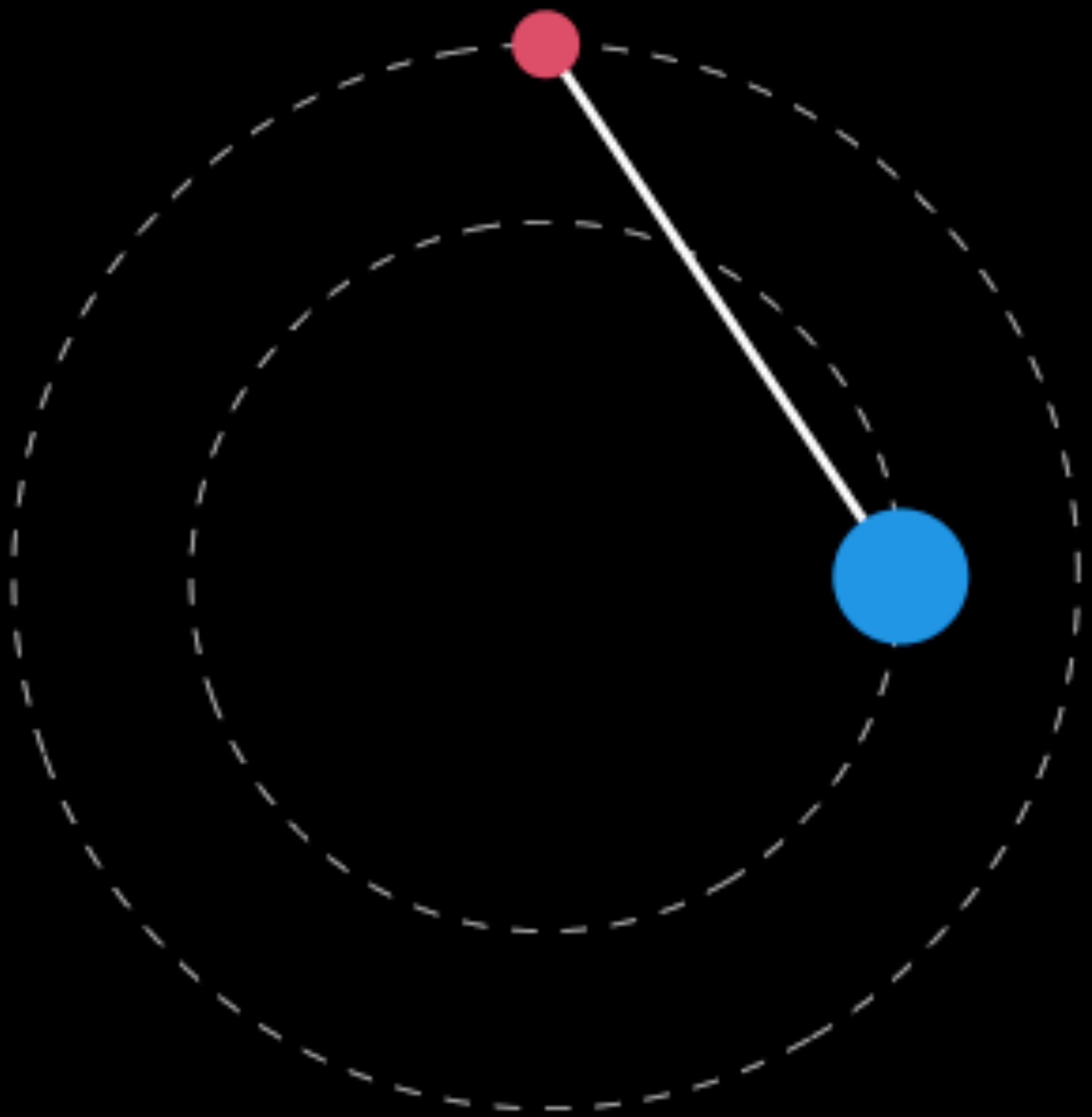
Statistical Rethinking

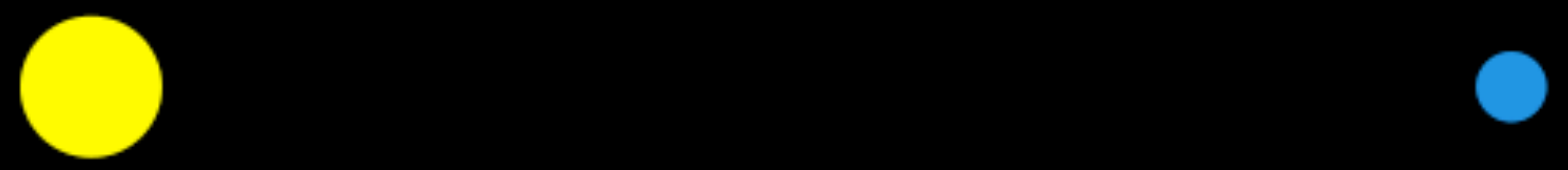
2022

07: Fitting Over and Under

Mikołaj Kopernik (1473–1543)



Copernican Model



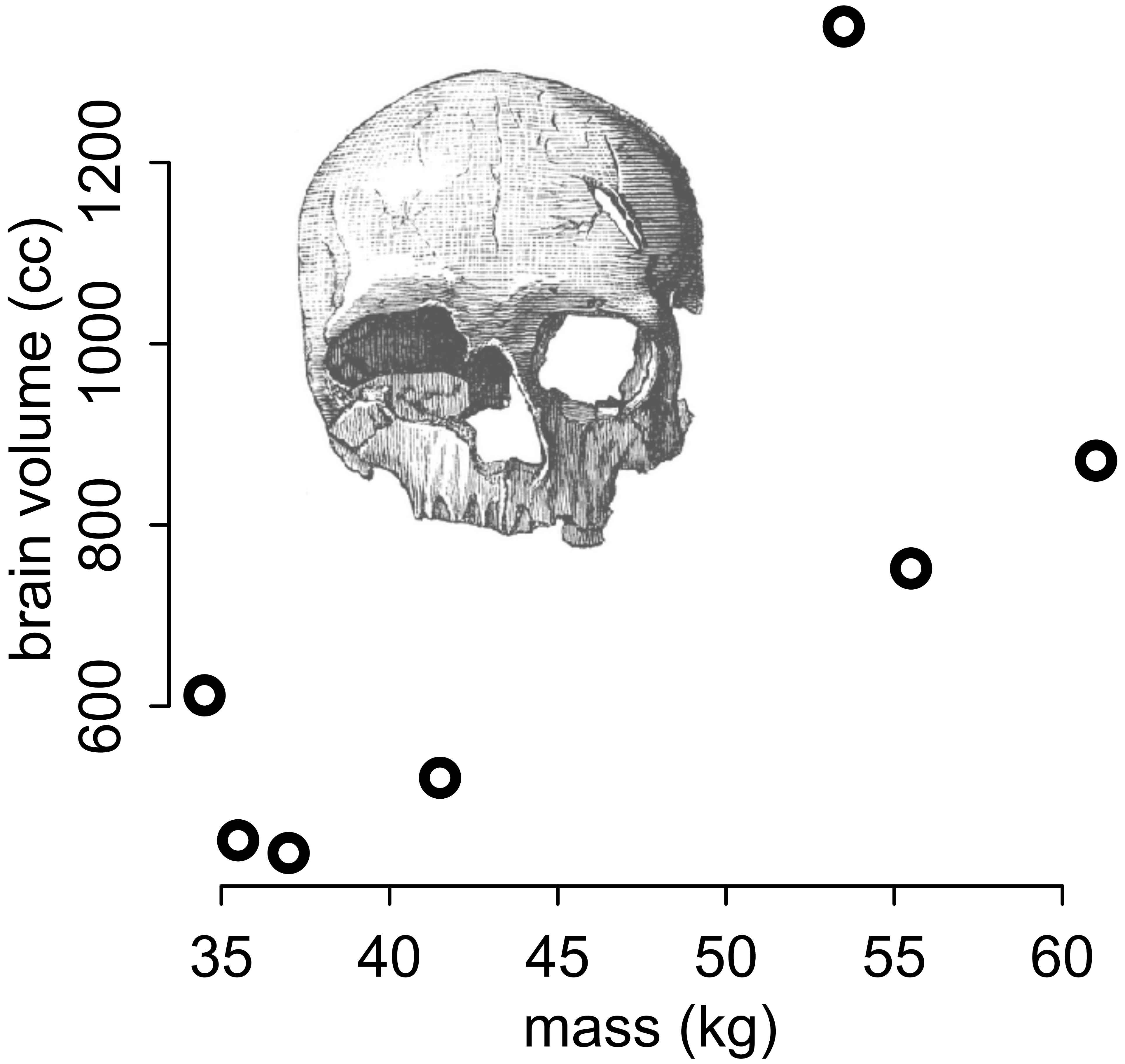
Problems of Prediction

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

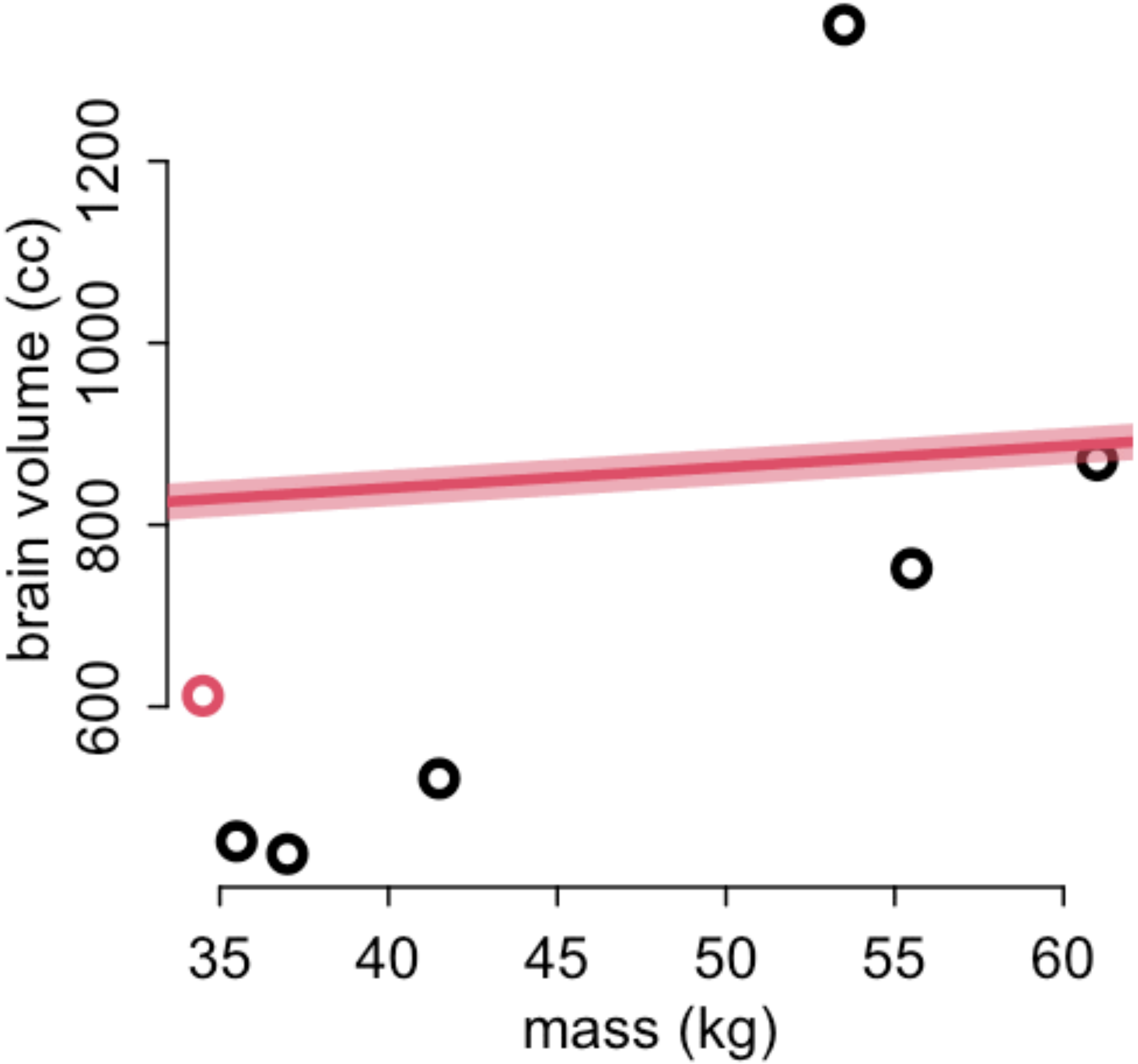
(1) Drop one point

(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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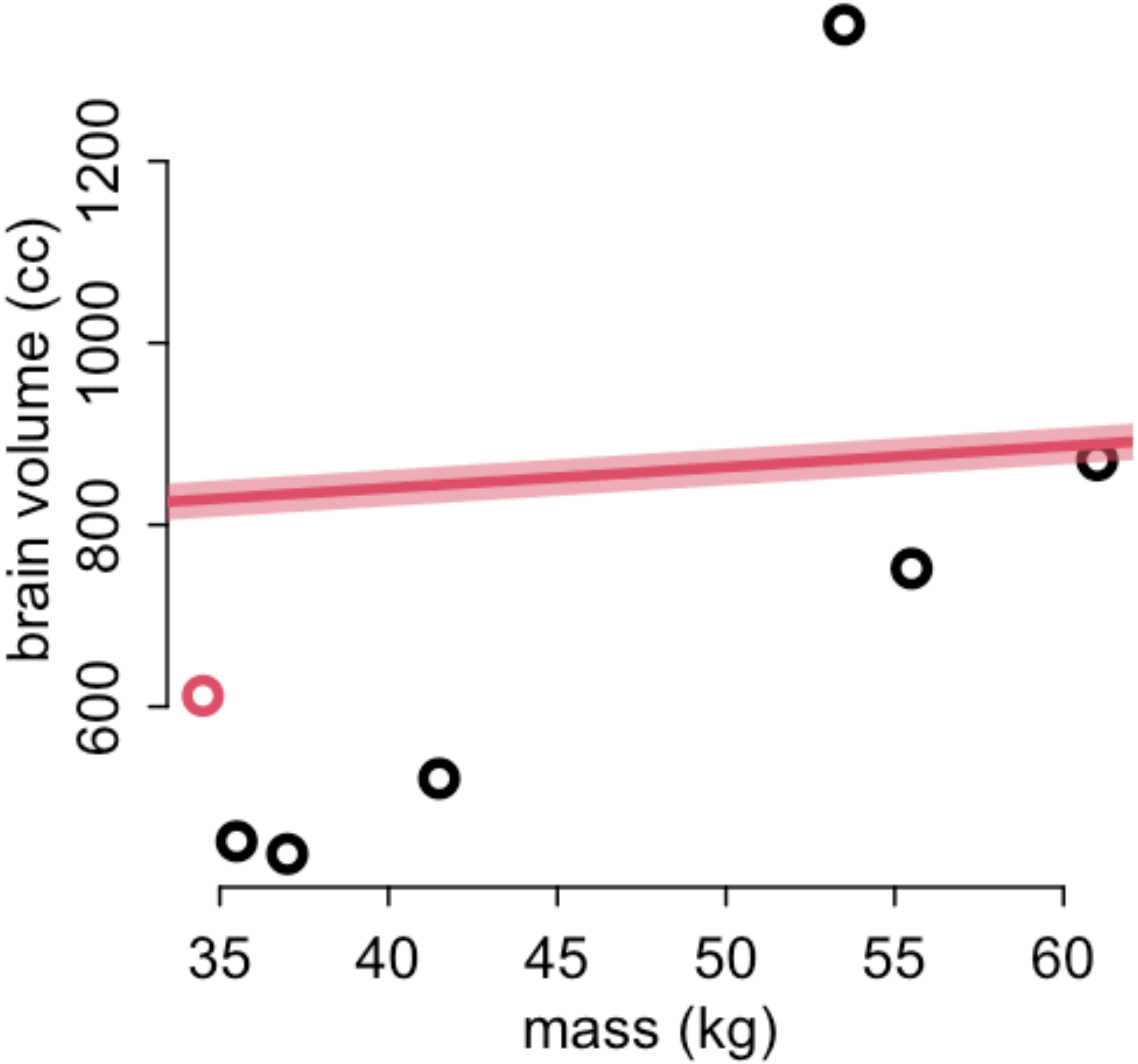

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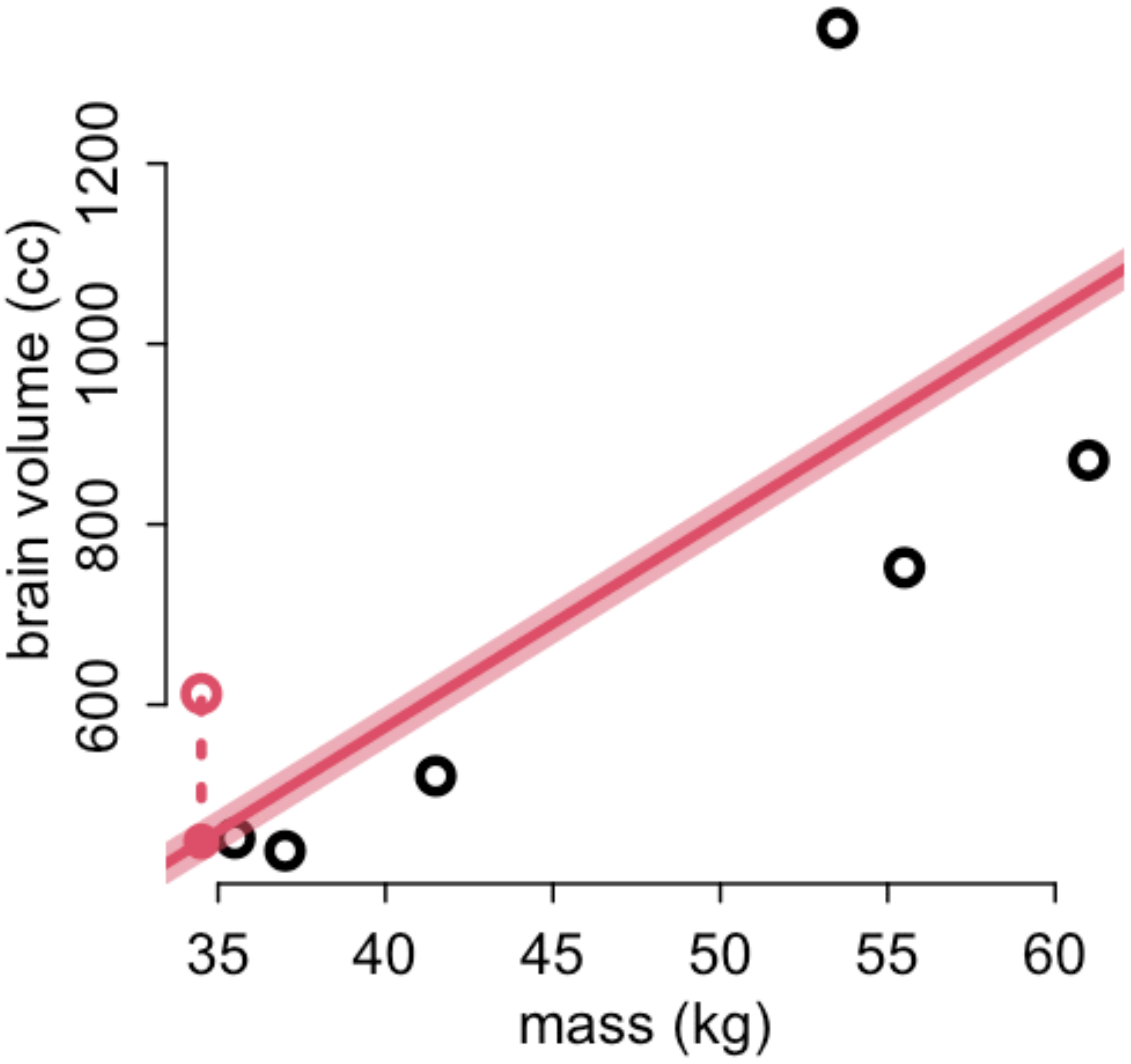

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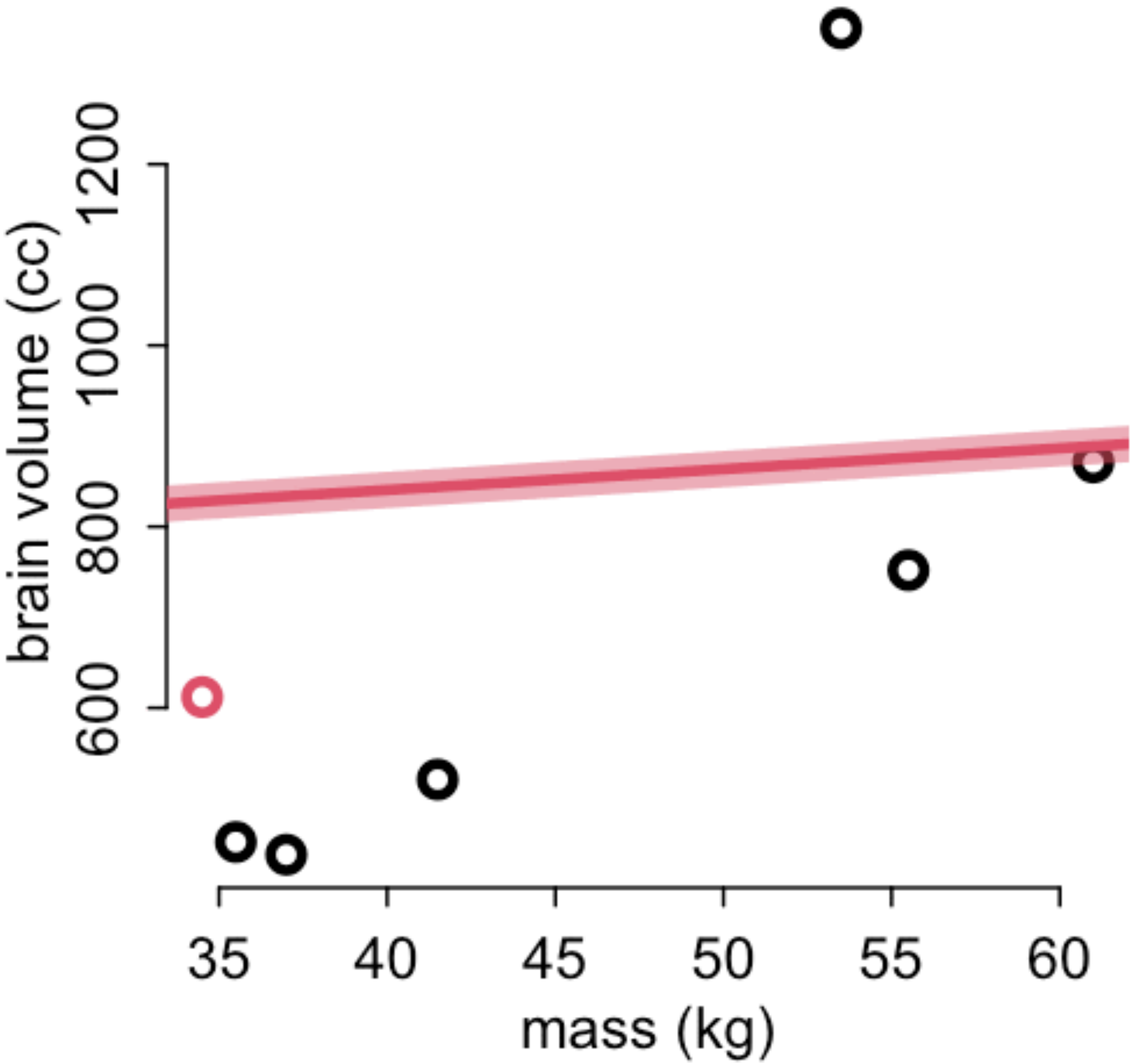

Leave-one-out cross-validation

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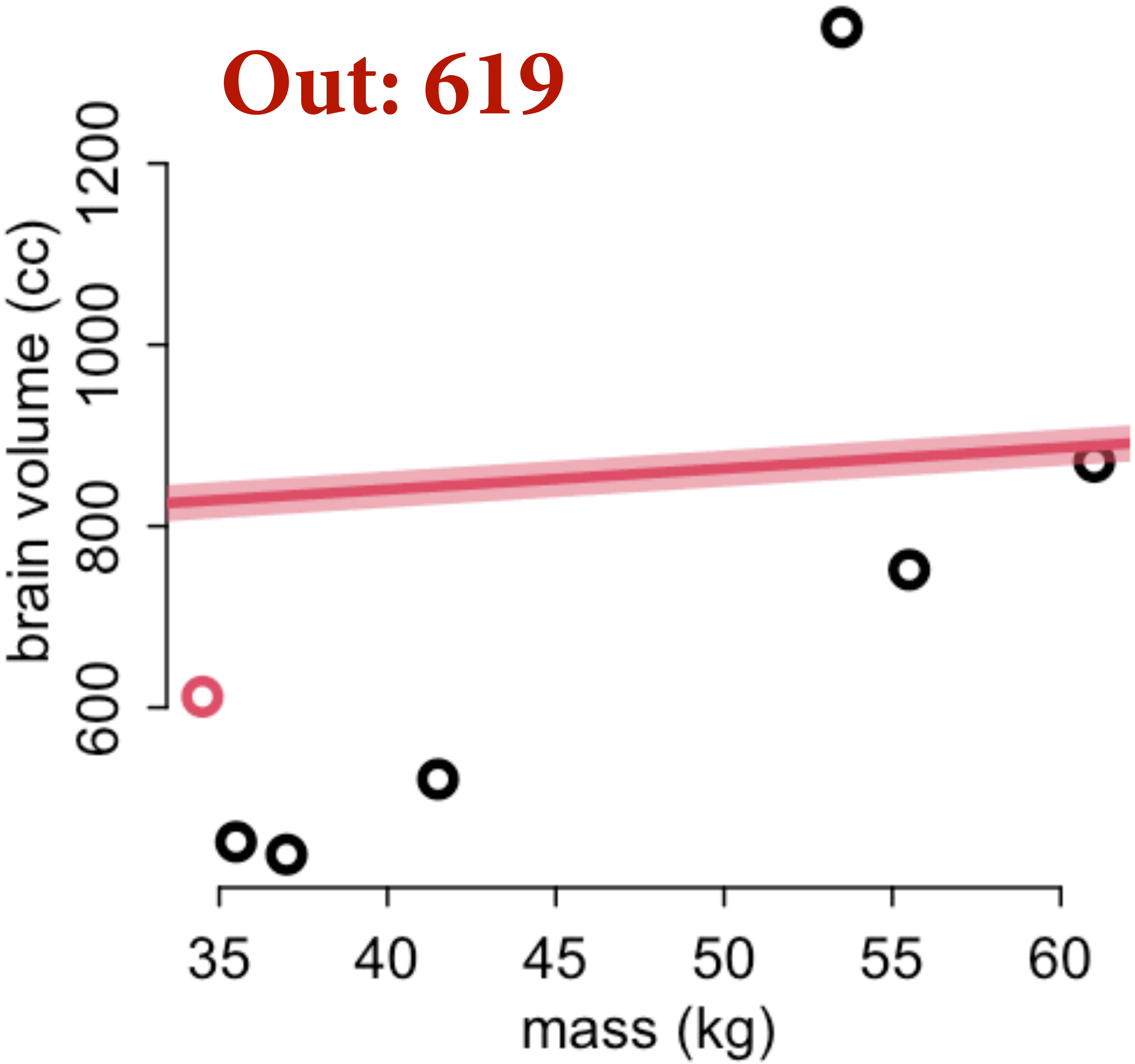
In: 318

Out: 619

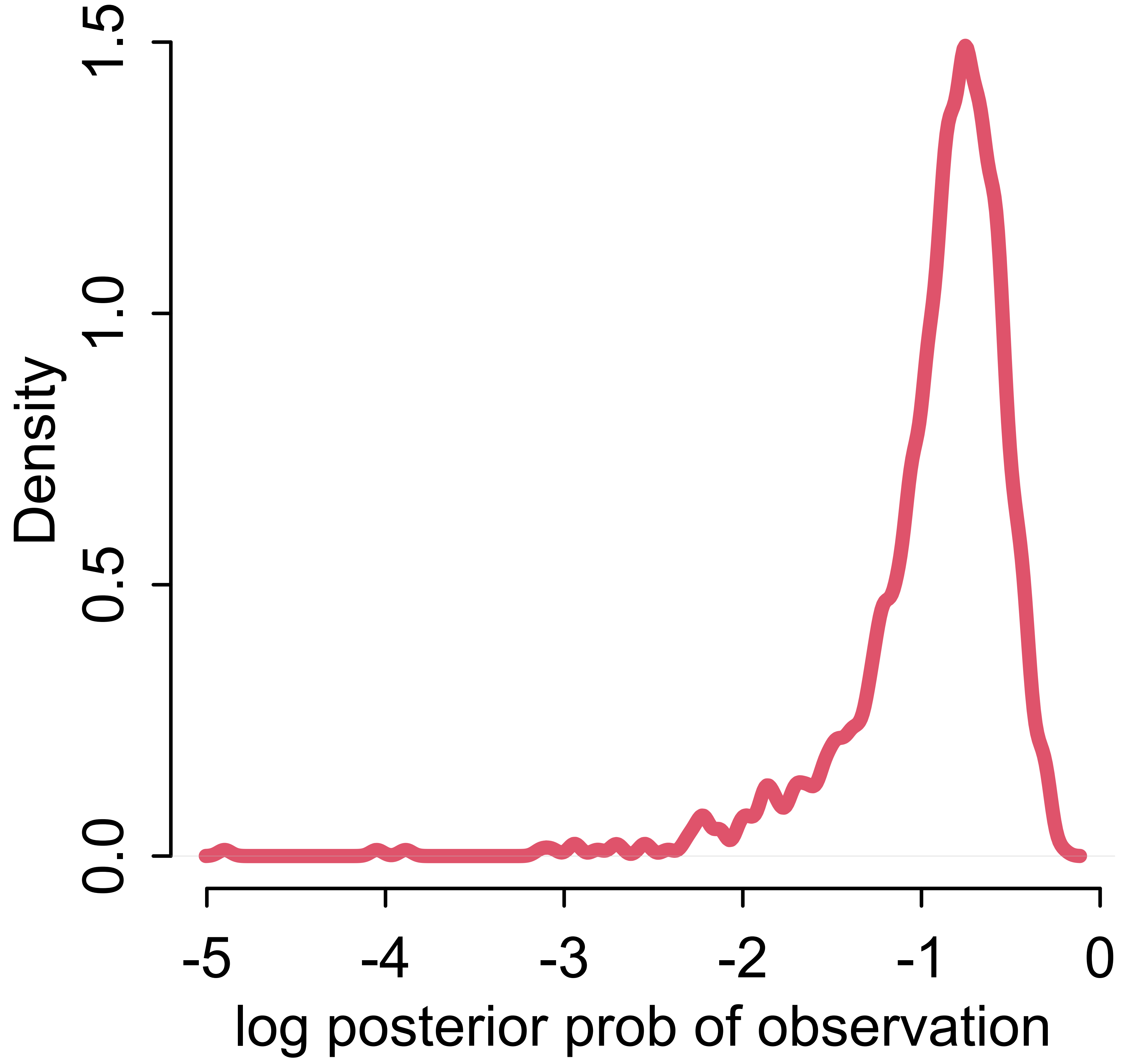


Bayesian Cross-Validation

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

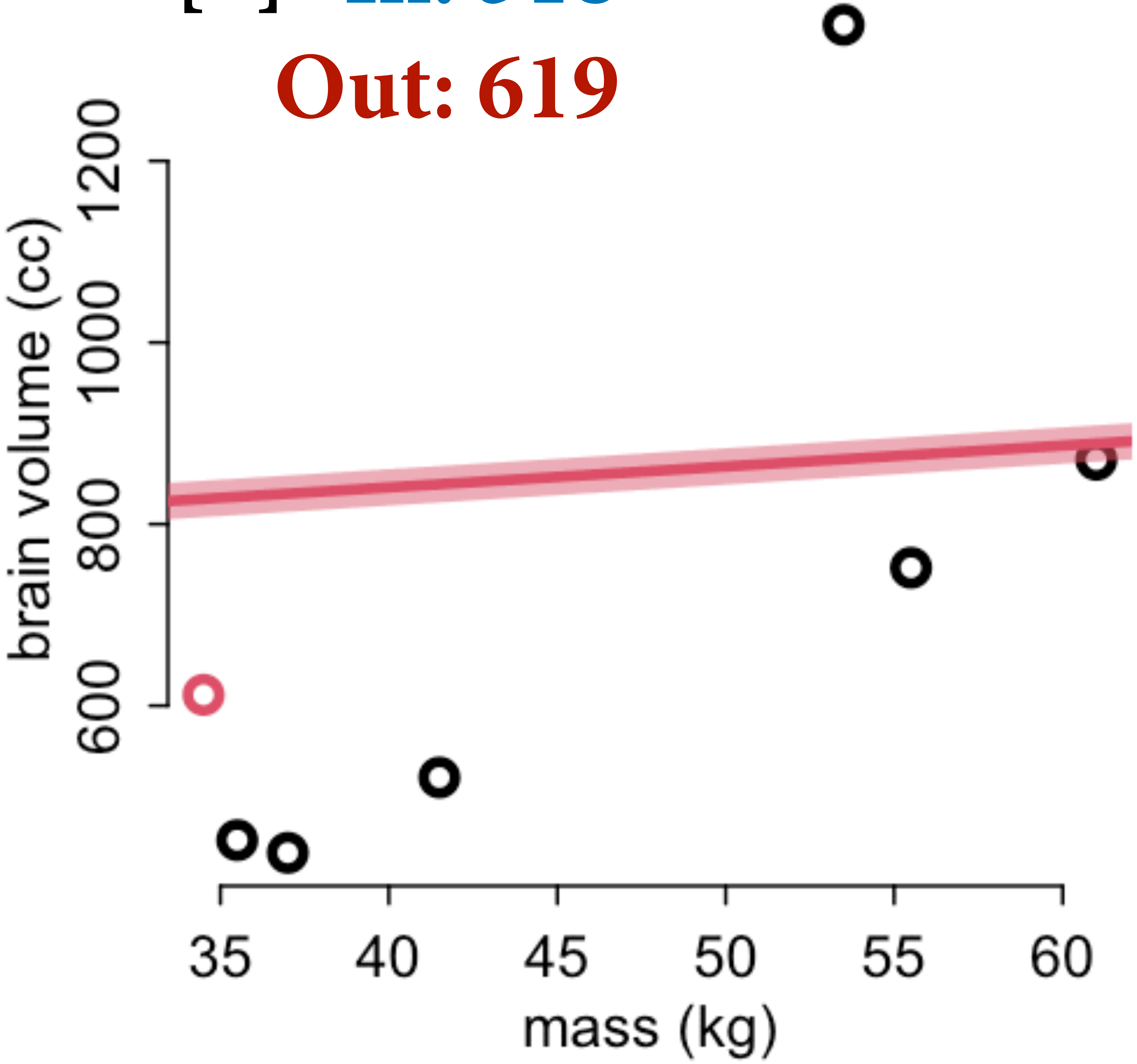
$$\text{lppd}_{\text{CV}} = \sum_{i=1}^{N} \underbrace{\frac{1}{S}\sum_{s=1}^{S} \underbrace{\log \Pr(y_i|\theta_{-i,s})}_{\textit{log probability of each point } i\textit{, computed with posterior that omits point } i}}_{\textit{average log probability for point } i}$$

average log probability for point i

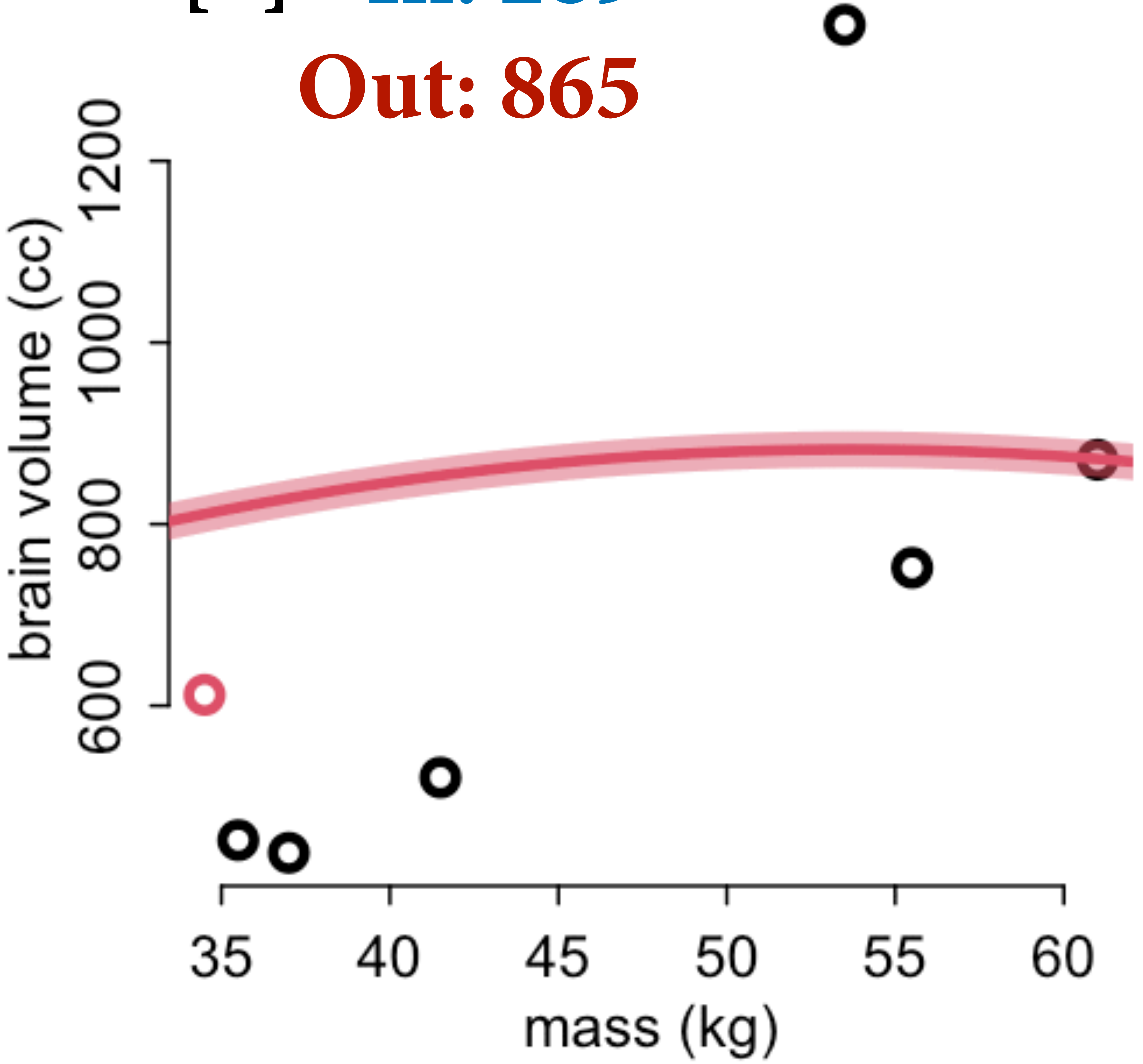
log probability of each point i, computed with posterior that omits point i

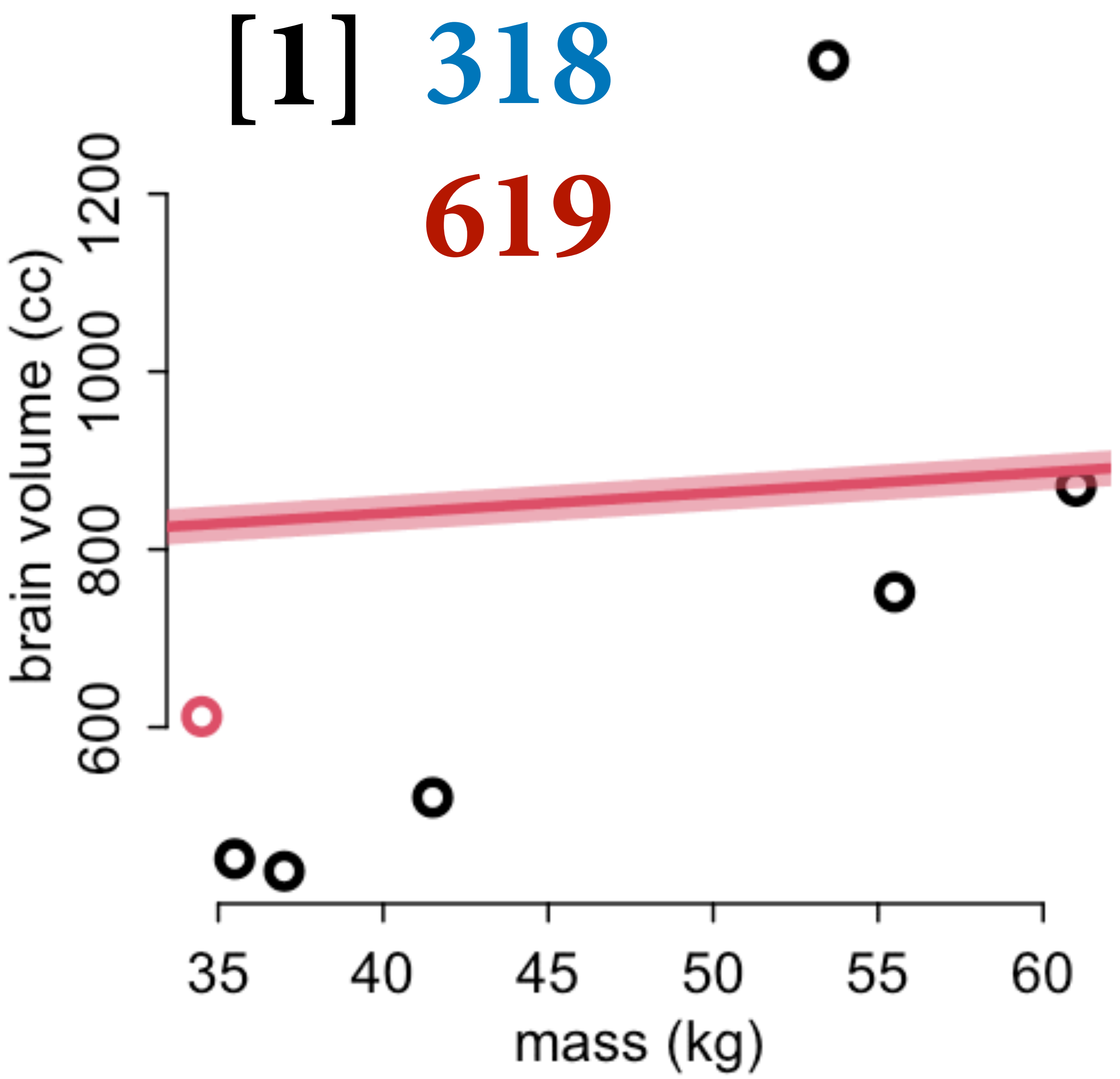
Pages 210 and 218

[1] In: 318
Out: 619



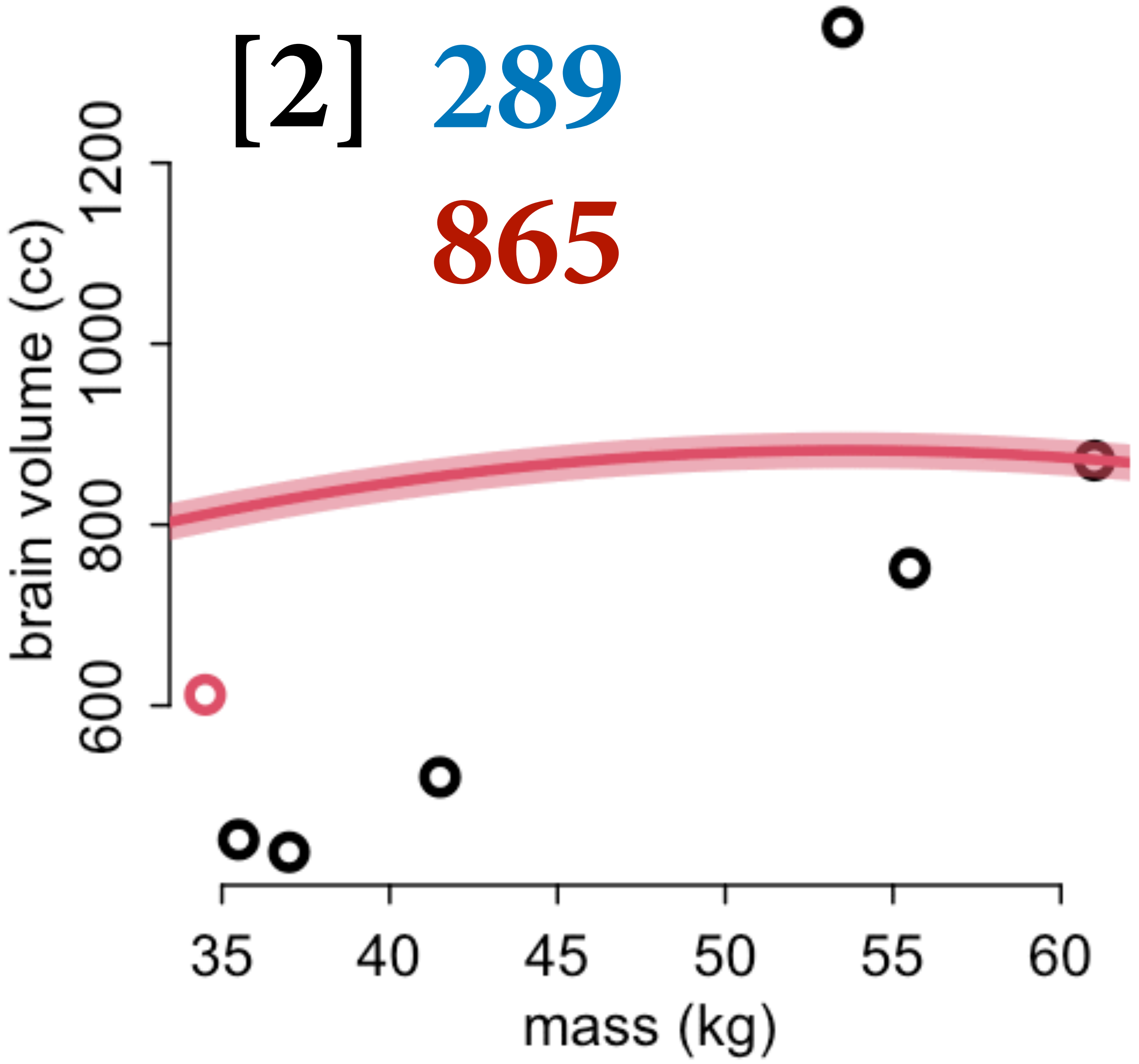
[2] In: 289
Out: 865





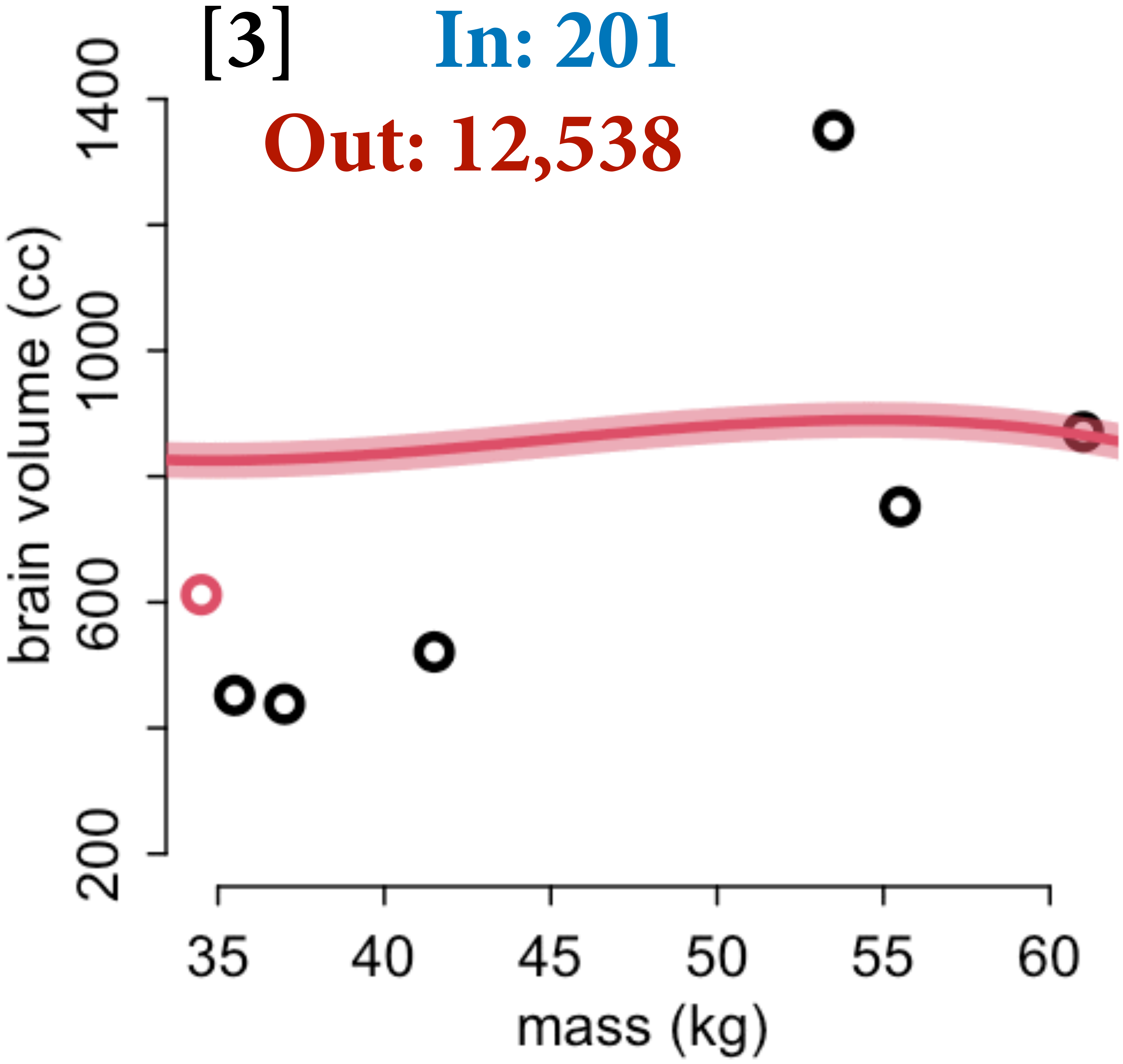
[1] 318

619



[2] 289

865

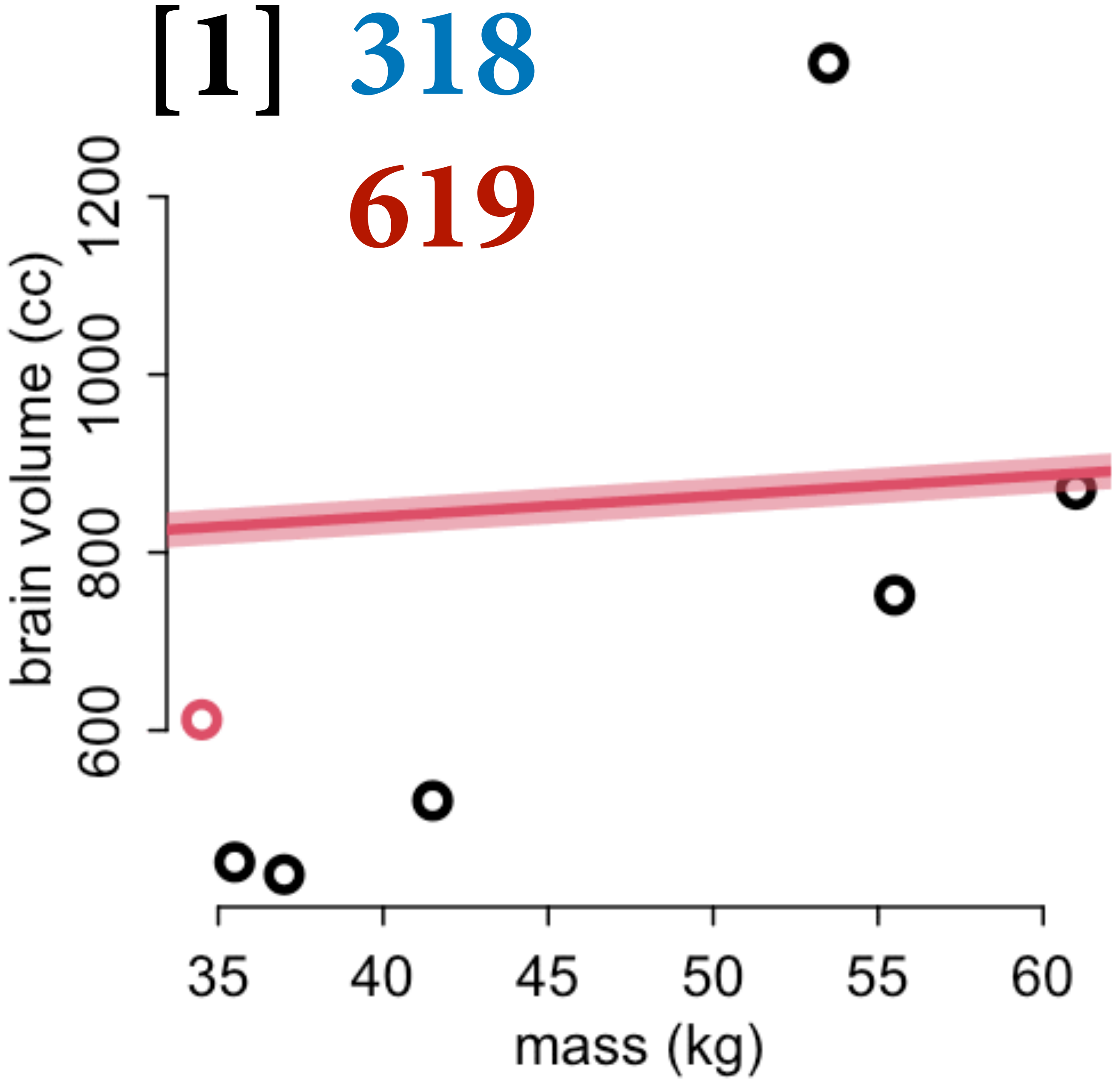


[3] In: 201

Out: 12,538

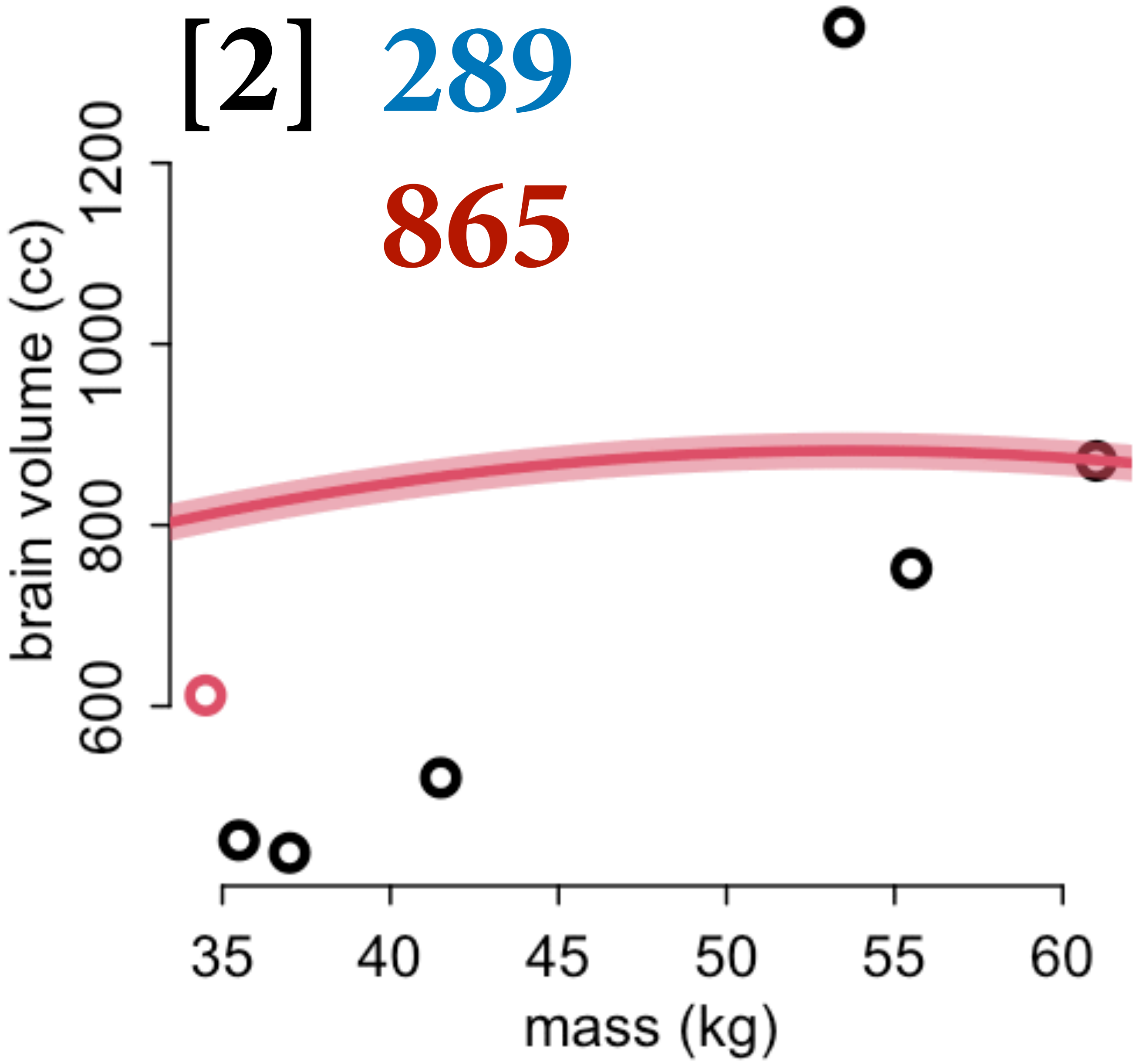
[1] 318

619



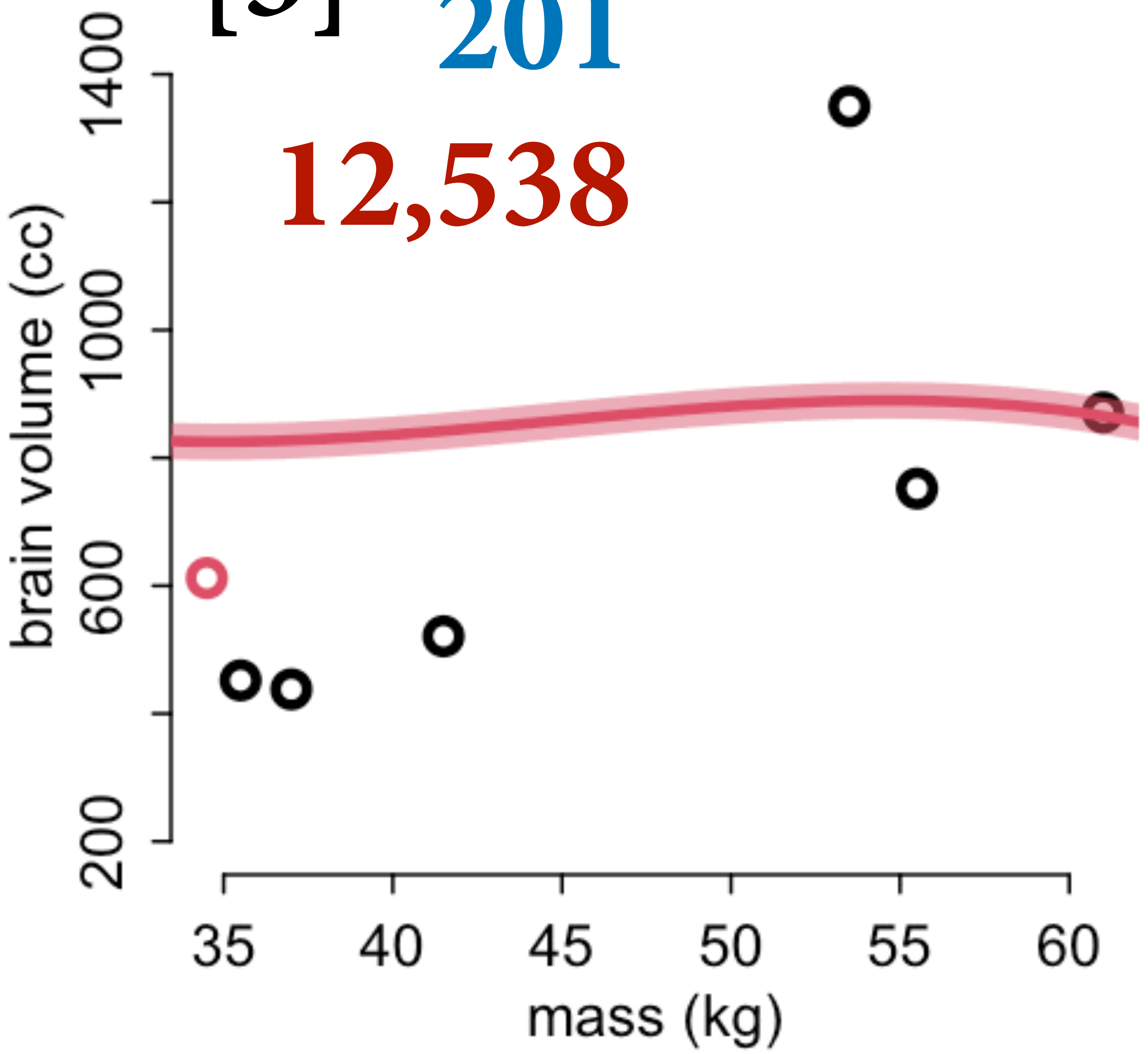
[2] 289

865



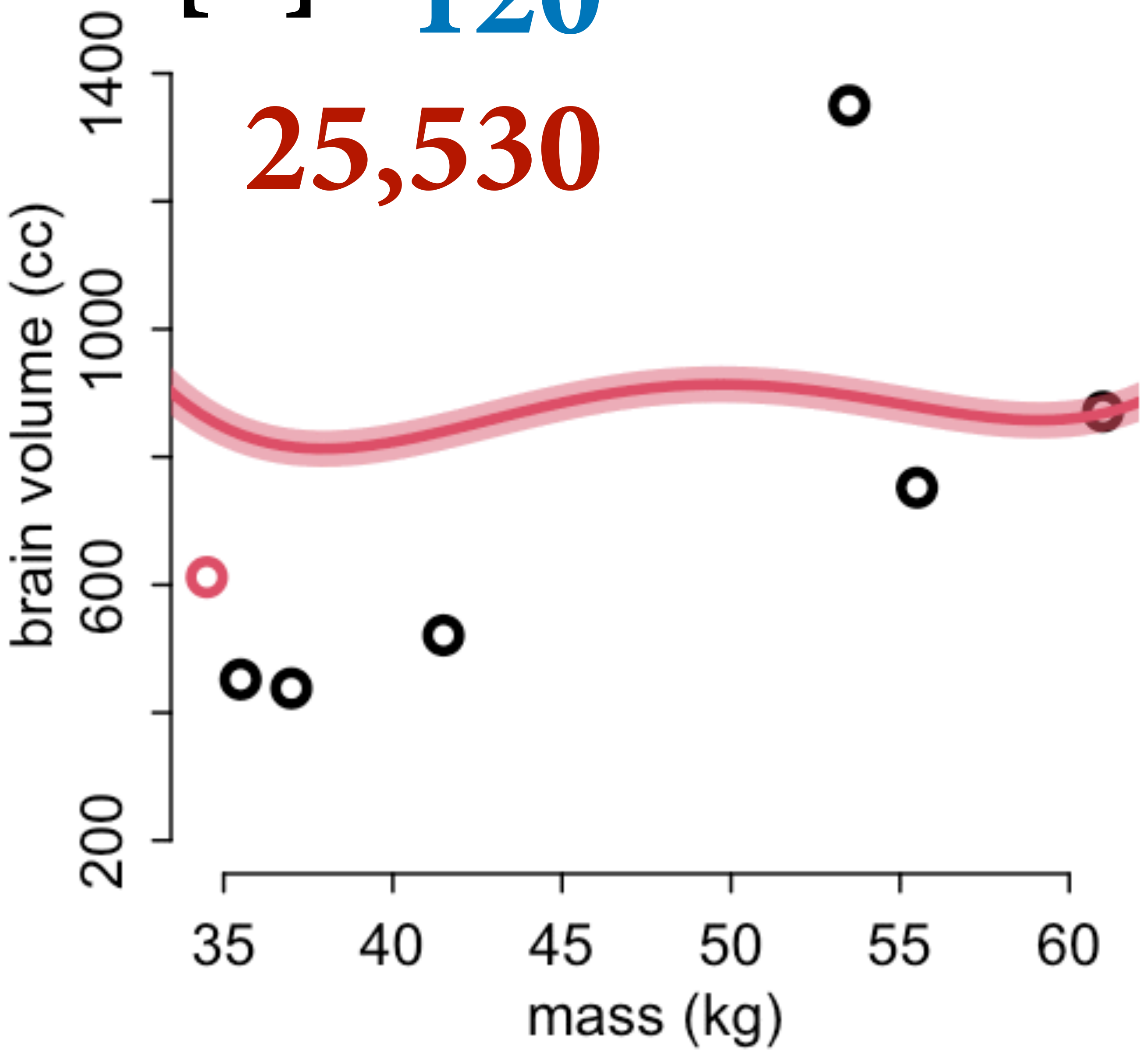
[3] 201

12,538



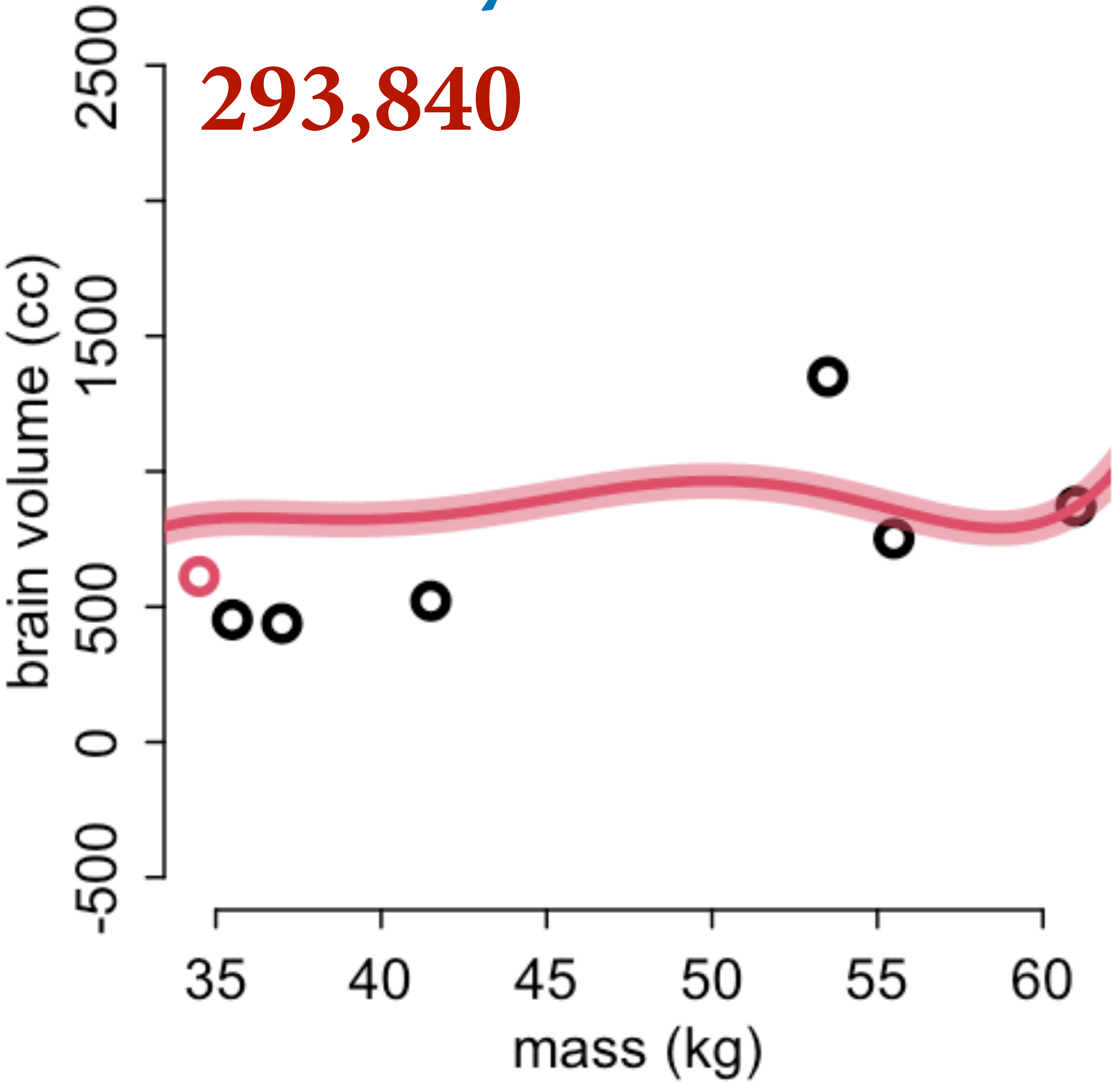
[4] 120

25,530



[5] 7

293,840

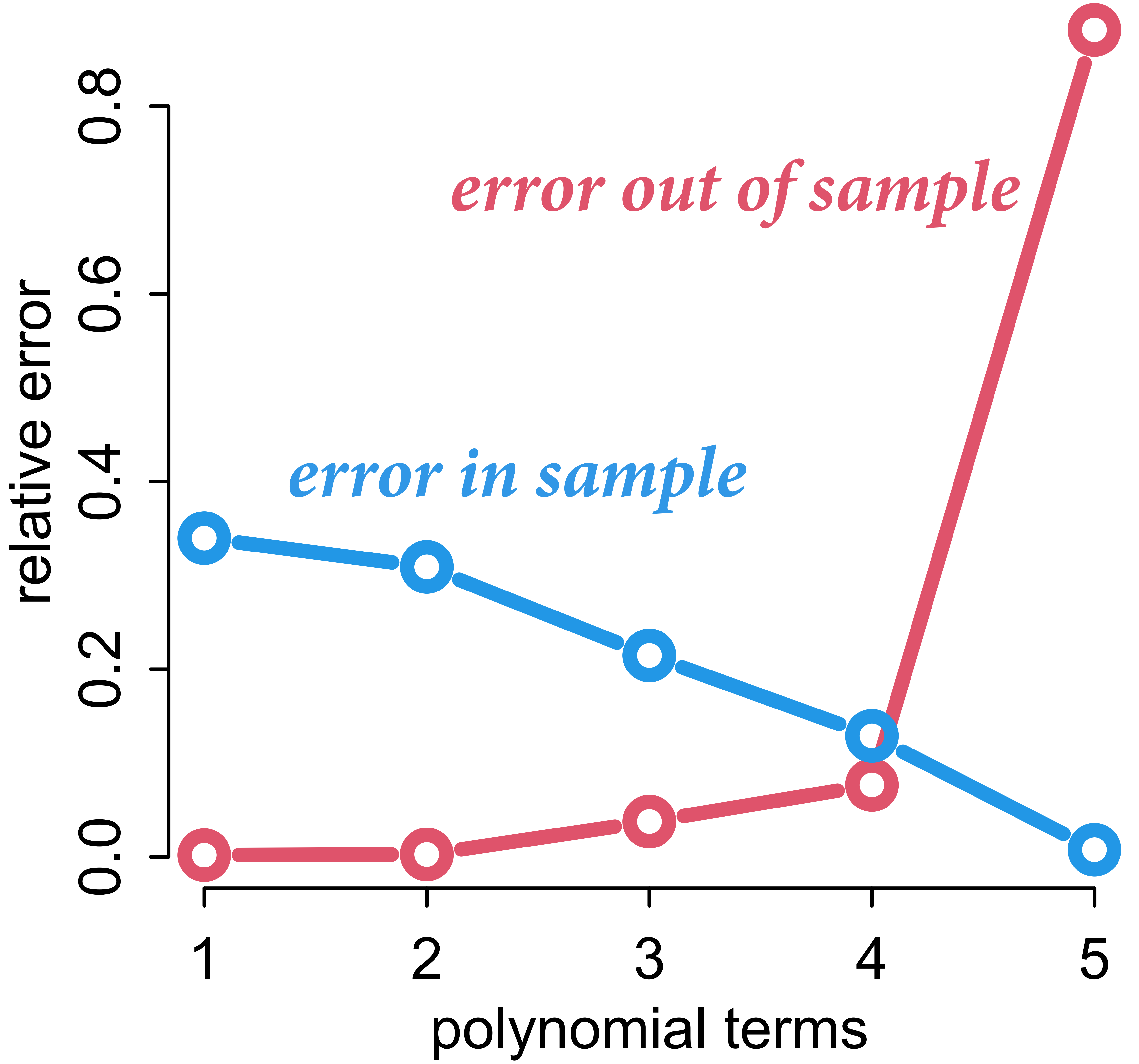


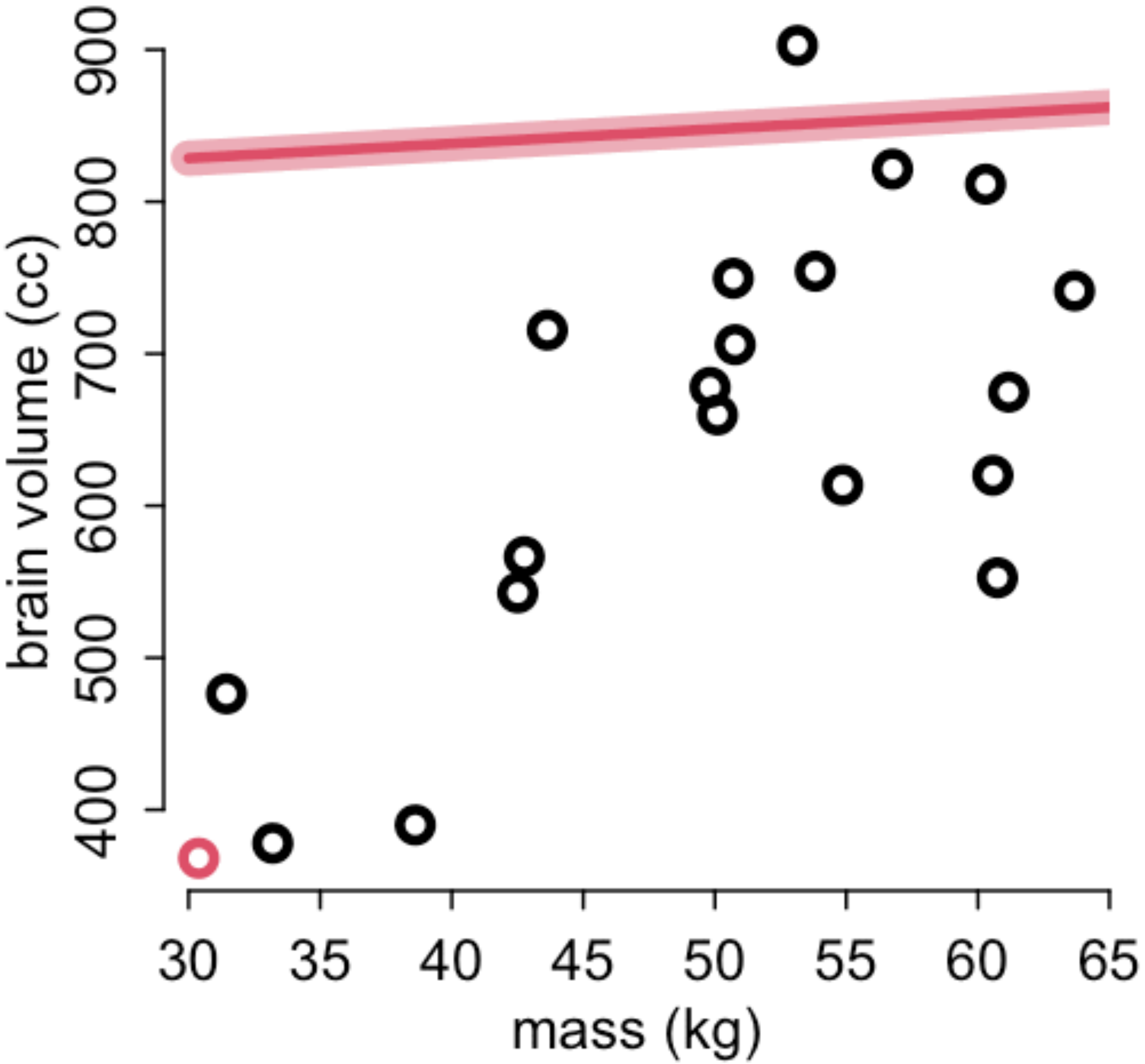
Cross-validation

For simple models, increasing parameters improves fit to sample

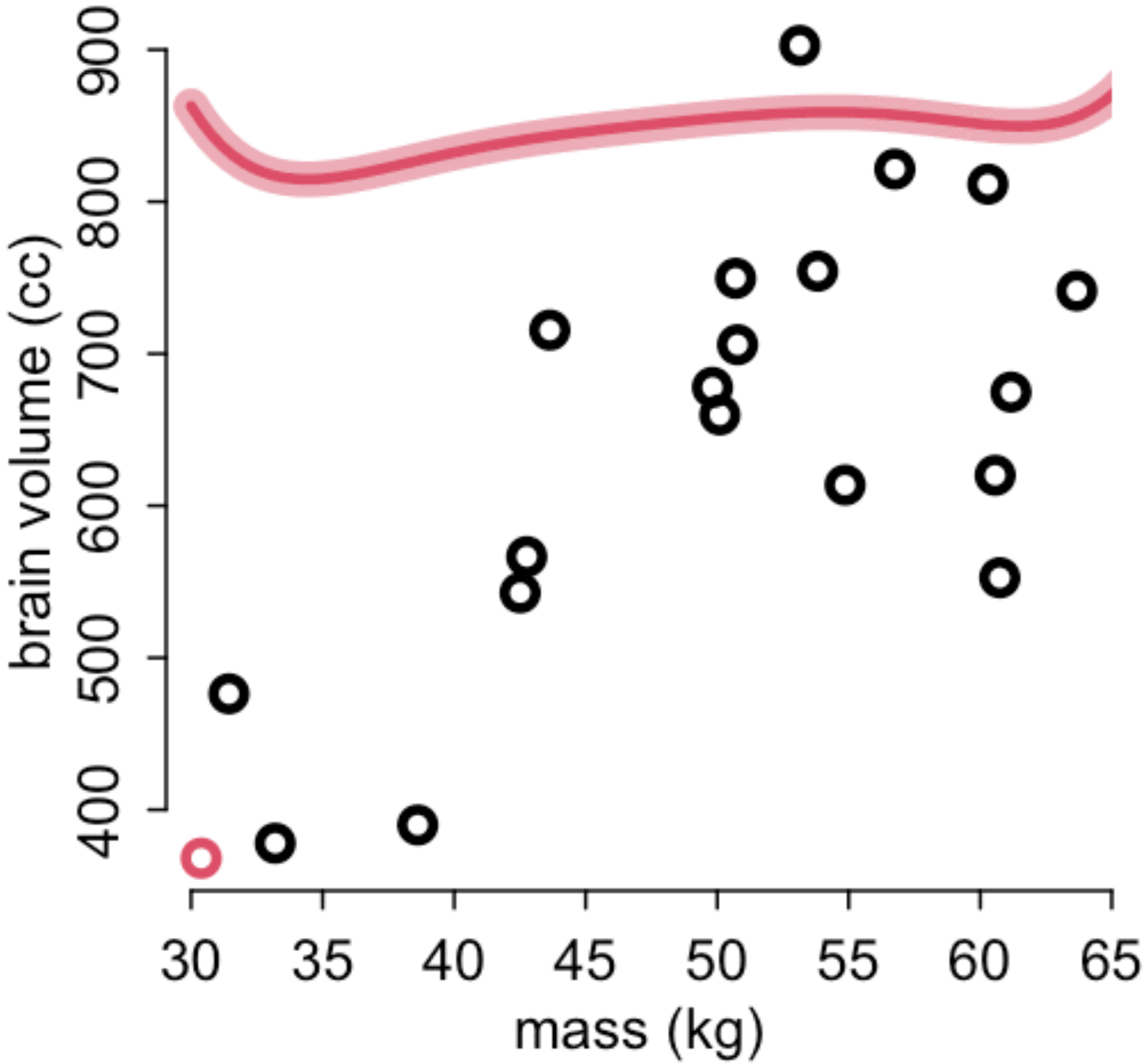
But may reduce accuracy of predictions out of sample

Most accurate model trades off flexibility with overfitting



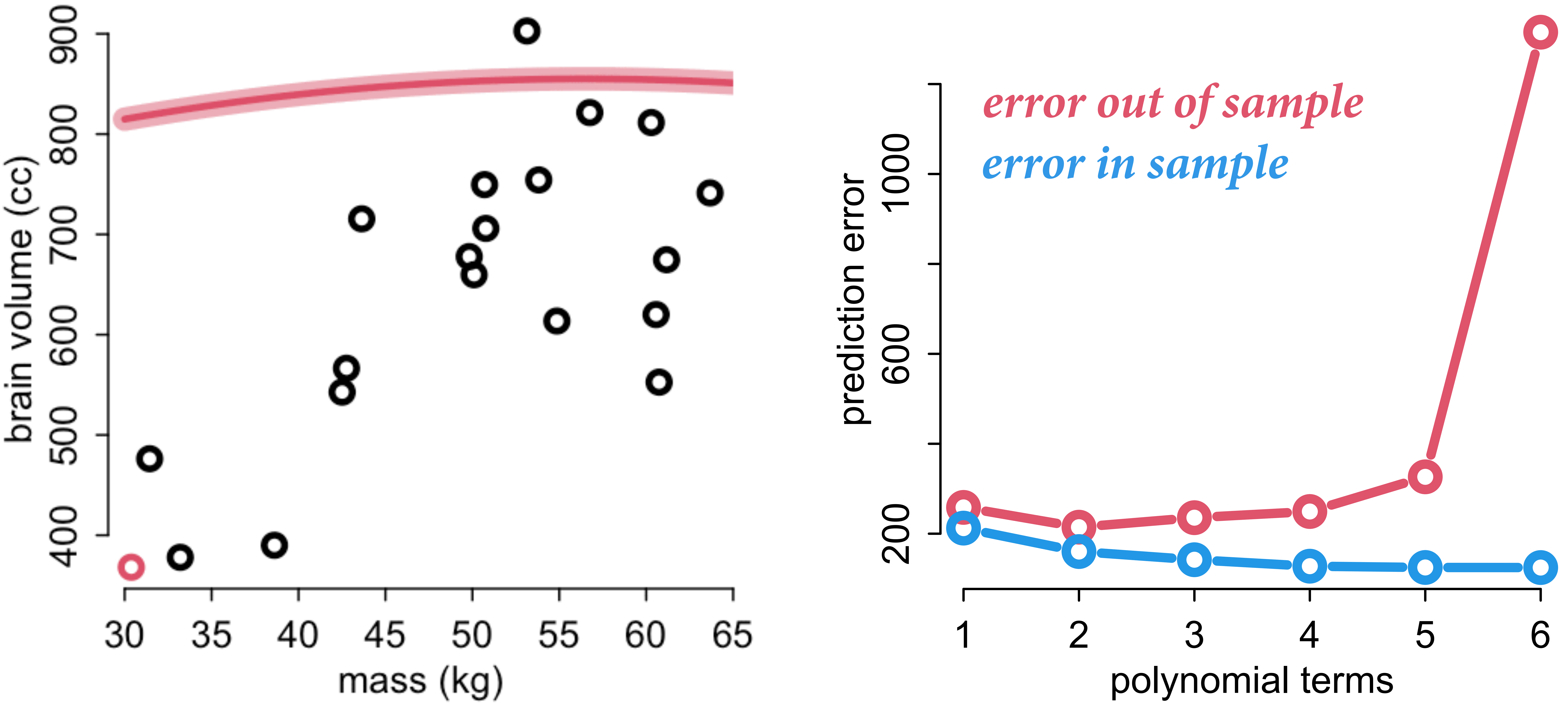


1st degree polynomial

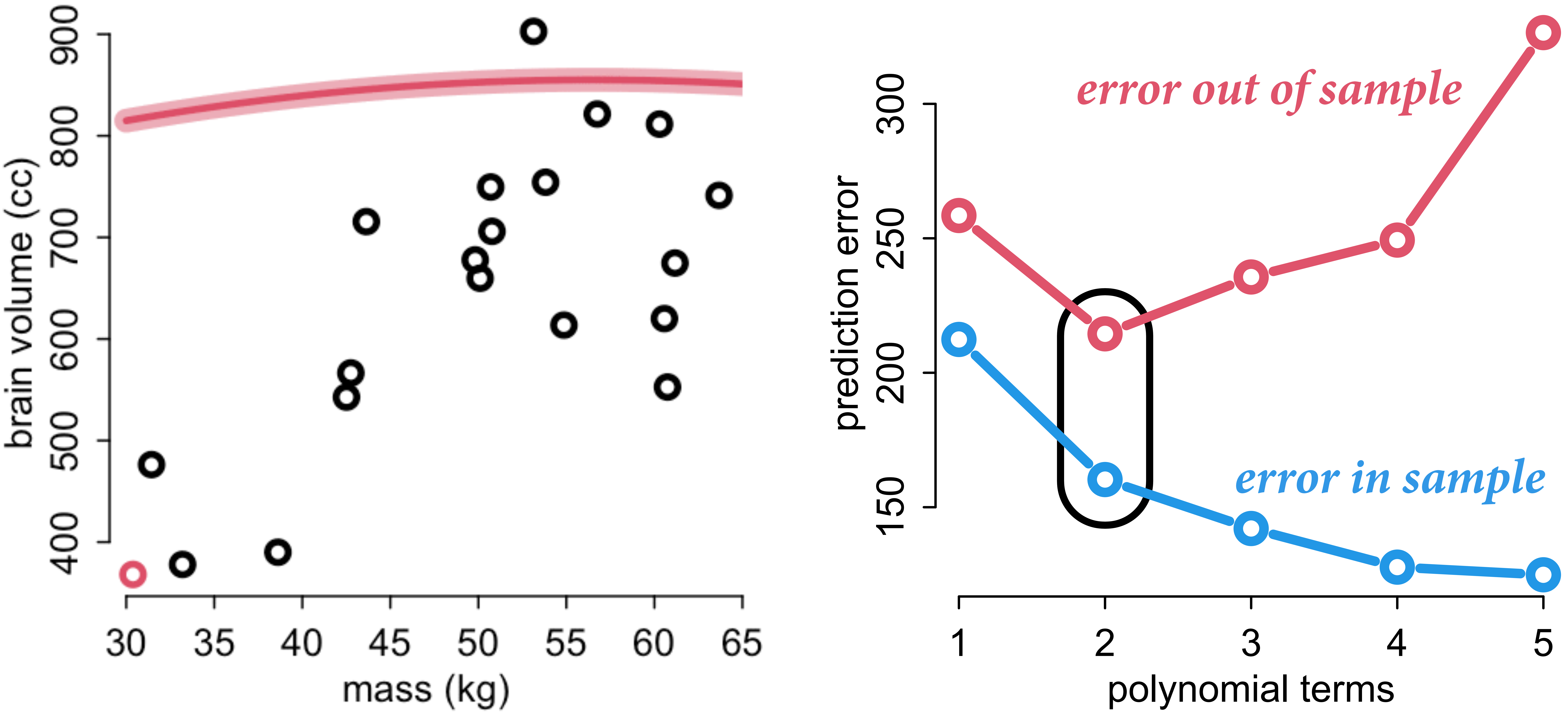


6th degree polynomial

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!

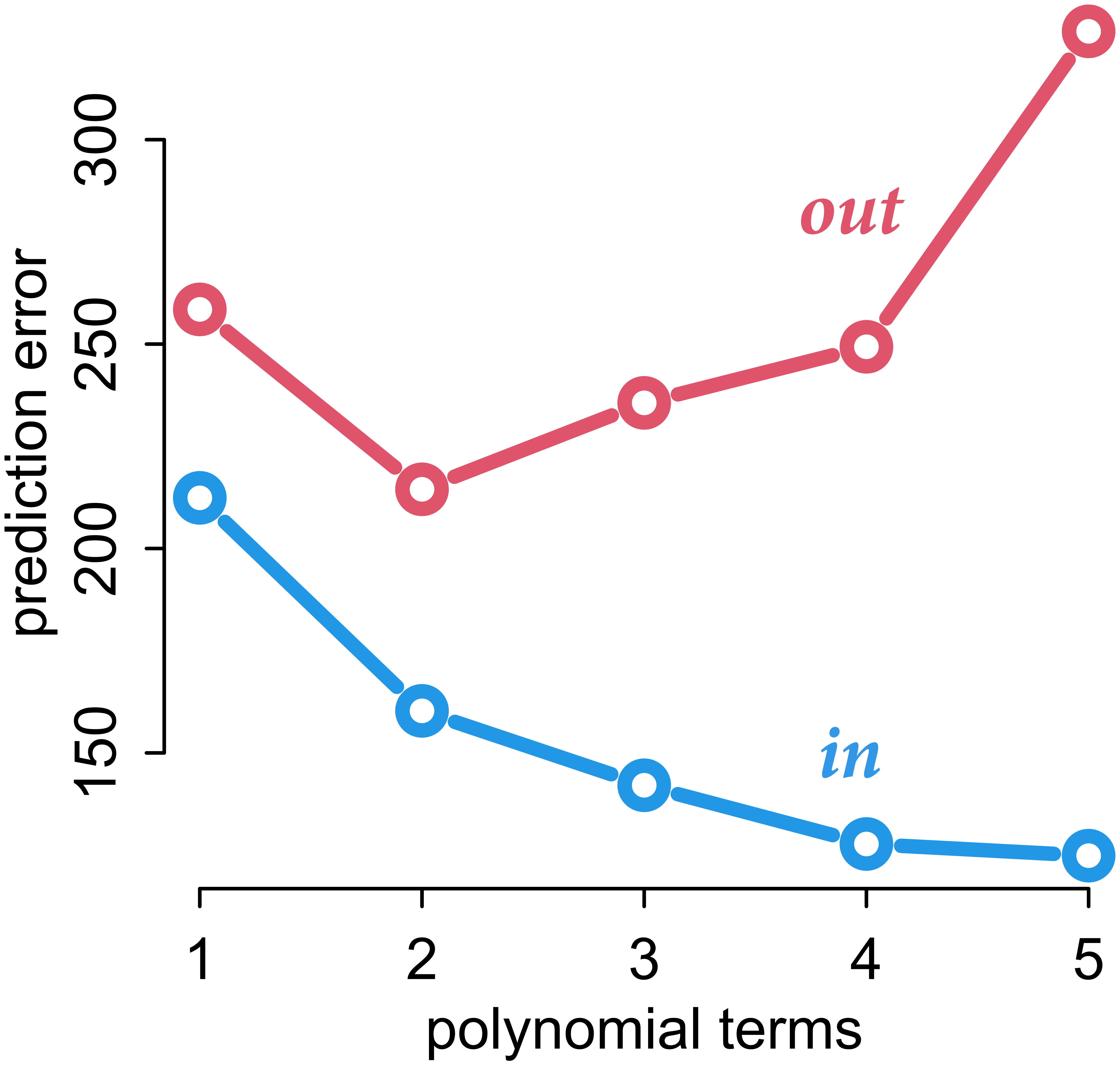
1 skeptischer Hamster zu verkaufen

20 €

25899 Niebüll >

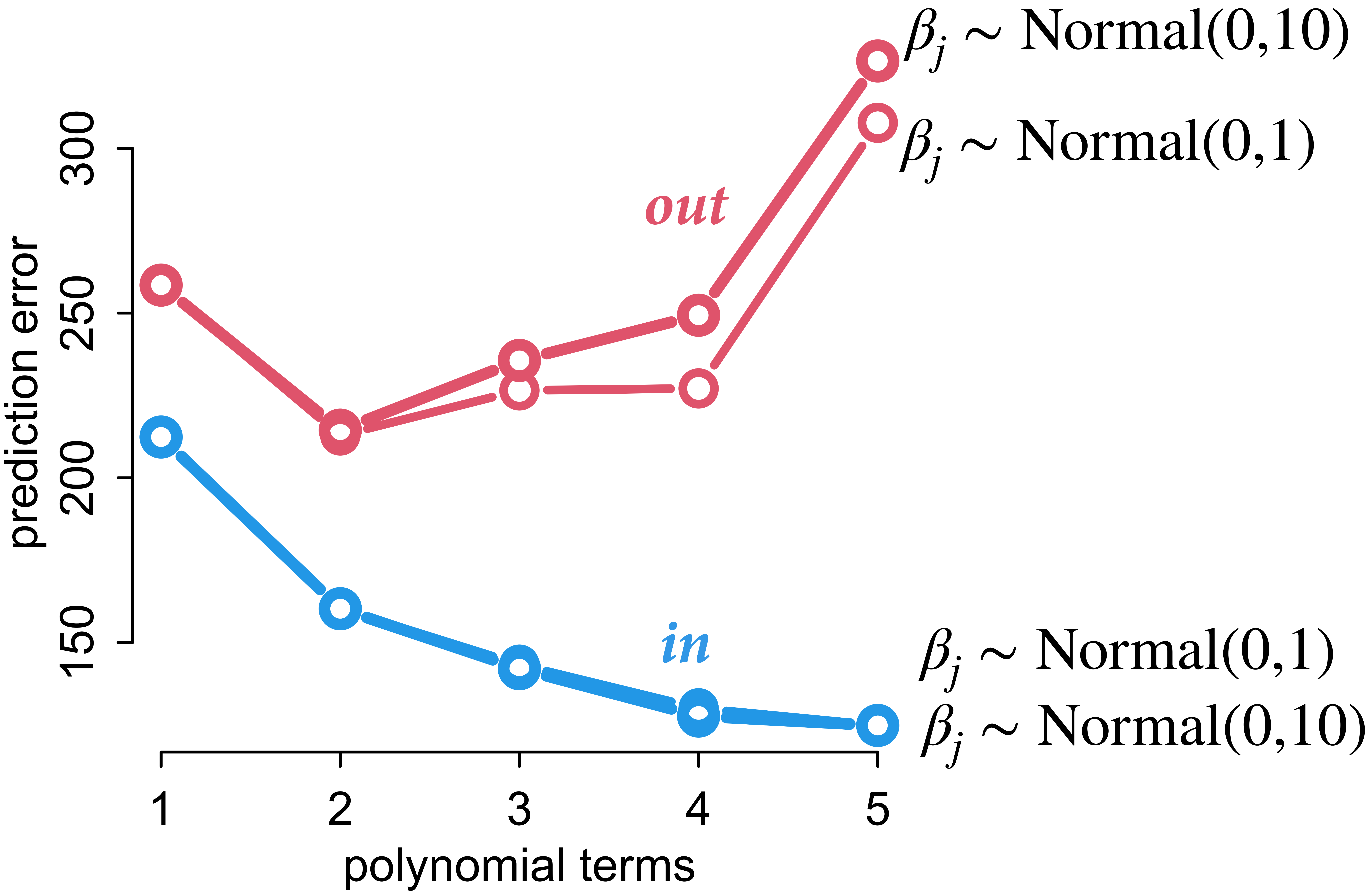
Art Hamster

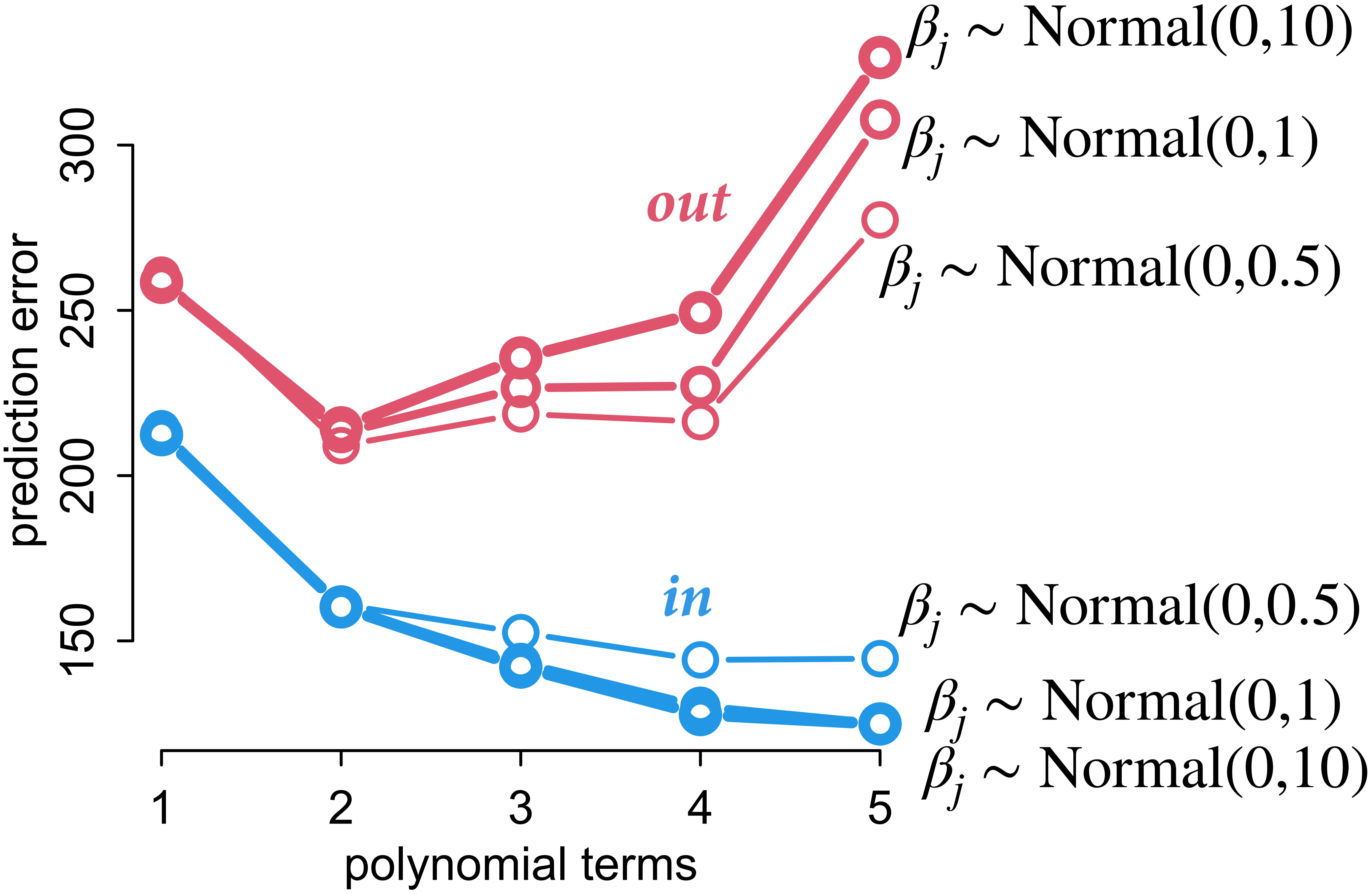
Er guckt einen skeptisch an, als würde man nichts richtig machen.
Es macht mich wahnsinnig, ich kann diesen vorwurfsvollen Blick nicht länger ertragen.
Sein Name ist Olaf.



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

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


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



prediction error
300
250
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1
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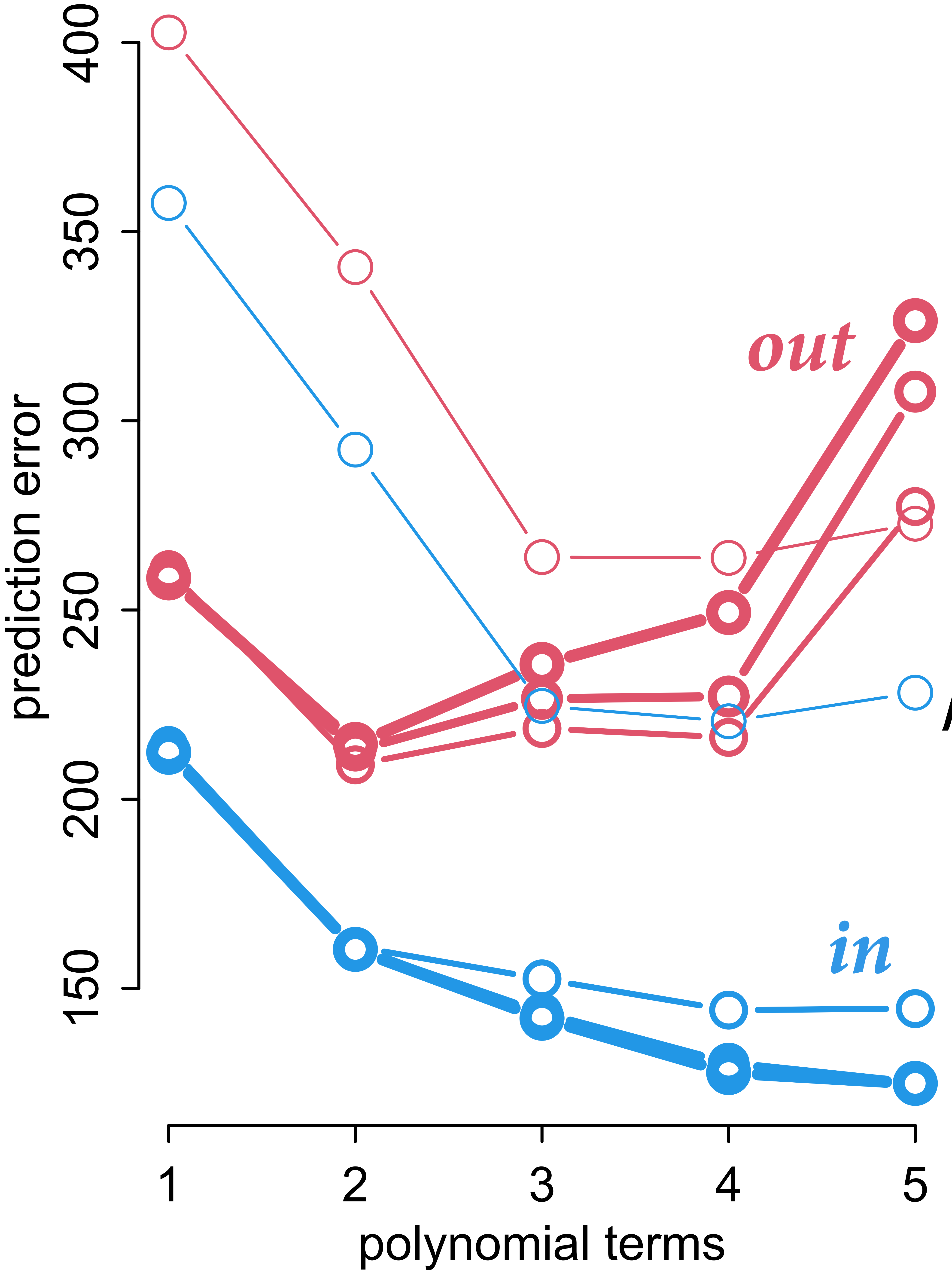
polynomial terms
out
in
$\beta_j \sim \text{Normal}(0,10)$
$\beta_j \sim \text{Normal}(0,1)$
$\beta_j \sim \text{Normal}(0,0.5)$
$\beta_j \sim \text{Normal}(0,0.5)$
$\beta_j \sim \text{Normal}(0,1)$
$\beta_j \sim \text{Normal}(0,10)$



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

Regularizing priors

How to choose width of prior?

For causal inference, use science

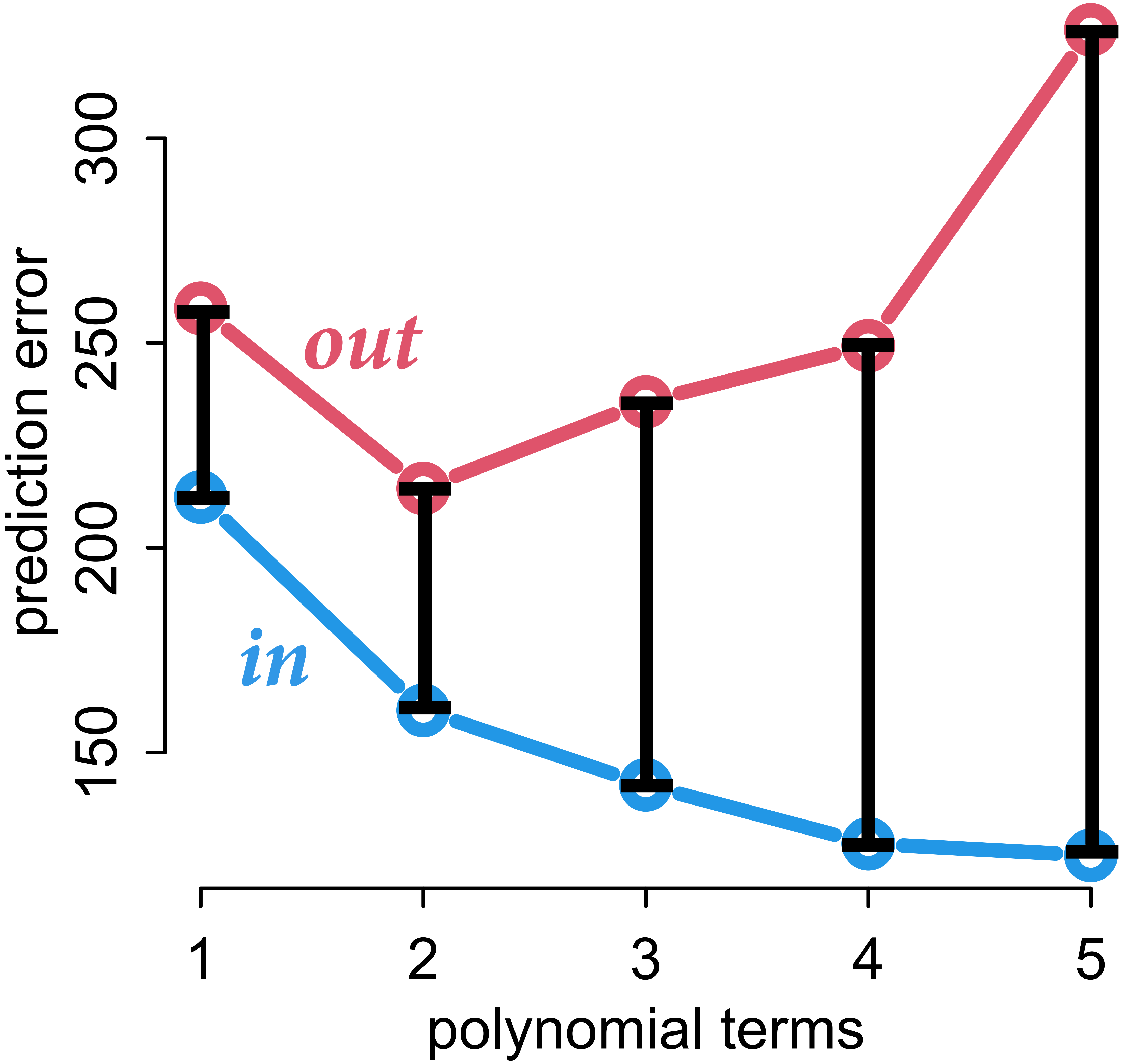
For pure prediction, can tune the prior using cross-validation

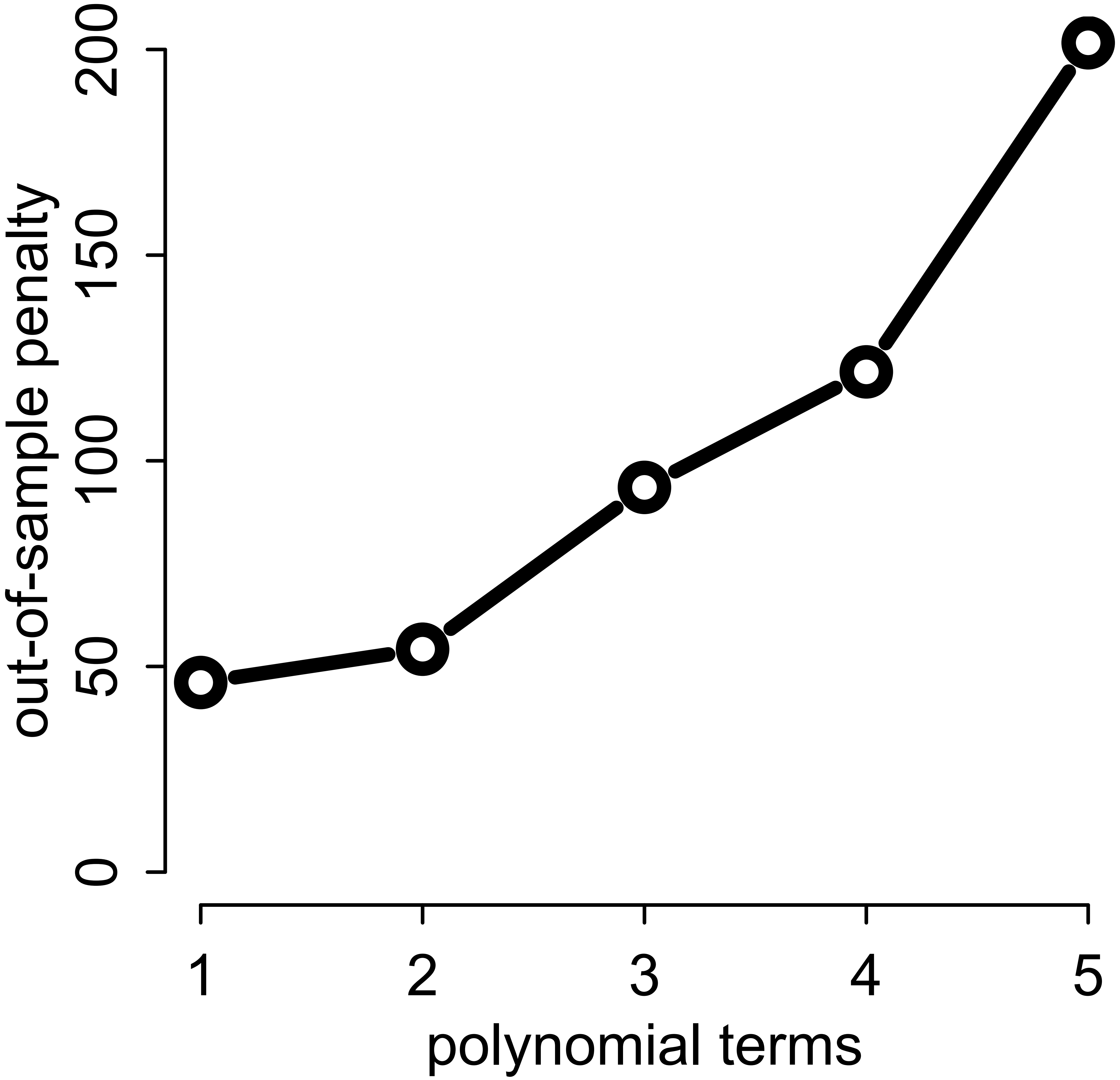
Many tasks are a mix of inference and prediction

No need to be perfect, just better

PAUSE

Prediction penalty





Penalty prediction

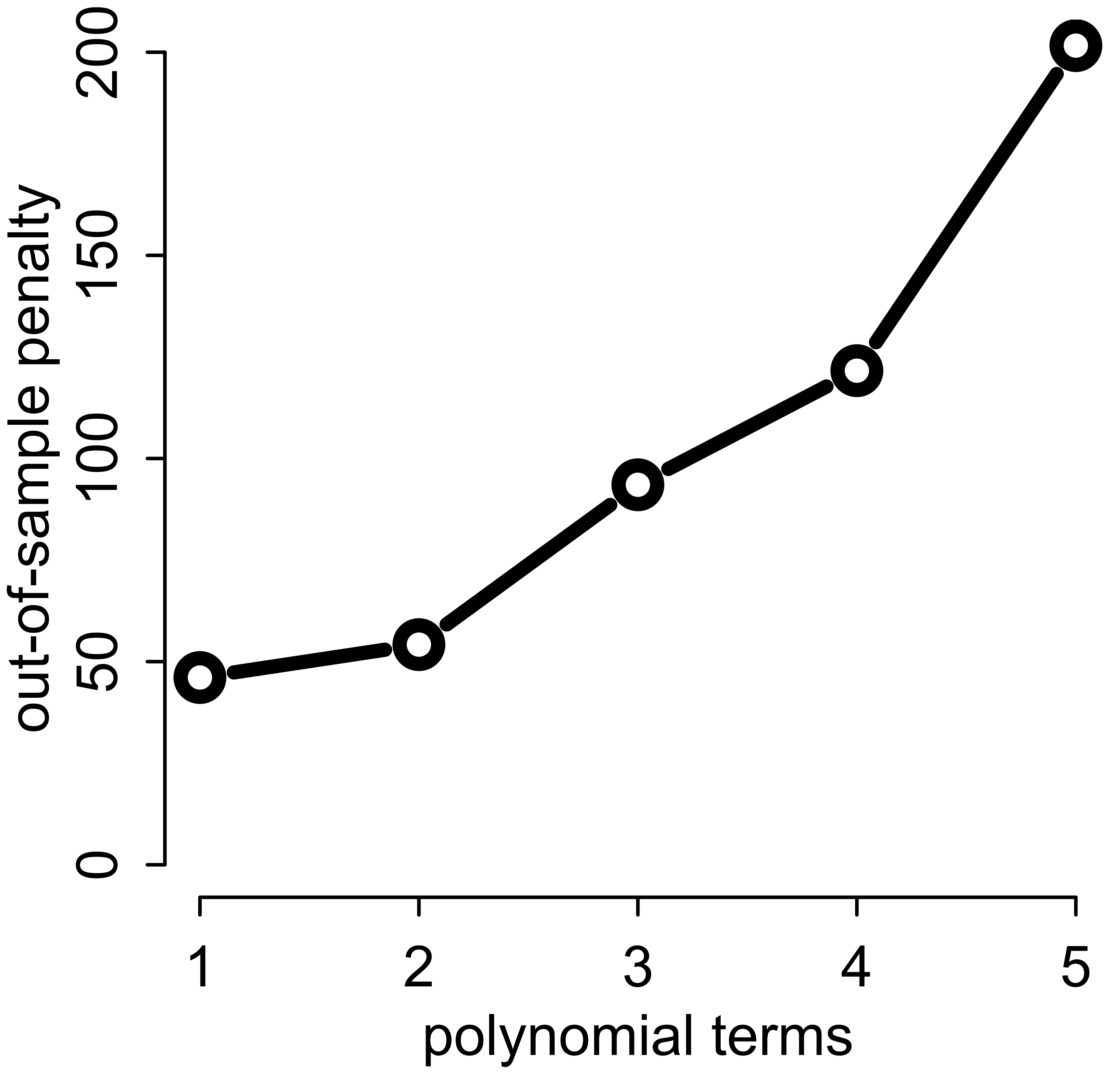
For *N* points, cross-validation requires fitting *N* models

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

Good news! You can:

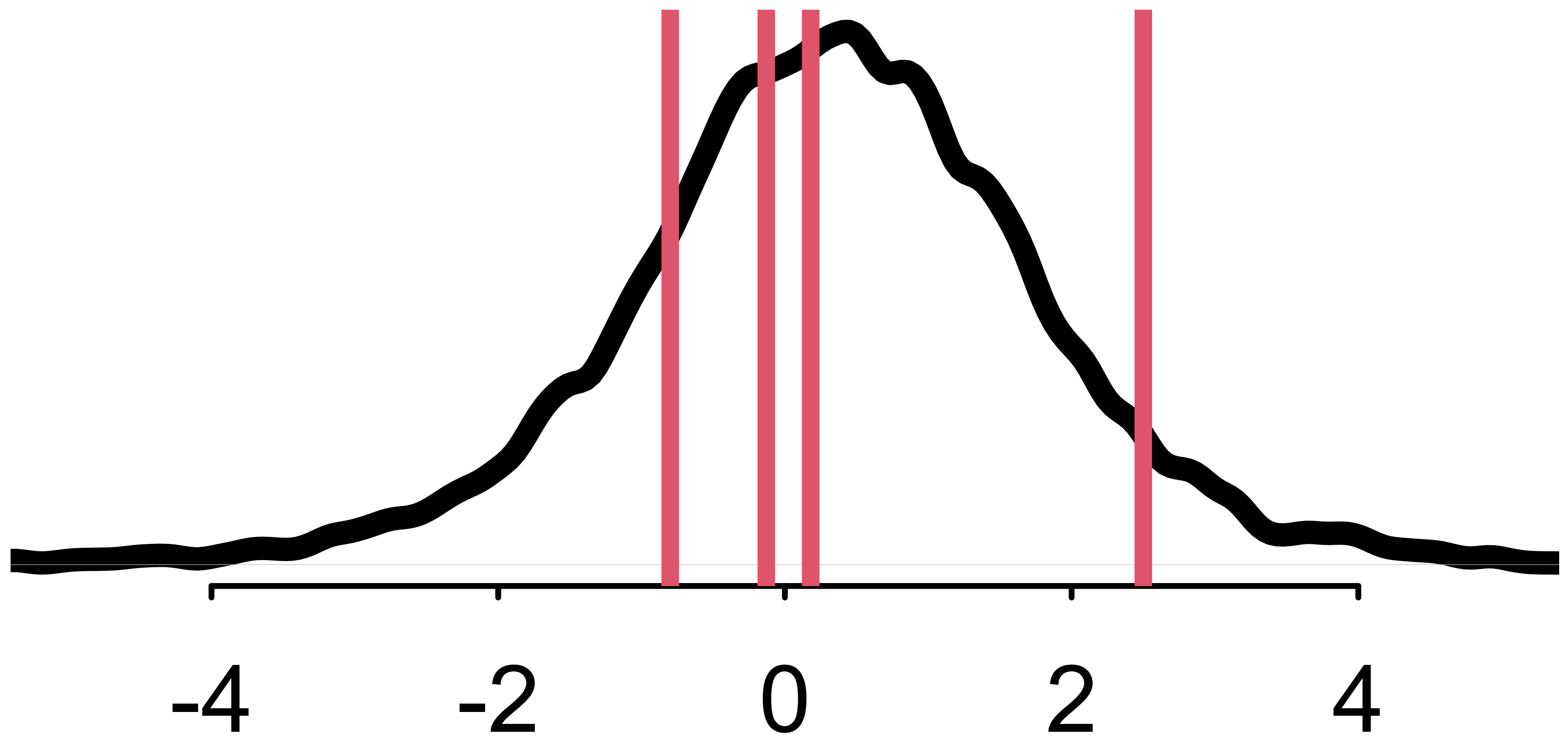
Importance sampling (PSIS)

Information criteria (WAIC)



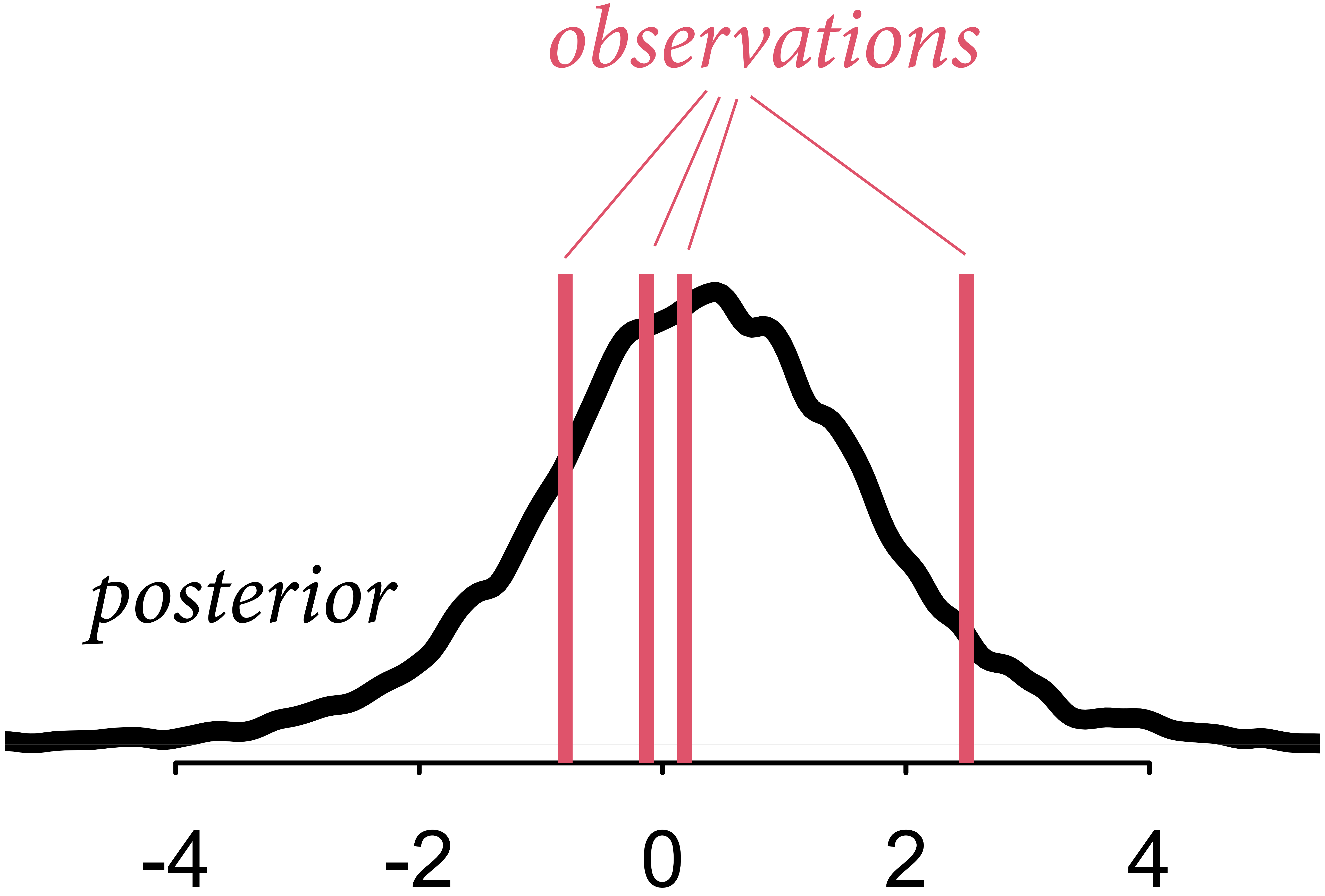
Importance Sampling

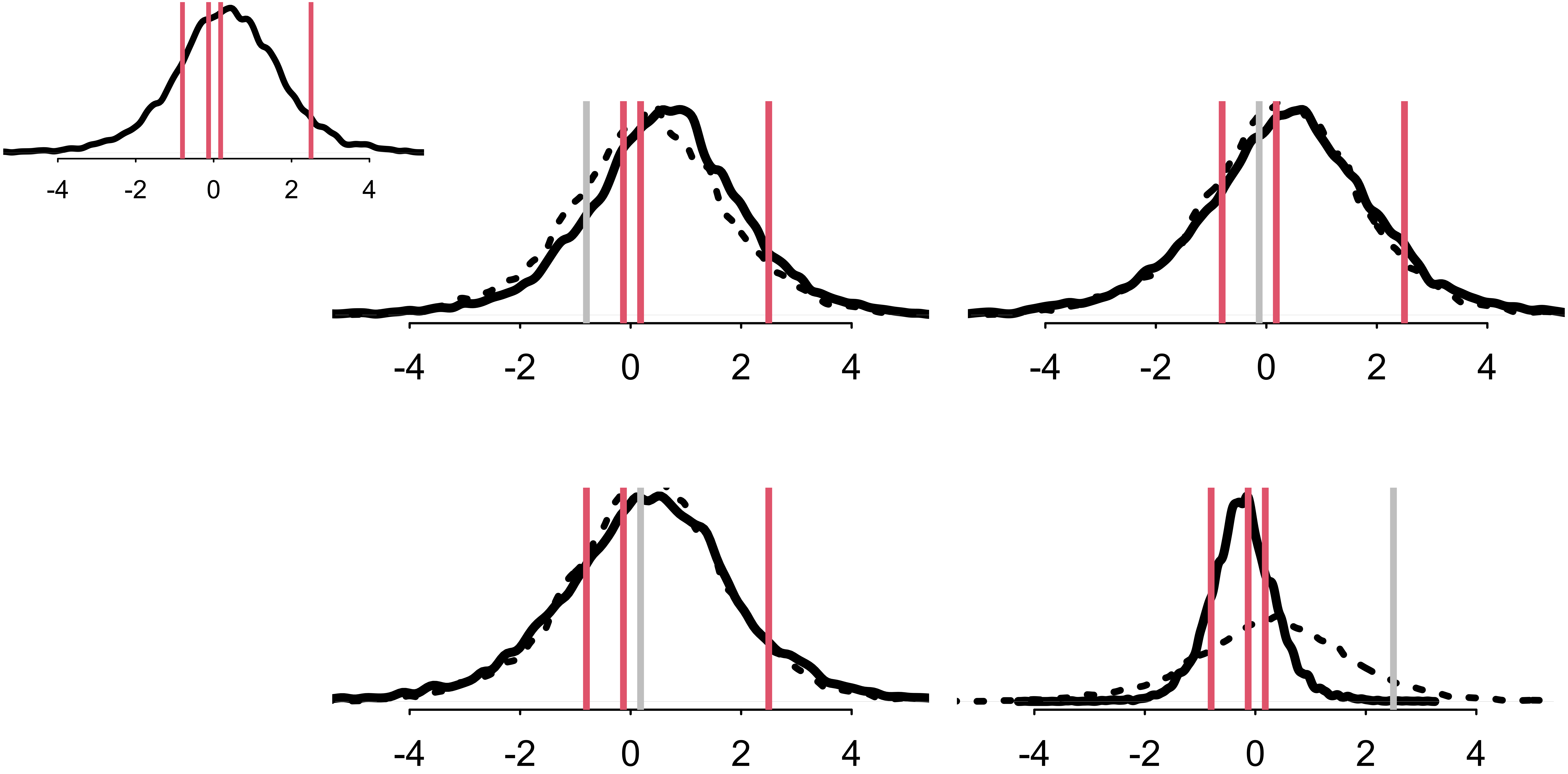
Importance sampling: Use a single posterior distribution for *N* points to sample from each posterior for *N*–1 points



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

Can use pointwise probabilities to reweight samples from posterior


observations
posterior
-4
-2
0
2
4


-4
-2
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2
4
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-4
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0
2
4

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

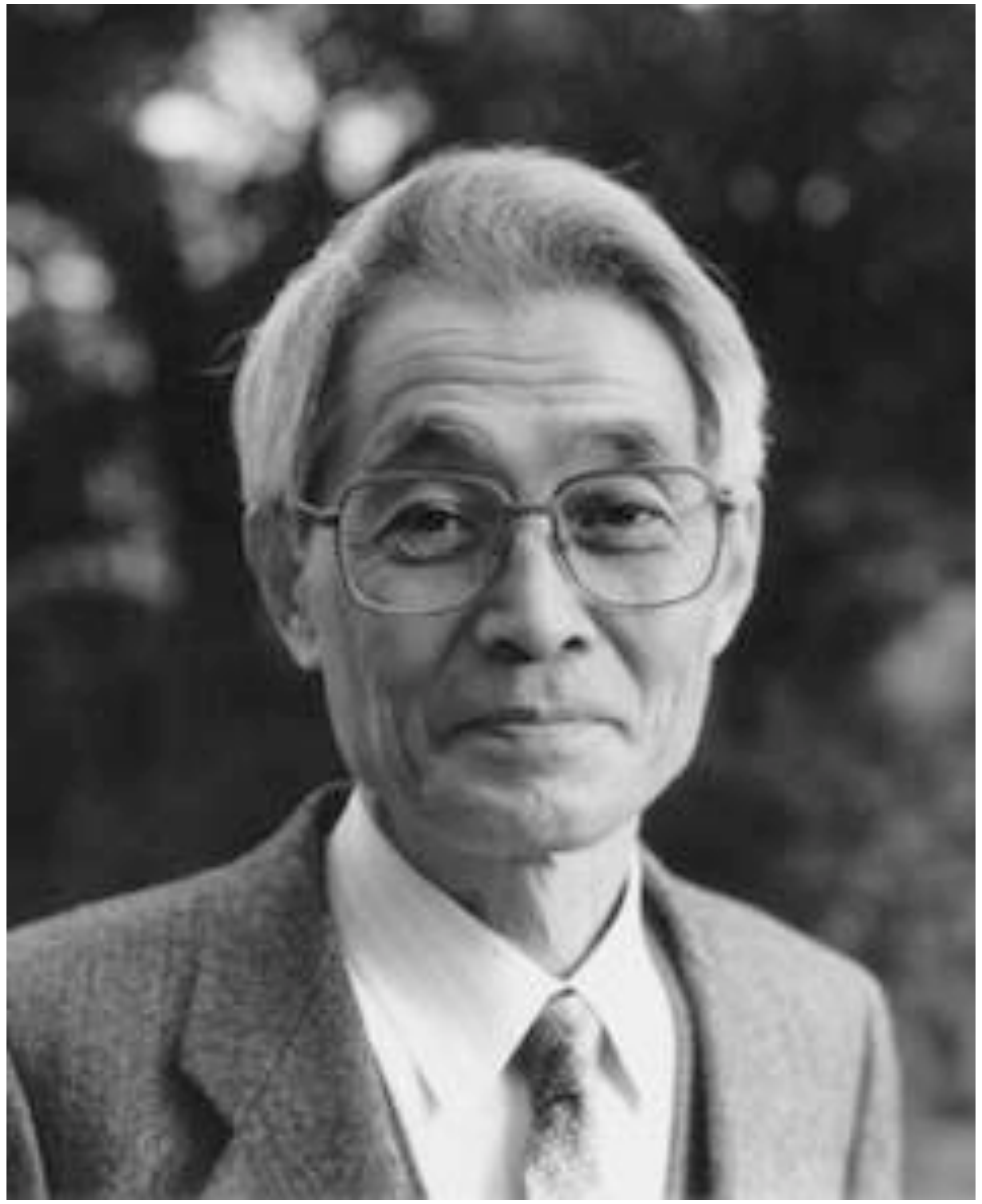
Akaike information criterion

[ah–ka–ee–kay]

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

For flat priors and large samples:

$$\mathrm{AIC} = (-2) \times \underbrace{\mathrm{lppd}}_{\textit{log pointwise predictive density}} + 2\underbrace{k}_{\textit{number of parameters}}$$



Hirotugu Akaike (1927–2009)

赤池弘次

Widely Applicable IC

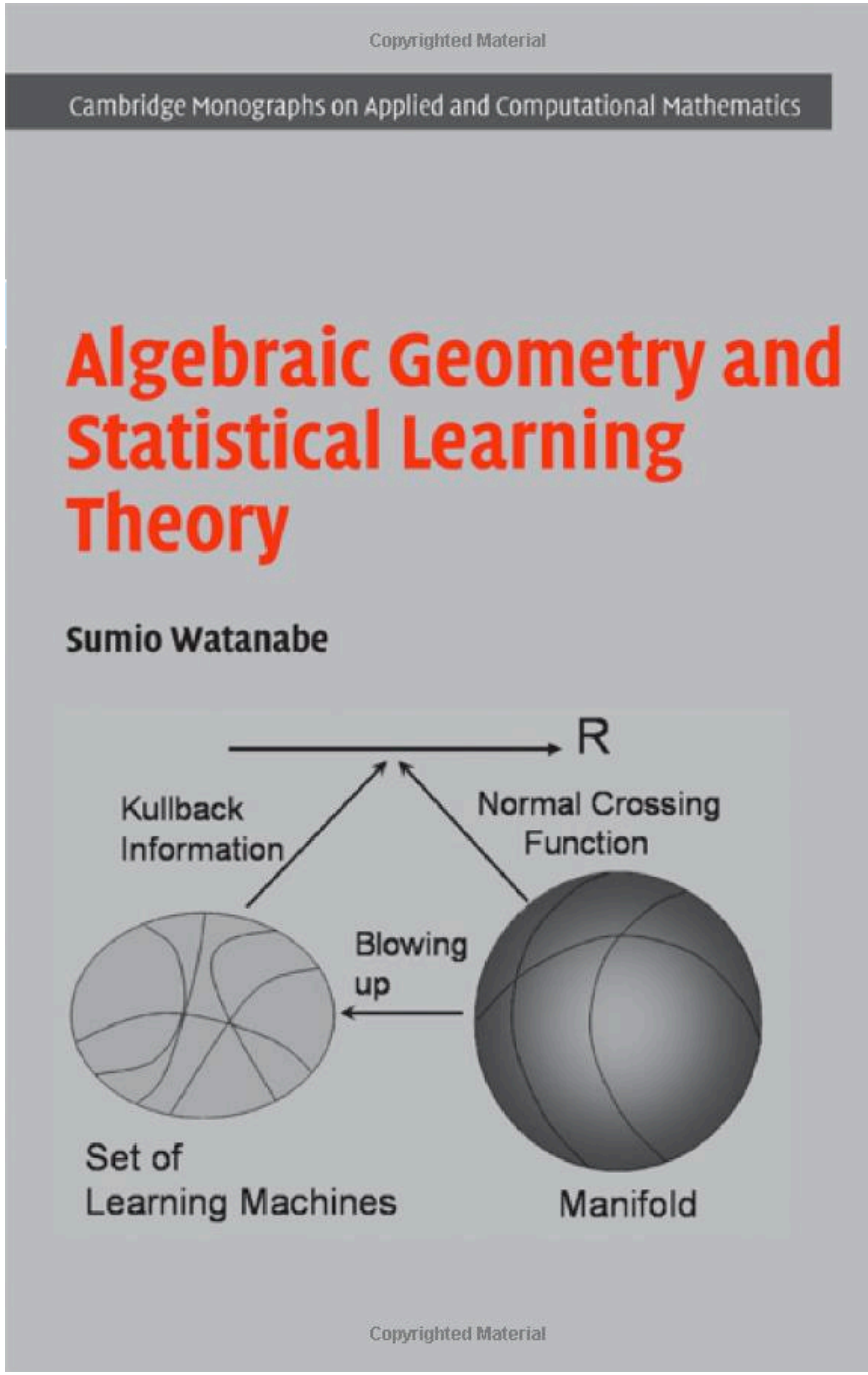
AIC of historical interest now

Widely Applicable Information Criterion (WAIC)

Sumio Watanabe (渡辺澄夫) 2010

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

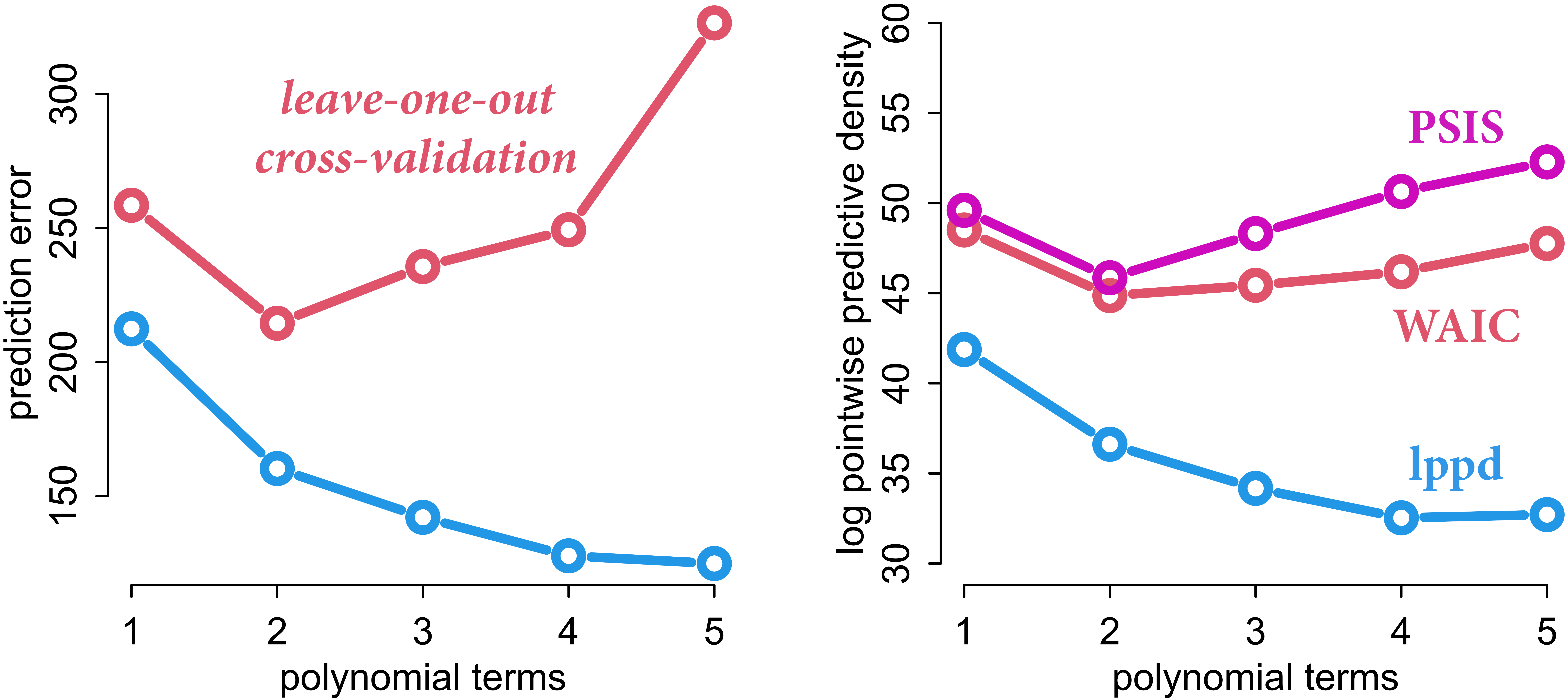
Very similar to PSIS score, but no automatic diagnostics



Cambridge Monographs on Applied and Computational Mathematics

Algebraic Geometry and Statistical Learning Theory

Sumio Watanabe


prediction error
150
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250
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leave-one-out
cross-validation
1
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4
5
polynomial terms
log pointwise predictive density
30
35
40
45
50
55
60
PSIS
WAIC
lppd
1
2
3
4
5
polynomial terms

WAIC,PSIS,CV measure overfitting

Regularization manages overfitting

None directly address causal inference

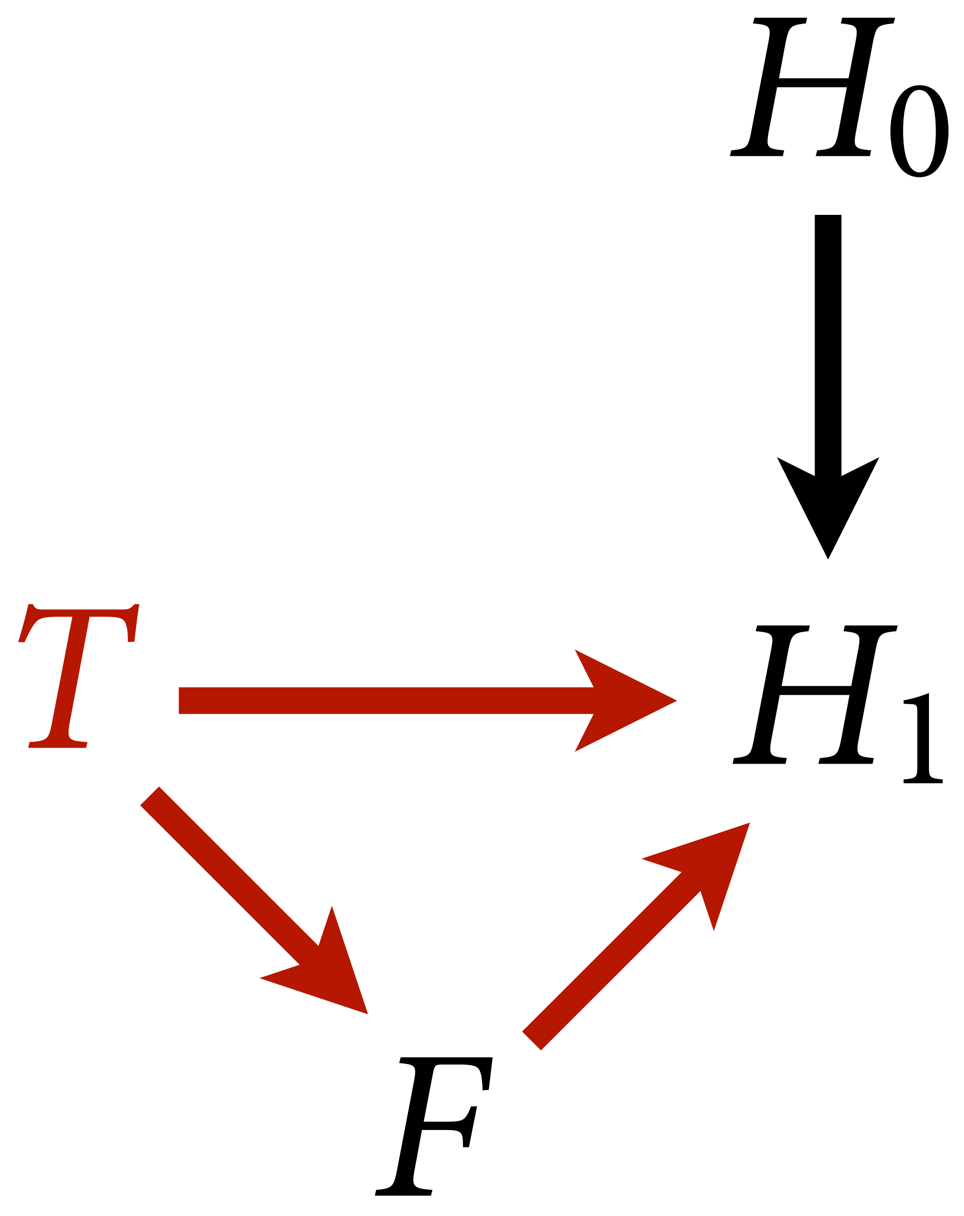
All important to understanding how statistical inference works

Model Mis-selection

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

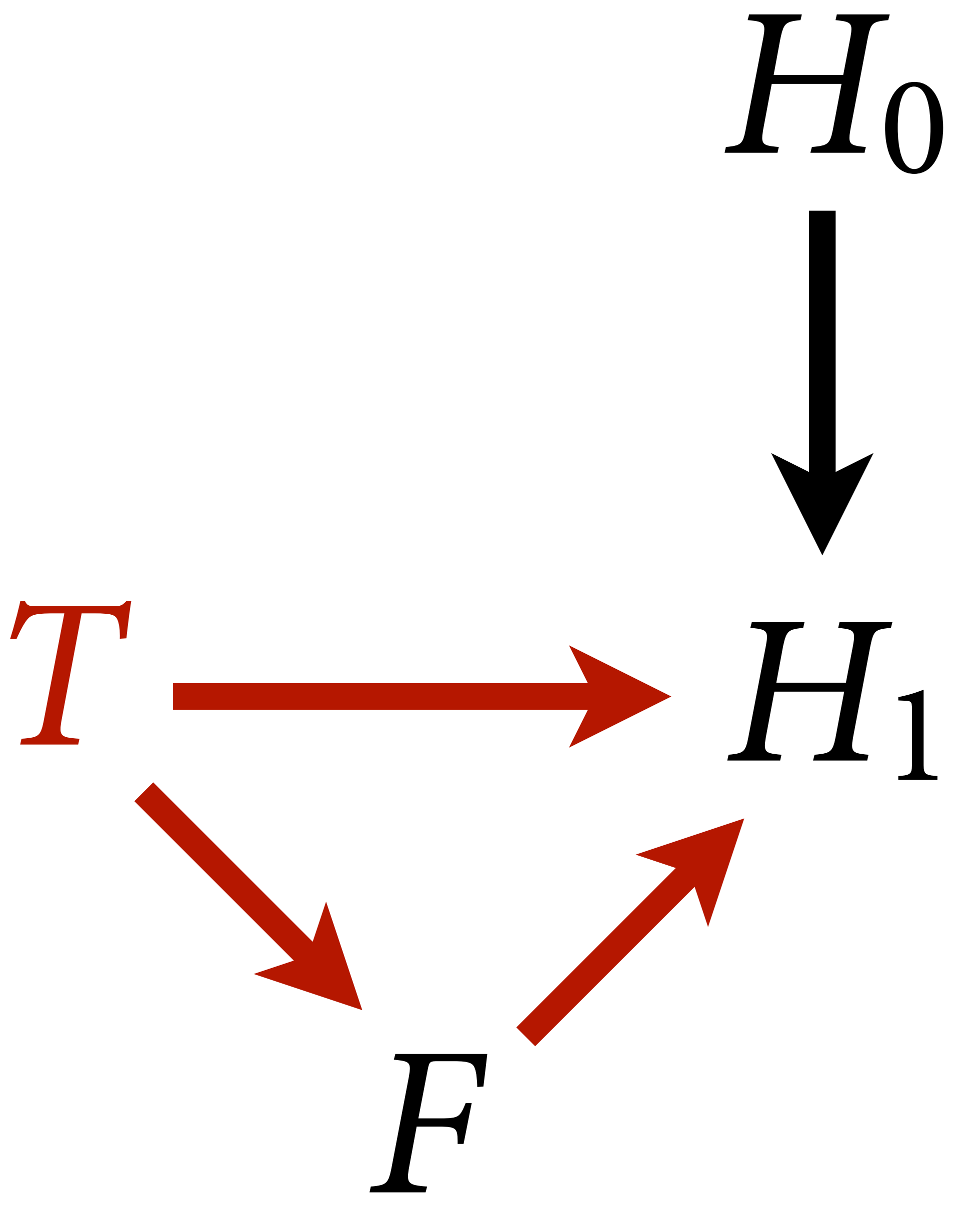
Predictive criteria actually prefer confounds & colliders

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)



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Correct adjustment set for total causal effect of treatment

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$$p_i = \alpha + \beta_T T_i + \beta_F F_i$$

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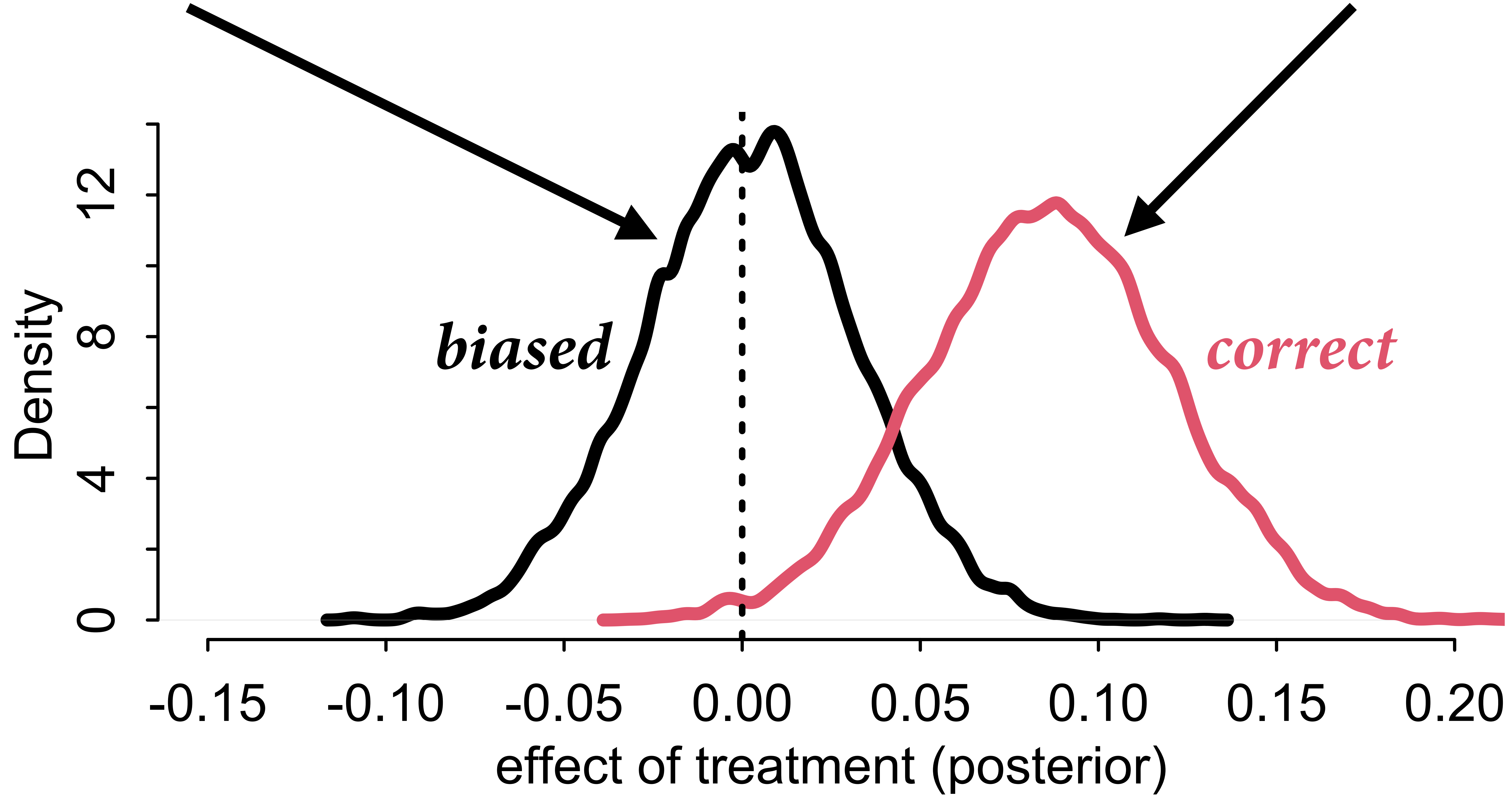

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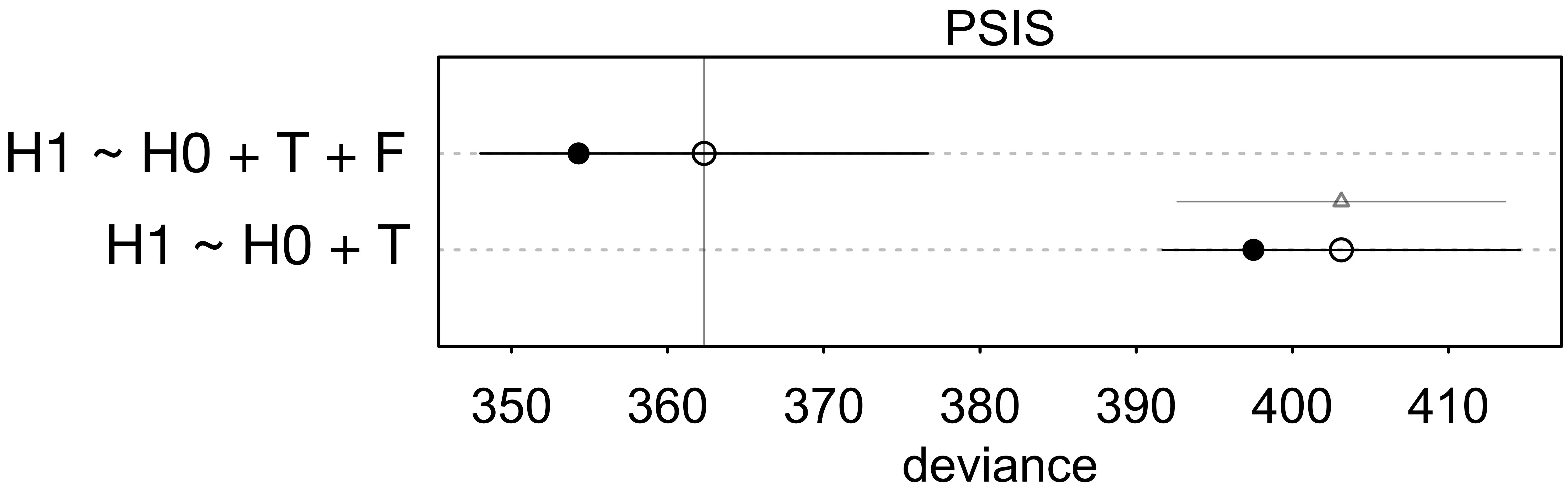
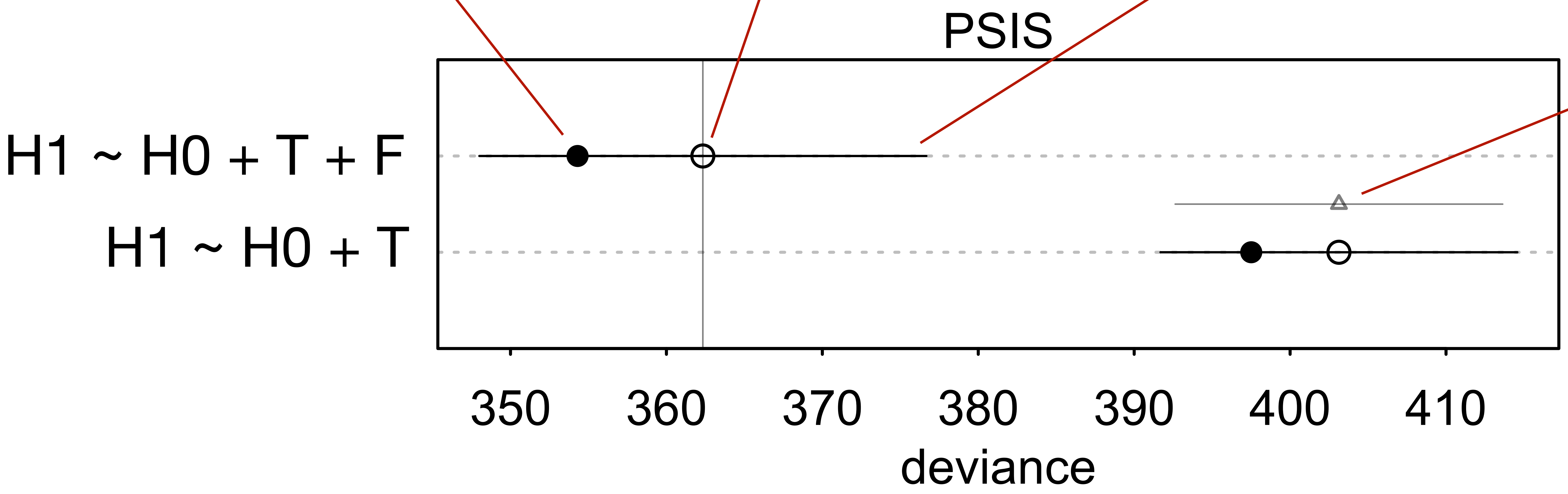


Wrong model wins at prediction



Score in sample

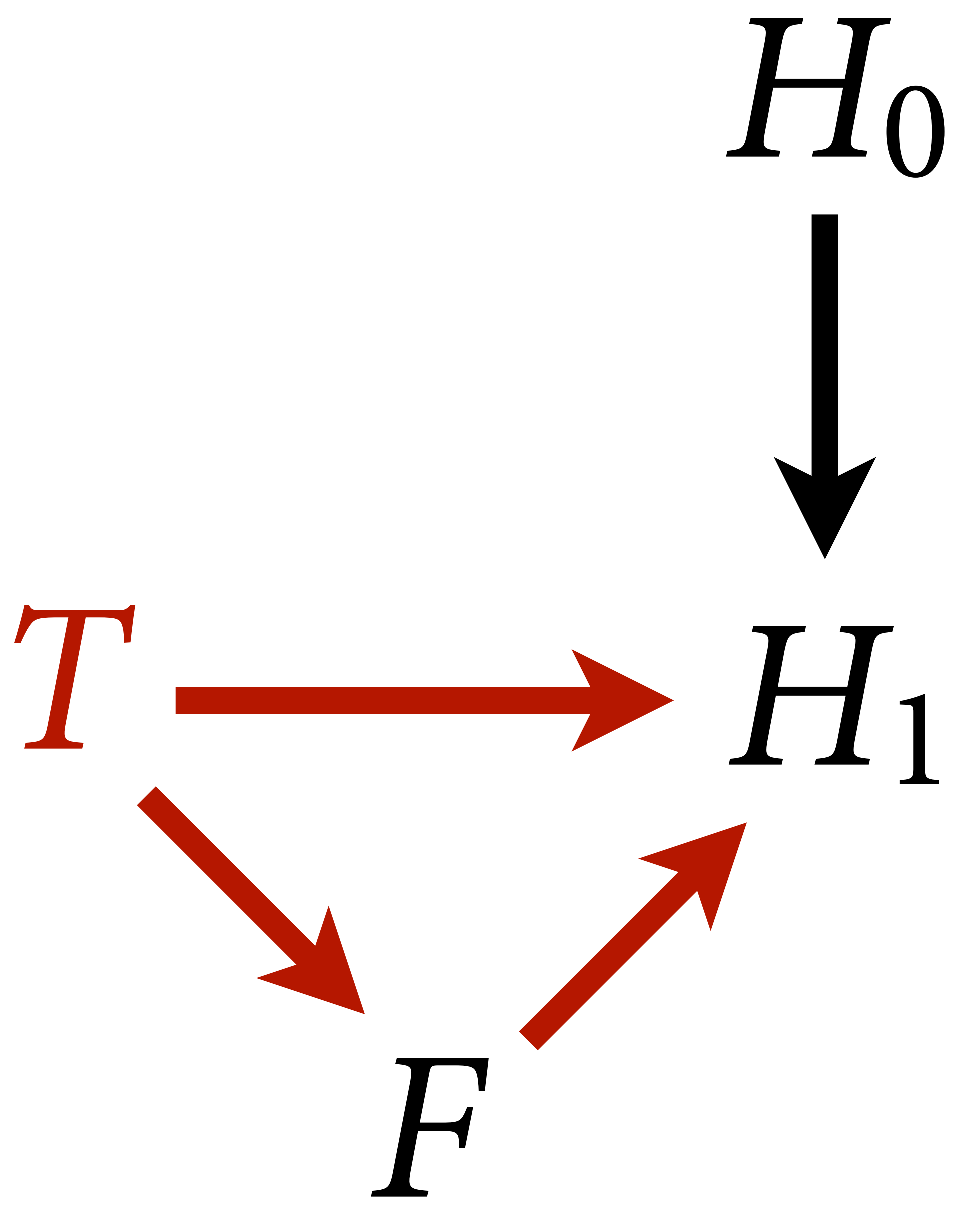
Score out of sample

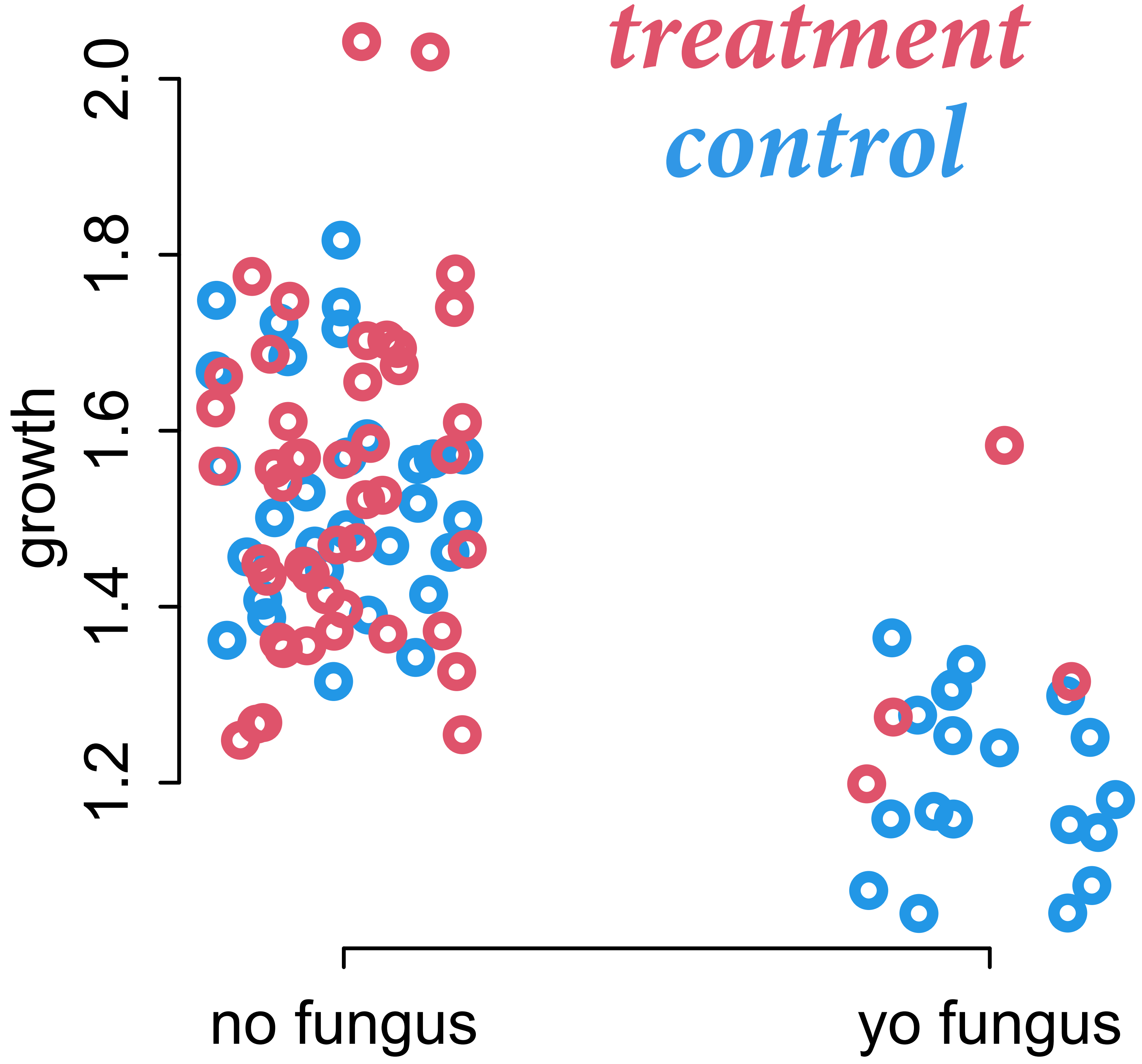
Standard error of score

PSIS contrast and standard error

Wrong model wins at prediction

Why does the wrong model win at prediction?





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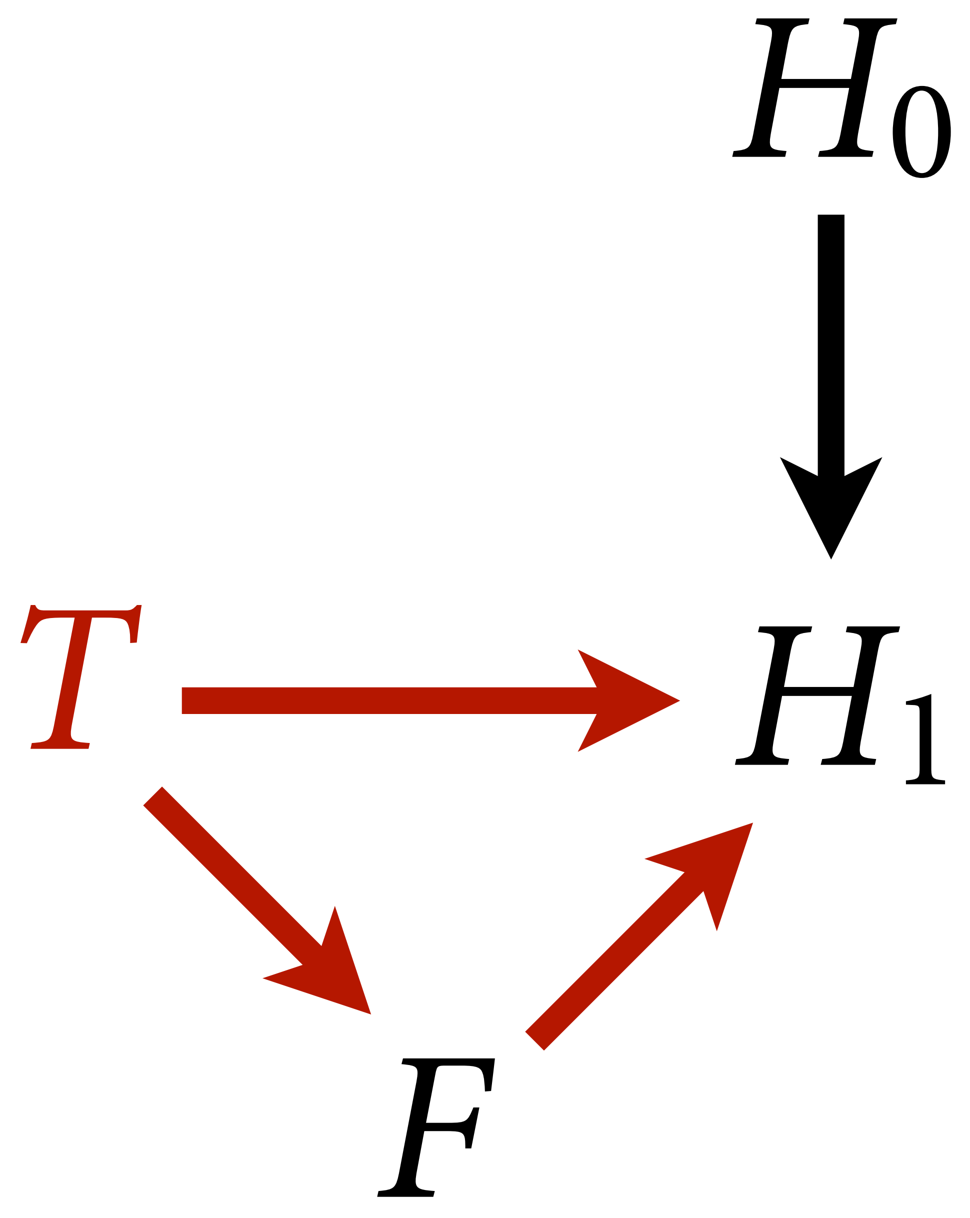
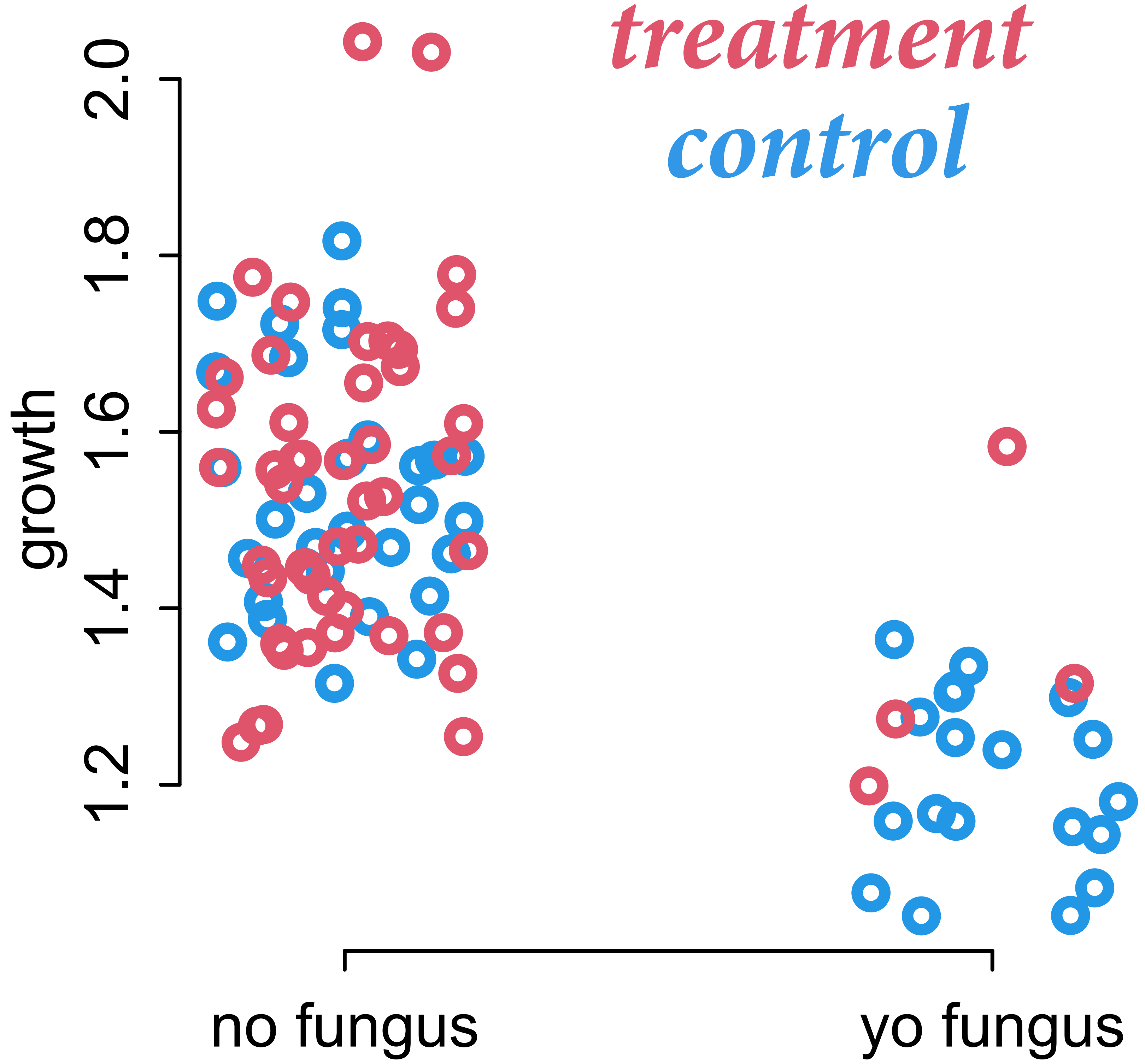
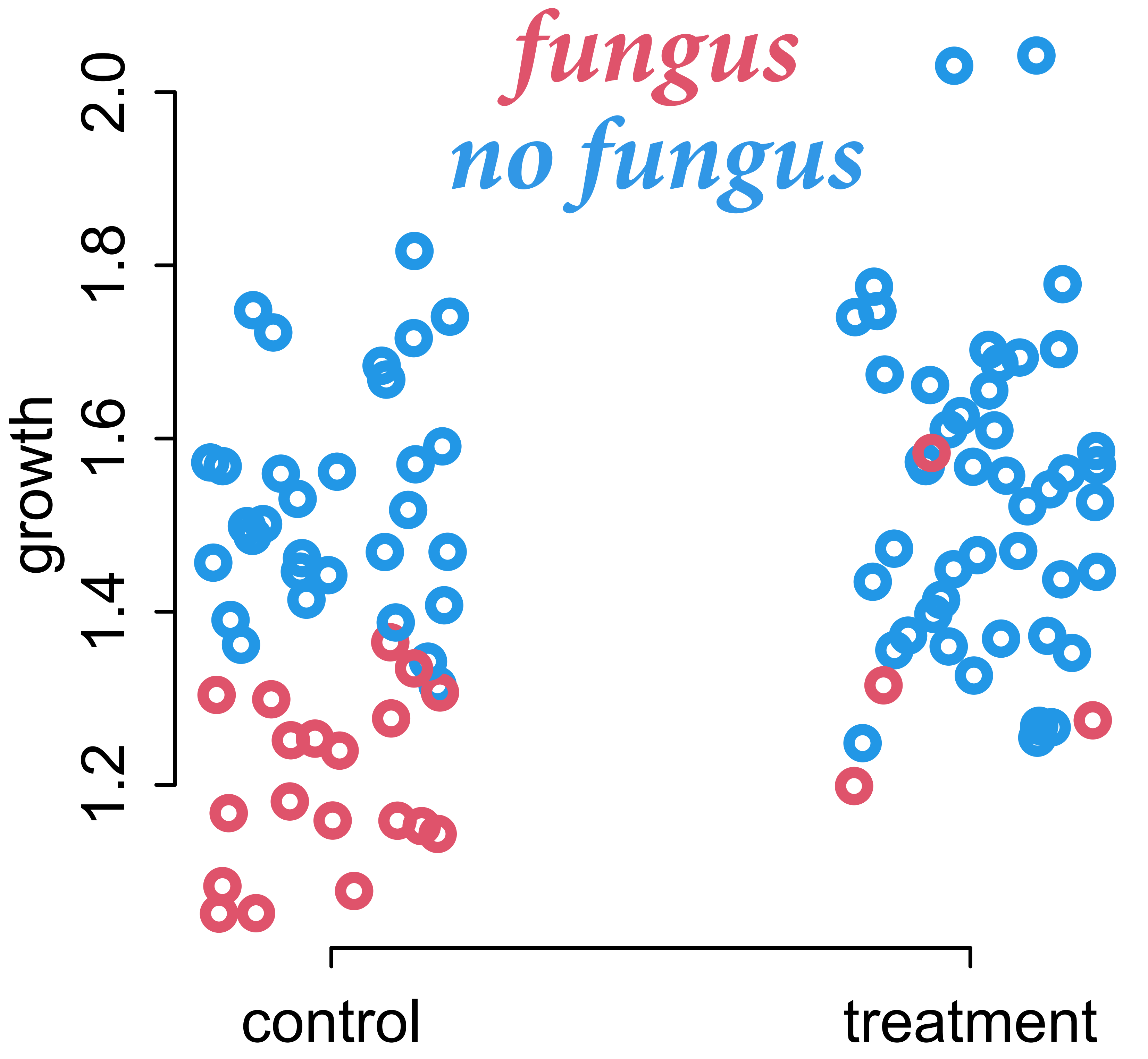






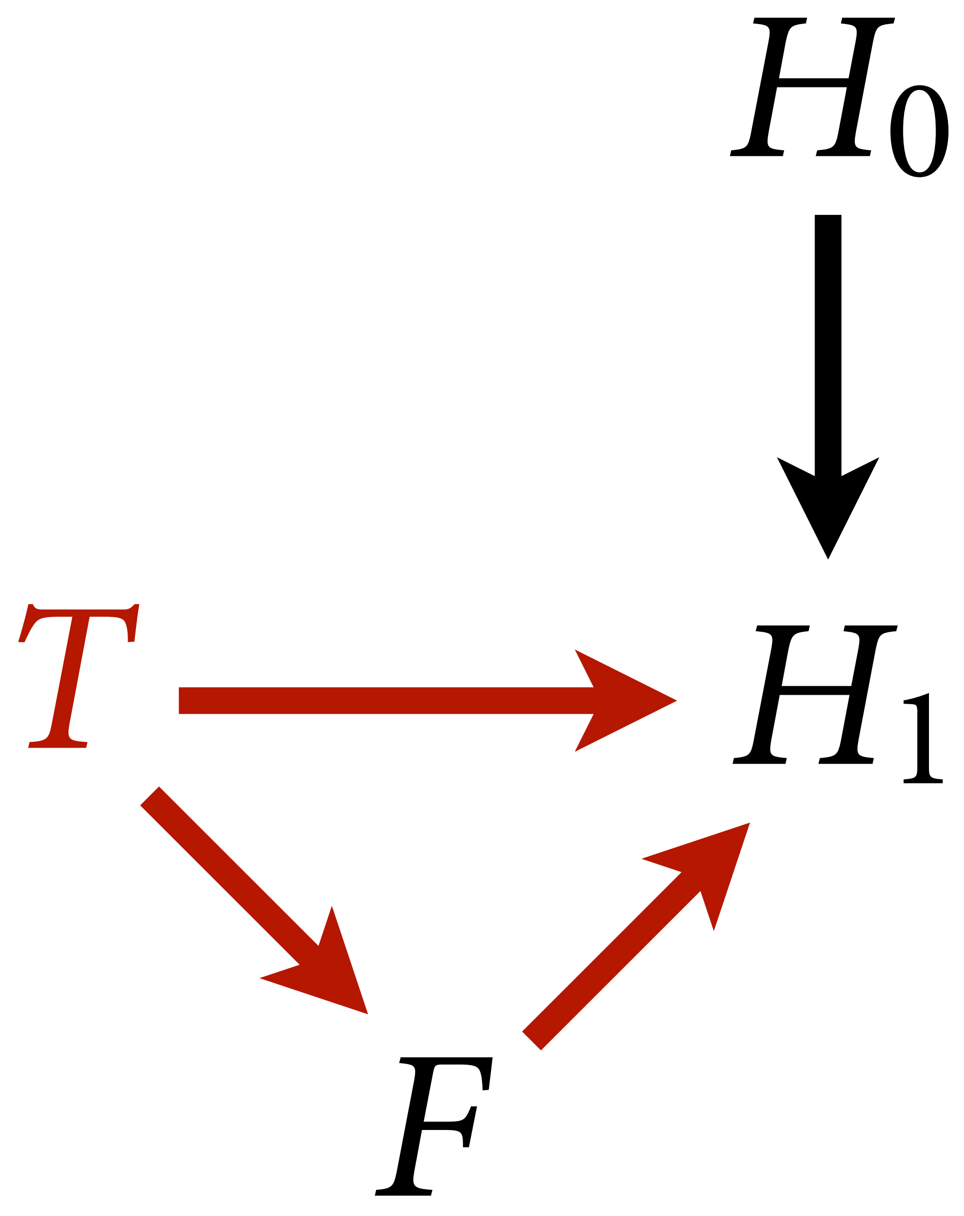
Fungus is in fact a better predictor than treatment

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



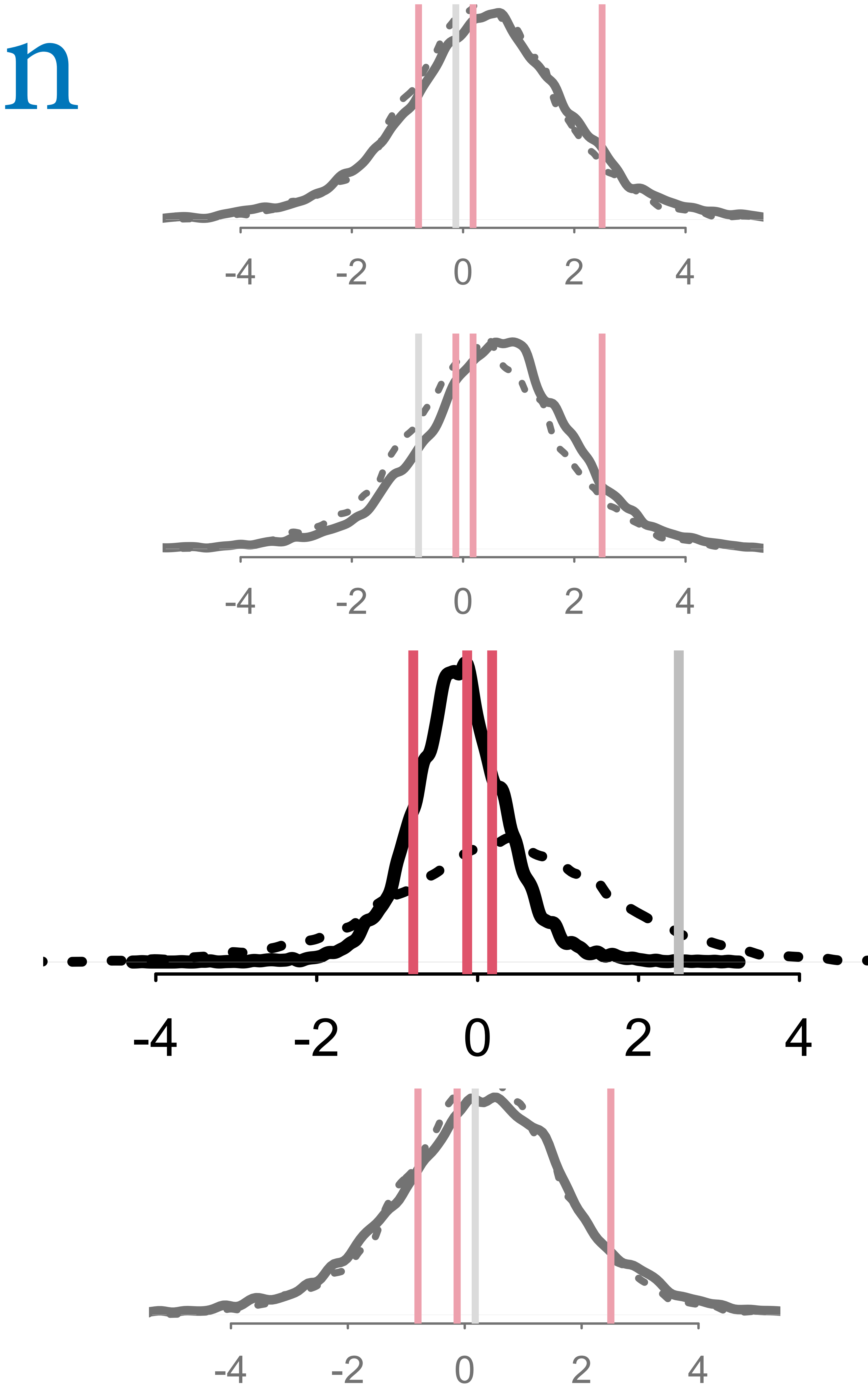
Outliers & Robust Regression

Some points are more influential than others

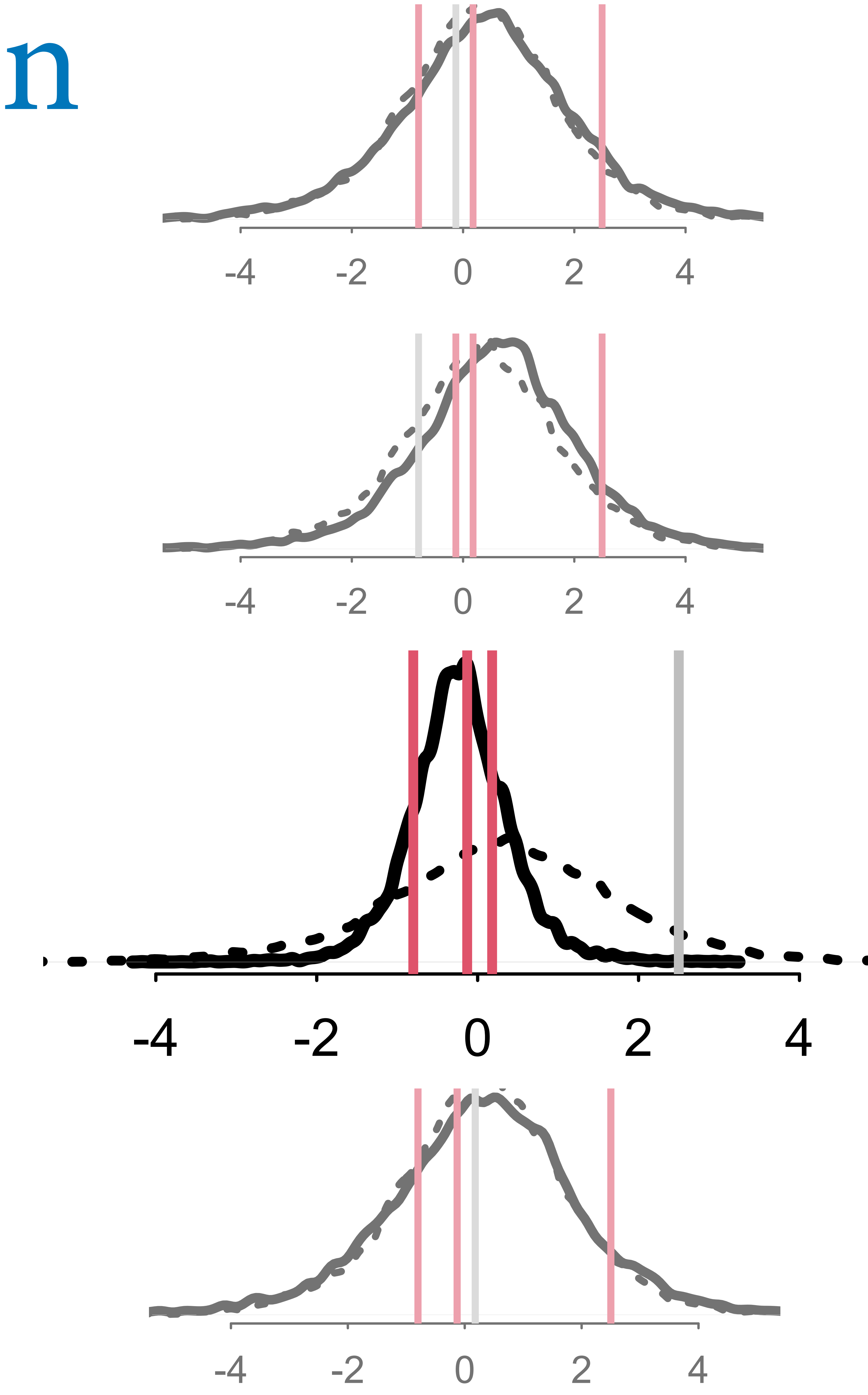
“Outliers”: Observations in the tails of predictive distribution

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)

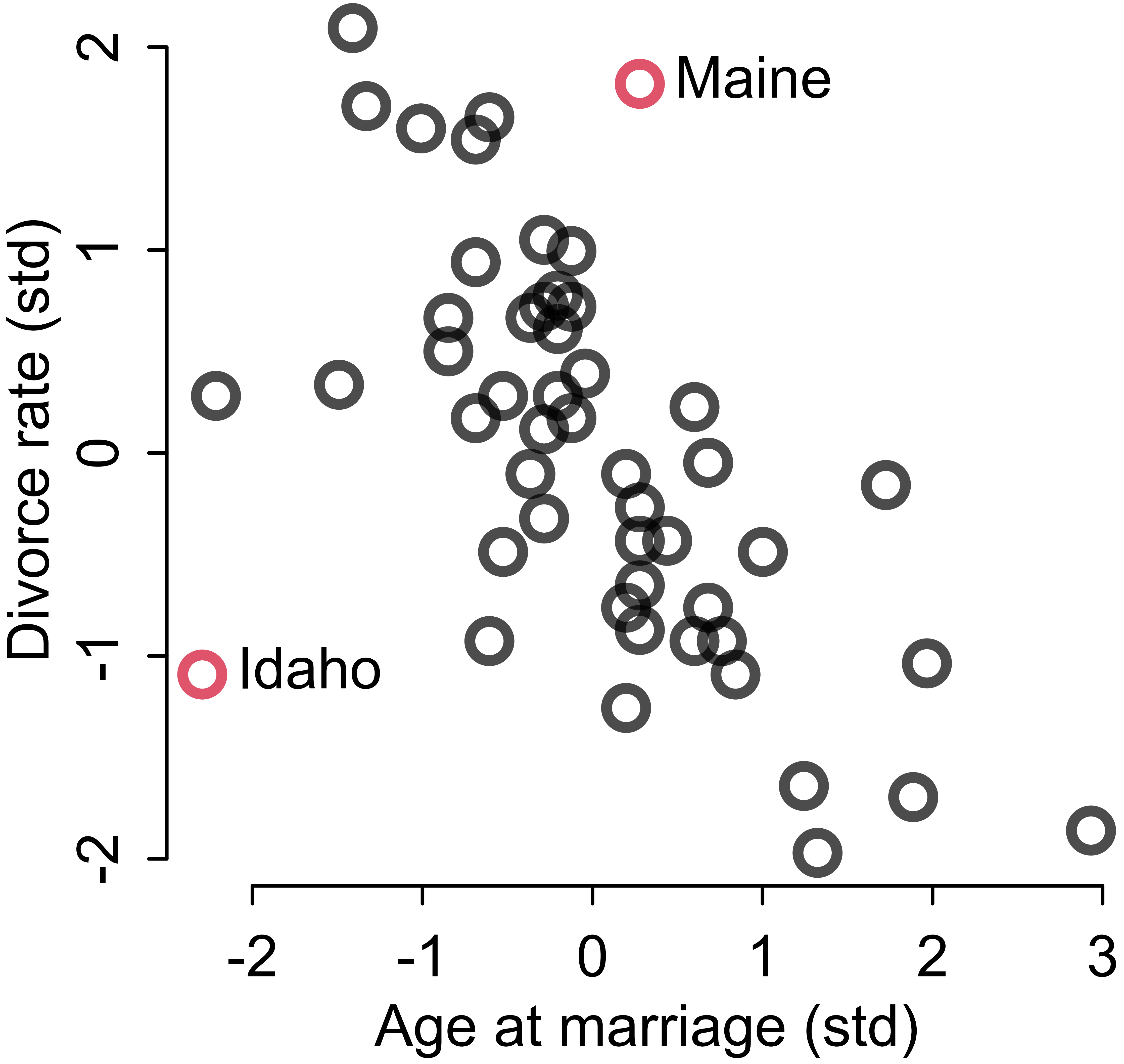
Outliers & Robust Regression

Divorce rate example

Maine and Idaho both highly unusual

Maine: high divorce for trend

Idaho: low divorce for trend

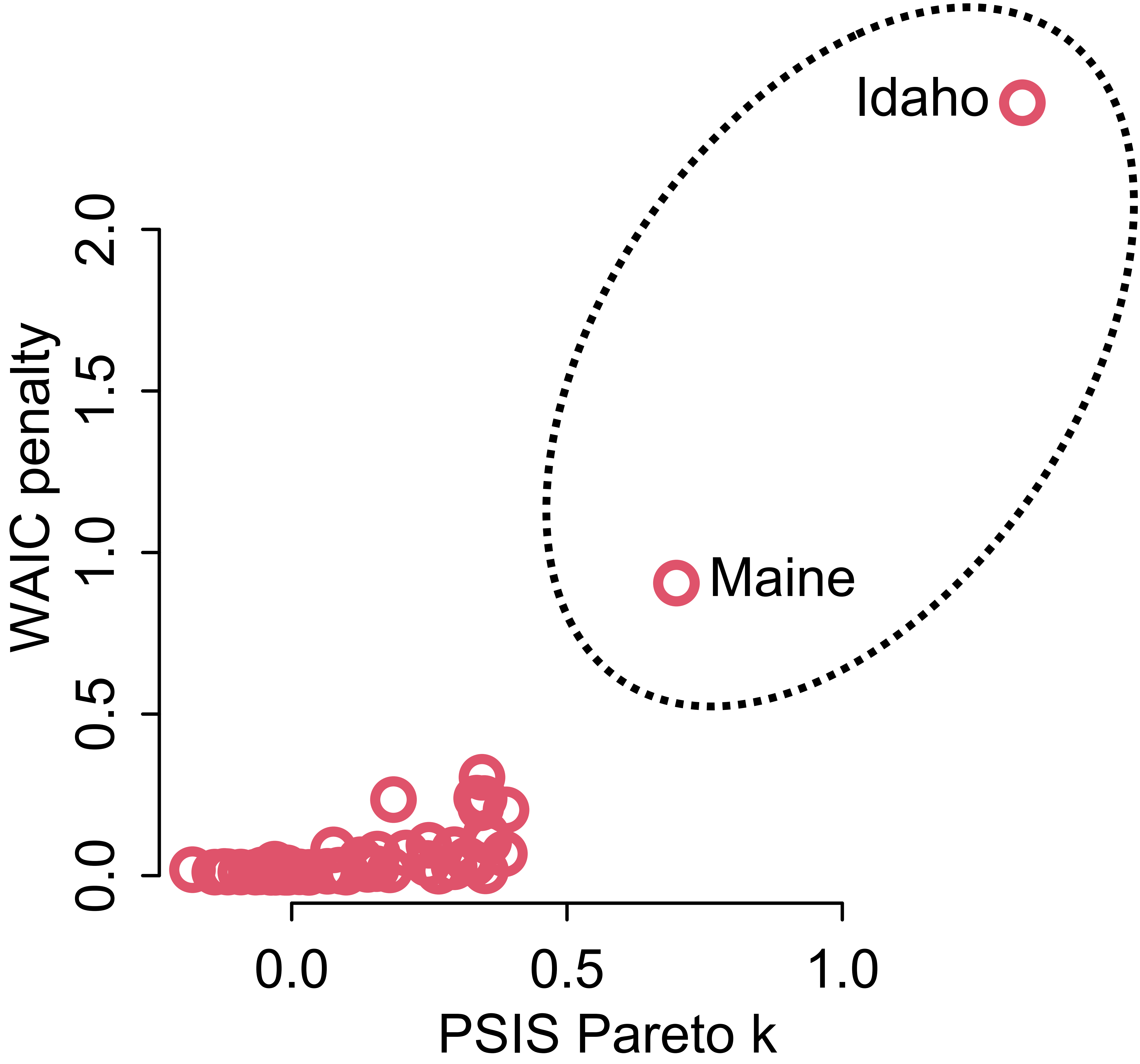


Outliers & Robust Regression

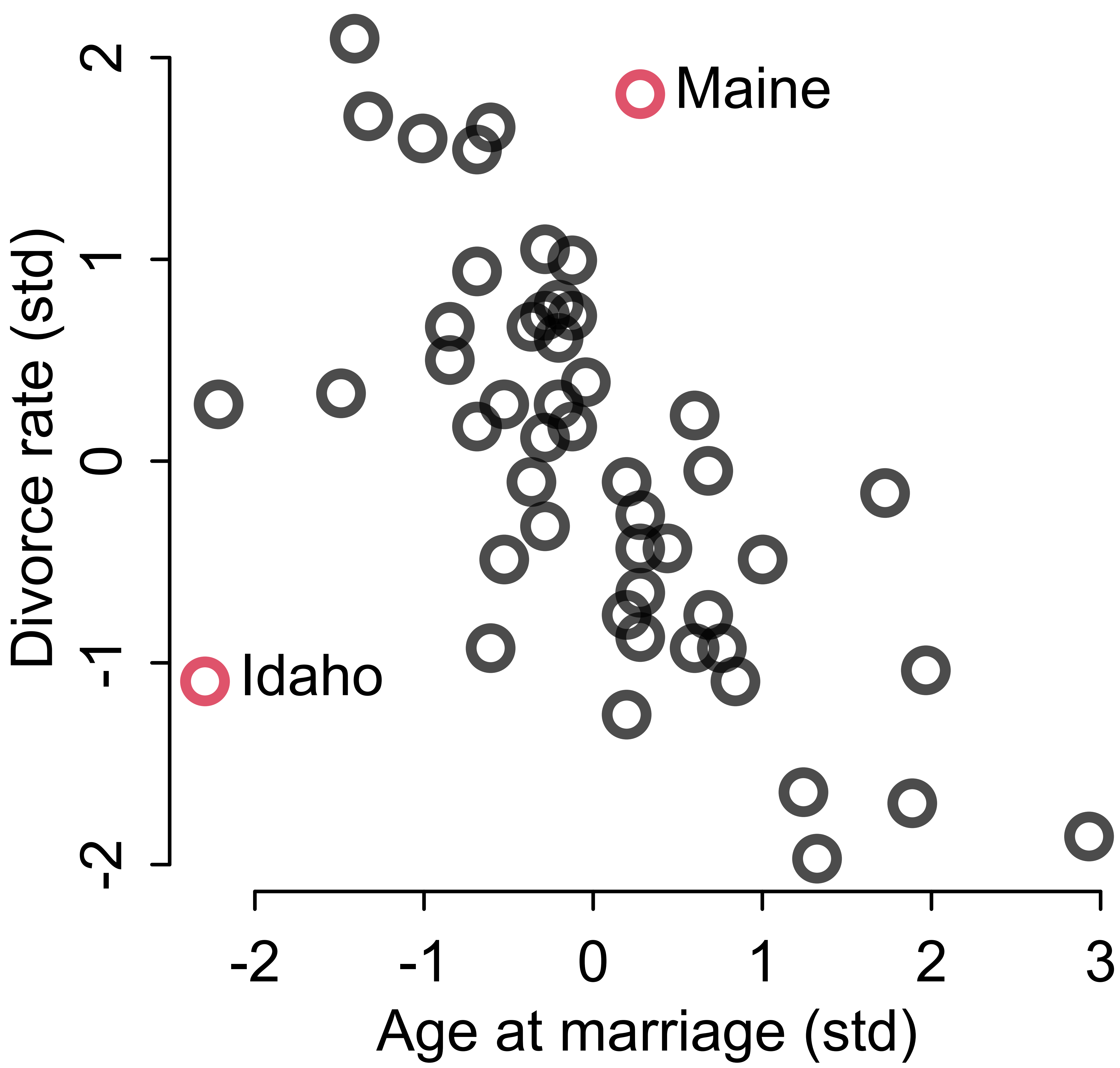
Quantify influence:

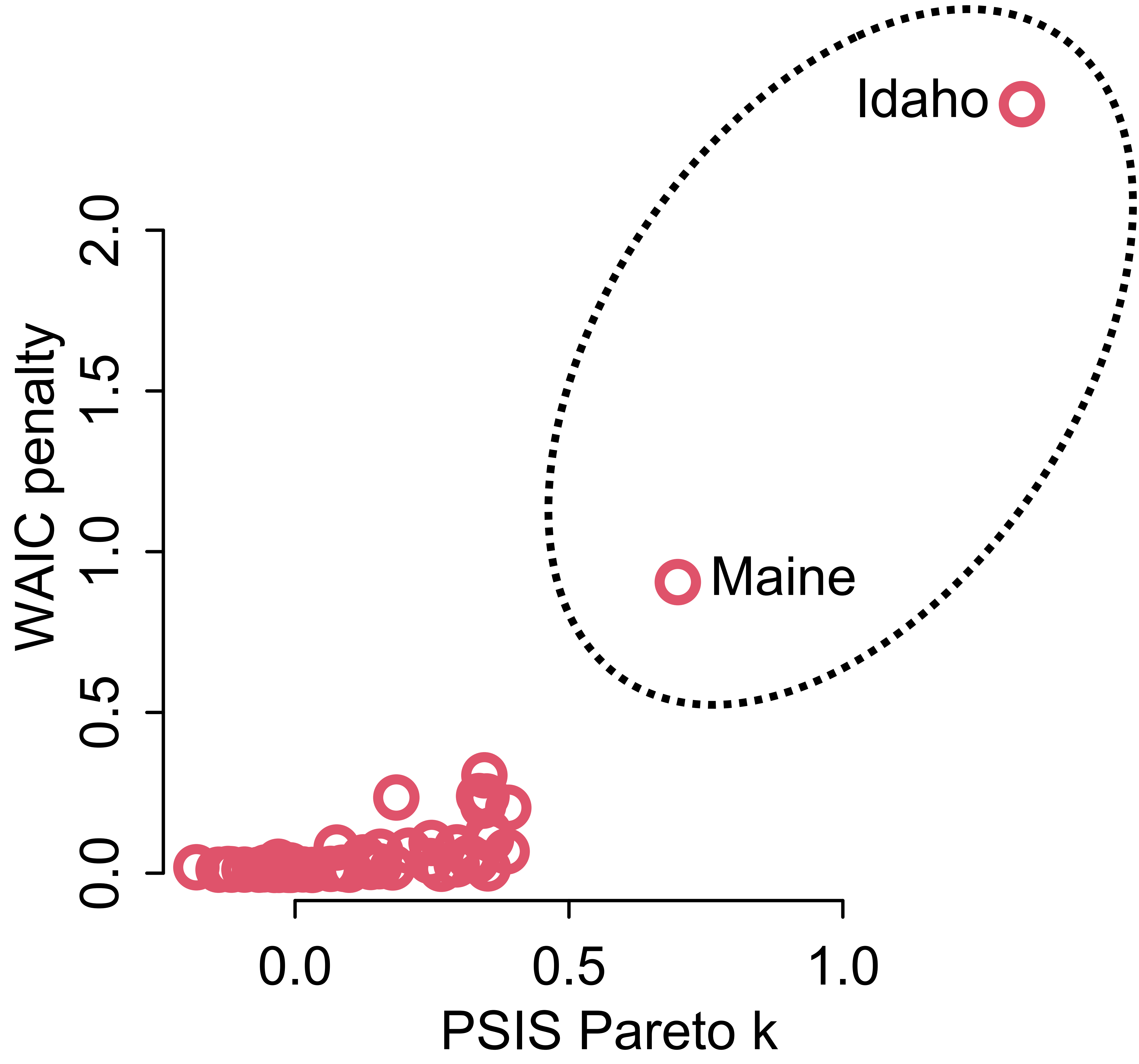
PSIS *k* statistic

WAIC penalty term ("effective number of parameters")

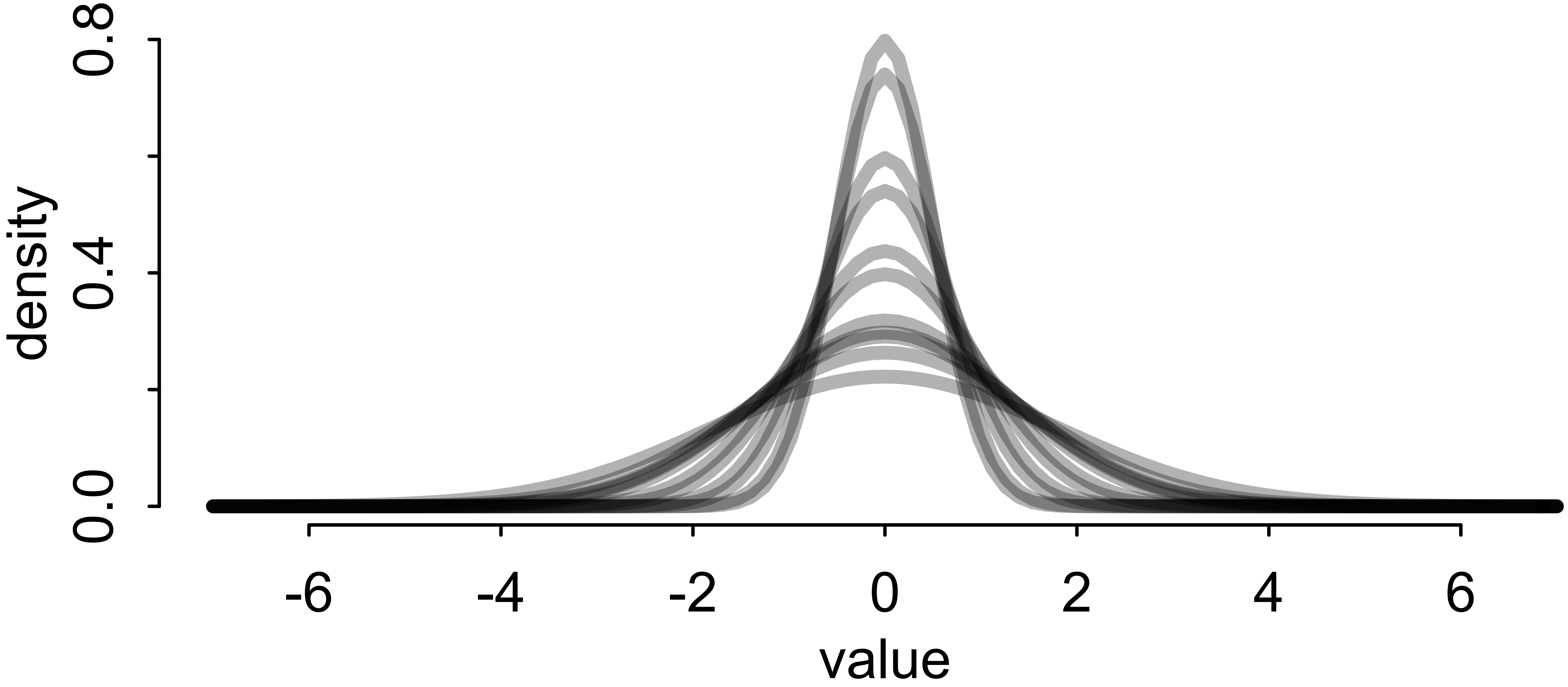


Outliers & Robust Regression

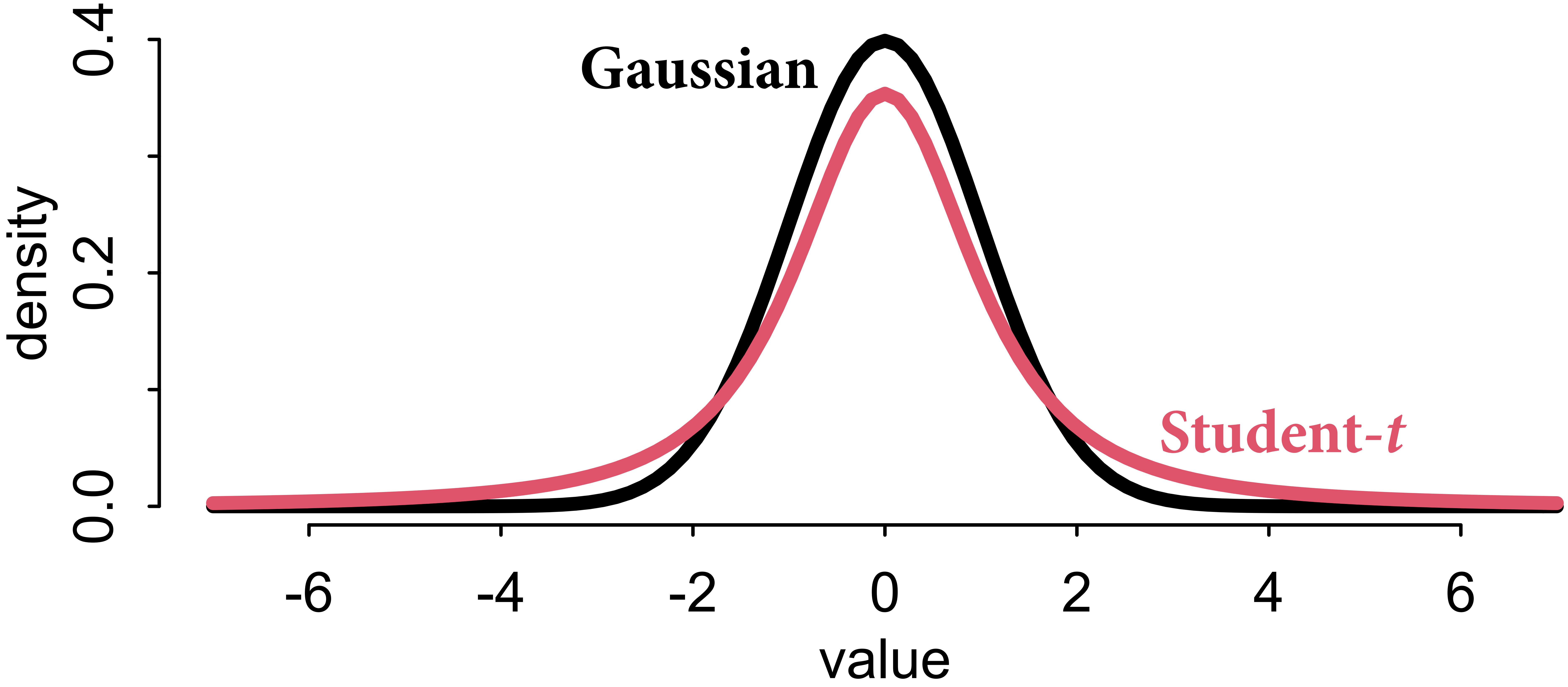




Mixing Gaussians



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 )
```

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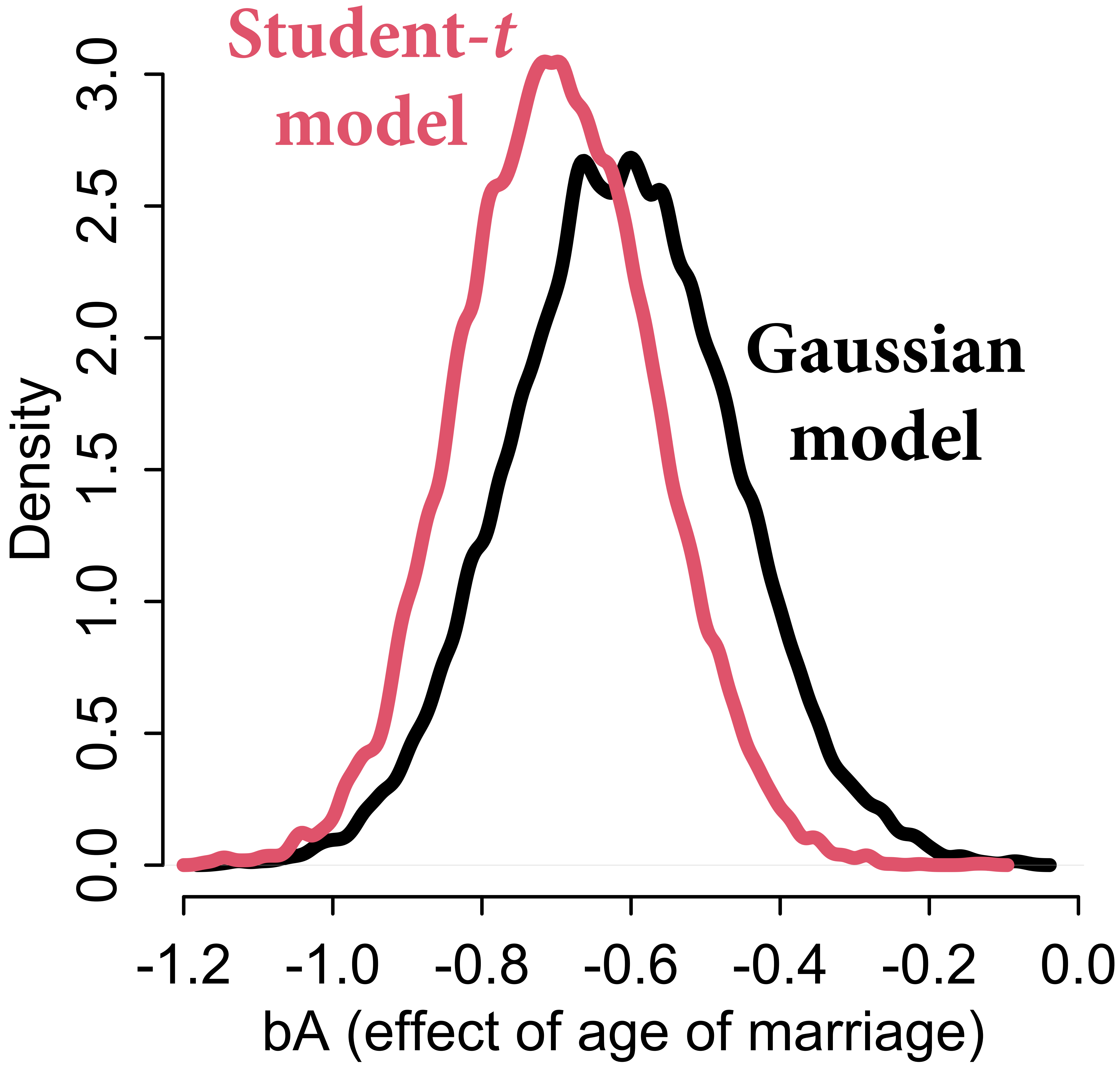
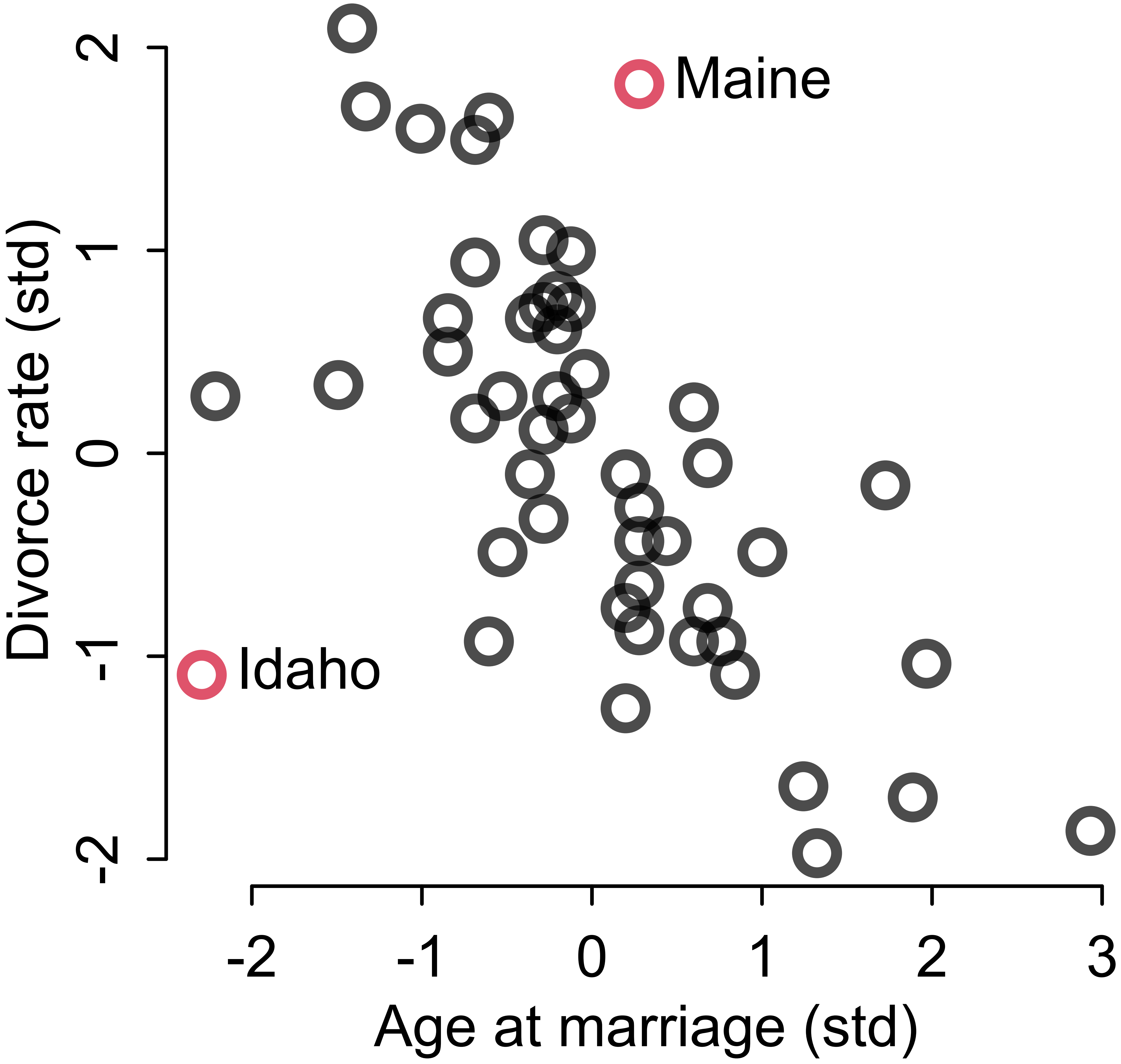



Robust Regressions

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



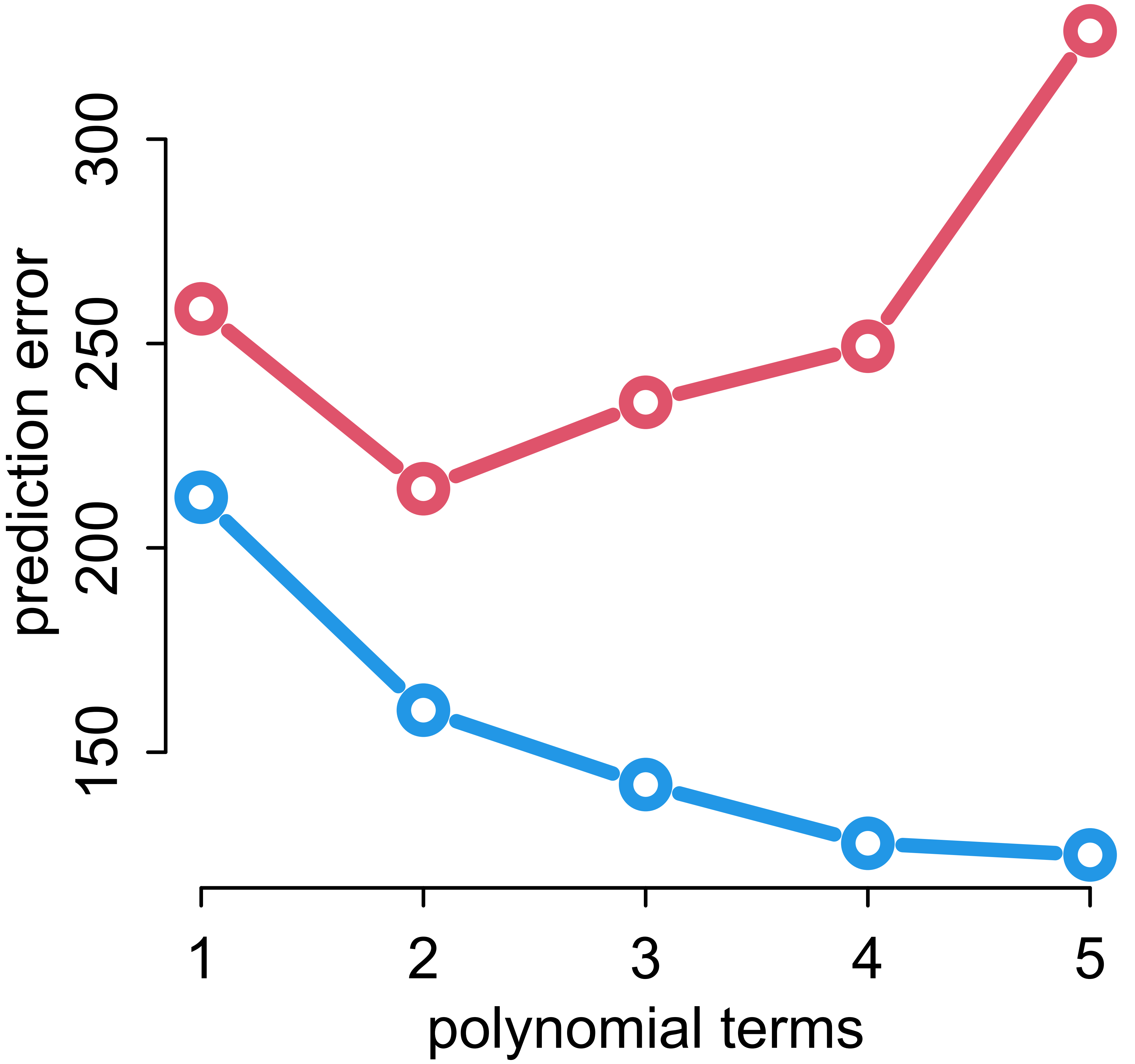
Problems of Prediction

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_2022`