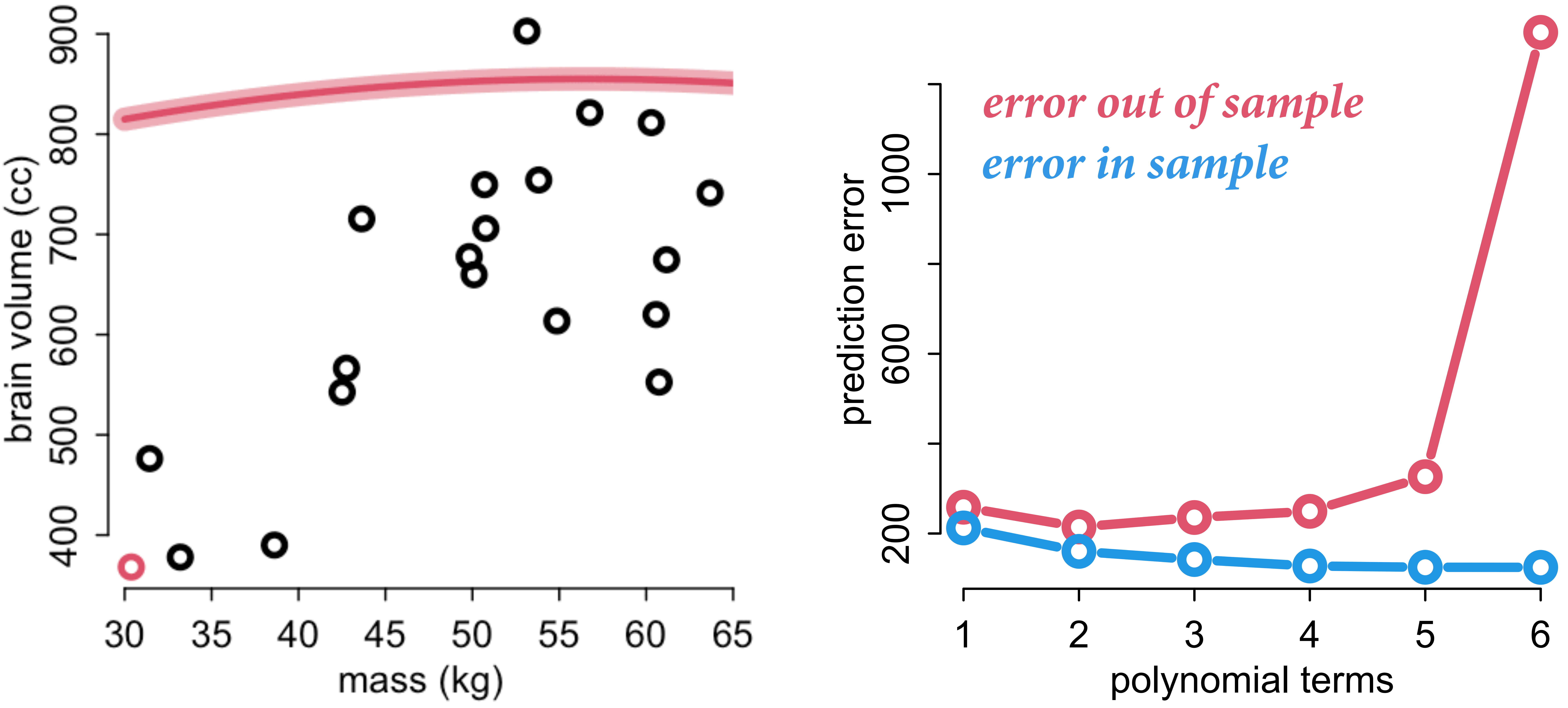
1st degree polynomial



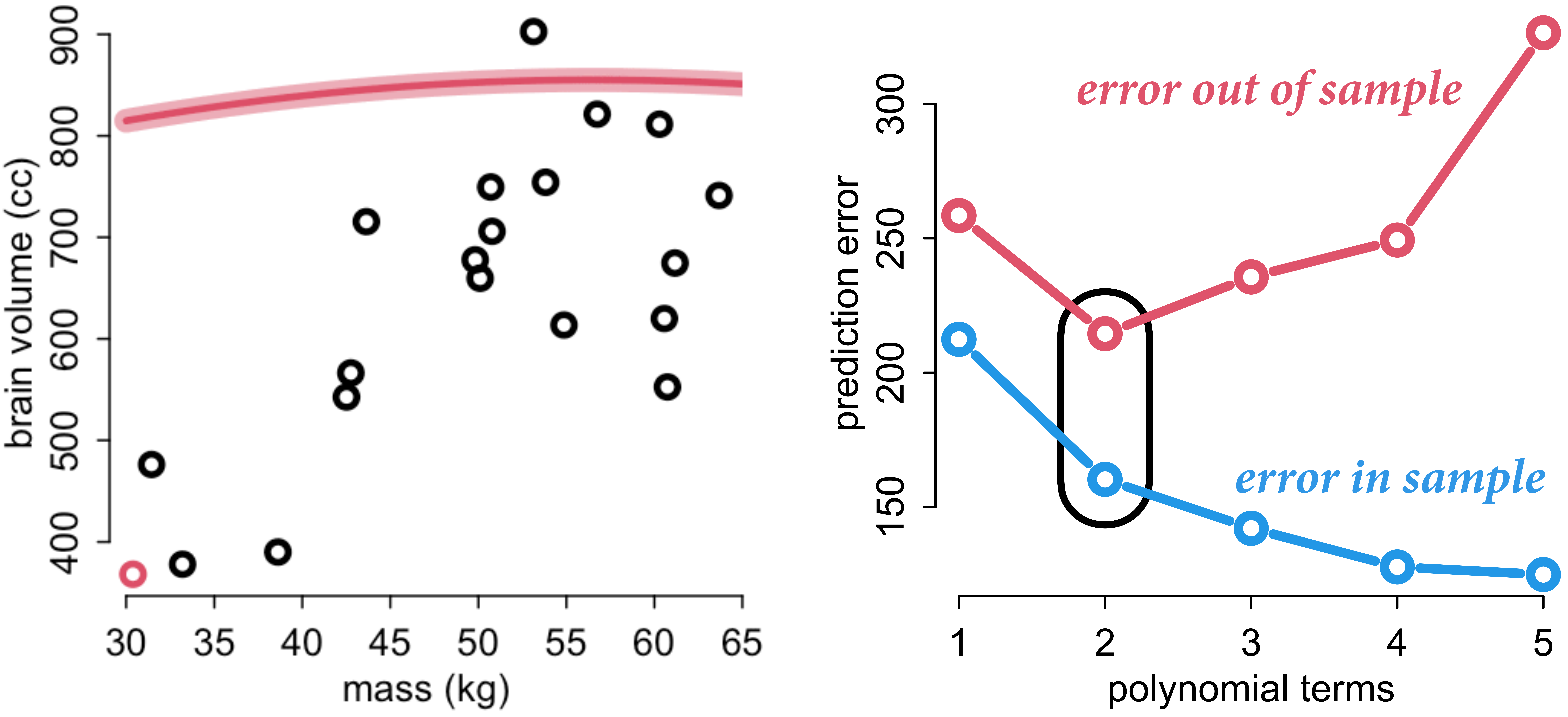
6th degree polynomial



2nd degree polynomial



2nd degree polynomial



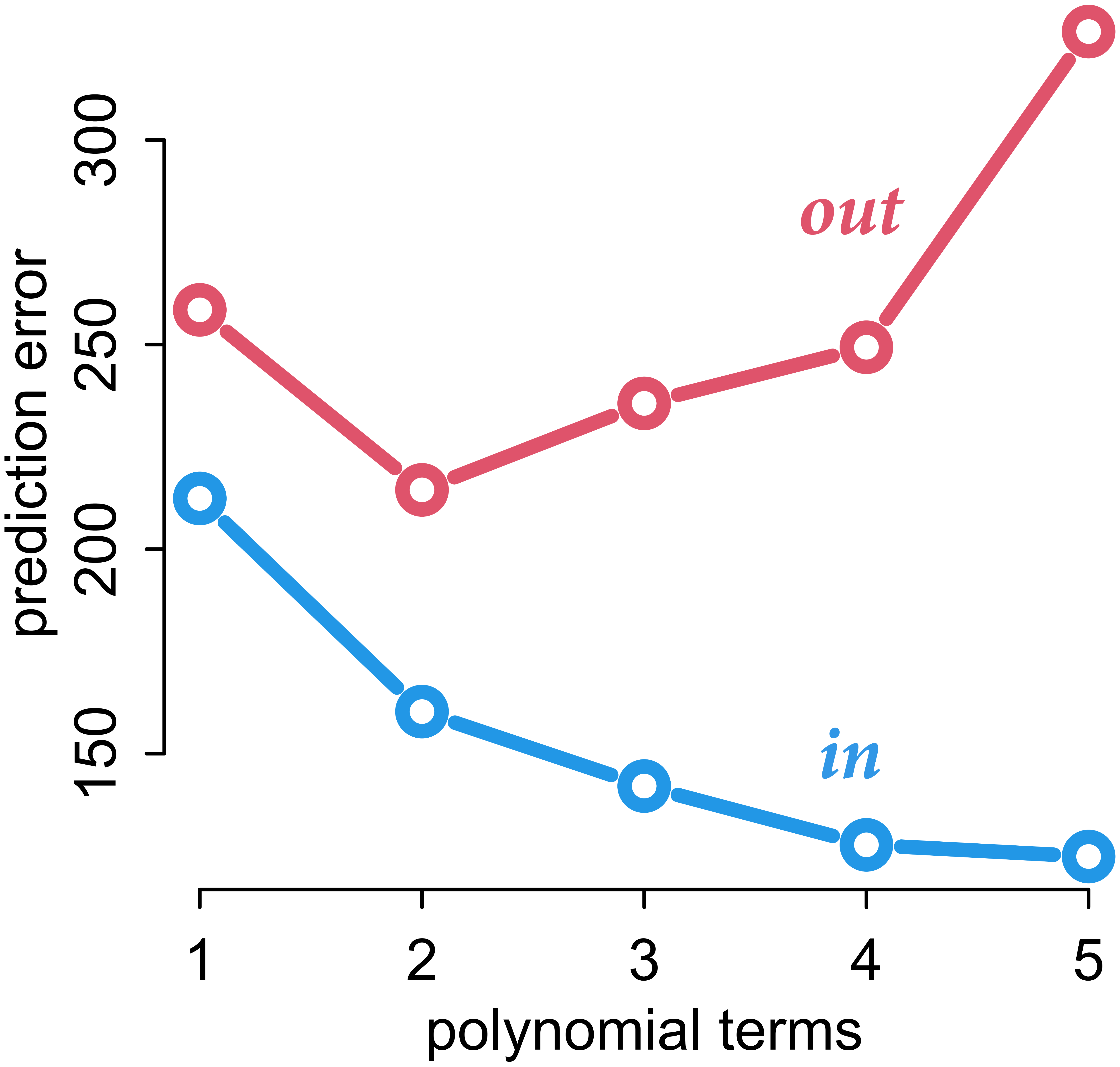
Regularization

Overfitting depends upon the priors

Skeptical priors have tighter variance, reduce flexibility

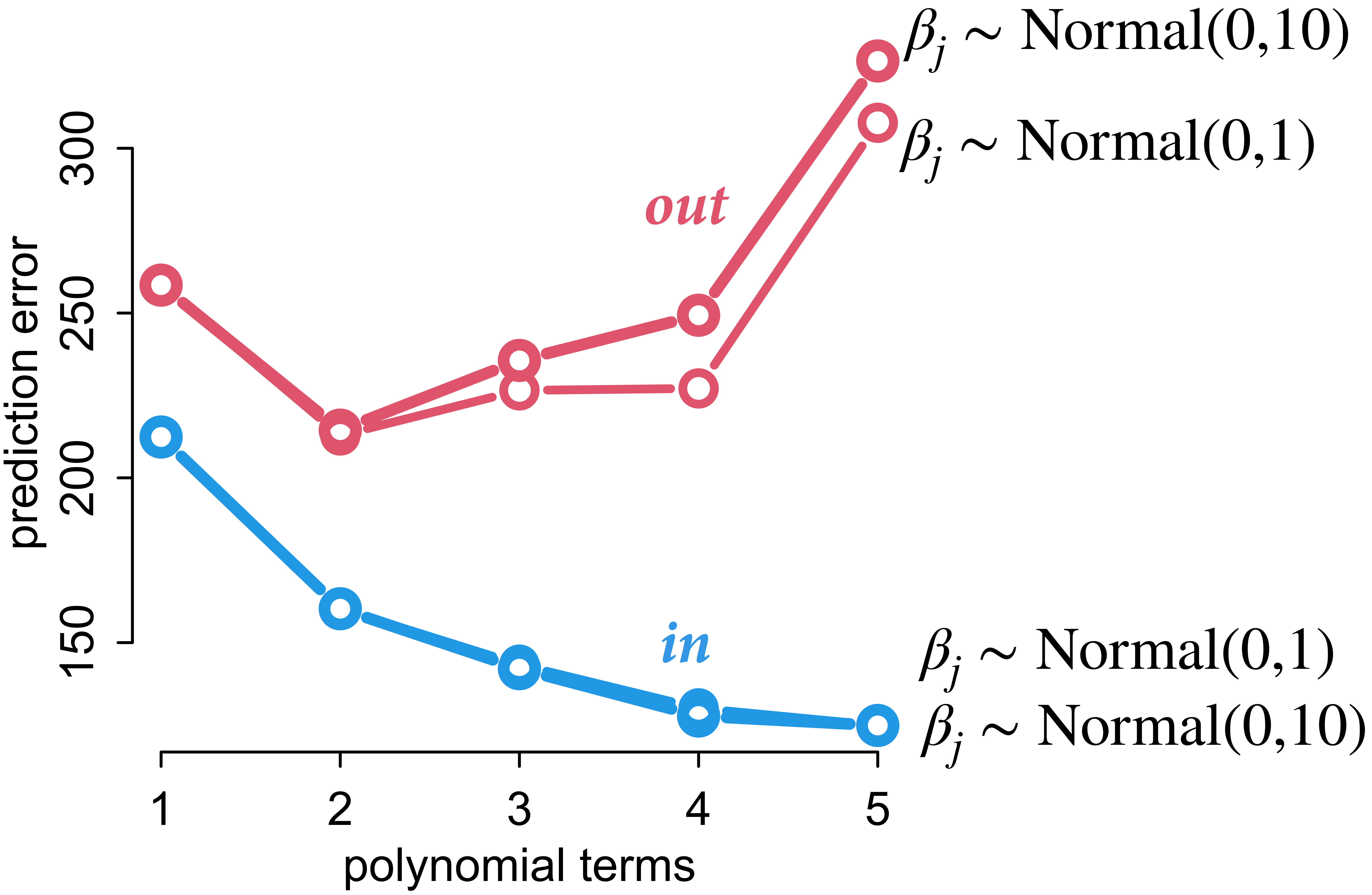
Regularization: Function finds regular features of process

Good priors are often tighter than you think!

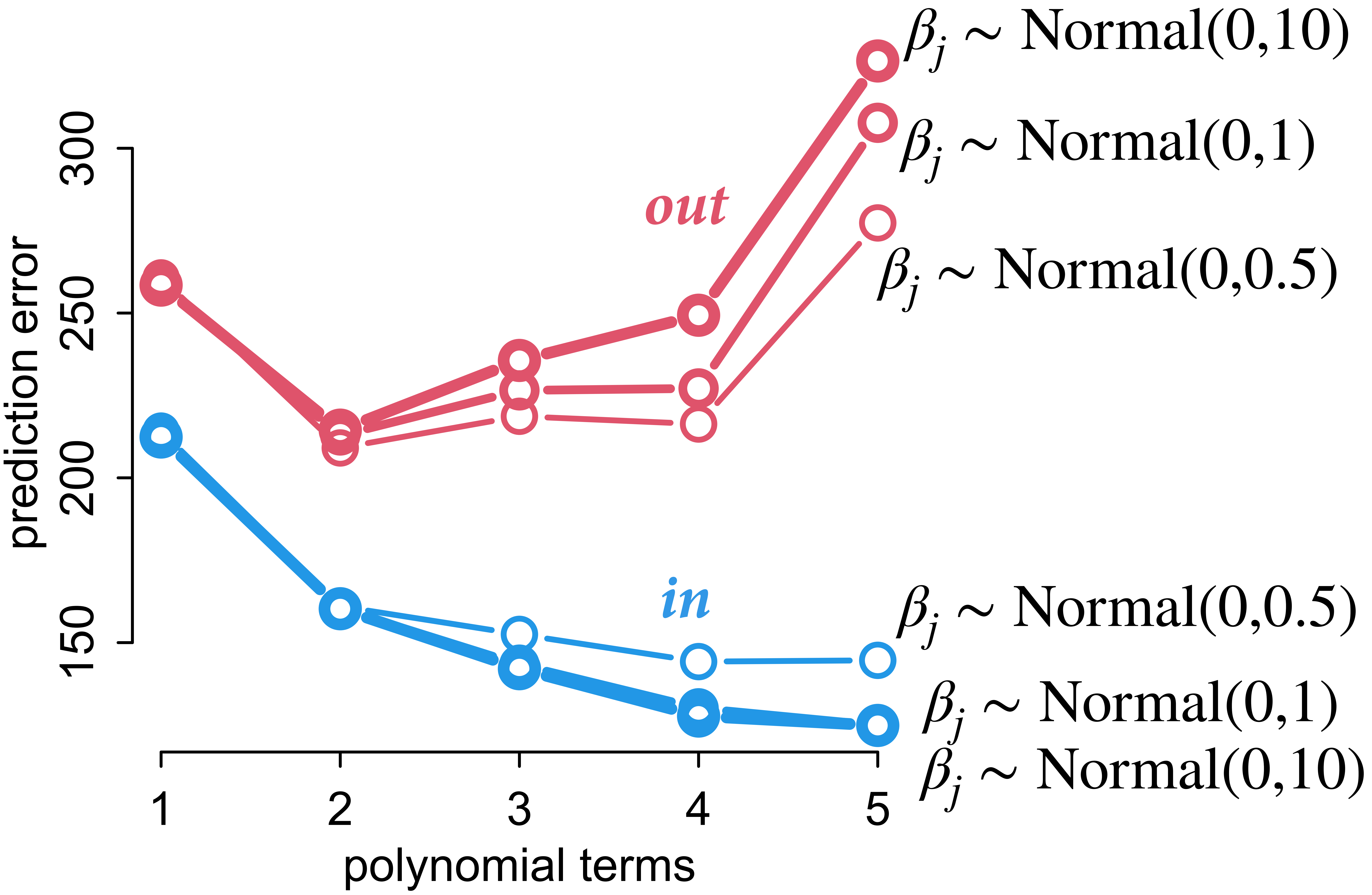


$$\mu_i = \alpha + \sum_{j=1}^{m} \beta_j x_i^j$$

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



$\beta_j \sim \text{Normal}(0,10)$
$\beta_j \sim \text{Normal}(0,1)$
out
in
$\beta_j \sim \text{Normal}(0,1)$
$\beta_j \sim \text{Normal}(0,10)$
prediction error
150
200
250
300
1
2
3
4
5
polynomial terms



$\beta_j \sim$ Normal(0,10)
$\beta_j \sim$ Normal(0,1)
$\beta_j \sim$ Normal(0,0.5)
out
in
$\beta_j \sim$ Normal(0,0.5)
$\beta_j \sim$ Normal(0,1)
$\beta_j \sim$ Normal(0,10)
prediction error
150
200
250
300
1
2
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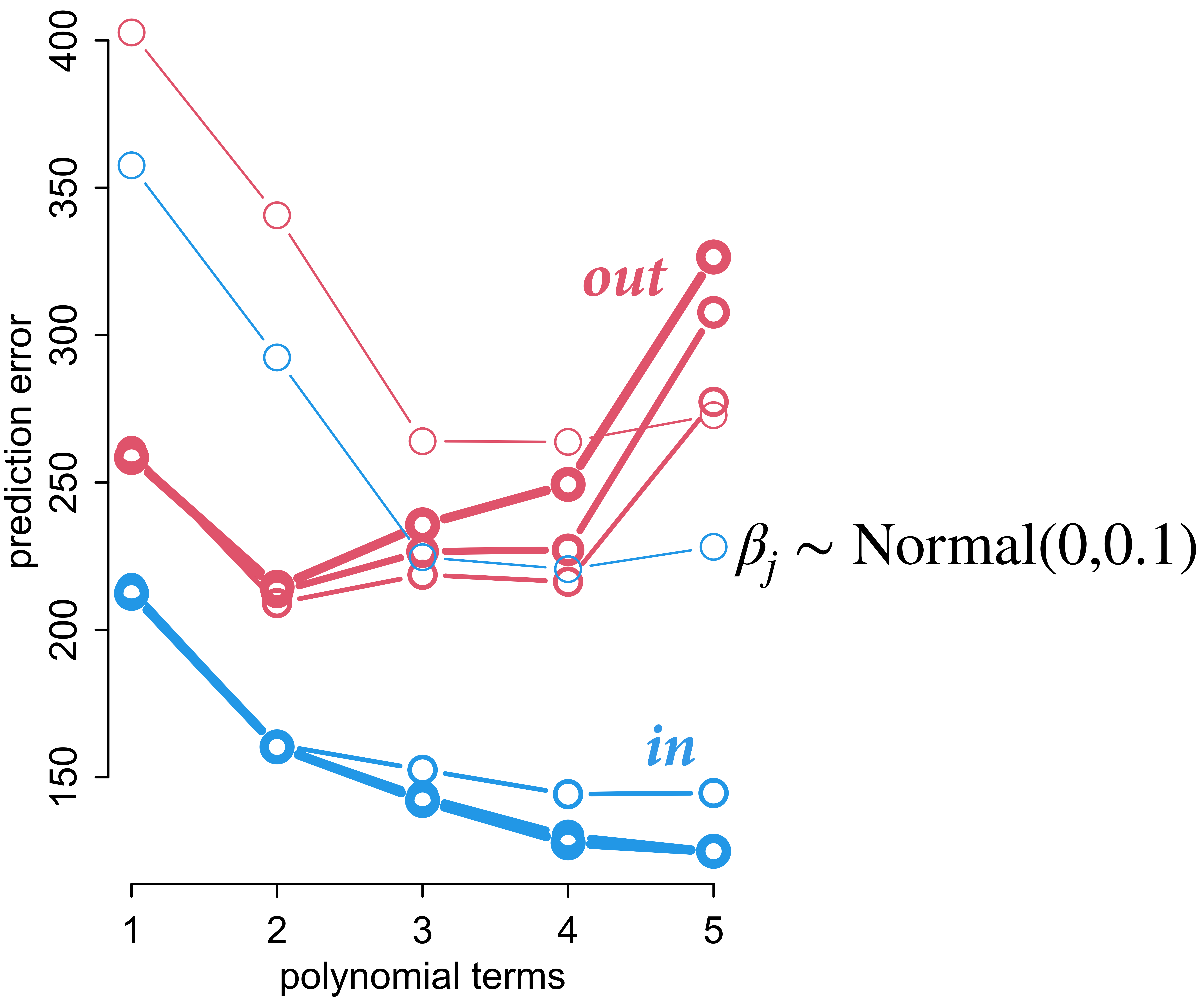

prediction error
400
350
300
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200
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polynomial terms
1
2
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out
in
$\beta_j \sim \text{Normal}(0,0.1)$

Regularizing priors

How to choose width of prior?

For causal inference, use science

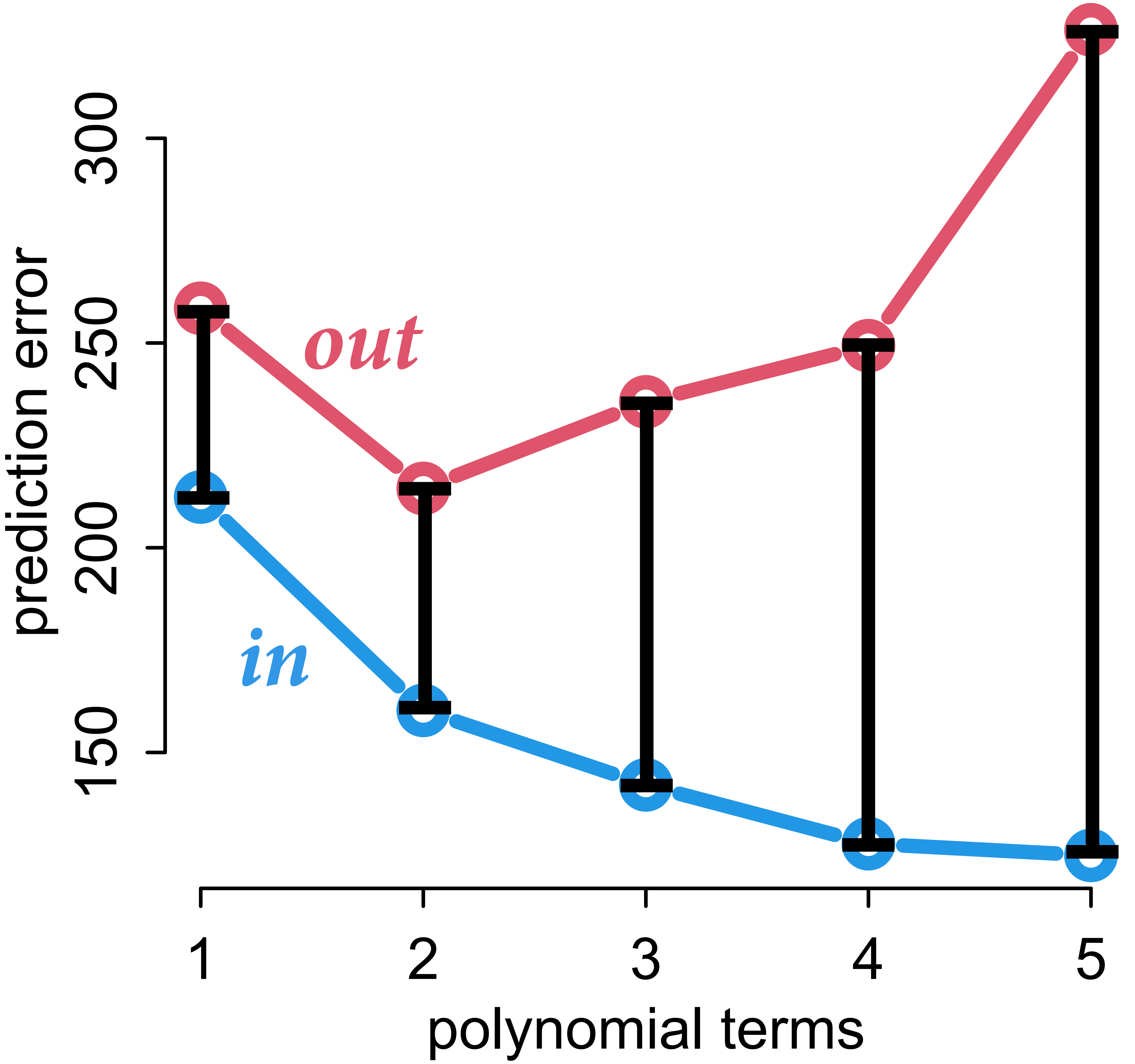
For pure prediction, can tune the prior using cross-validation

Many tasks are a mix of inference and prediction

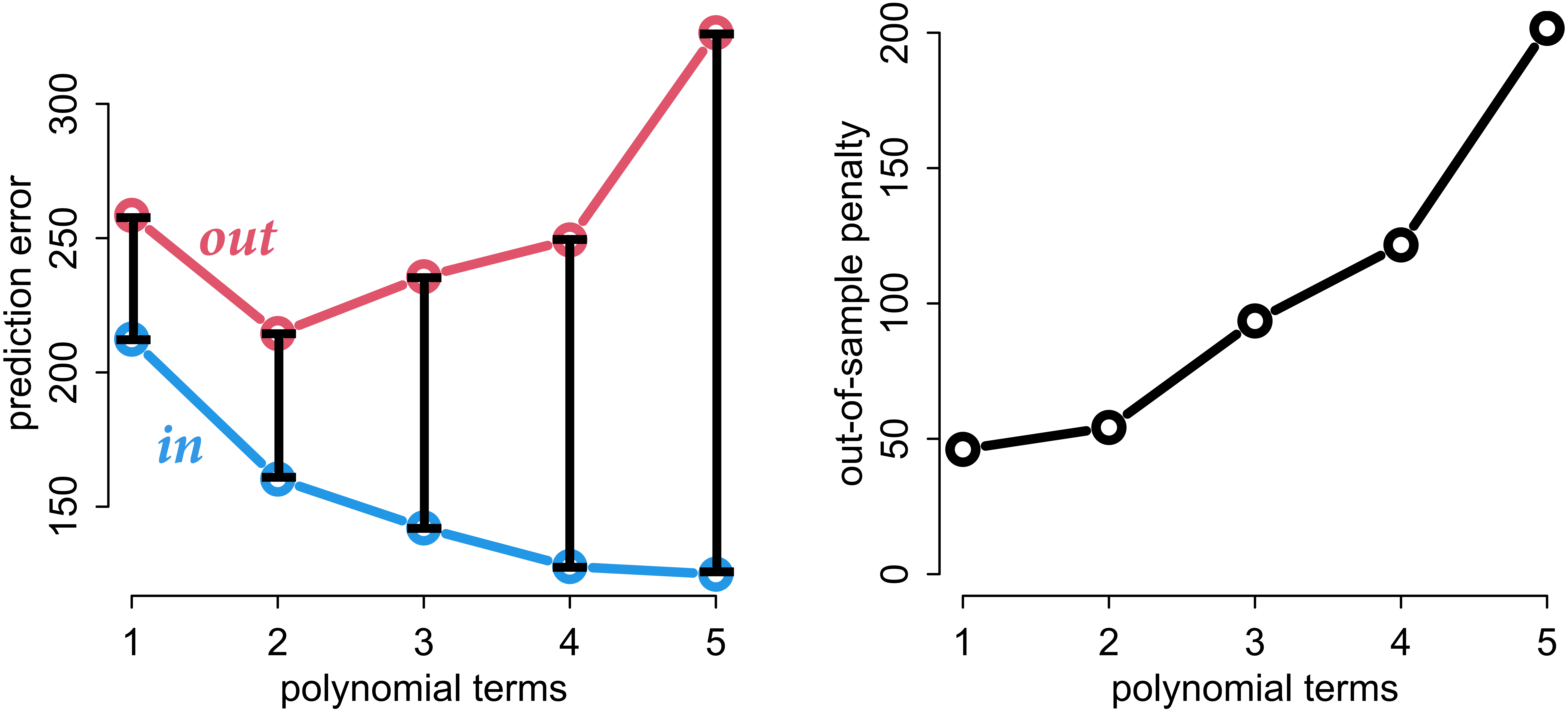
No need to be perfect, just better

PAUSE

Prediction penalty



Prediction penalty



Penalty prediction

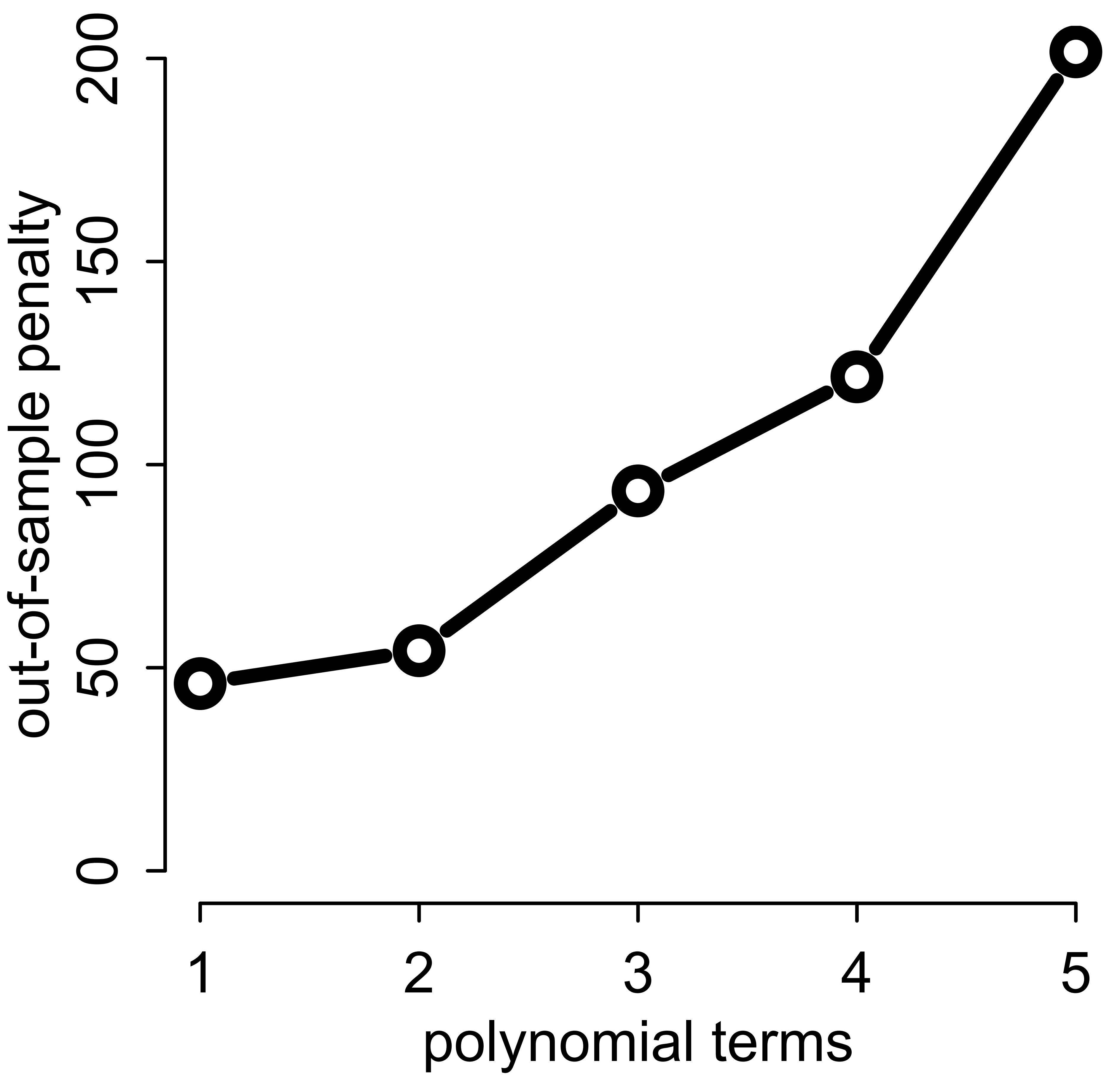
For *N* points, cross-validation requires fitting *N* models

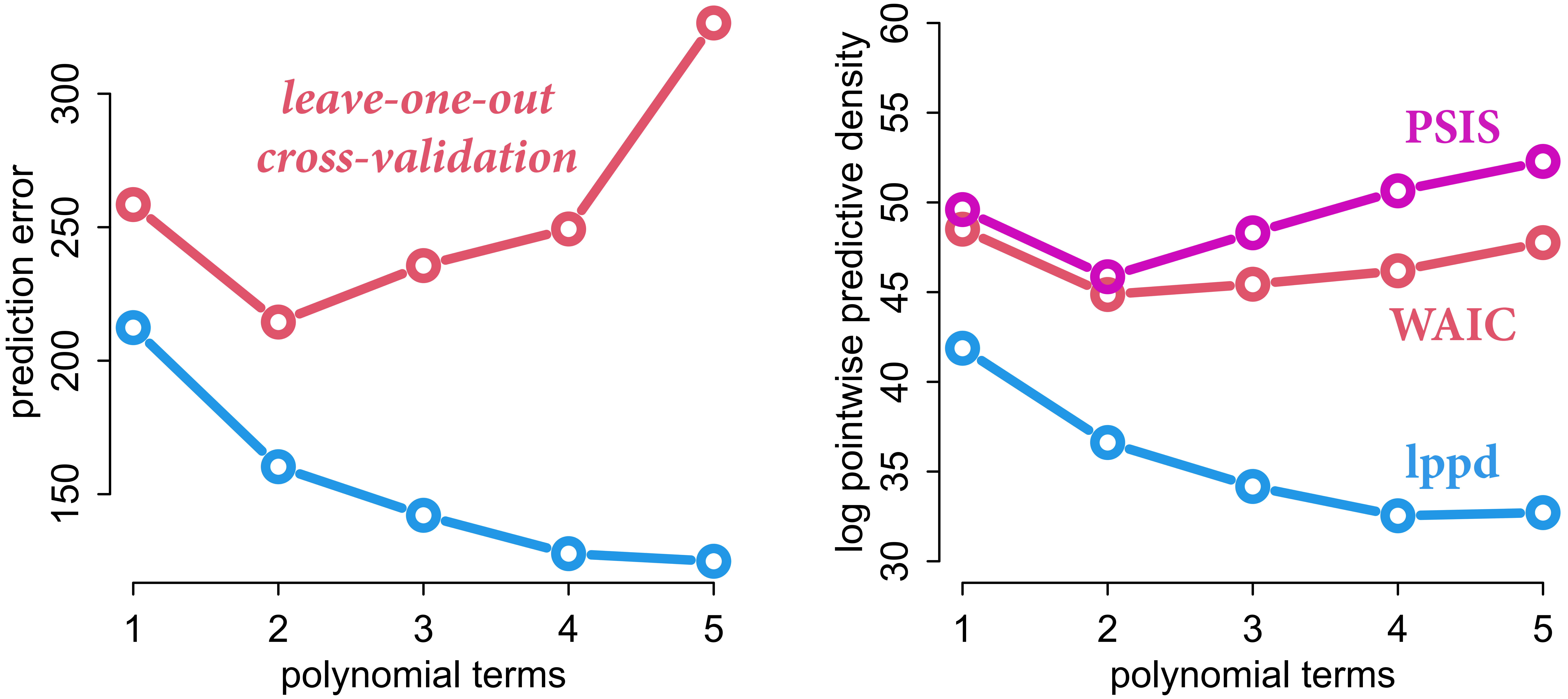
What if you could estimate the penalty from a single model fit?

Good news! You can:

Importance sampling (PSIS)

Information criteria (WAIC)





leave-one-out
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60
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35
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PSIS
WAIC
lppd
1
2
3
4
5
polynomial terms

WAIC,PSIS,CV measure overfitting

Regularization manages overfitting

None directly address causal inference

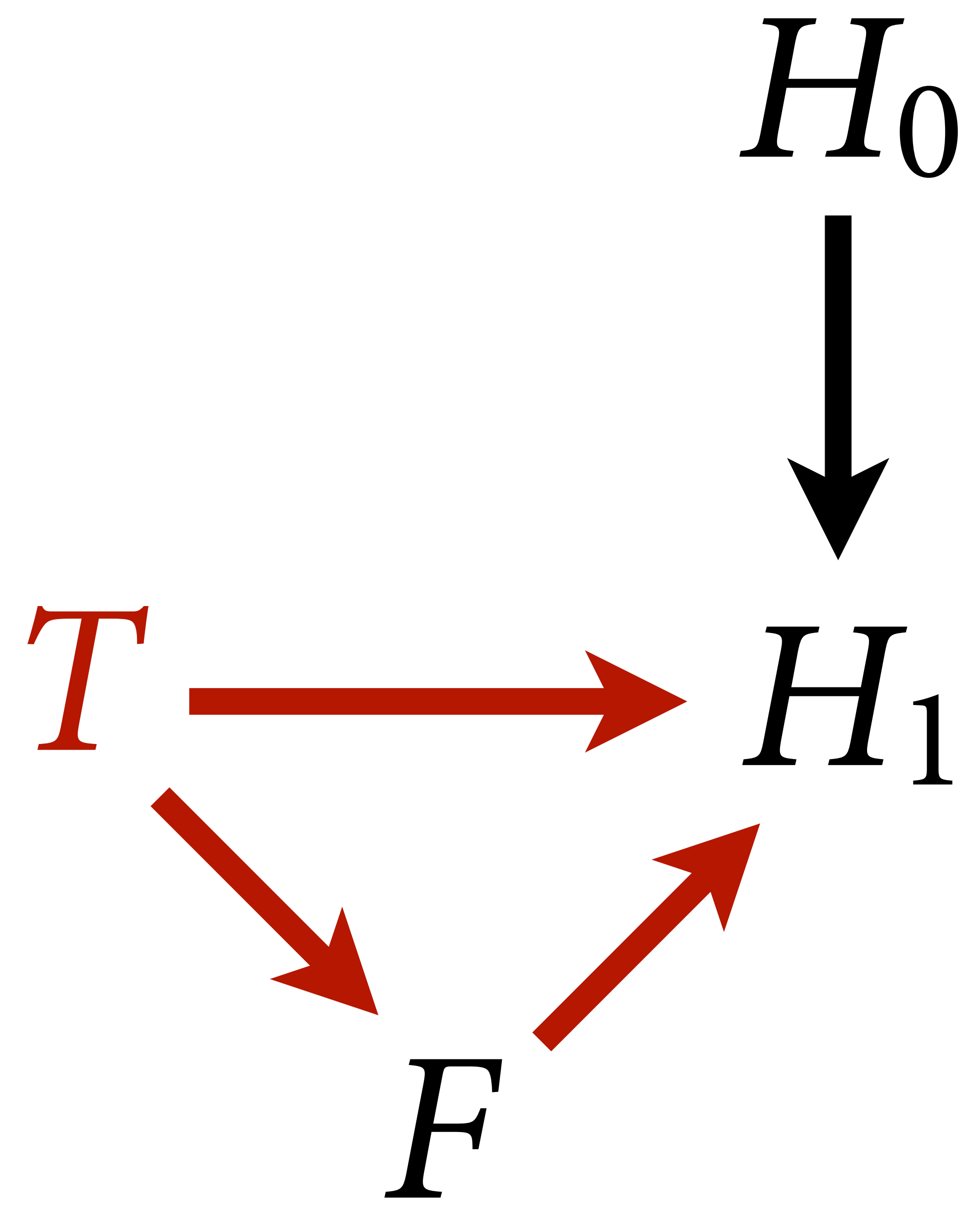
Important for understanding statistical inference

Model Mis-selection

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

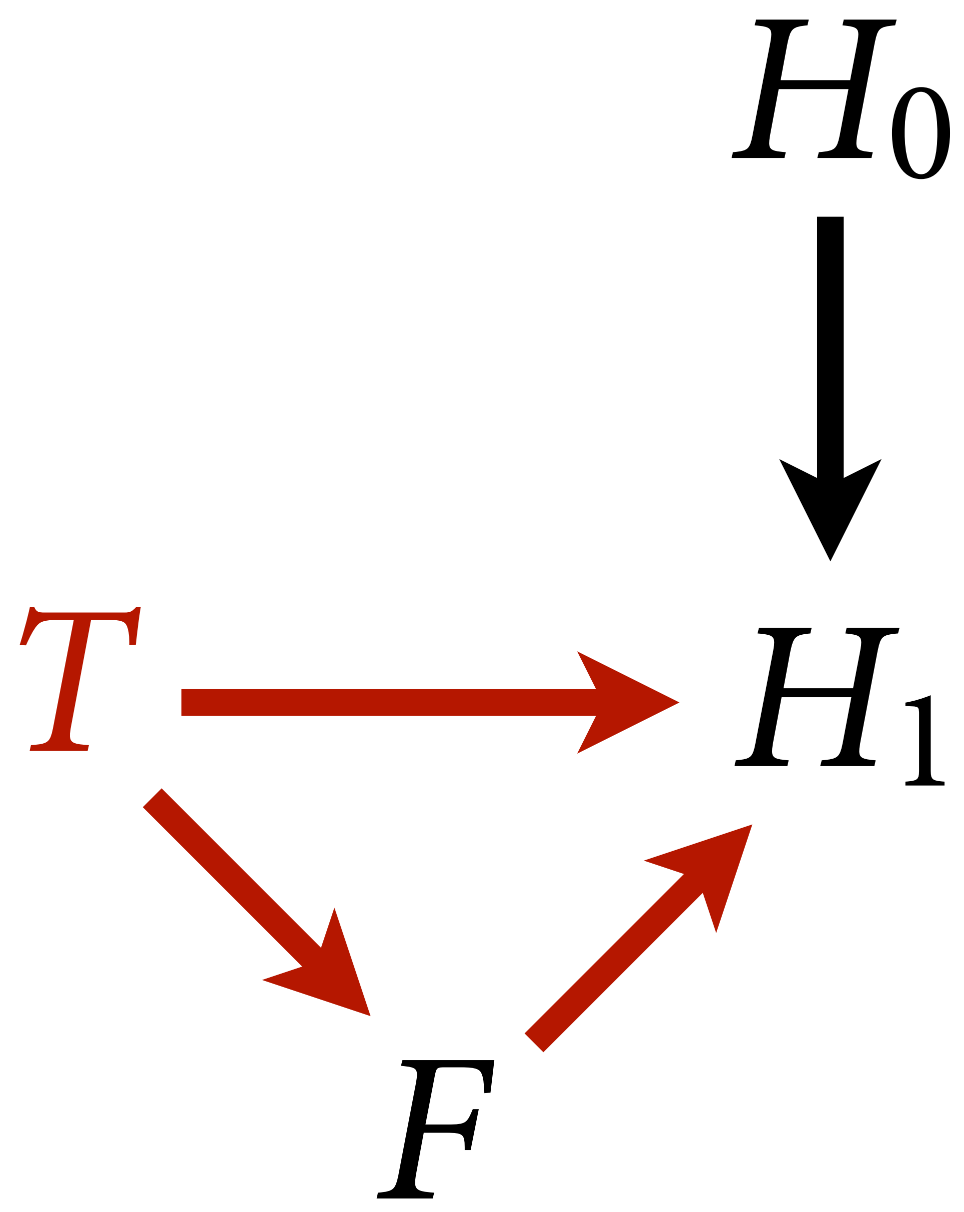
Predictive criteria actually prefer confounds & colliders

Example: Plant growth experiment



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

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



$$H_1 \sim \text{Normal}(\mu_i, \sigma)$$
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Correct adjustment set for total causal effect of treatment

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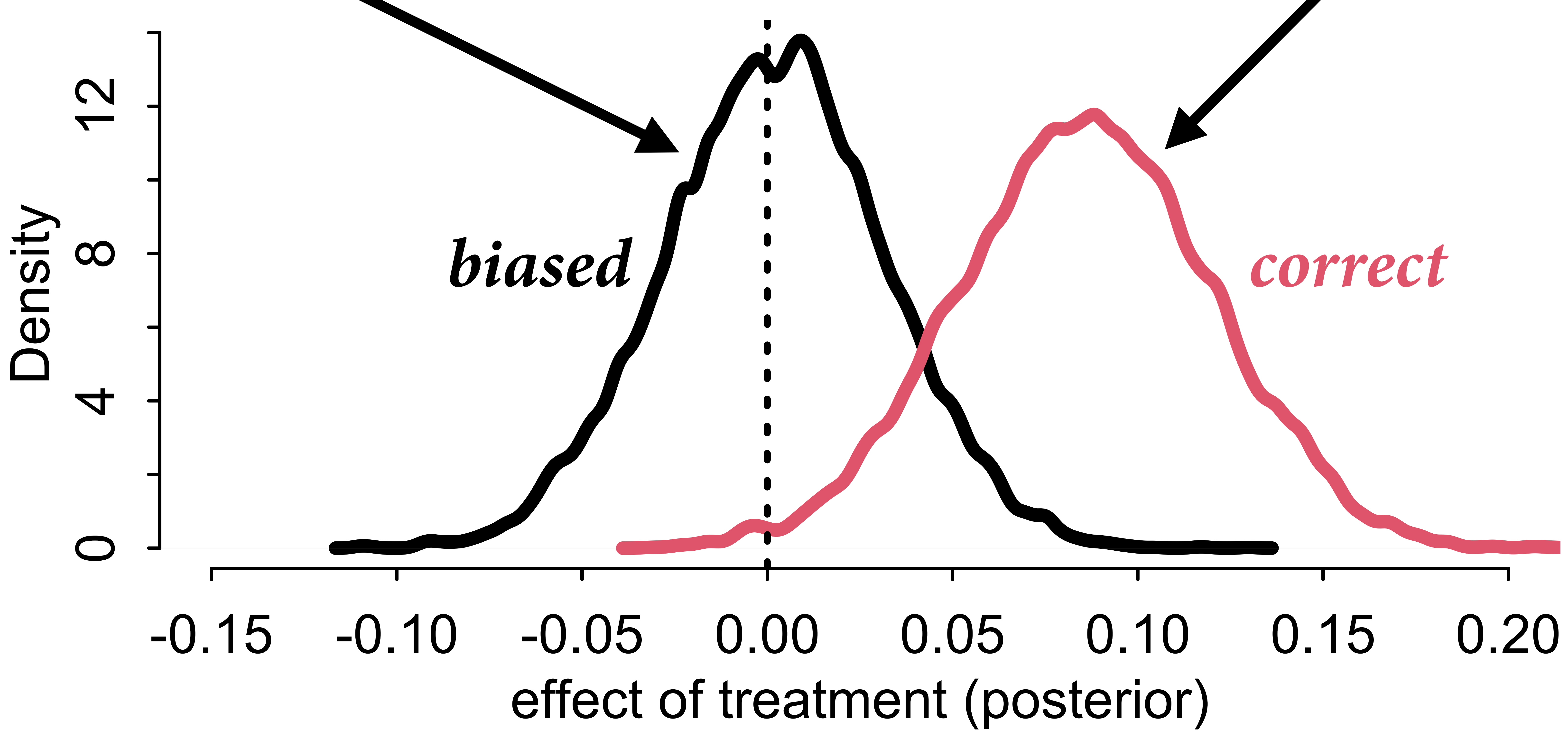

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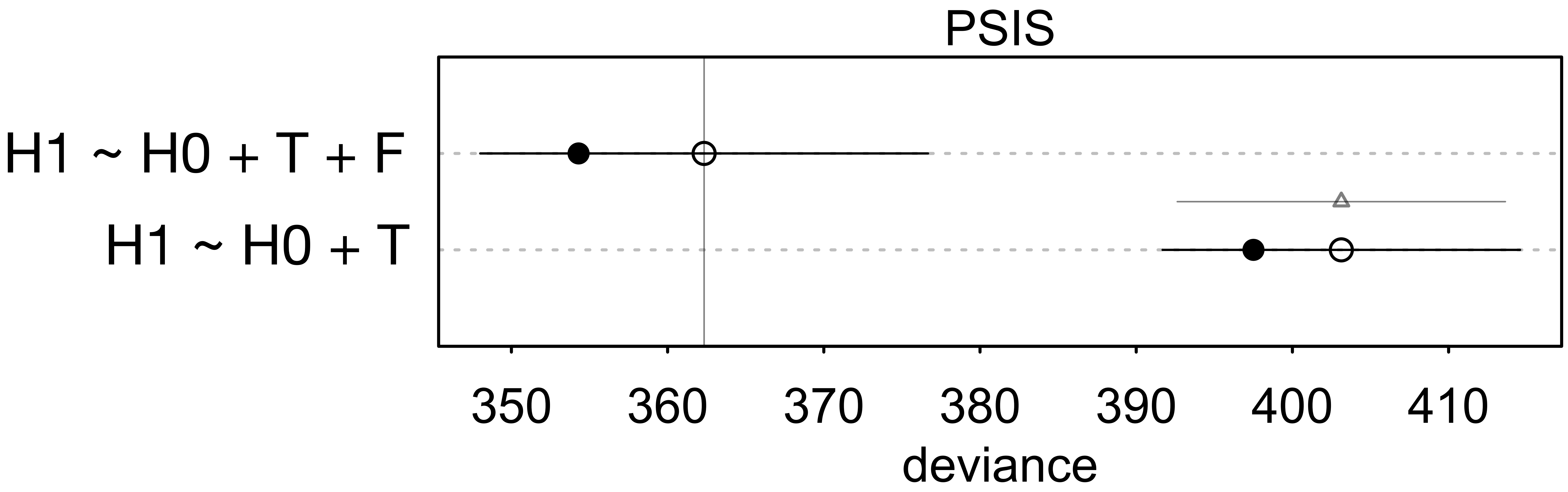
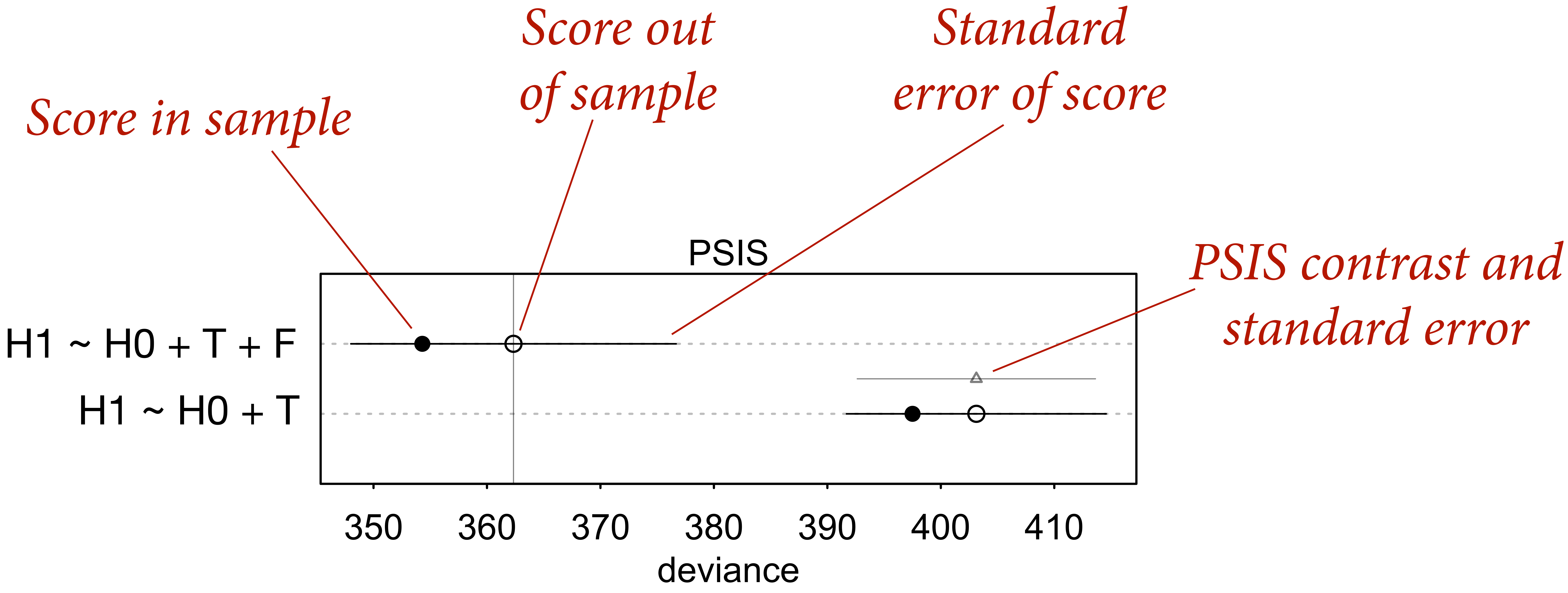
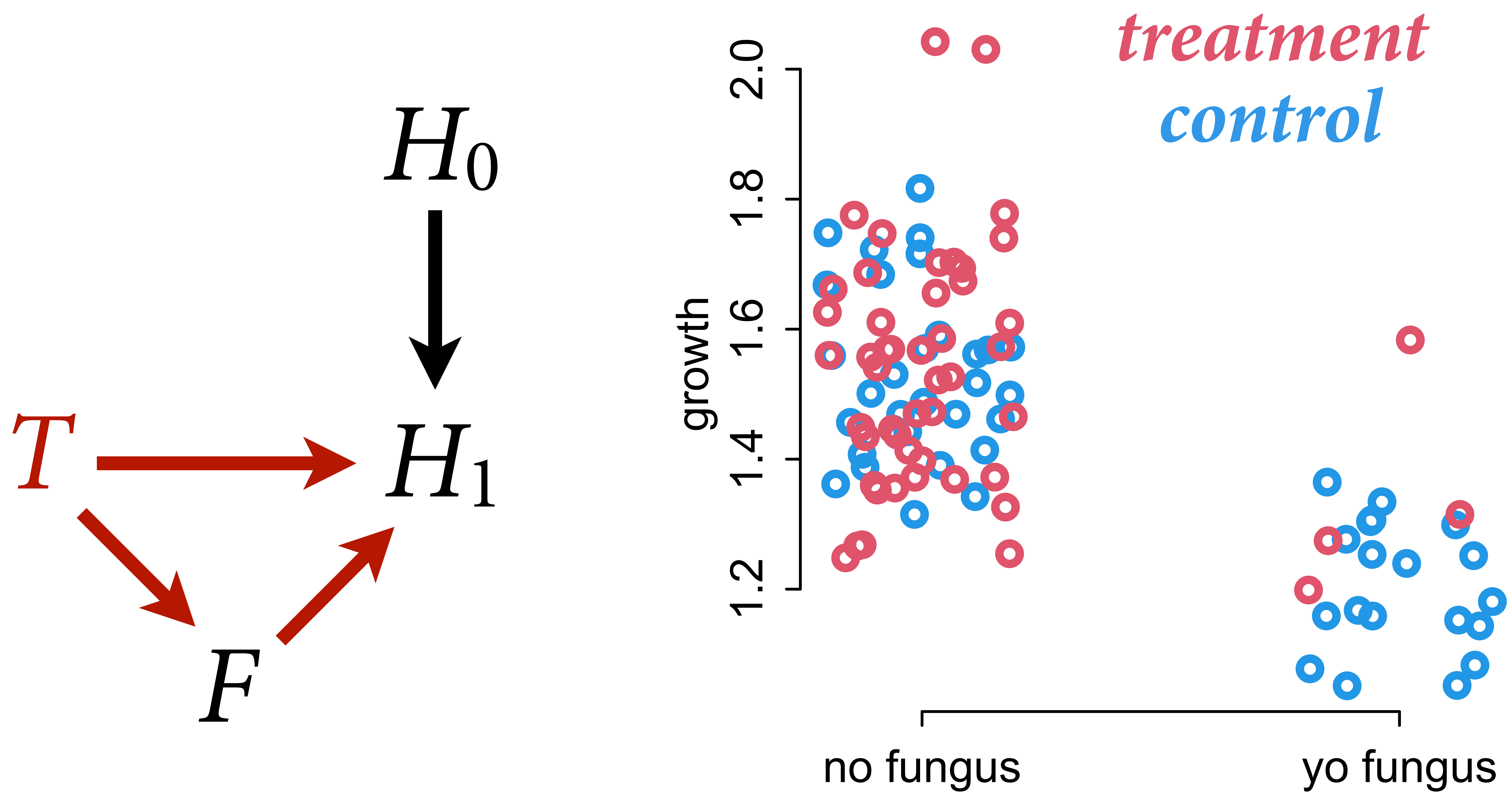


Wrong model wins at prediction



Wrong model wins at prediction

Why does the wrong model win at prediction?



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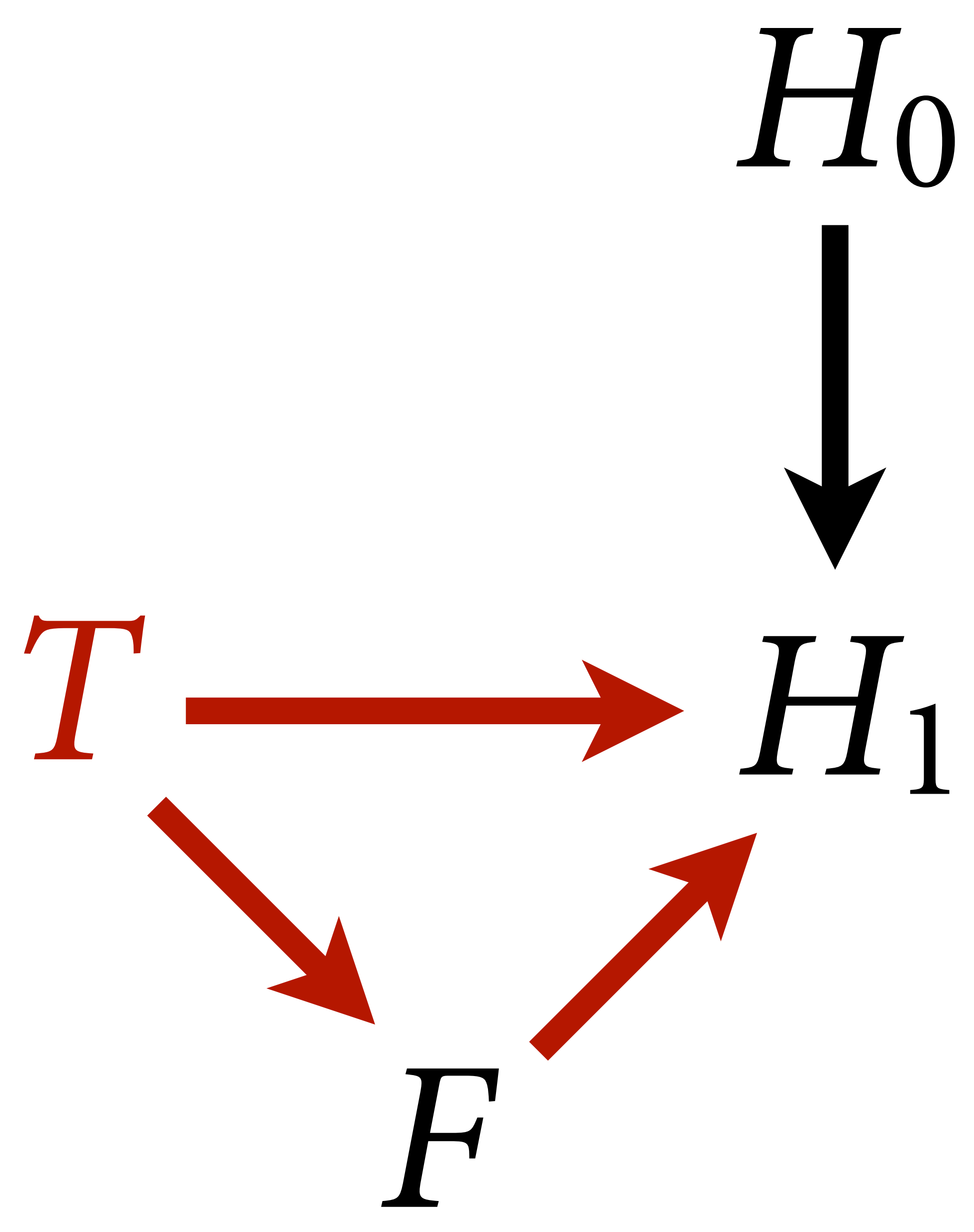
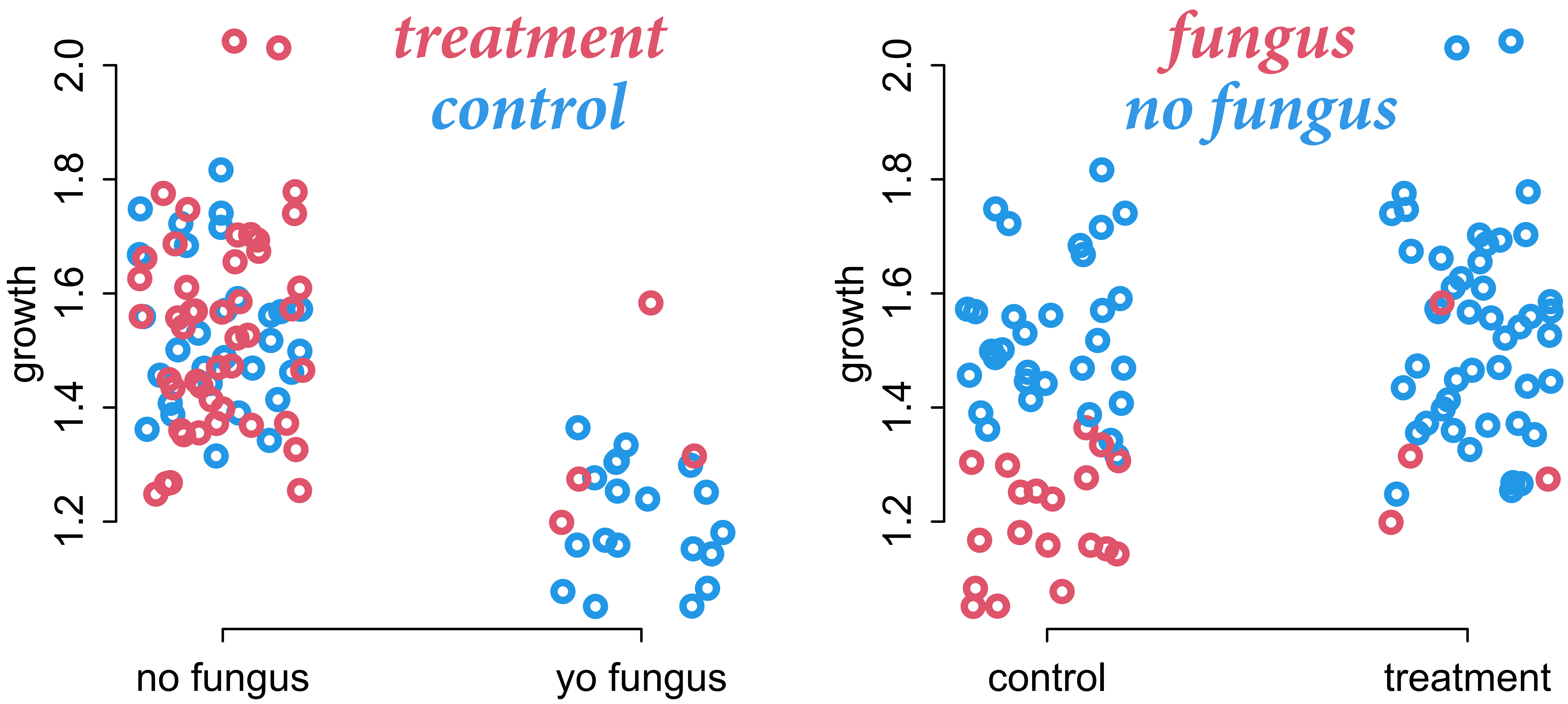




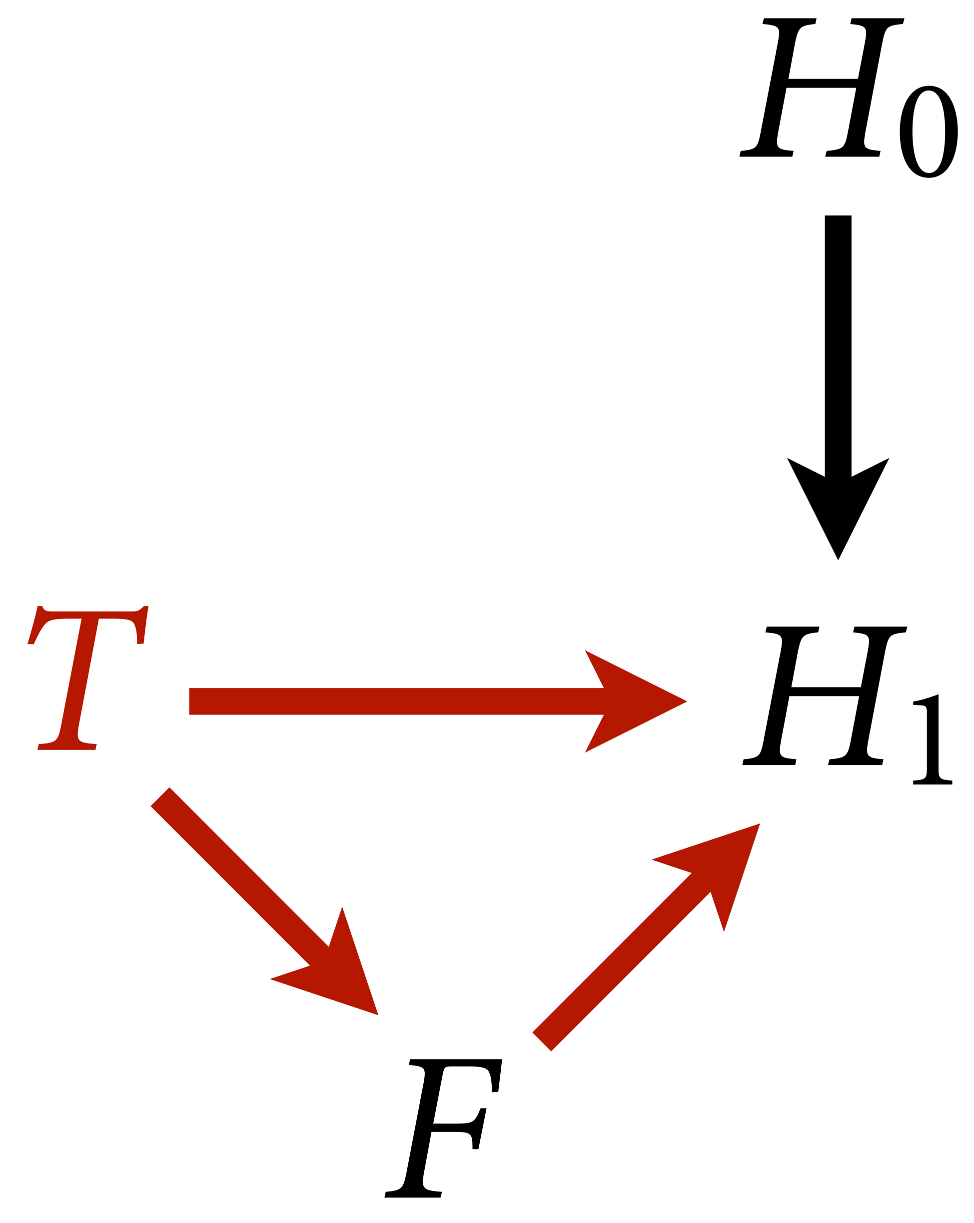
Fungus is in fact a better predictor than treatment

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



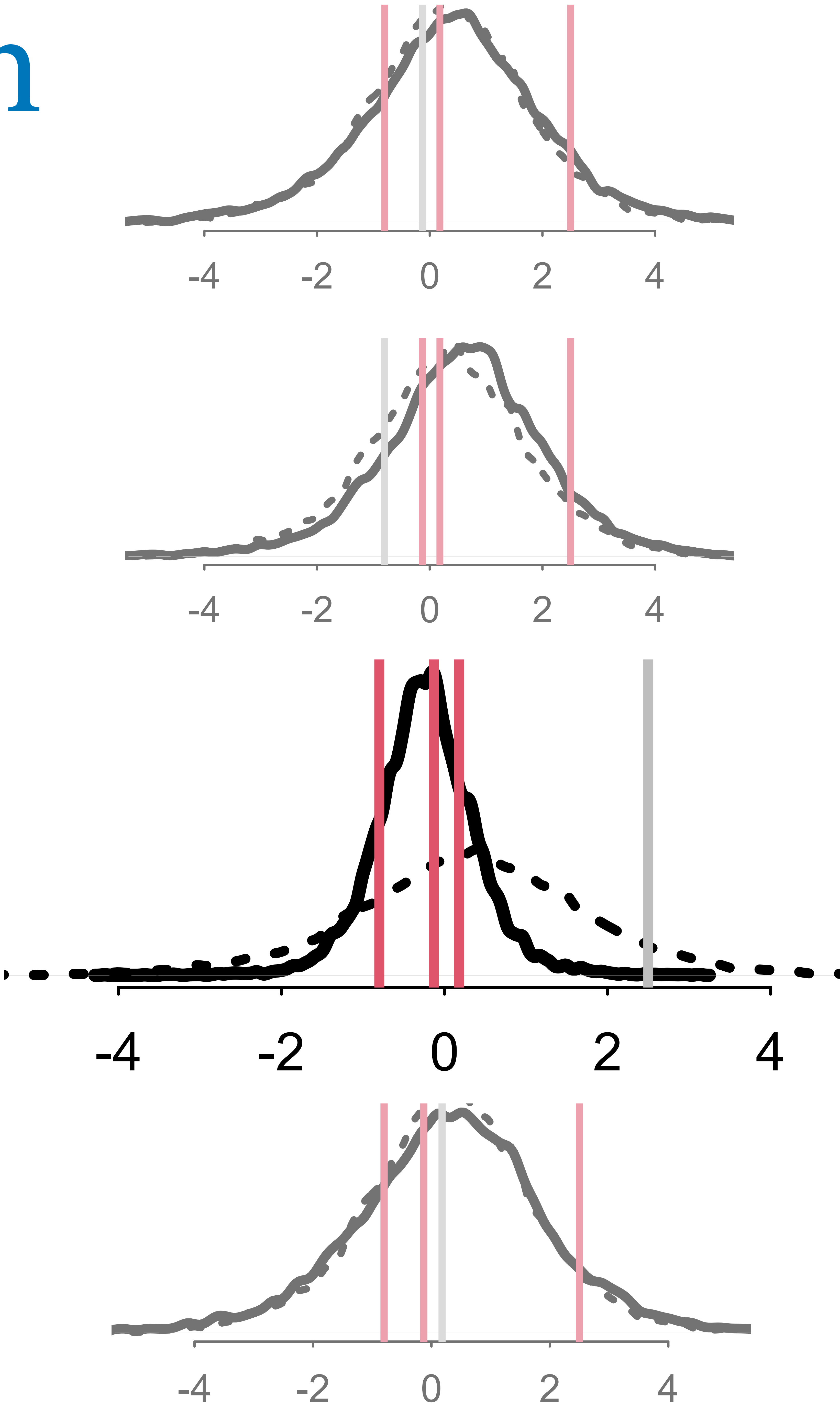
Outliers & Robust Regression

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



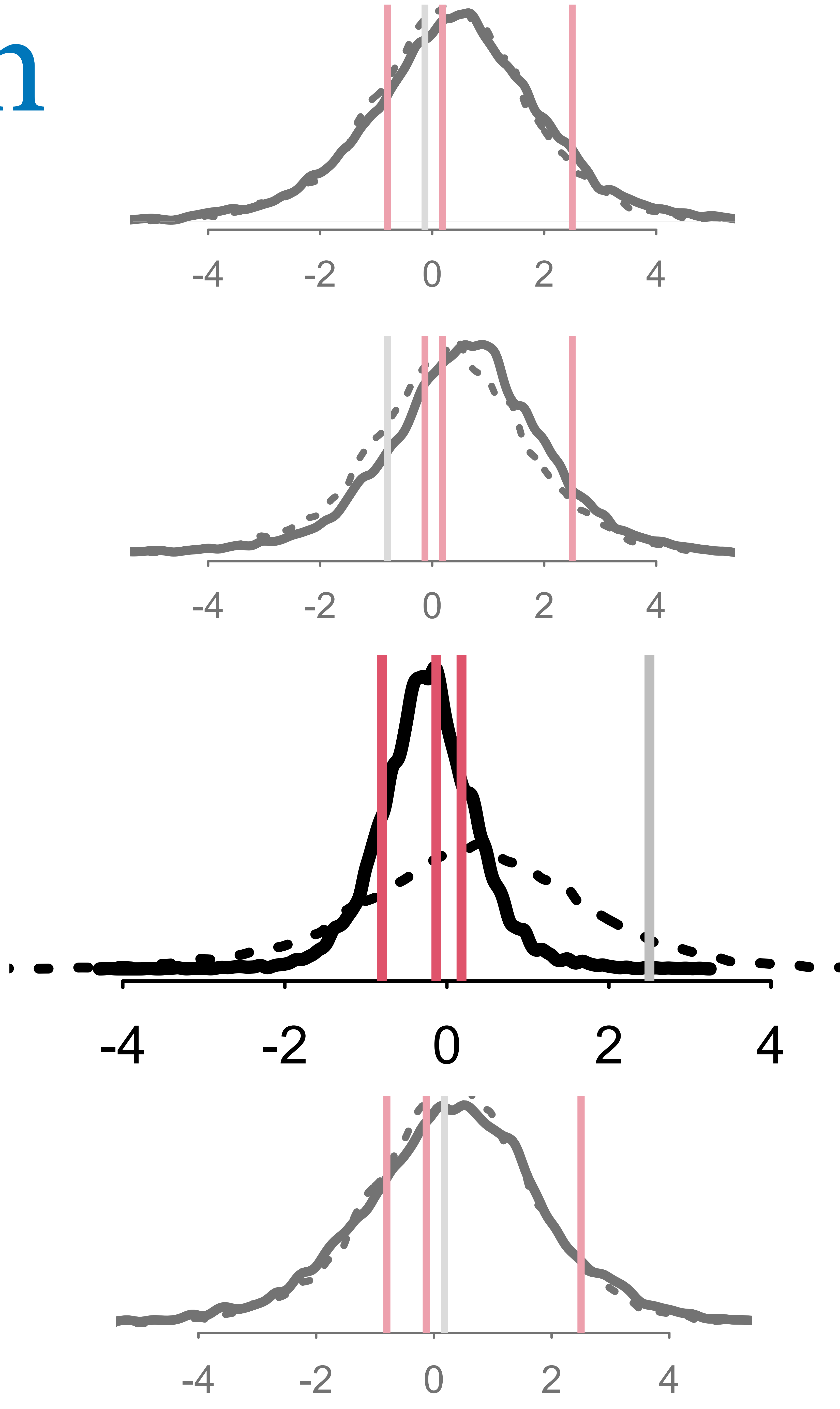
Outliers & Robust Regression

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)



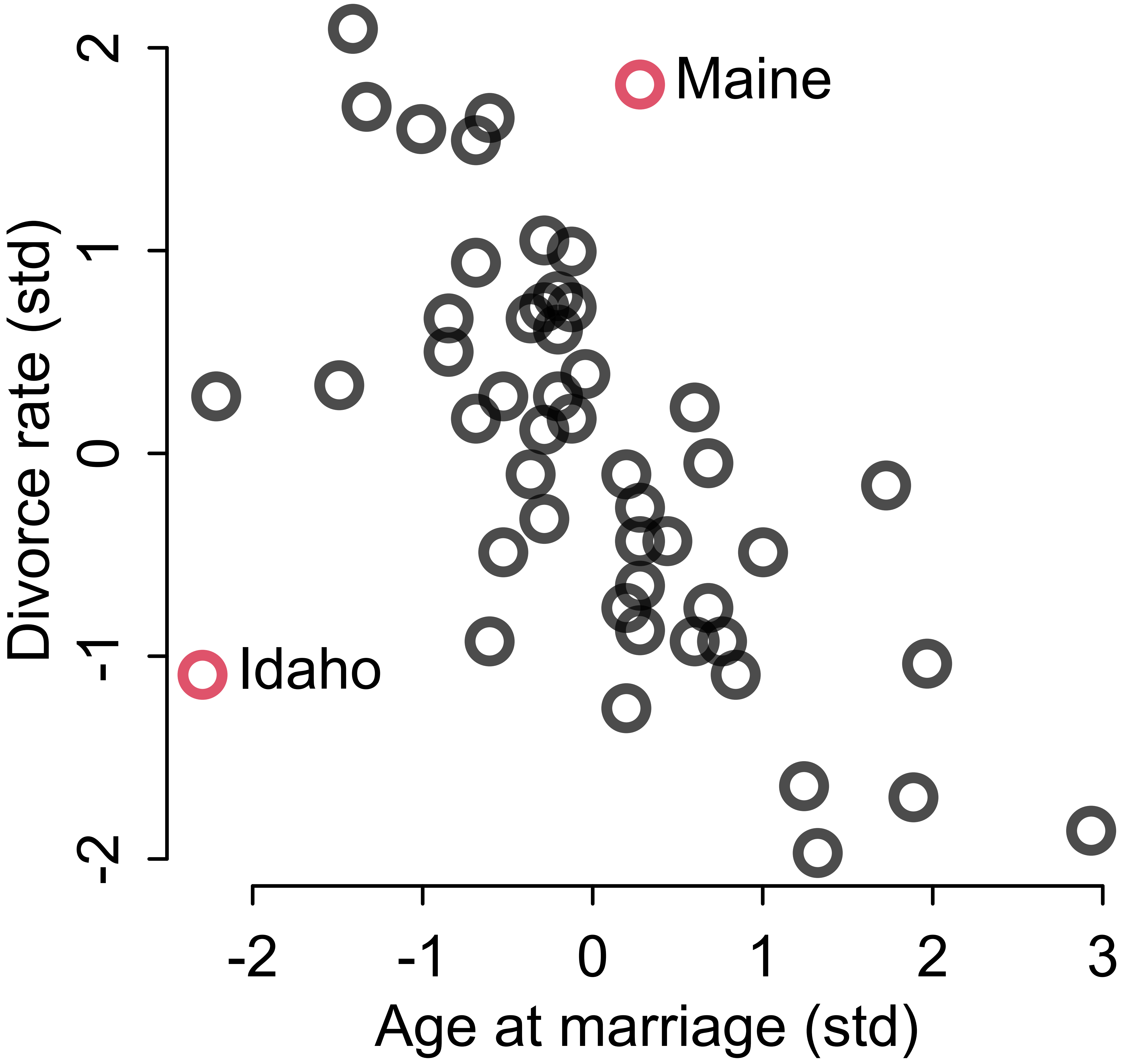
Outliers & Robust Regression

Divorce rate example

Maine and Idaho both unusual

Maine: high divorce for trend

Idaho: low divorce for trend

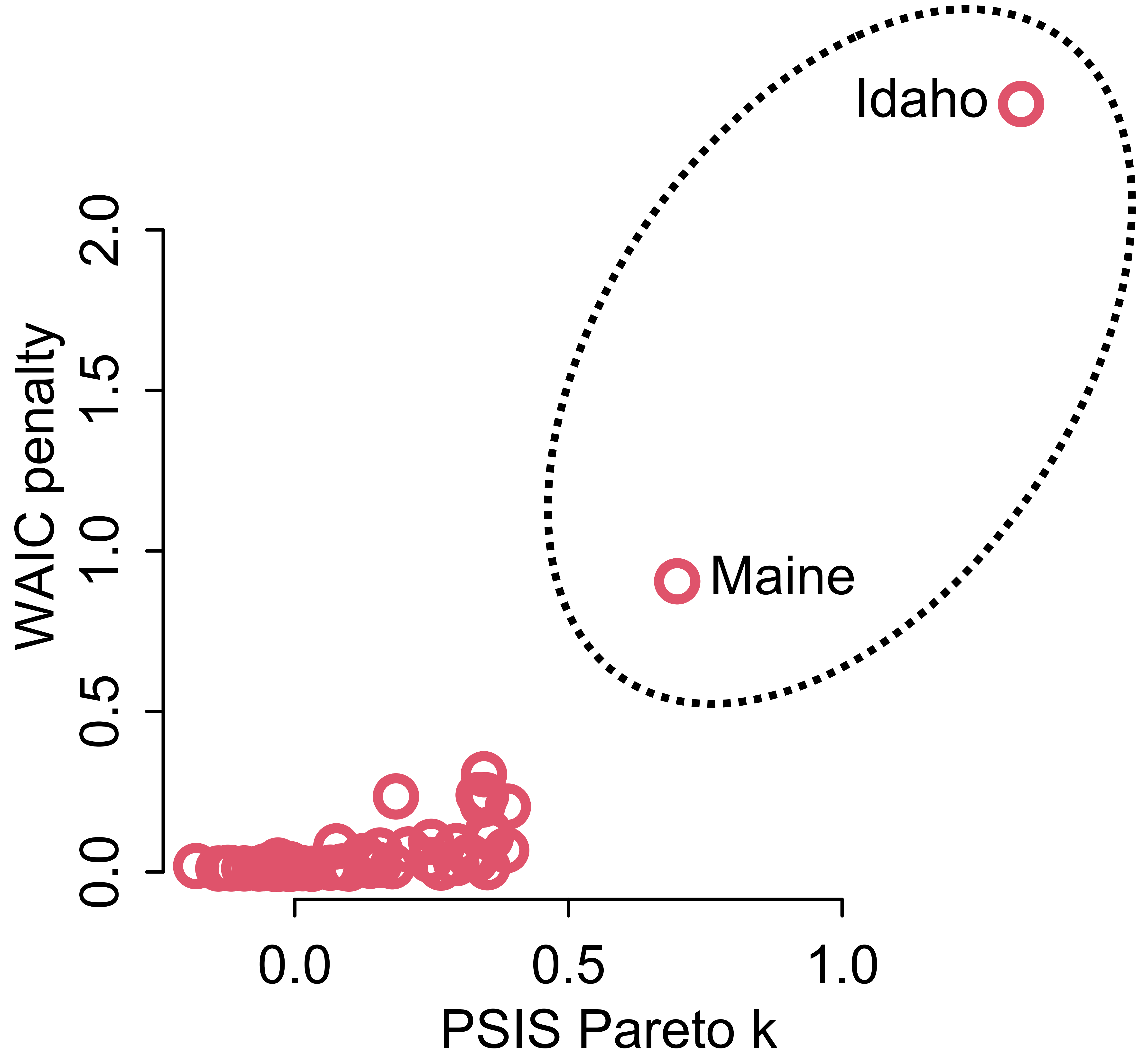


Outliers & Robust Regression

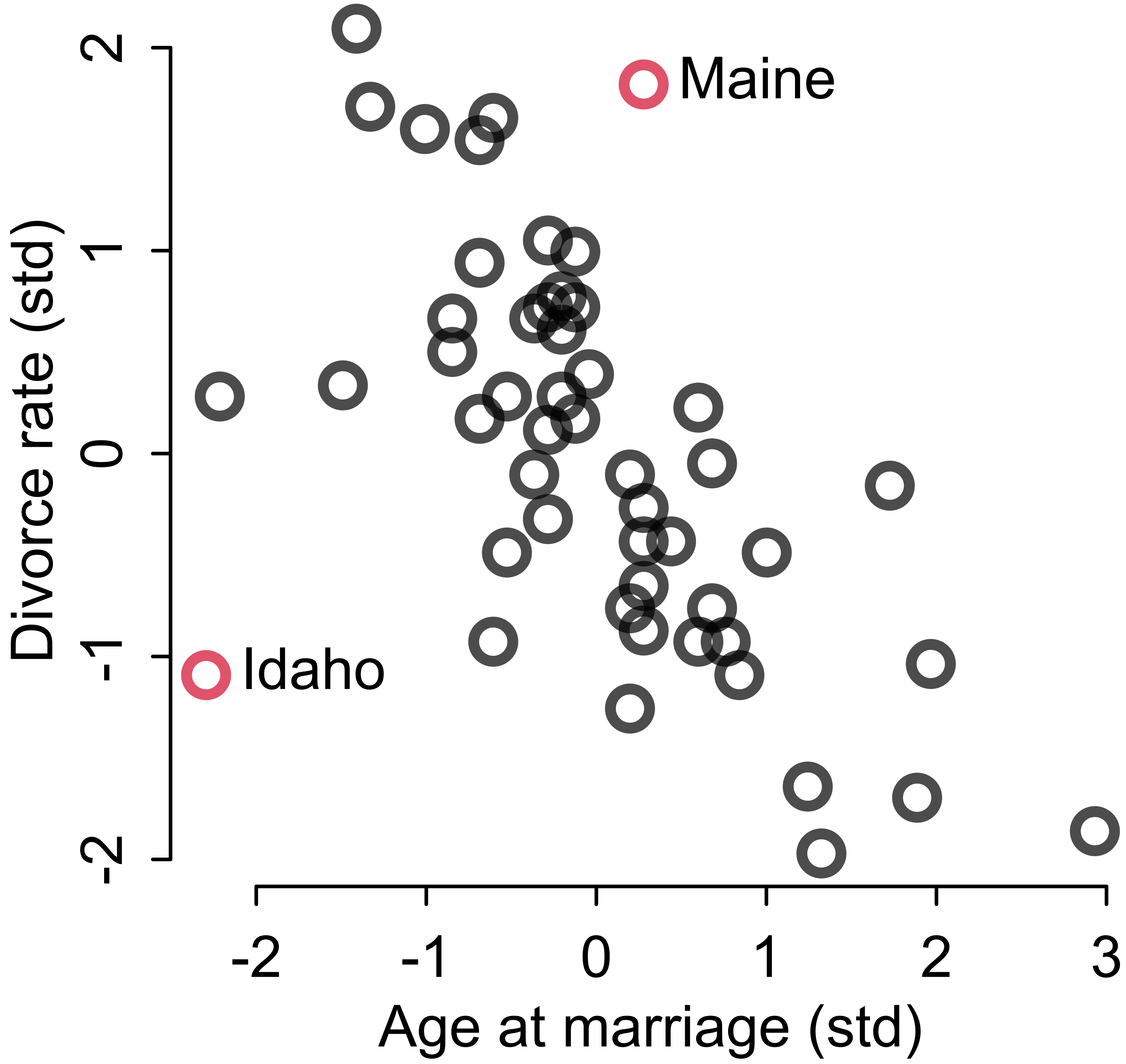
Quantify influence:

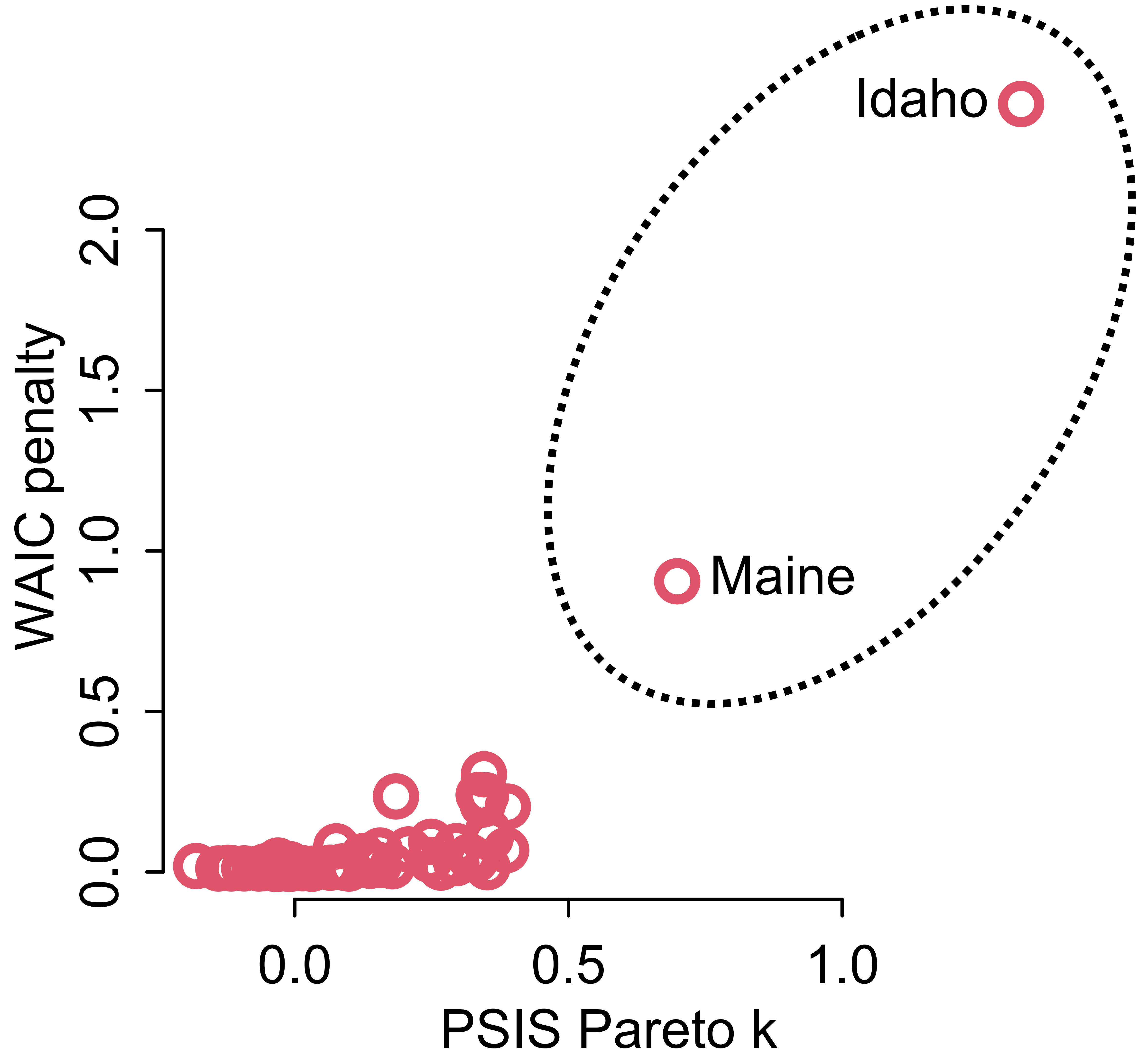
PSIS k statistic

WAIC penalty term ("effective number of parameters")

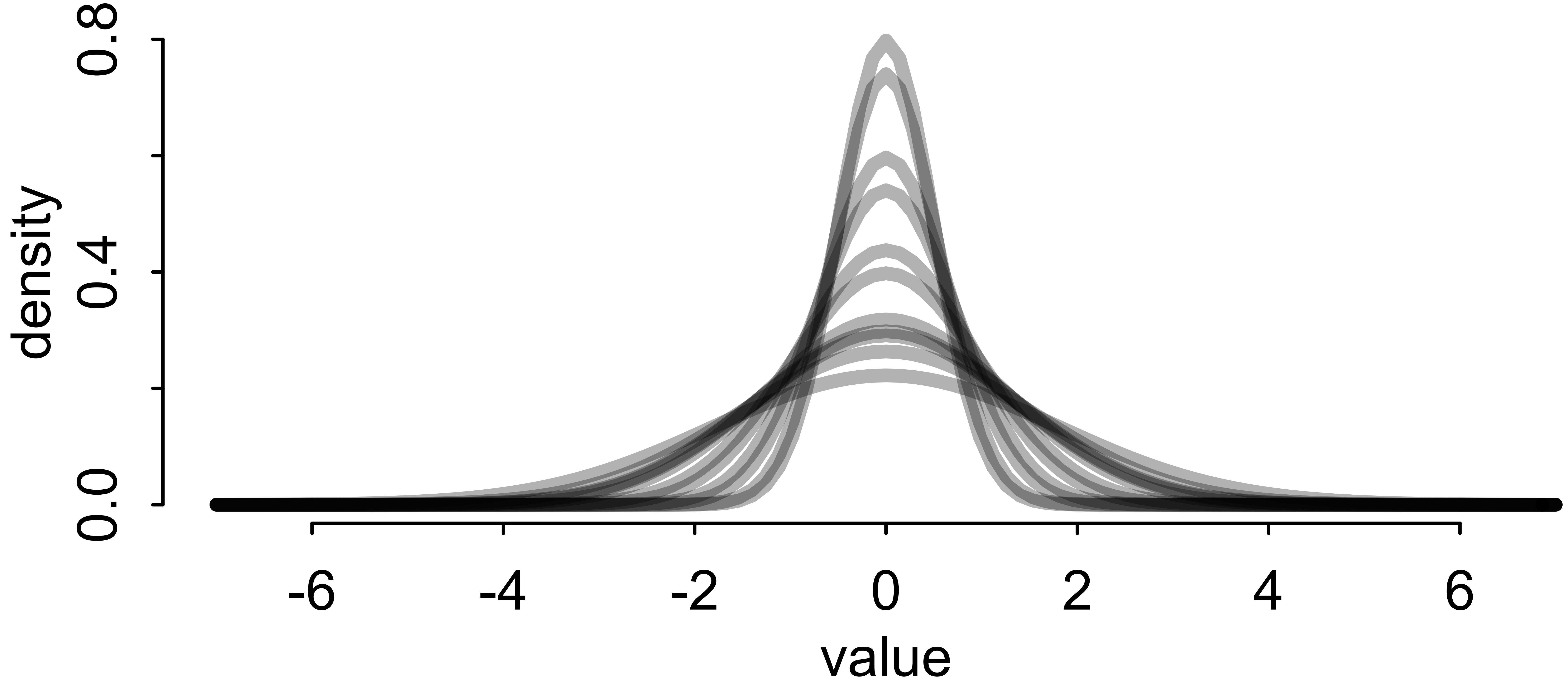


Outliers & Robust Regression

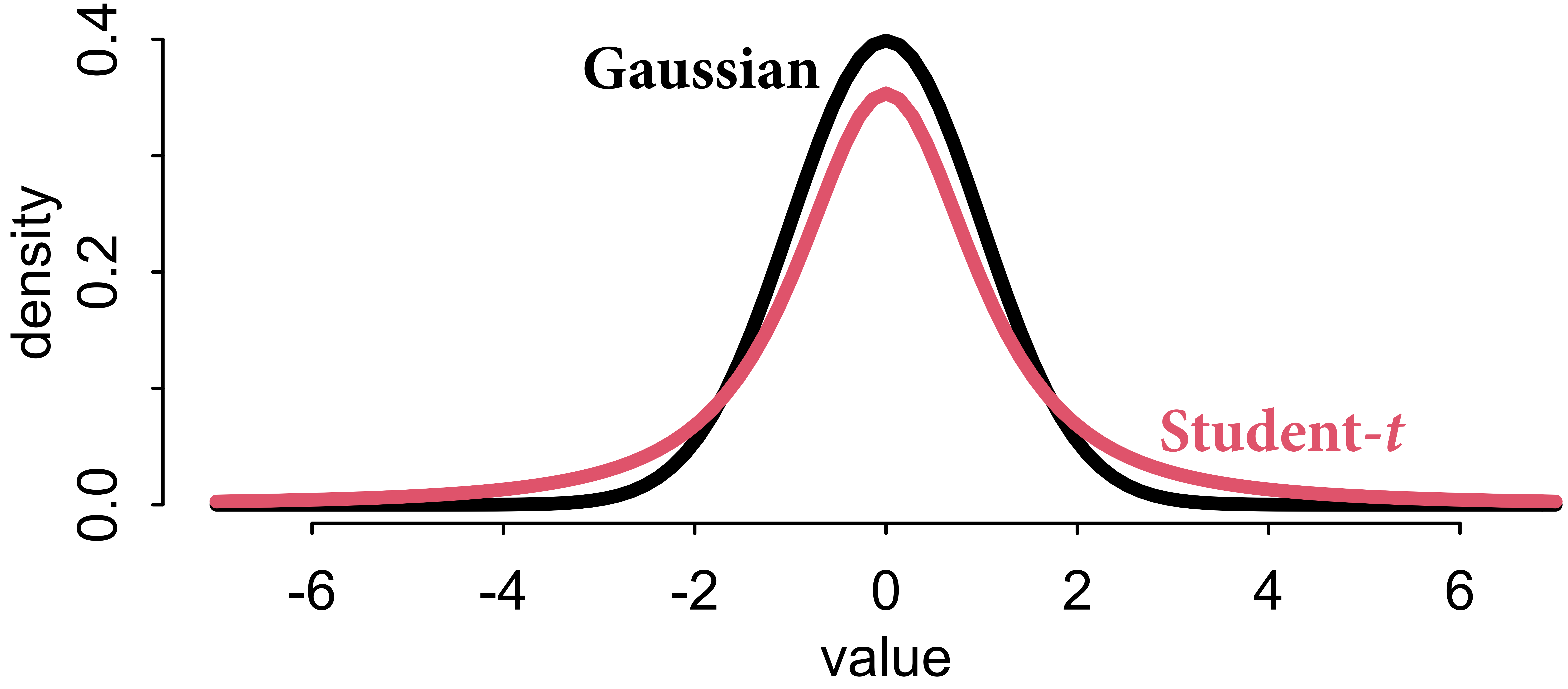




Mixing Gaussians



Mixing Gaussians



```
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 ) ,
        bA ~ dnorm( 0 , 0.5 ) ,
        sigma ~ dexp( 1 )
    ) , data = dat )
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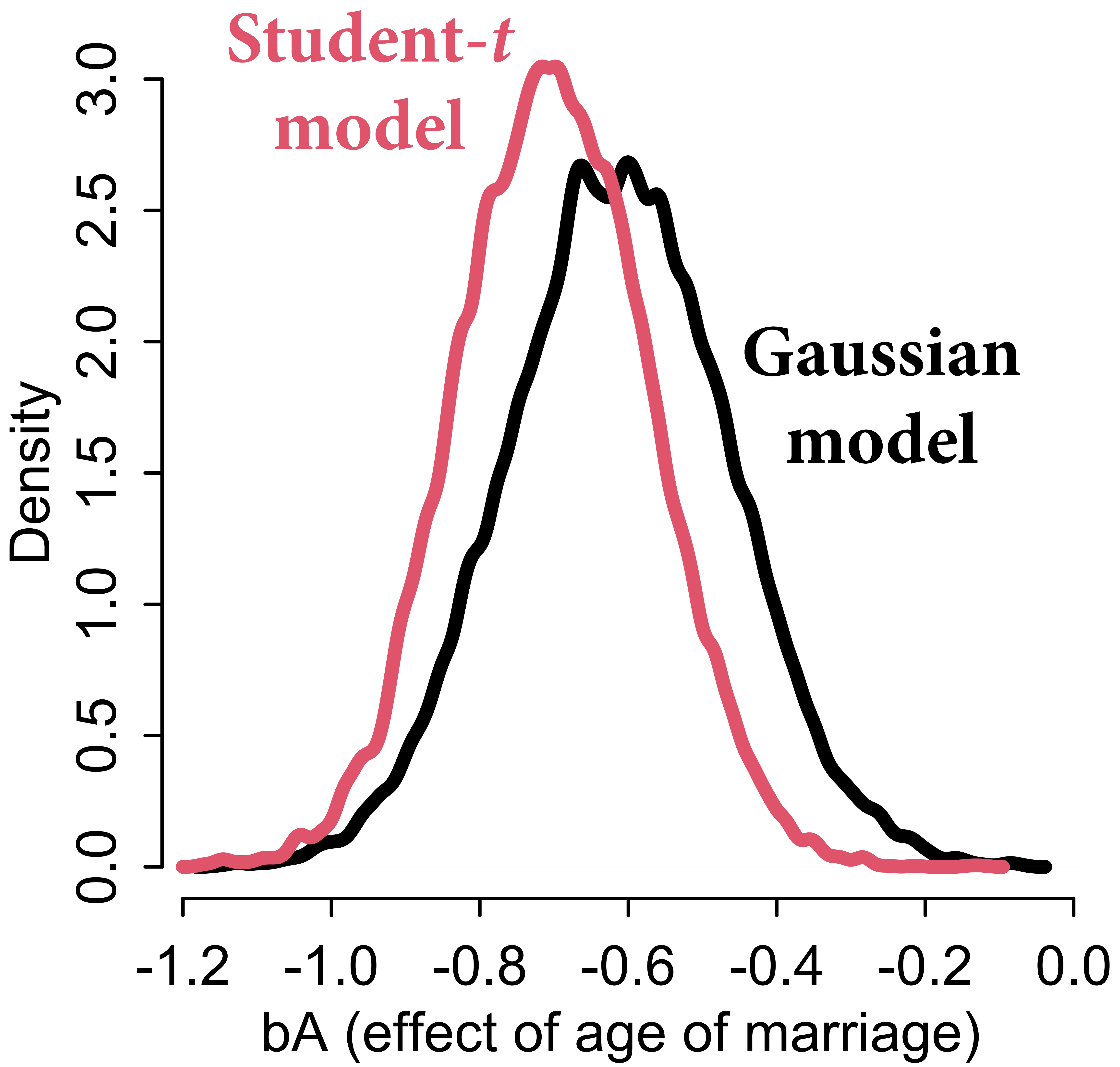


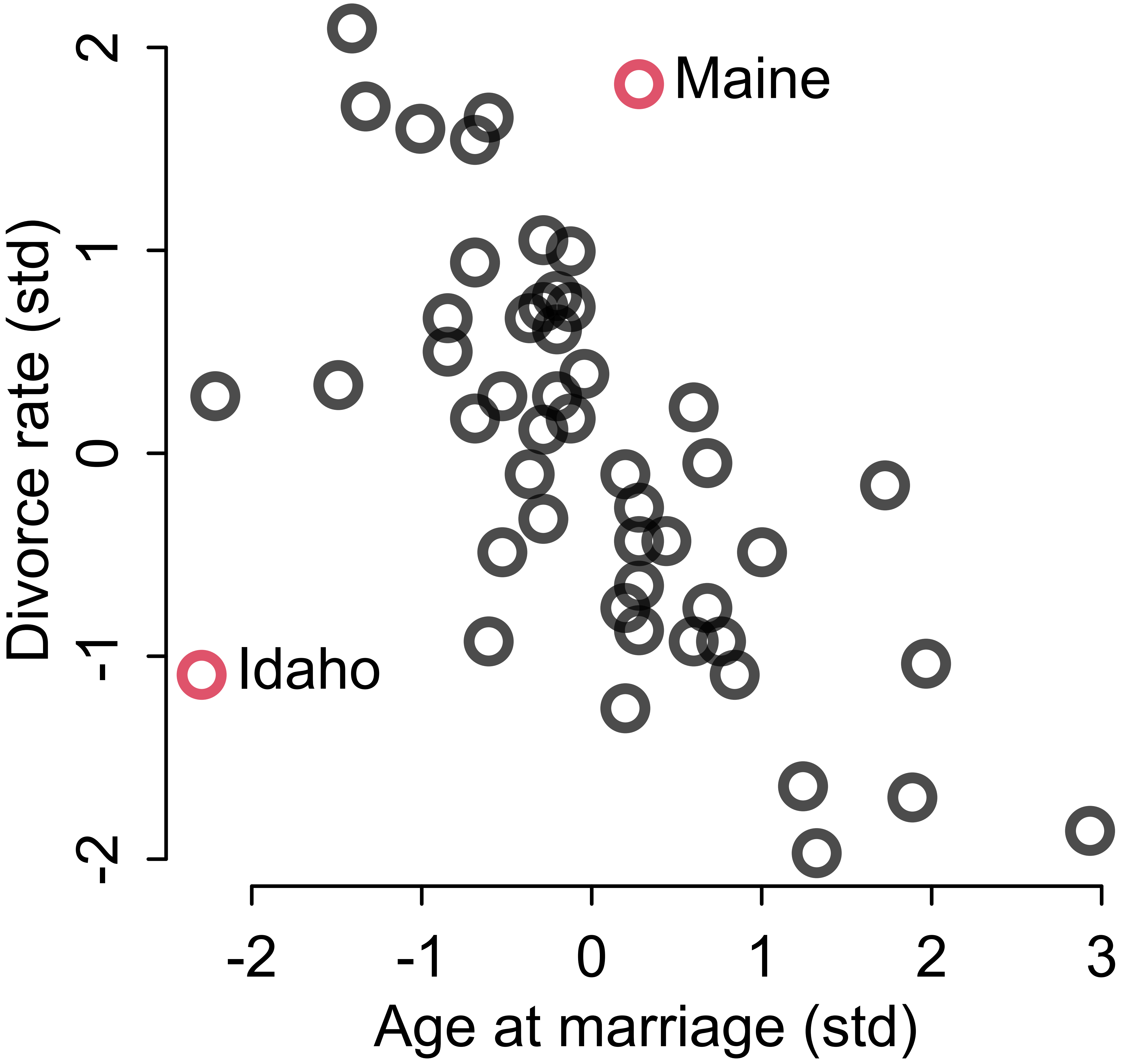
Robust Regressions

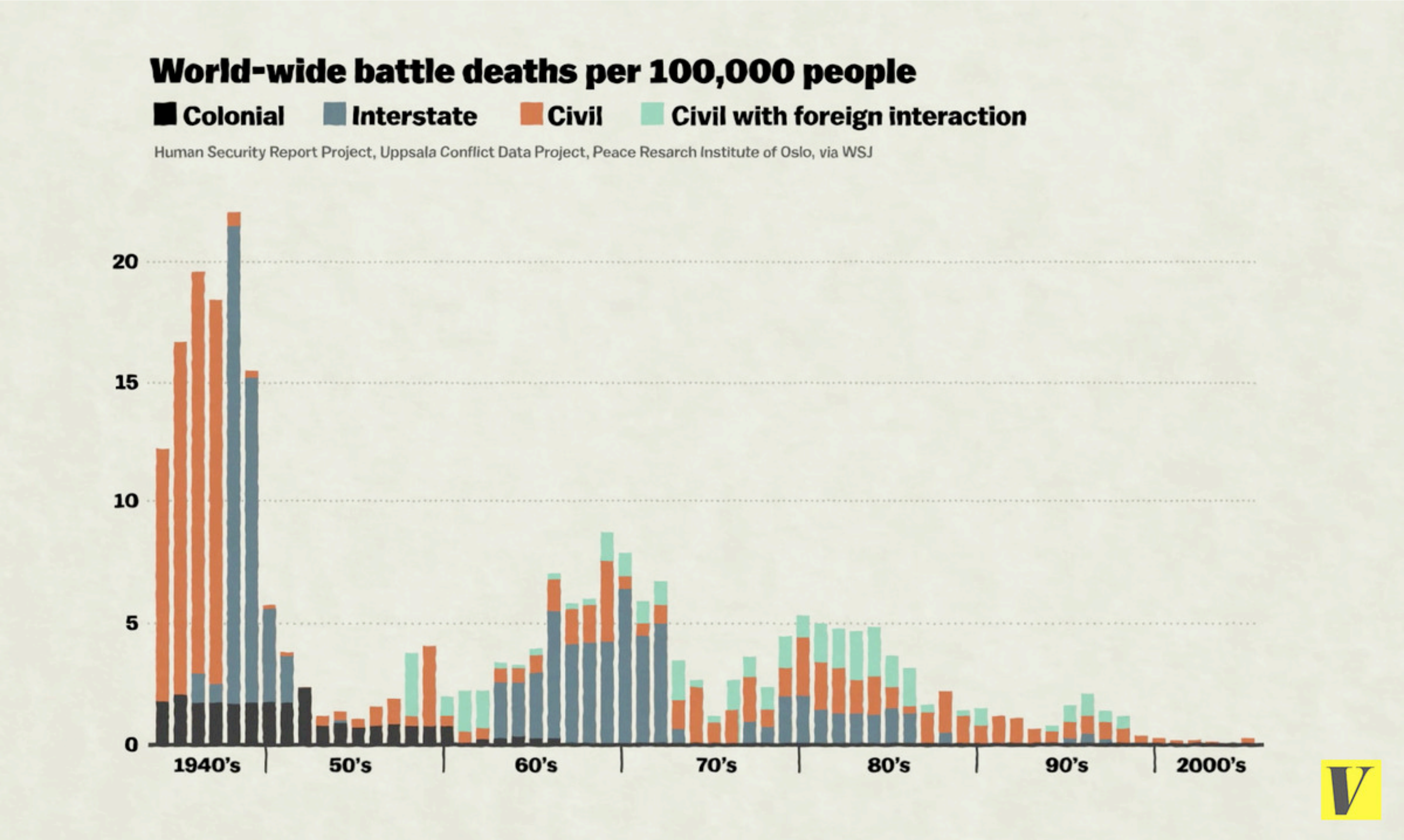
Unobserved heterogeneity => mixture of Gaussians

Thick tails means model is less surprised by extreme values

Usually impossible to estimate distribution of extreme values

Student-*t* regression as default?





https://www.vox.com/2015/5/21/8635369/pinker-taleb

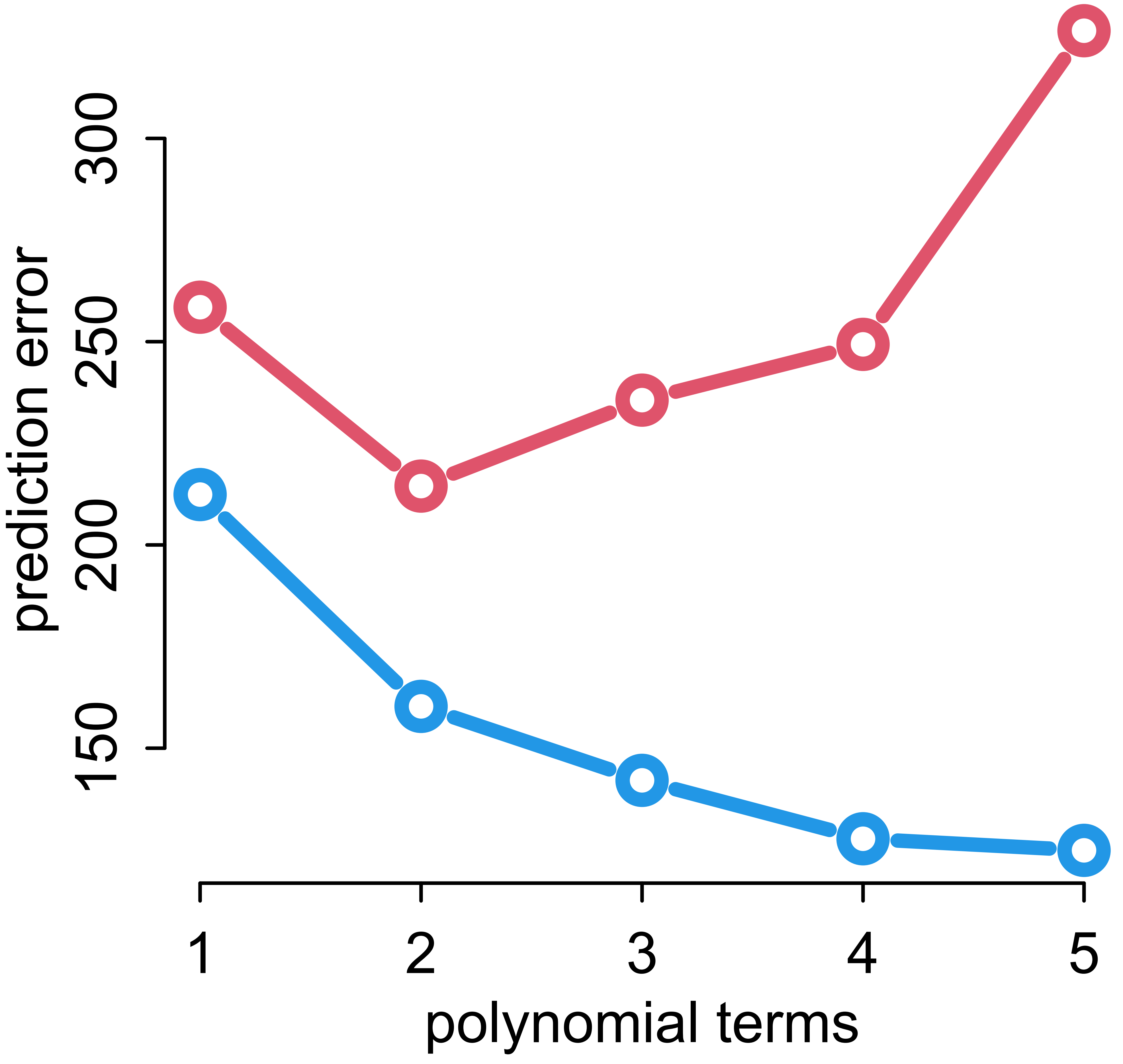
Problems of Prediction

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



Course Schedule

Week 1	Bayesian inference	Chapters 1, 2, 3
Week 2	Linear models & Causal Inference	Chapter 4
Week 3	Causes, Confounds & Colliders	Chapters 5 & 6
Week 4	Overfitting / MCMC	Chapters 7, 8, 9
Week 5	Generalized Linear Models	Chapters 10, 11
Week 6	Integers & Other Monsters	Chapters 11 & 12
Week 7	Multilevel models I	Chapter 13
Week 8	Multilevel models II	Chapter 14
Week 9	Measurement & Missingness	Chapter 15
Week 10	Generalized Linear Madness	Chapter 16

https://github.com/rmcelreath/stat_rethinking_2023