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Bayesian Statistics and Data Analysis
Lecture 8b

Måns Magnusson
Department of Statistics, Uppsala University
Thanks to Aki Vehtari, Aalto University

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Section 1

Model assessment and selection

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Predictive performance

- Modeling complex phenomena with models that are simplified
  All models are wrong... but some are useful.

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  All models are wrong... but some are useful.
- True predictive performance is found out by using it to make predictions and comparing predictions to true observations
  - external validation

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- Modeling complex phenomena with models that are simplified
  All models are wrong... but some are useful.
- True predictive performance is found out by using it to make predictions and comparing predictions to true observations
  - external validation
- Expected predictive performance
  - approximates the external validation

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Goal of model evaluation

- Model choice is a (model-)decision-theoretic problem

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- Evaluate the utility of a model M for new unseen data $\tilde{y}$:

$$U = \int u(\tilde{y}) p_{\text{true}}(\tilde{y}) d\tilde{y} \,,$$

where $\tilde{y}$ is an unseen observation generated from the true data generating process $p_{\text{text}}(\tilde{y})$, and y are observed data and $u(\tilde{y})$ is a utility function.

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- The expectation is with respect to p_{true} (f in BDA3)

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- The expectation is with respect to p_{true} (f in BDA3)
- Choose the model function to maximize our utility

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Model choice utility

- Application specific utility/cost functions are important
  - eg. money, life years, quality adjusted life years, etc.

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- General utility: overall in the goodness of the predictive distribution
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$$\log p_M(y^{\text{rep}}|y)$$

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$$\log p_M(y^{\text{rep}}|y)$$

- We want the "best" model to explain the data

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Subsection 1

Measures of predictive accuracy

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(Bayesian) Points Prediction Accuracy

- Point residuals

$$e_i = y_i - E(\tilde{y}_i|y)\,,$$

where

$$E(\tilde{y}|y) = \int \tilde{y}_i p(\tilde{y}_i|y) d\tilde{y}\,,$$

i.e. the expected predicted value

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i.e. the expected predicted value

- Mean squared (prediction) error (MSE)

$$\text{MSE} = \frac{1}{n}\sum_i^n [y_i - E(\tilde{y}_i|y)]^2\,.$$

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Probabilistic predictions

- The log score (a local and proper scoring rule)*

$$\log p(y|\theta)$$

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Probabilistic predictions

- The log score (a local and proper scoring rule)*

$$\log p(y|\theta)$$

- The log predictive density (lpd)

$$\begin{aligned} \text{lpd} &= \log p(y|y) \\ &= \log \int p(y|\theta)p(\theta|y)d\theta \end{aligned}$$

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Probabilistic predictions

- The lpd is usually approximated with the log point predictive density (lppd or just lpd)

$$\begin{aligned}\text{lppd} &= \sum_{i}^{n} \log\, p(y_i|y) \\ &\approx \log p(y|y)\end{aligned}$$

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- Estimation using MCMC

$$\text{lppd} = \sum_{i}^{n} \log \left(\frac{1}{S} \sum_{s}^{S} p(y_i|\theta_s) \right)$$

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Subsection 2

Model selection

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Model selection

- Evaluate how model M generalizes to unseen data $\tilde{y}$ (the *expected log predictive density*):

$$\text{elpd}_M = \int \log p_M(\tilde{y}|y) p_{\text{true}}(\tilde{y}) d\tilde{y} \,,$$

  where $\tilde{y}$ is an unseen observation generated from the true data generating process $p_{\text{true}}(\tilde{y})$, and y are observed data.
- $\log p_M(\tilde{y}|y)$ is the log score (the utility of the model)

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- p_{true} is (almost always) unknown

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- The expectation is with respect to p_{true}
- p_{true} is (almost always) unknown
- The utility function is the log scoring rule.

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Section 2

Cross-validation

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Leave-one-out cross-validation (LOO-CV)

- Evaluate how model M *generalizes* to unseen data (the *expected log predictive density*):

$$\text{elpd}_M = \int \log p_M(\tilde{y}_i|y) p_{\text{true}}(\tilde{y}_i) d\tilde{y}_i \,,$$

where $\tilde{y}_i$ is an unseen observation generated from the true data generating process $p_{\text{true}}(\tilde{y}_i)$, and y are observed data.

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Leave-one-out cross-validation (LOO-CV)

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  where $\tilde{y}_i$ is an unseen observation generated from the true data generating process $p_{\text{true}}(\tilde{y}_i)$, and y are observed data.
- Can we approximate $p_{\text{true}}(\tilde{y}_i)$?

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Leave-one-out cross-validation (LOO-CV)

- Approximate $p_{\text{true}}(\tilde{y}_i)$ with data y

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Leave-one-out cross-validation (LOO-CV)

- Approximate $p_{\text{true}}(\tilde{y}_i)$ with data y
- Hold out observation i and try to predict y_i based on $\mathbf{y}_{-i}$
- Estimation of elpd_M using leave-one-out cross-validation

$$\begin{aligned}\text{elpd}_{\text{loo}} &= \sum_{i=1}^{n} \log p_M(y_i|\mathbf{y}_{-i}) \\ &= \sum_{i=1}^{n} \log \int p_M(y_i|\theta)p(\theta|\mathbf{y}_{-i})d\theta\end{aligned}$$

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- Analogy: Monte Carlo approximation using our data
- Similar to jack-knife resampling

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- Analogy: Monte Carlo approximation using our data
- Similar to jack-knife resampling
- The elpd, lpd and efficient number of parameters (p_{loo})

$$\text{elpd}_{\text{loo}} = \text{lpd} + p_{\text{loo}}$$

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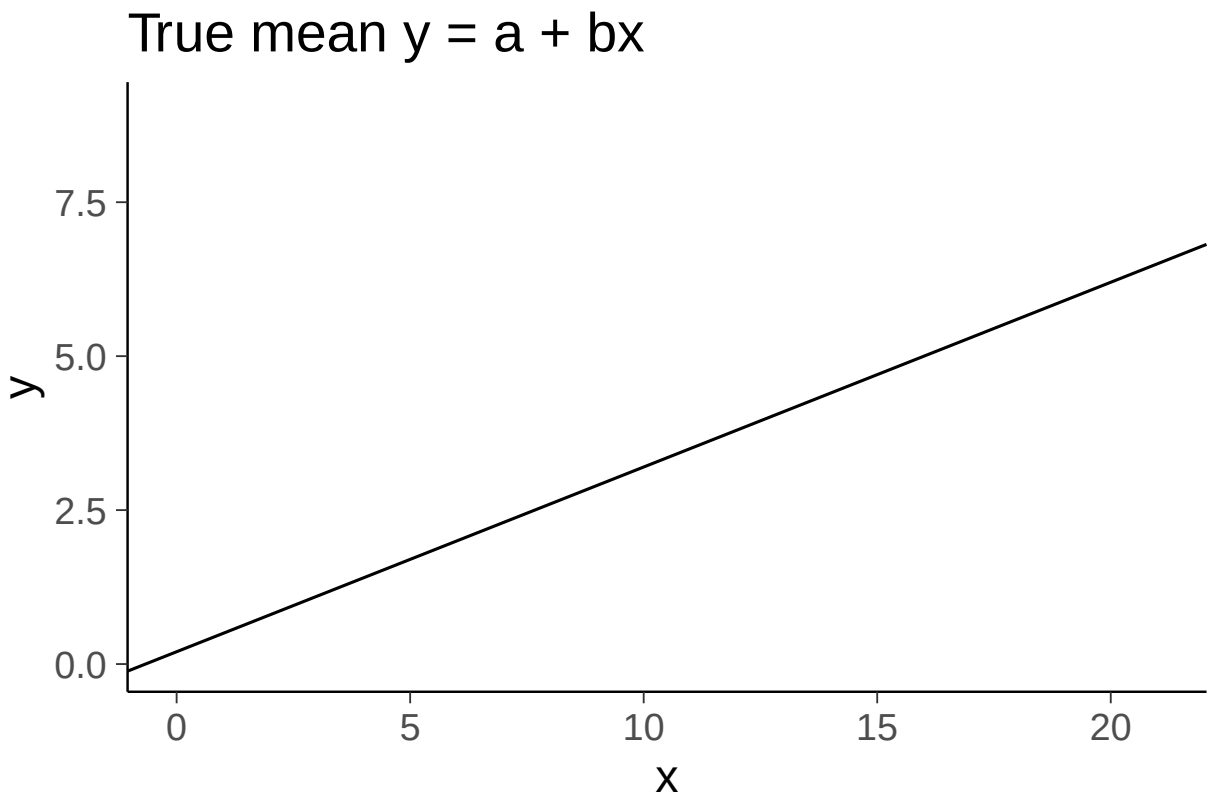

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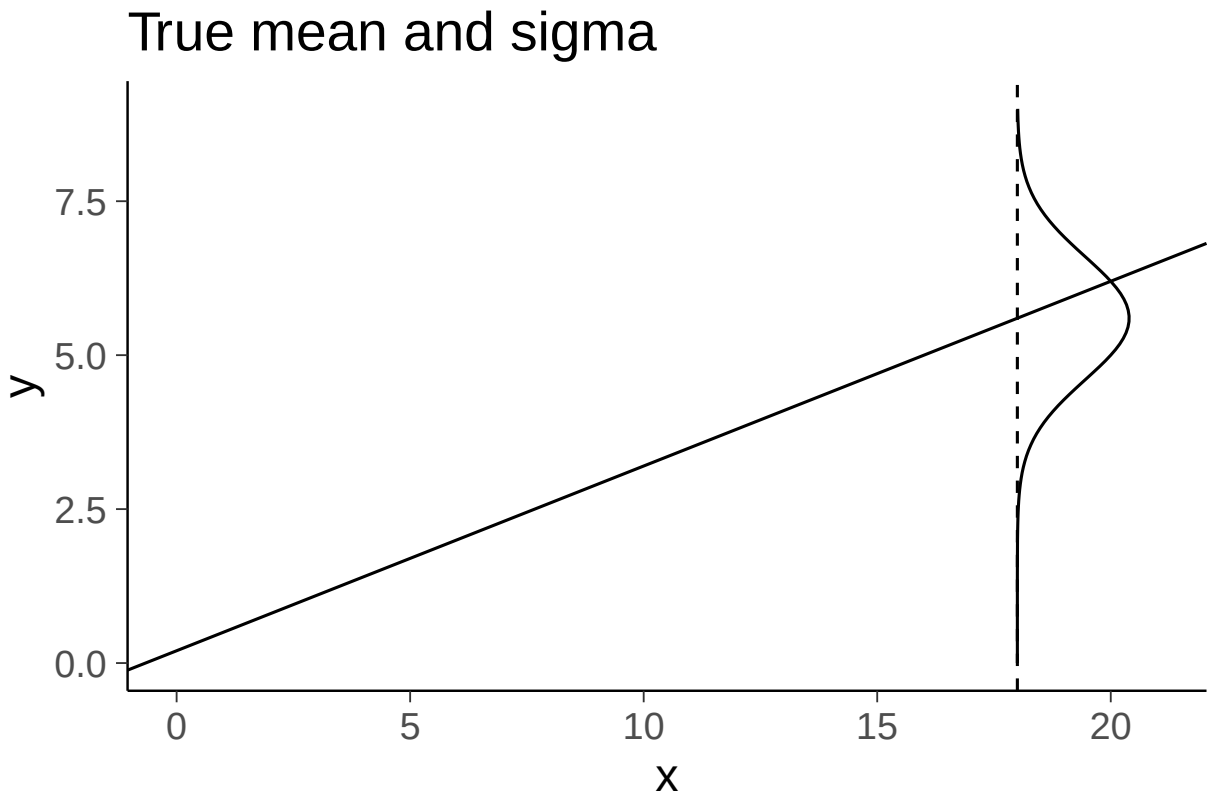

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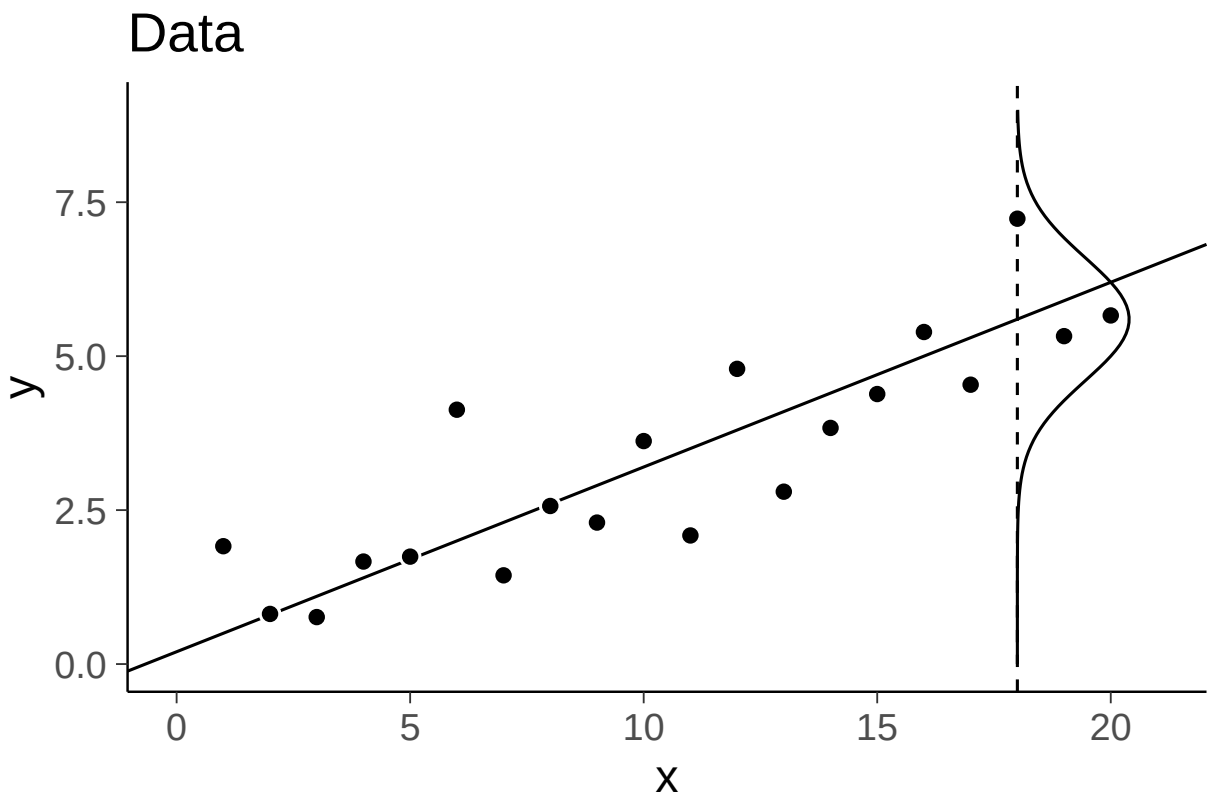

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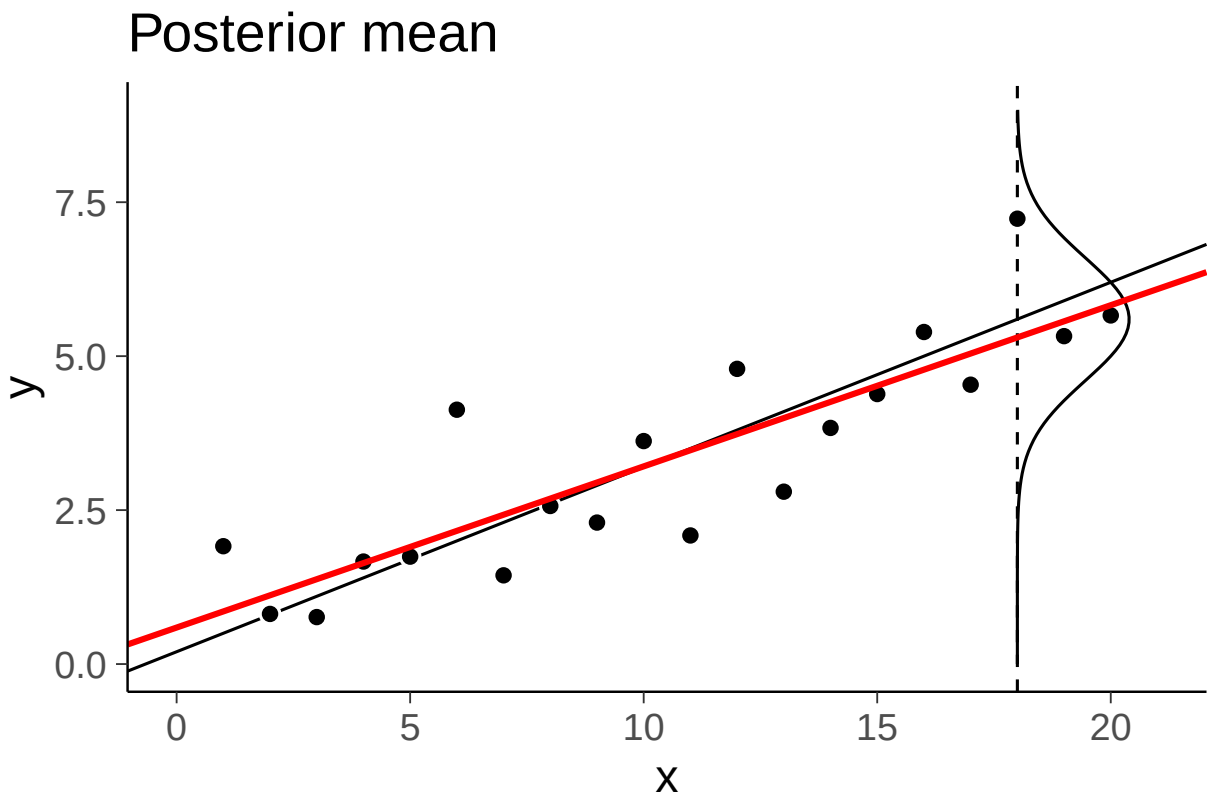

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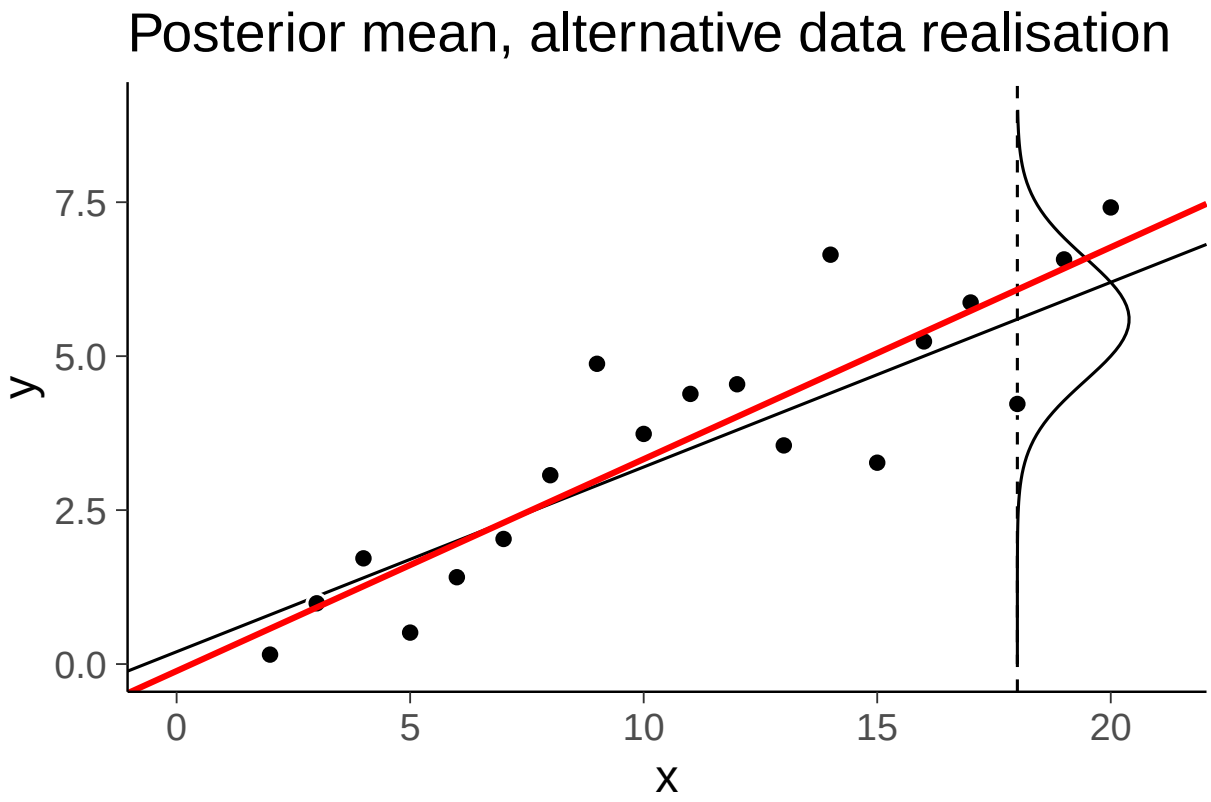

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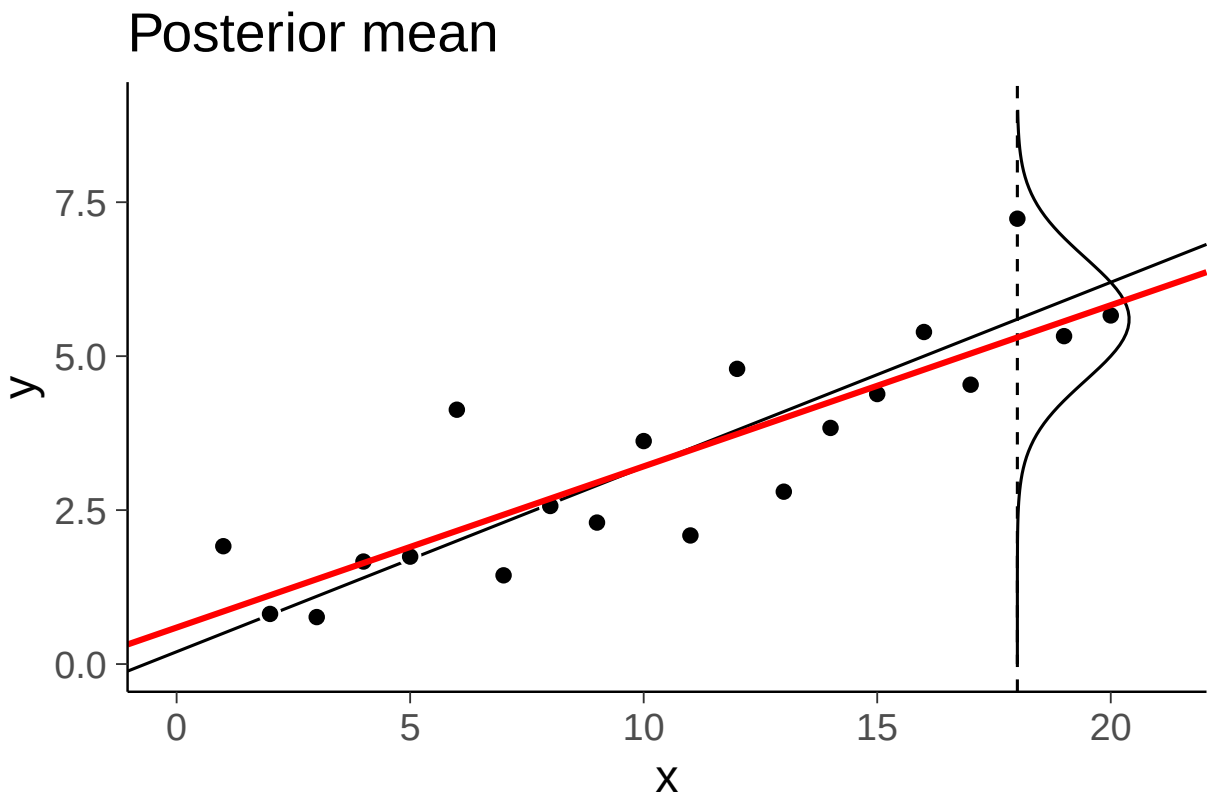

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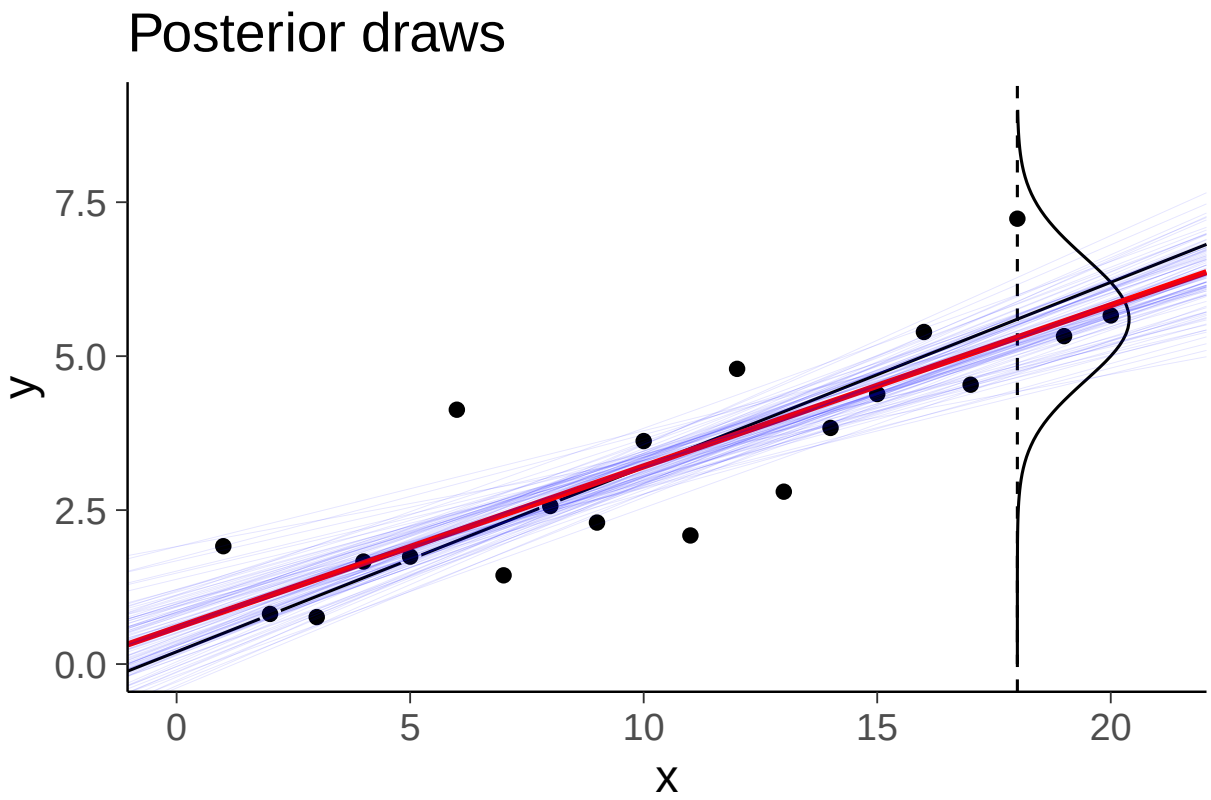

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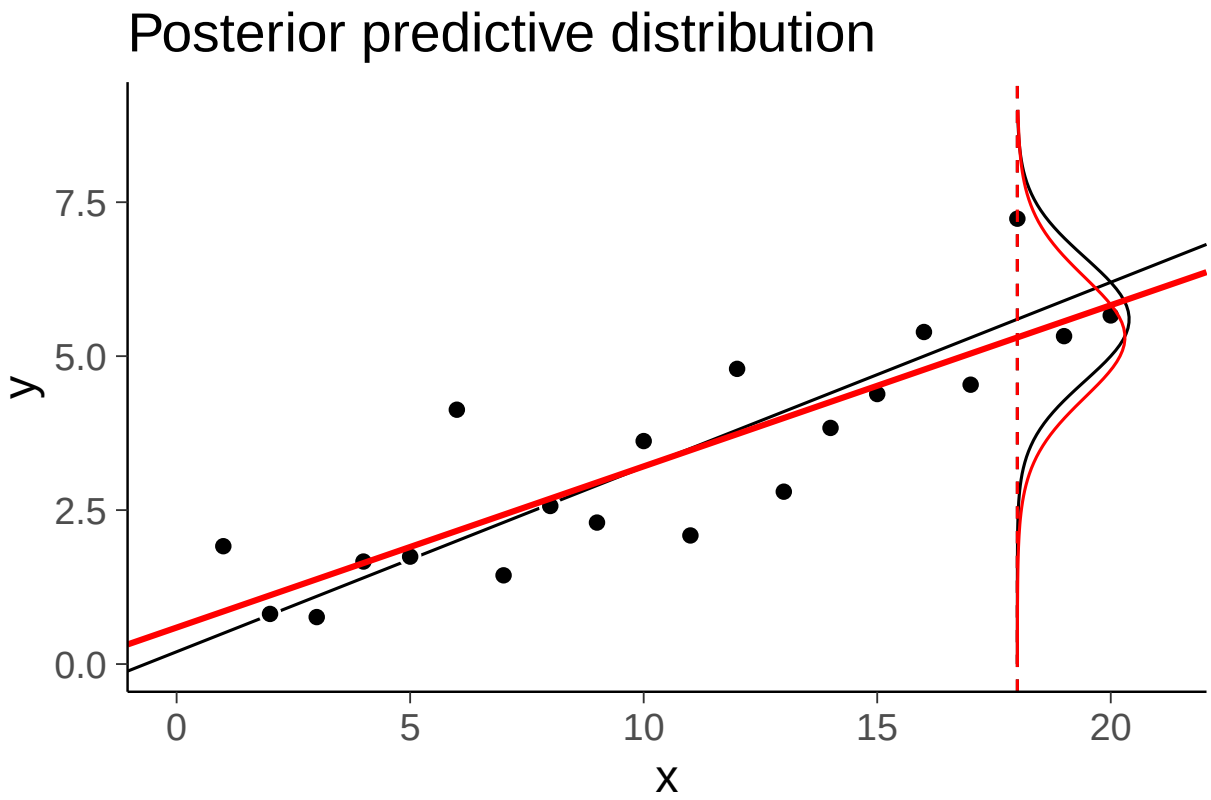

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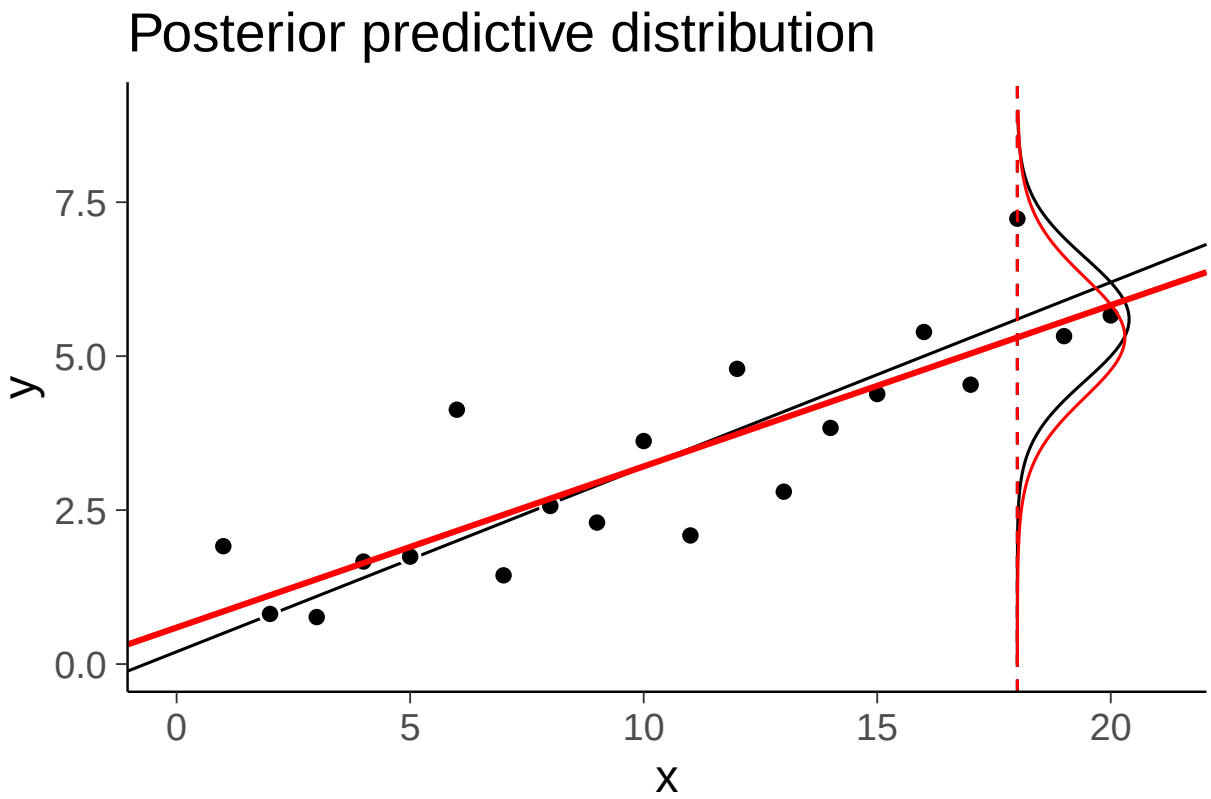

$$p(\tilde{y}|\tilde{x} = 18, x, y) = \int p(\tilde{y}|\tilde{x} = 18, \theta) p(\theta|x, y) d\theta$$

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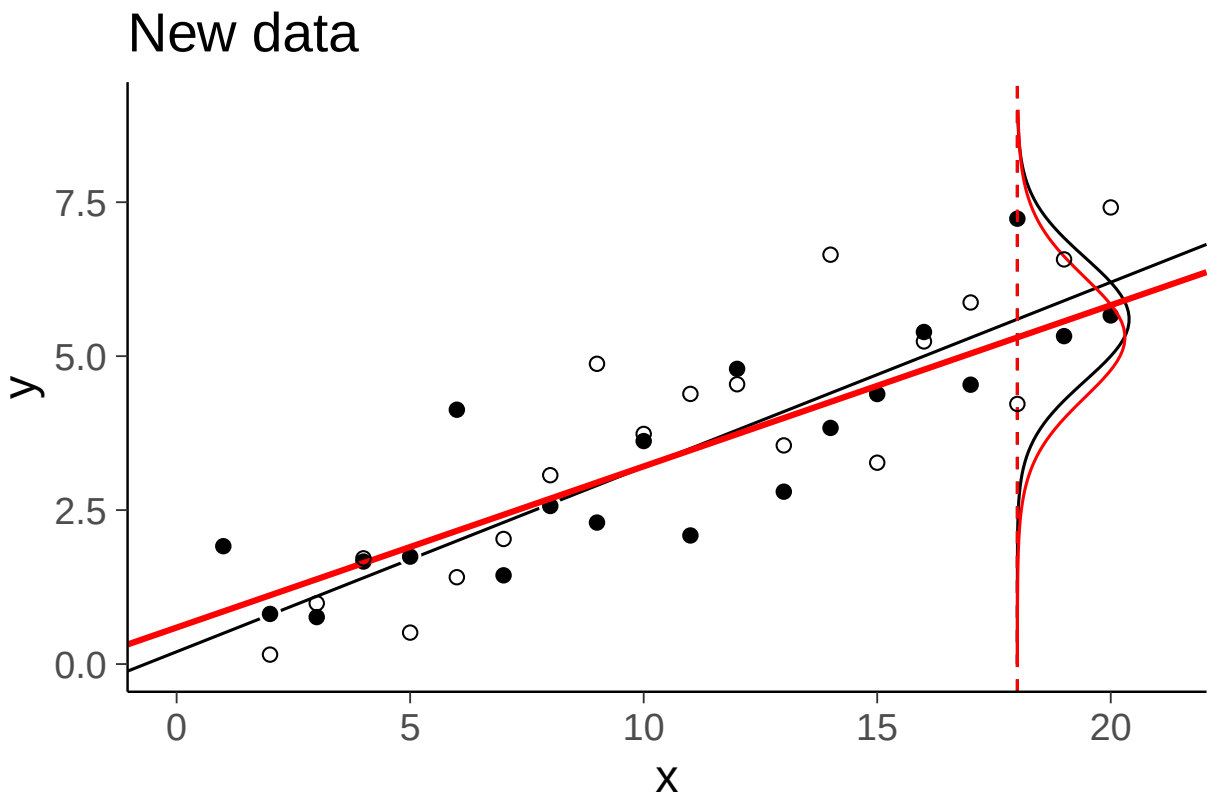

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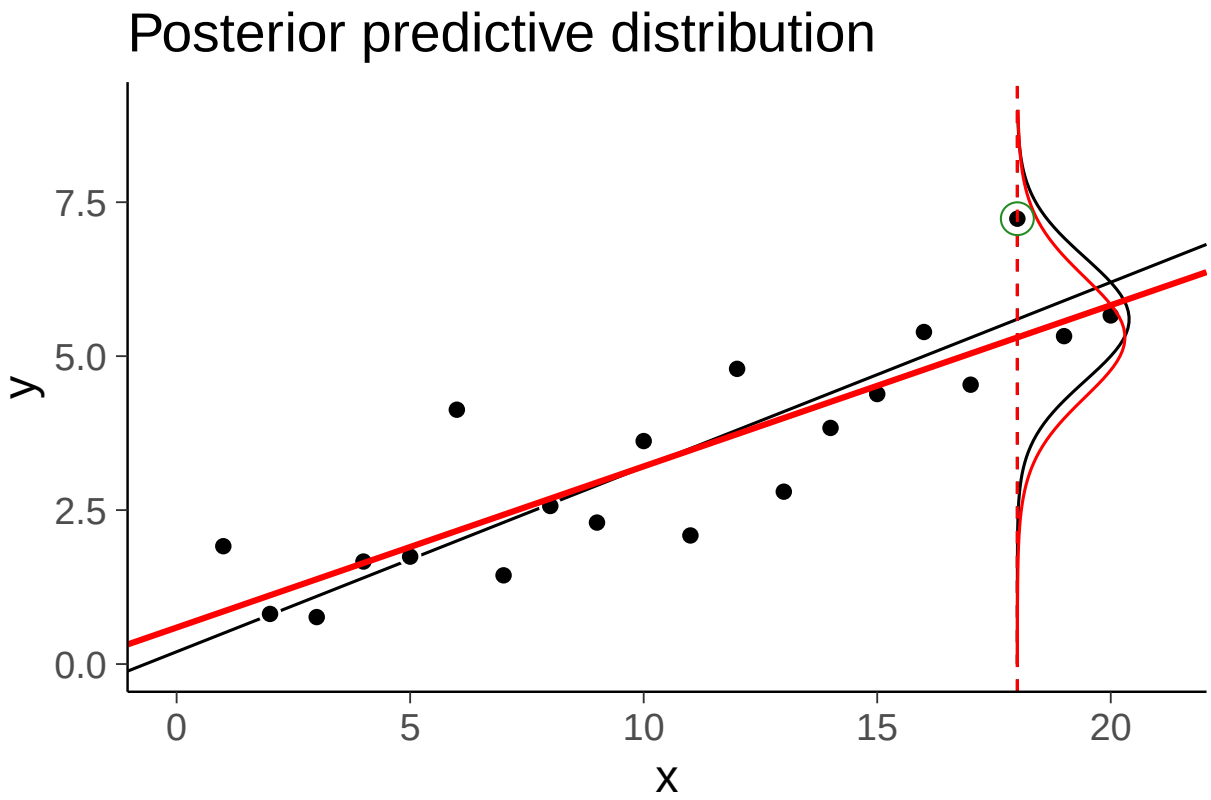

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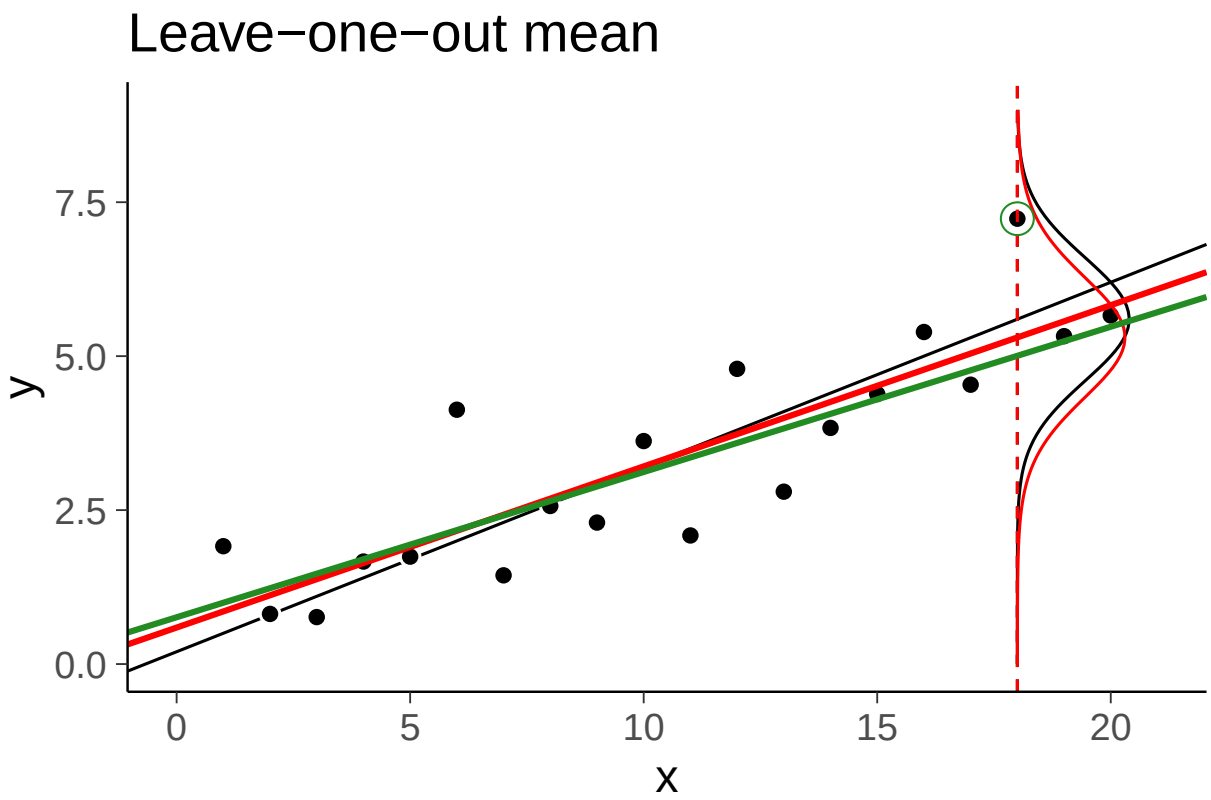

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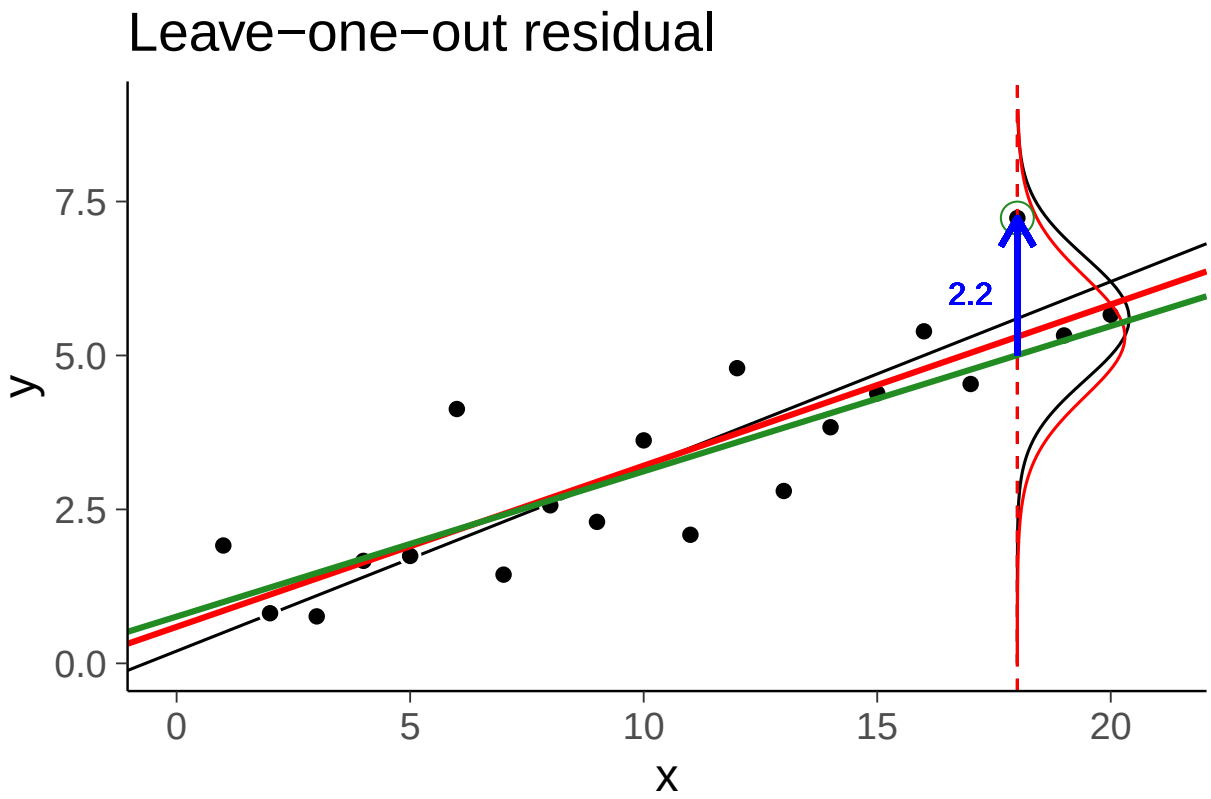

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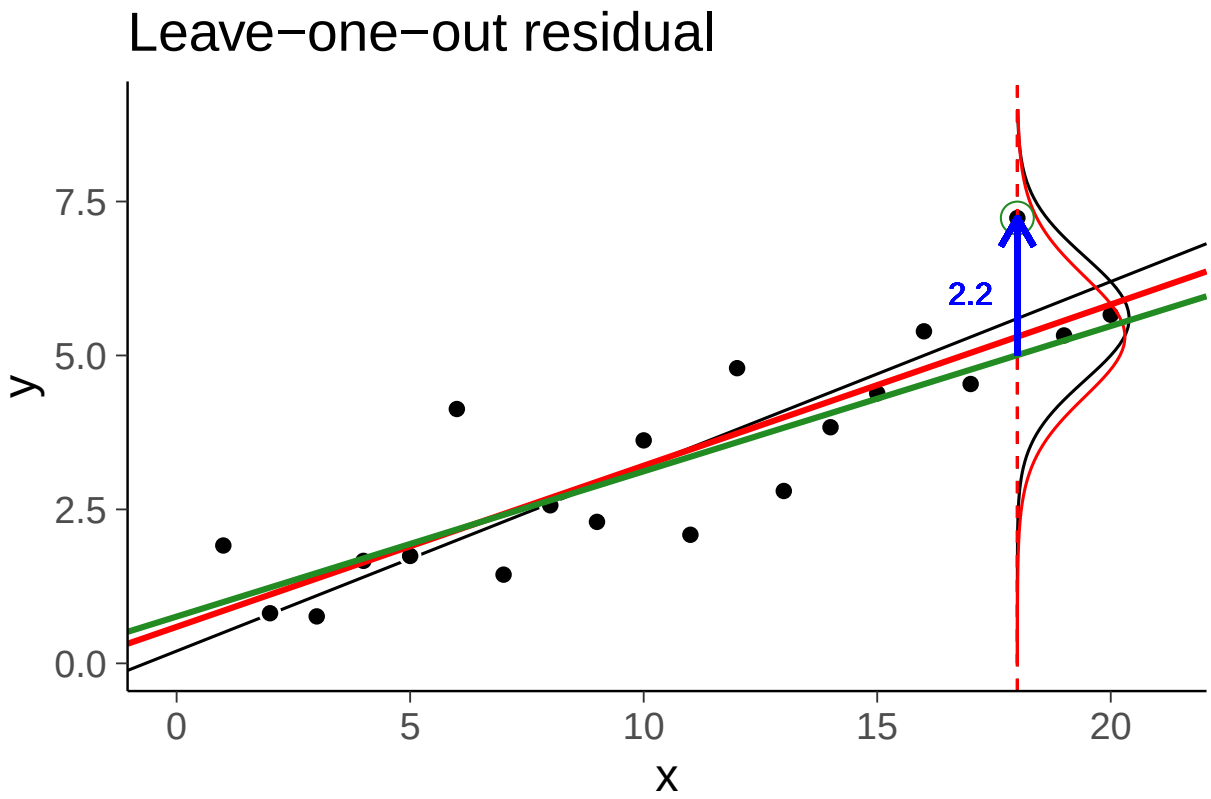

$$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$$

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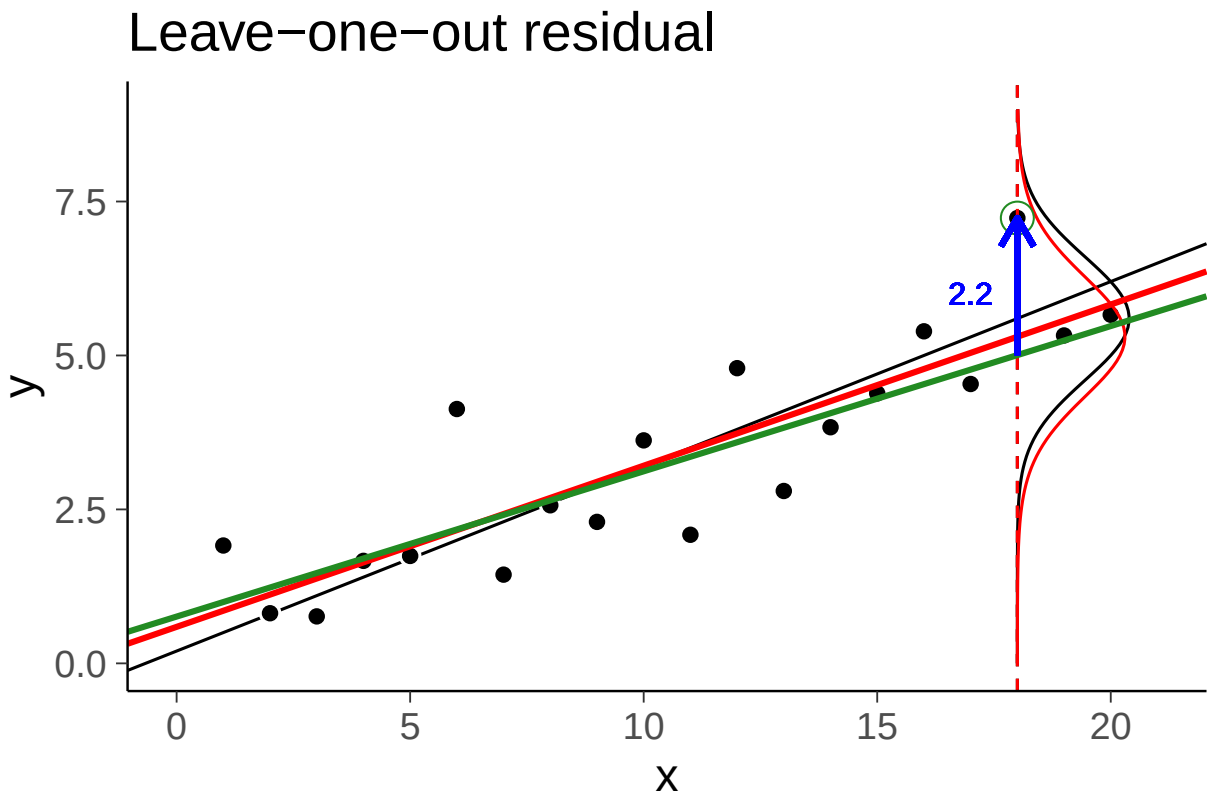

$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$

Can be use to compute, e.g., RMSE, R^2, 90% error

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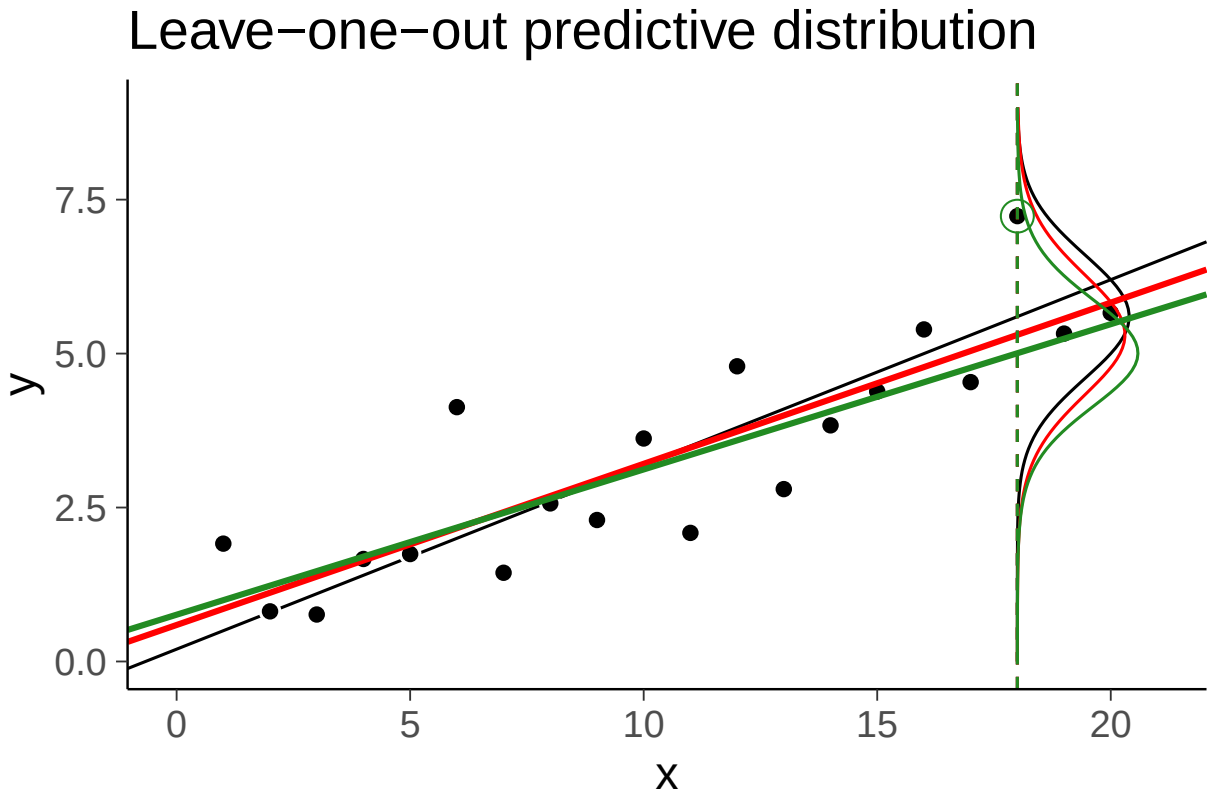

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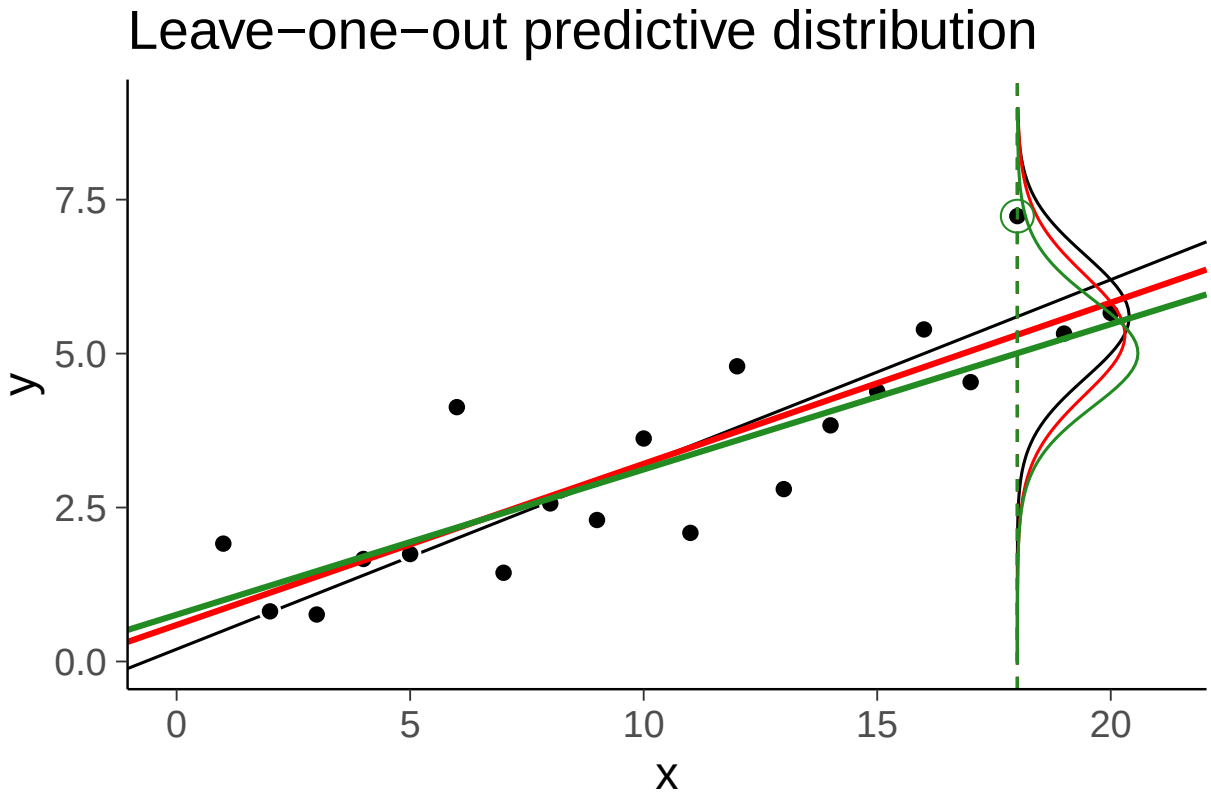

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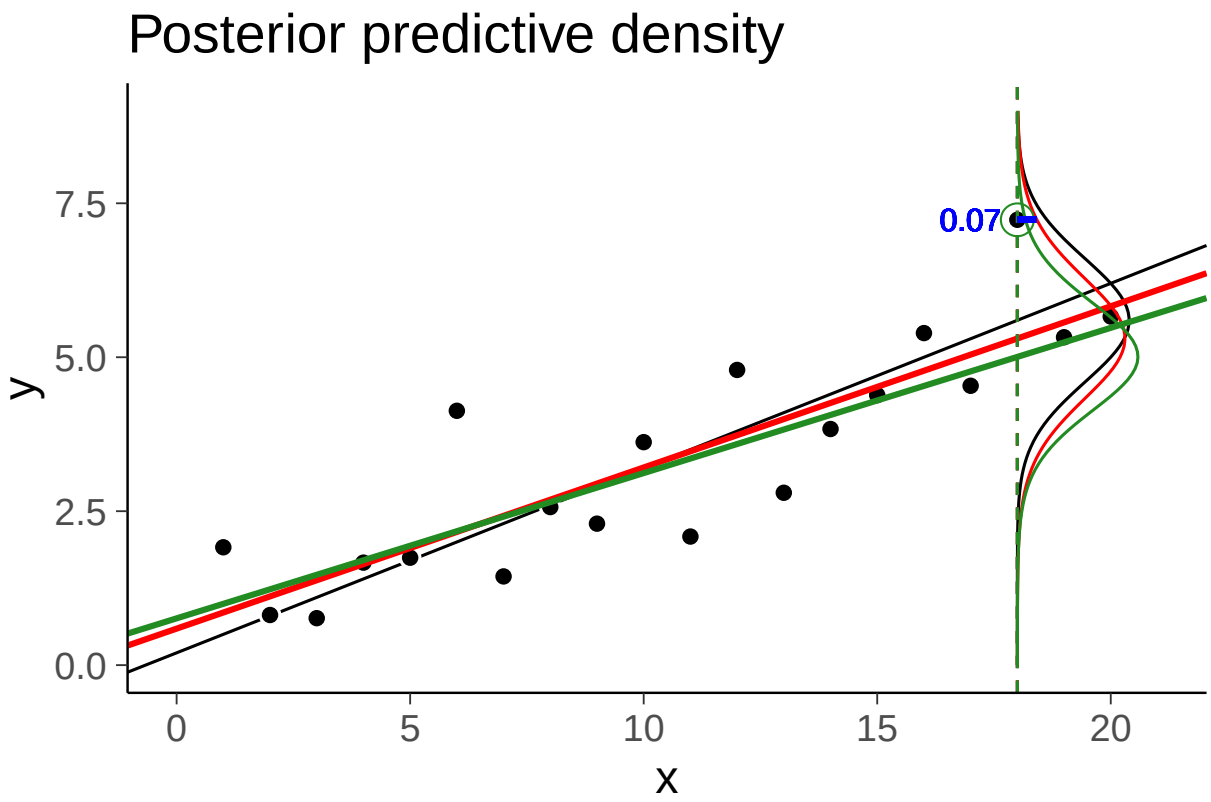

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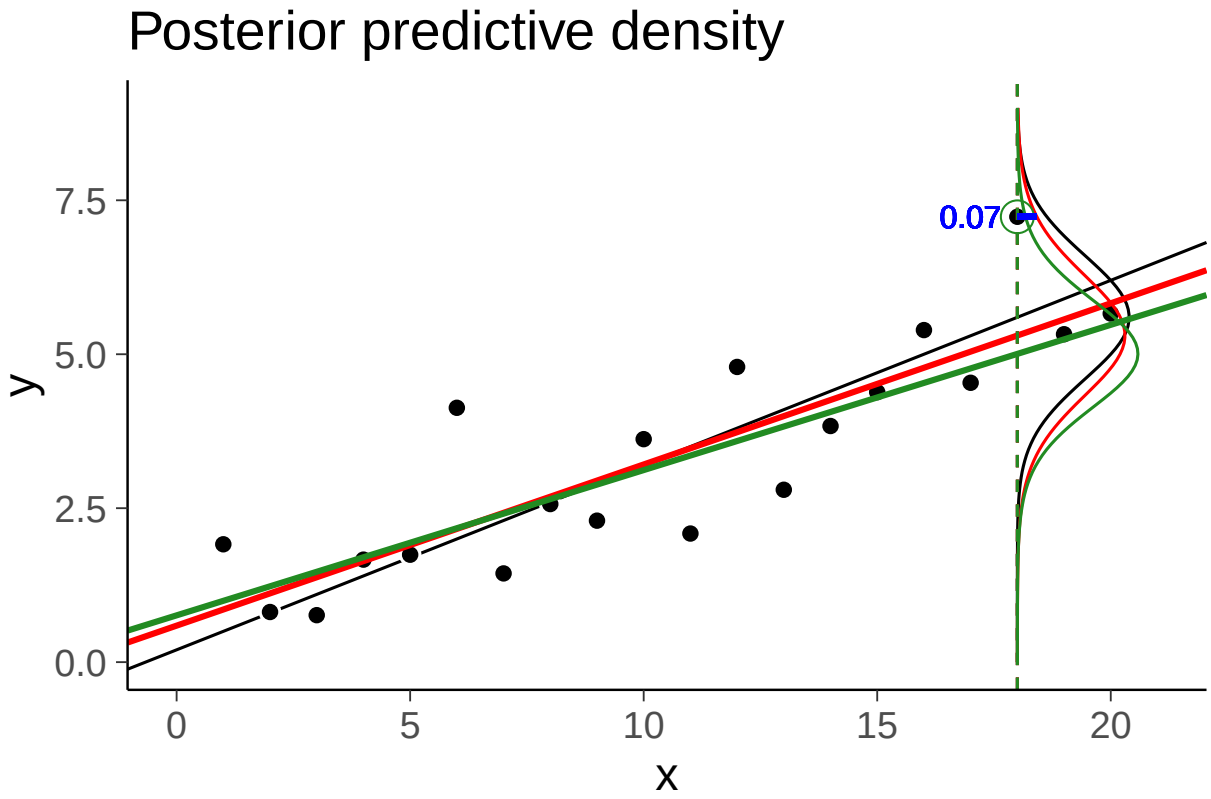

$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$$

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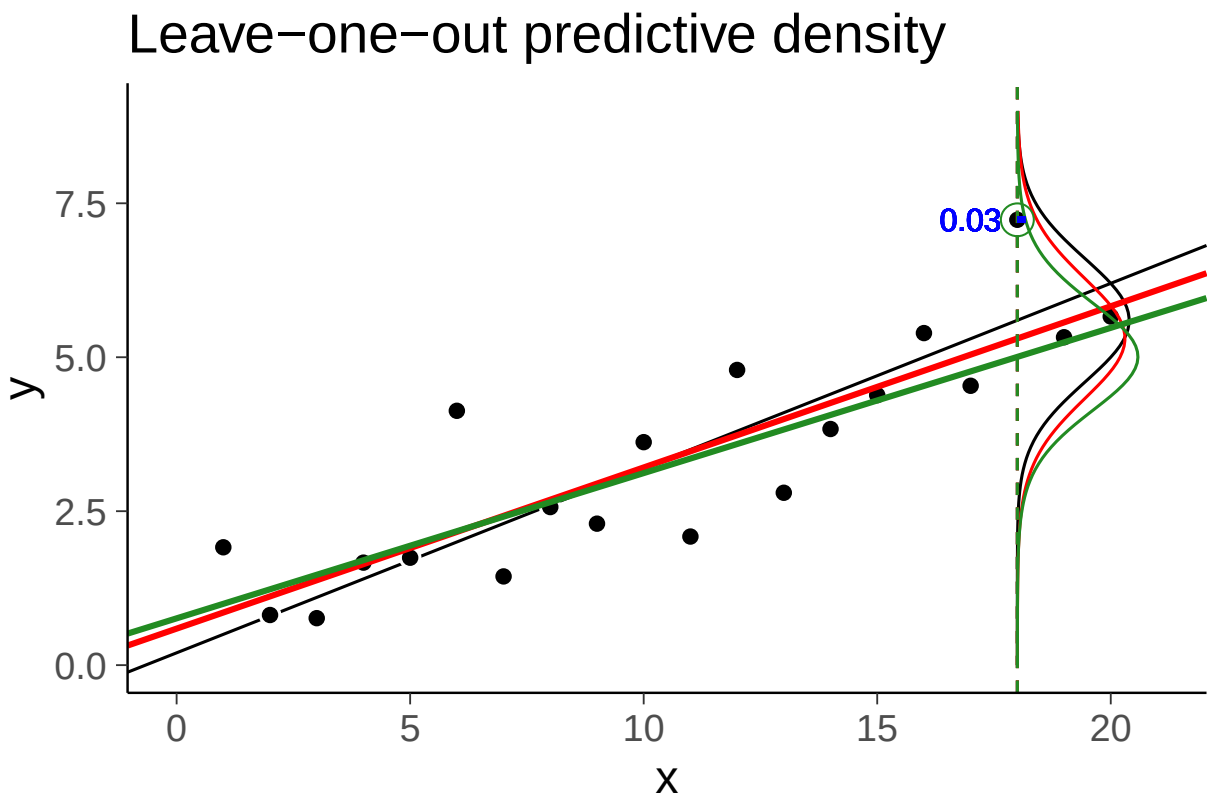

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$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$$

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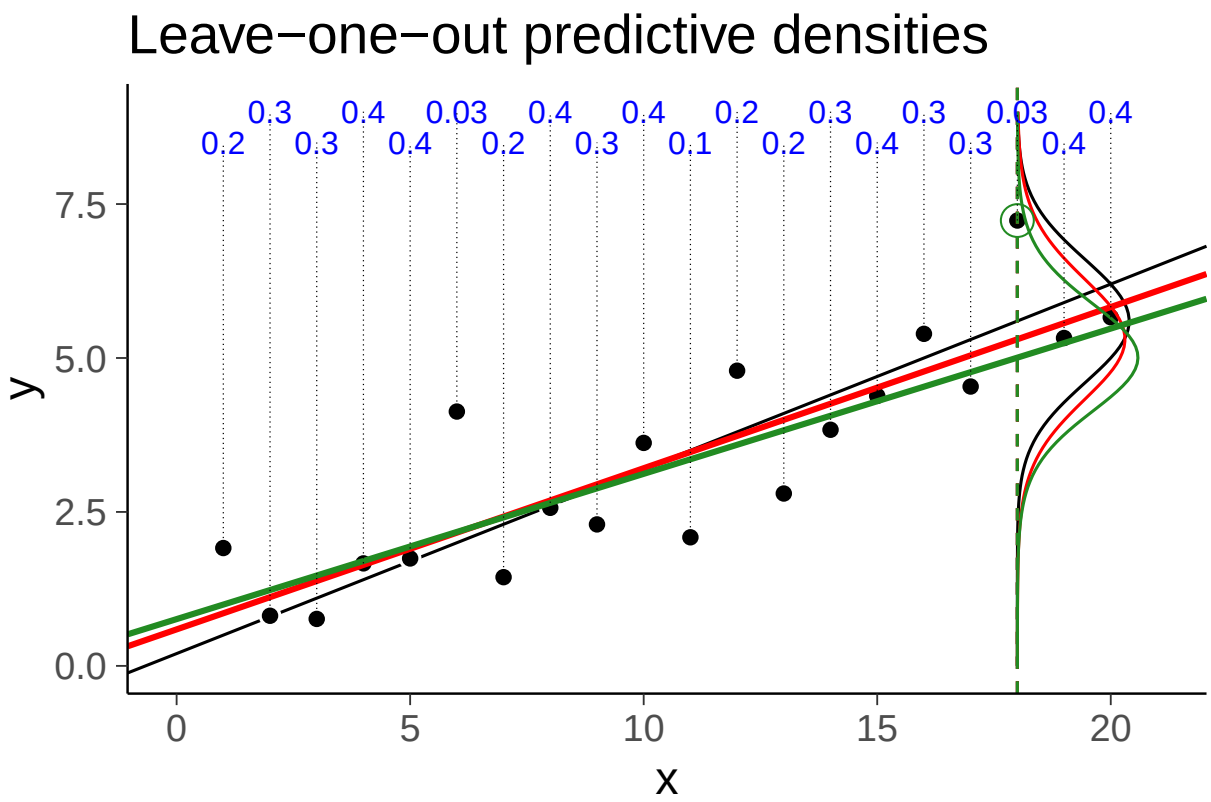

$$p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$$

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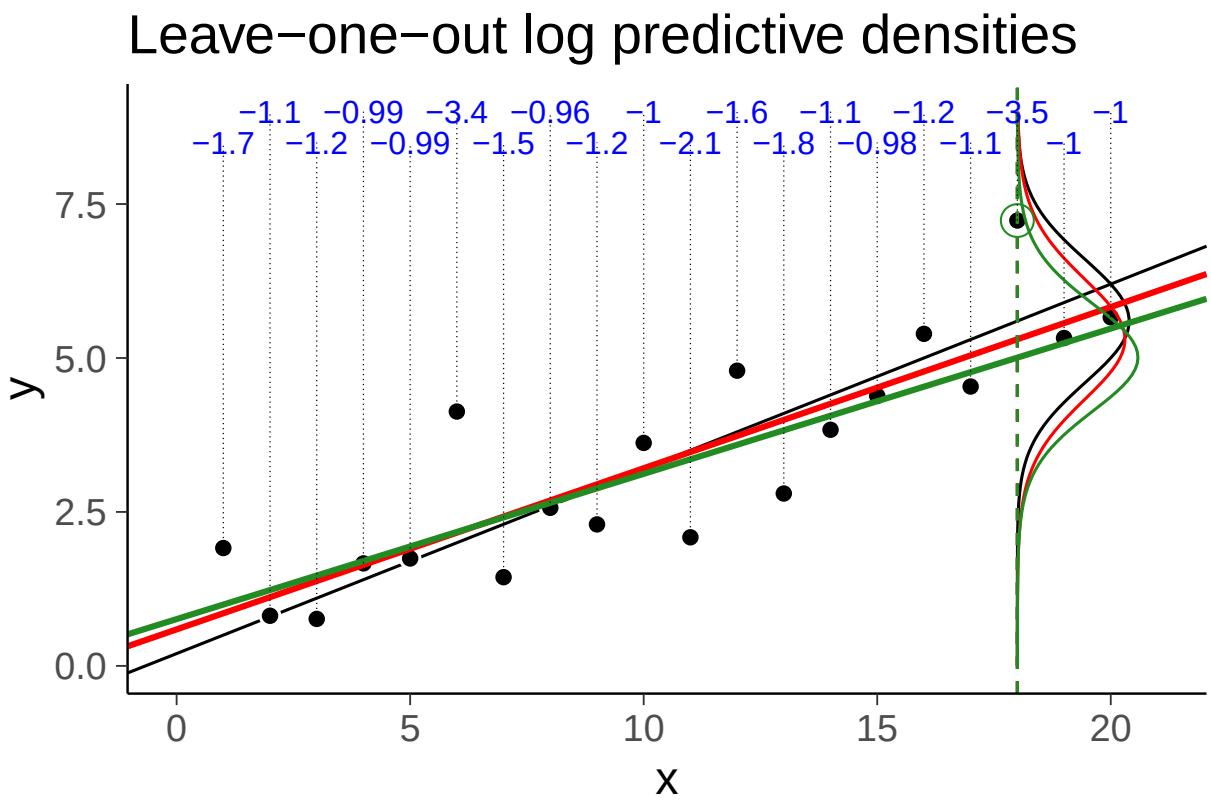

$$\log p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$$

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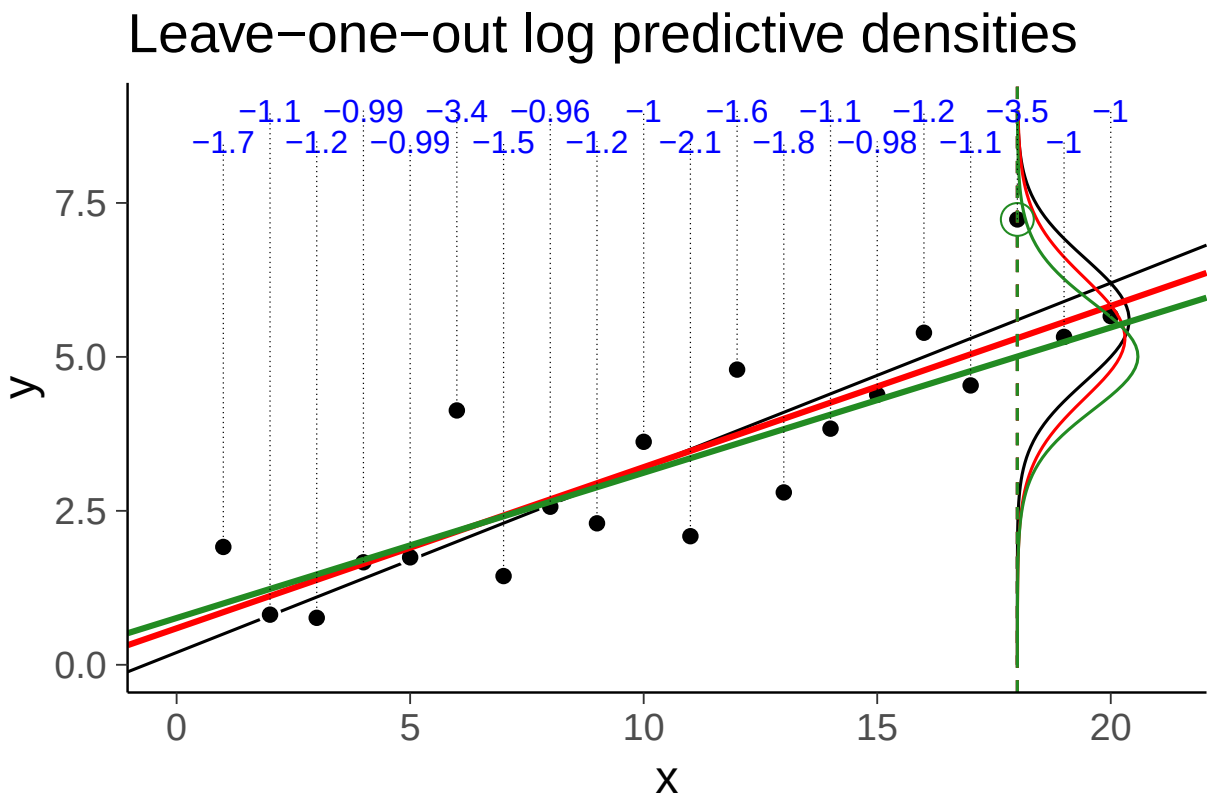

$\sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

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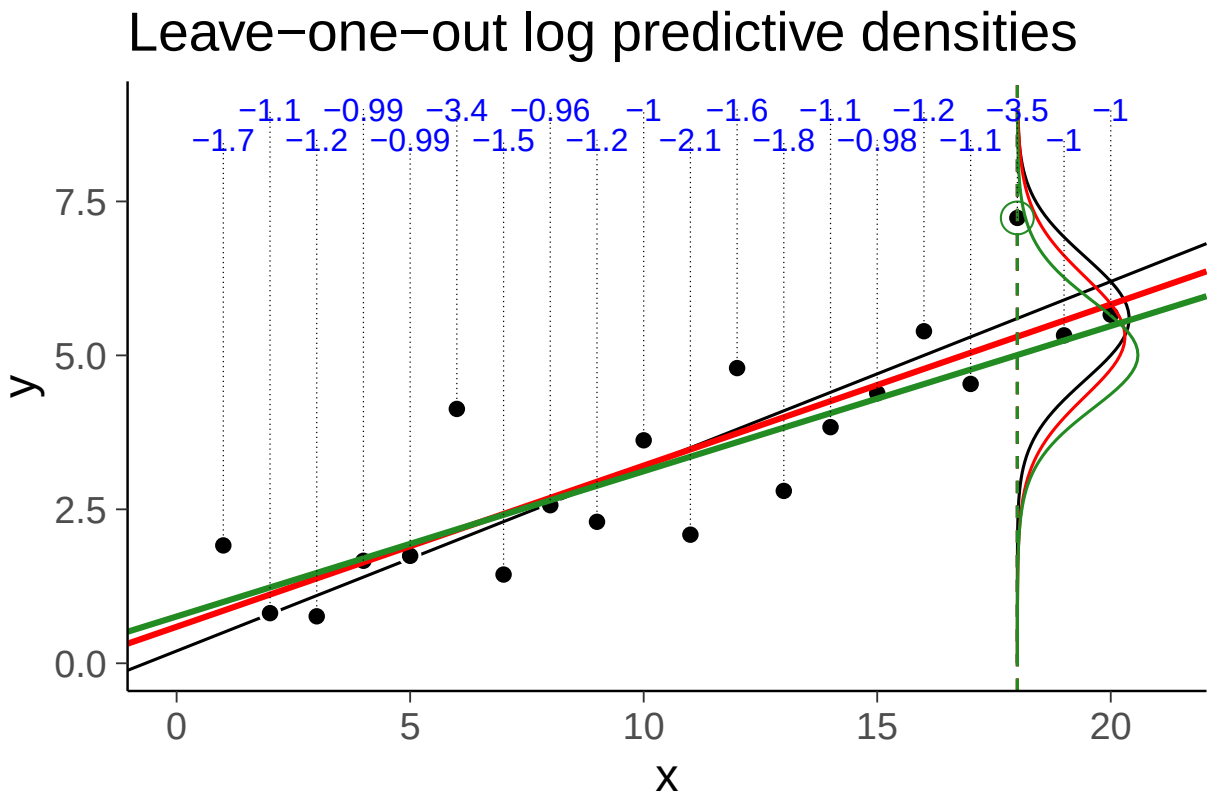

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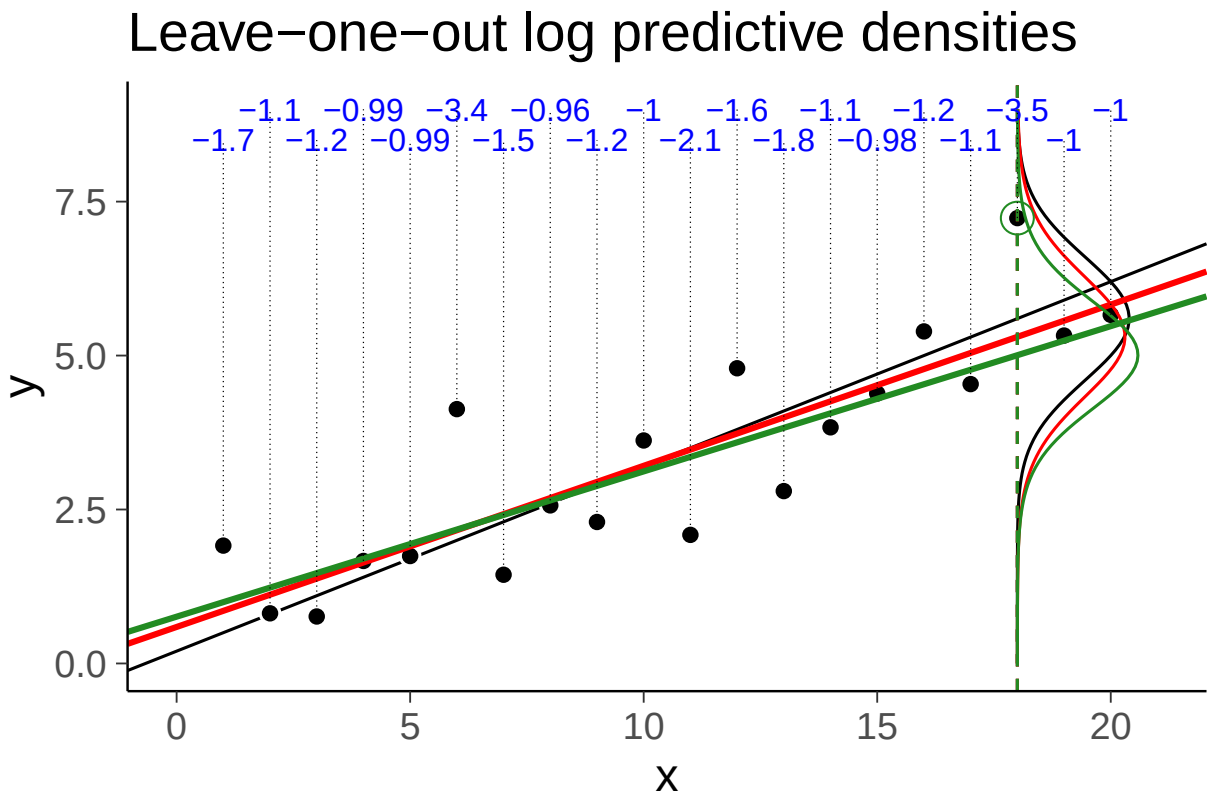

$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

unbiased estimate of log posterior pred. density for new data

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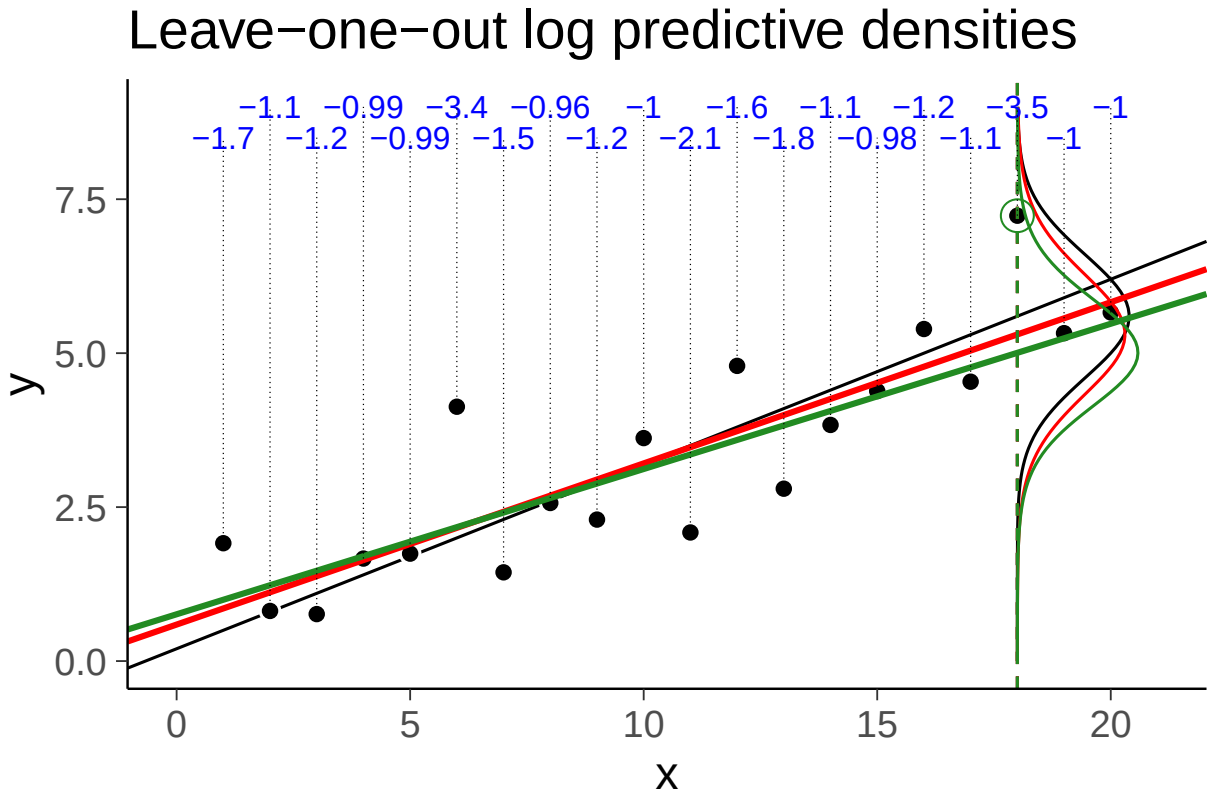

$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$$

$$\text{lpd} = \sum_{i=1}^{20} \log p(y_i|x_i, x, y) \approx -26.8$$

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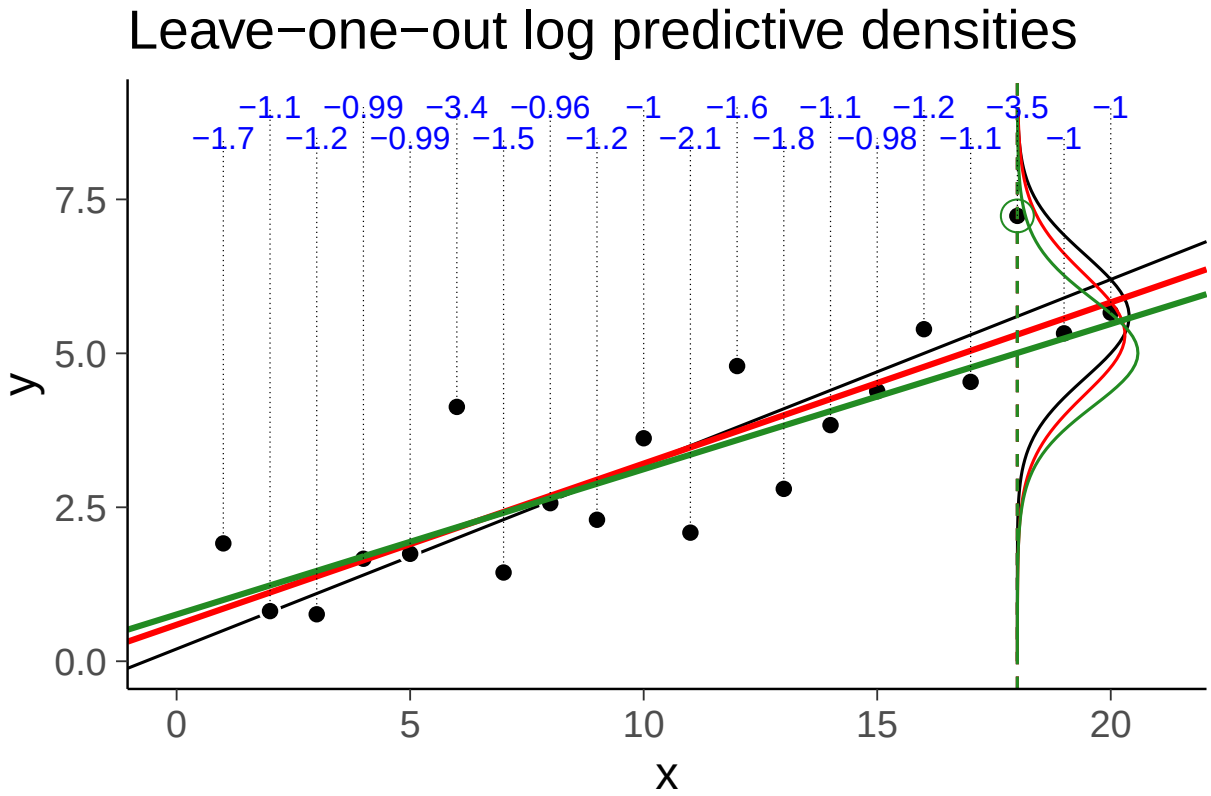

$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$$

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$$\text{p\_loo} = \text{lpd} - \text{elpd\_loo} \approx 2.7$$

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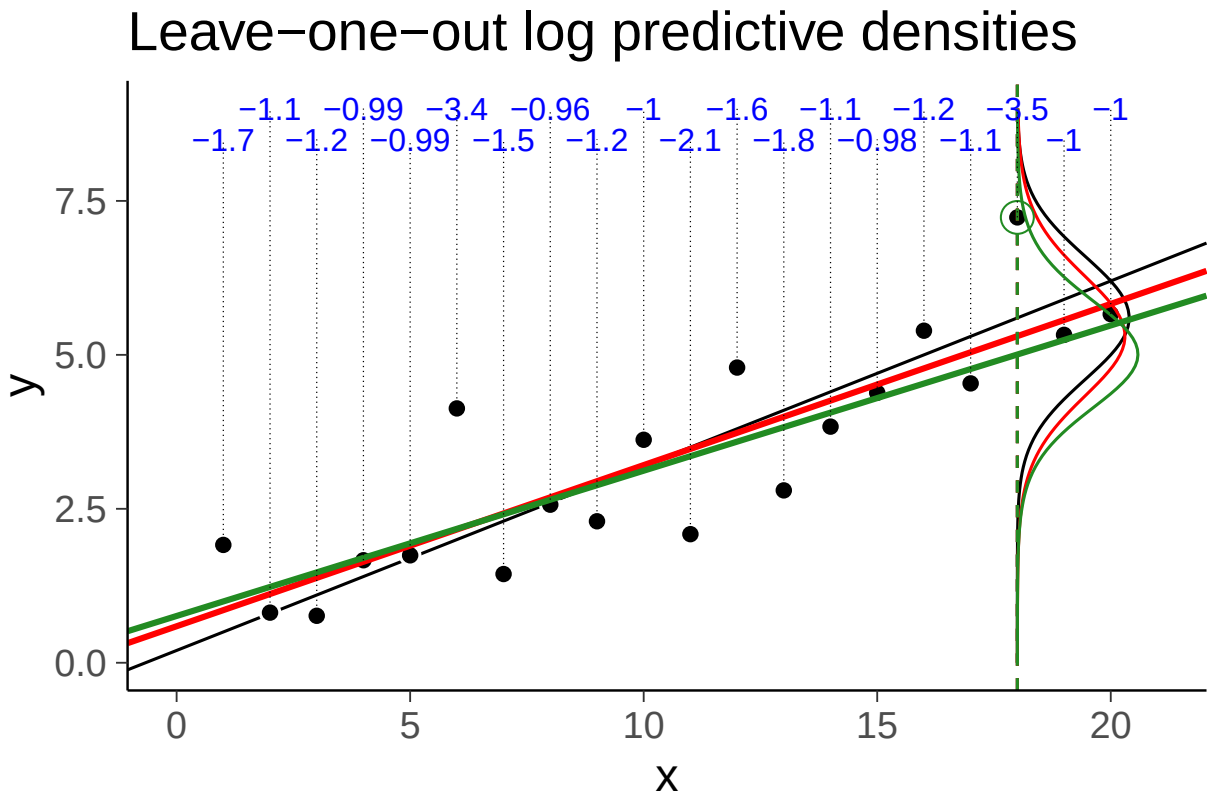

$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$$

$$\text{SE} = \text{sd}(\log p(y_i|x_i, x_{-i}, y_{-i})) \cdot \sqrt{20} \approx 3.3$$

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Stan and loo package

```
 Computed from 4000 by 20 log-likelihood matrix

          Estimate  SE
elpd_loo    -29.5 3.3
p_loo         2.7 1.0
------

Monte Carlo SE of elpd_loo is 0.1.

Pareto k diagnostic values:
                         Count Pct.    Min. n_eff
(-Inf, 0.5]   (good)     18    90.0%   899
 (0.5, 0.7]   (ok)        2    10.0%   459
   (0.7, 1]   (bad)       0     0.0%   <NA>
   (1, Inf)   (very bad)  0     0.0%   <NA>

All Pareto k estimates are ok (k < 0.7).
See help('pareto-k-diagnostic') for details.
```

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Subsection 1

When is LOO applicable

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Pro and cons with LOO-CV

\+ Intuitive

\+ Robust

\+ Good theoretical properties

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Pro and cons with LOO-CV

\+ Intuitive

\+ Robust

\+ Good theoretical properties

\- Can be costly (naive LOO-CV mean n posterior computations)

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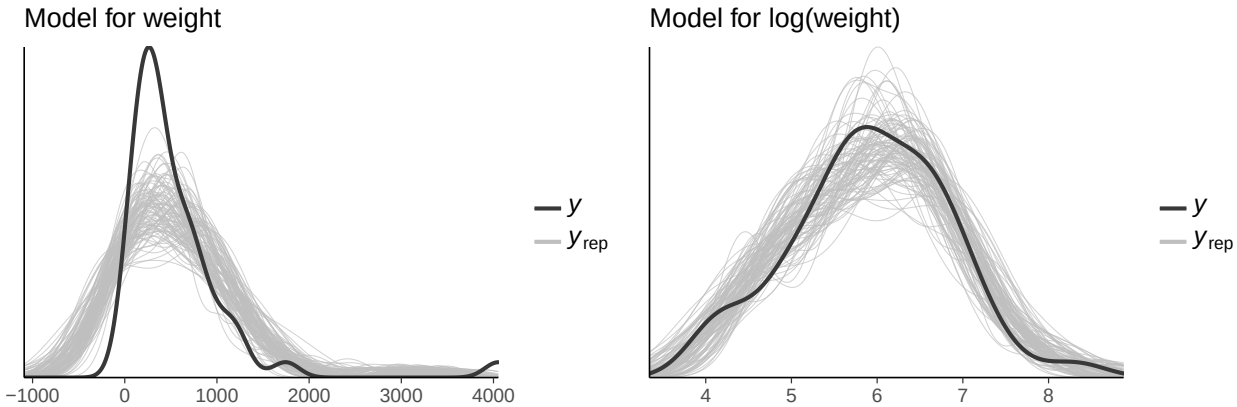
Sometimes cross-validation is not needed

- Posterior predictive checking can be sufficient



Predicting the yields of mesquite bushes.

Gelman, Hill & Vehtari (2020, Ch. 11)

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Sometimes cross-validation is not needed

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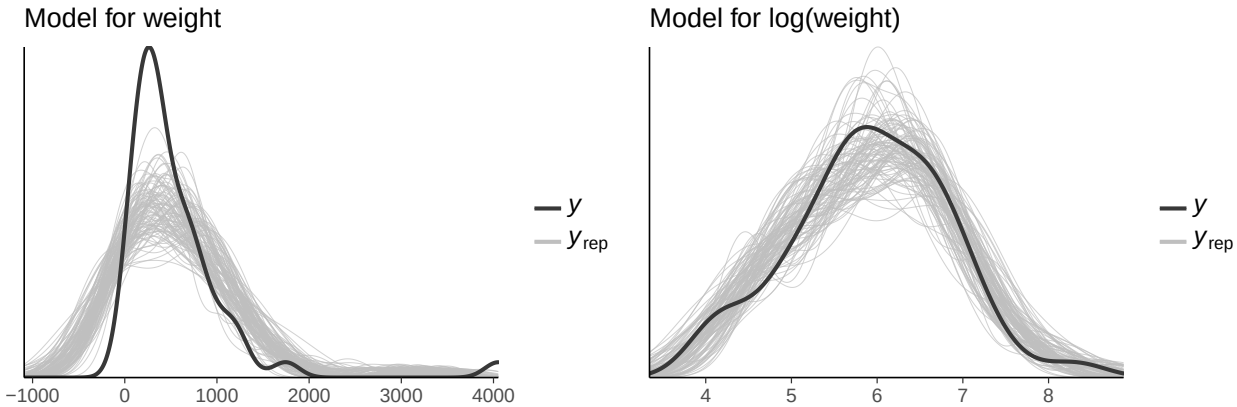

Predicting the yields of mesquite bushes.

Gelman, Hill & Vehtari (2020, Ch. 11)

- In nested case, often easier and more accurate to analyse posterior distribution of more complex model directly

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Data generating mechanisms and prediction tasks

1. You have to make some assumptions on data generating mechanism p_{true}

$$\text{elpd}_M = \int \log p_M(\tilde{y}|y) p_{\text{true}}(\tilde{y}) d\tilde{y} \,,$$

2. Use the knowledge of the prediction task if available
3. Cross-validation can be used to analyse different parts, even if there is no clear prediction task

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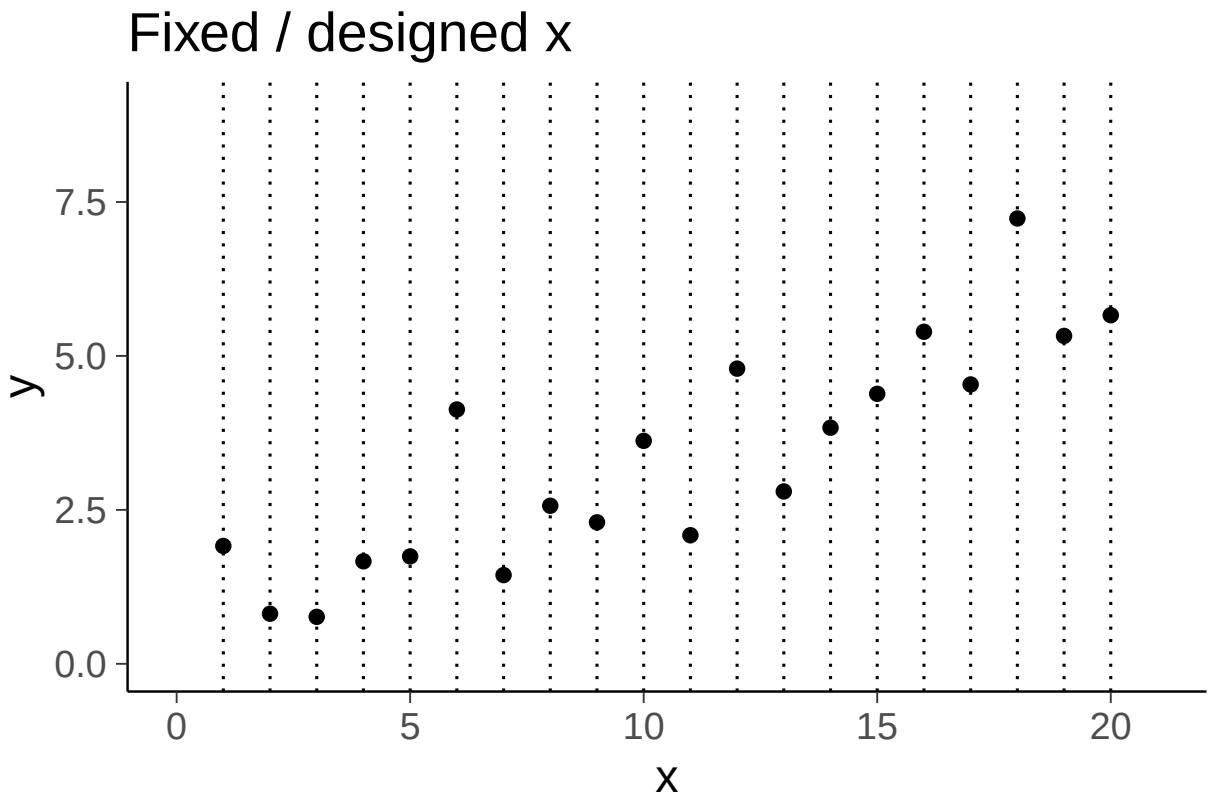
x in p_{true}



LOO is ok for fixed / designed x. SE is uncertainty about $y|x$.

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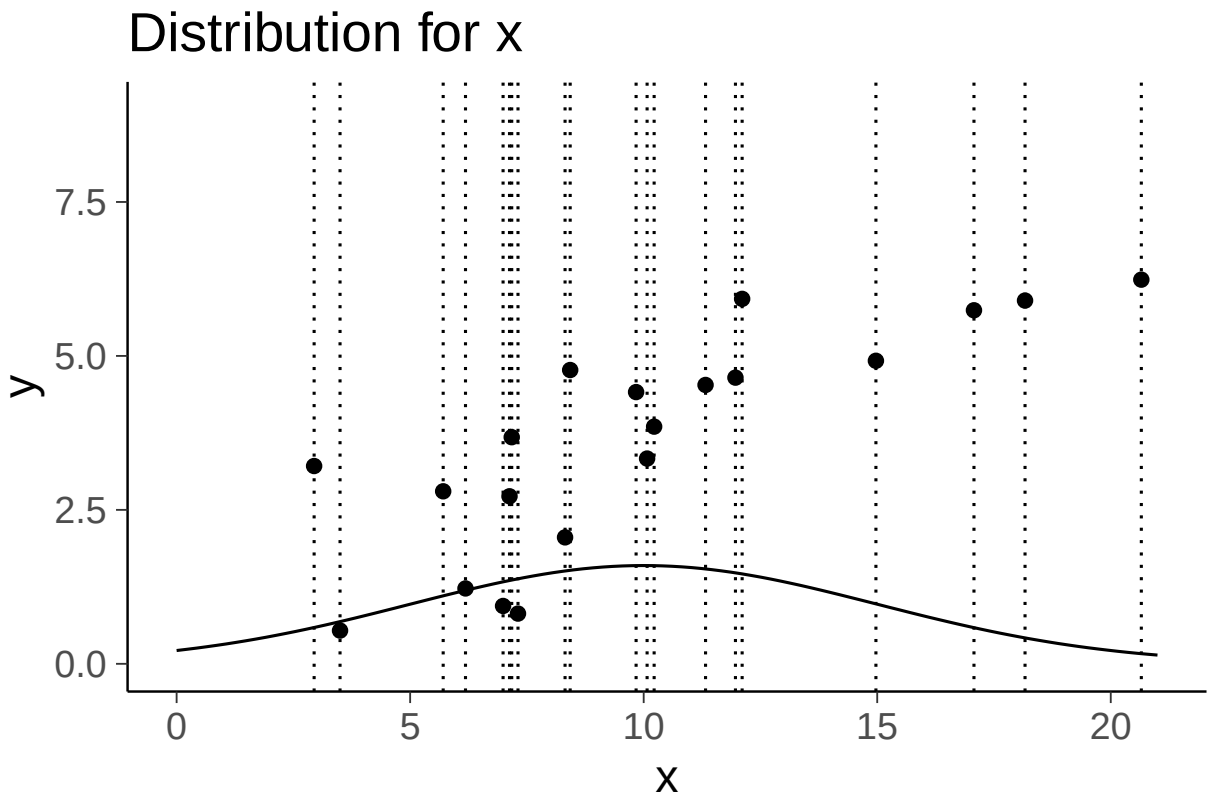
x in p_{true}



LOO is ok for random x. SE is uncertainty about $y|x$ and x.

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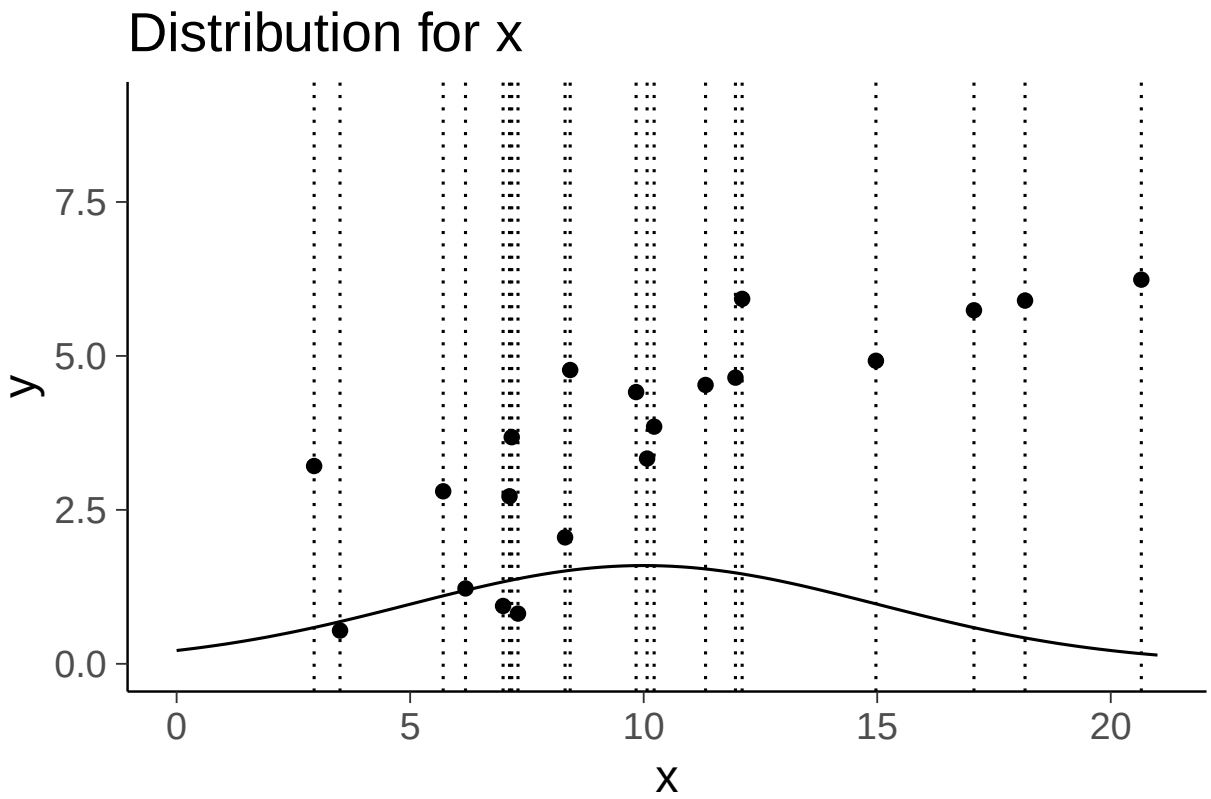
x in p_{true}



LOO is ok for random x. SE is uncertainty about $y|x$ and x.

Covariate shift can be handled with importance weighting or modelling

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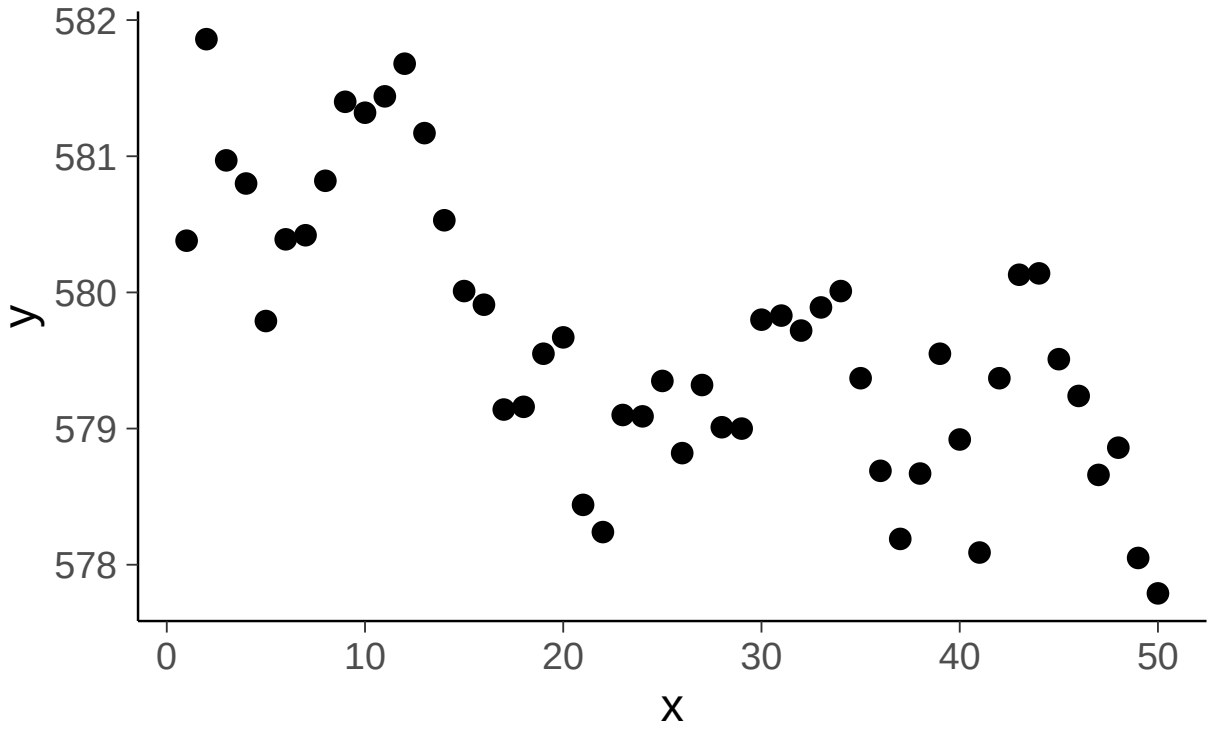

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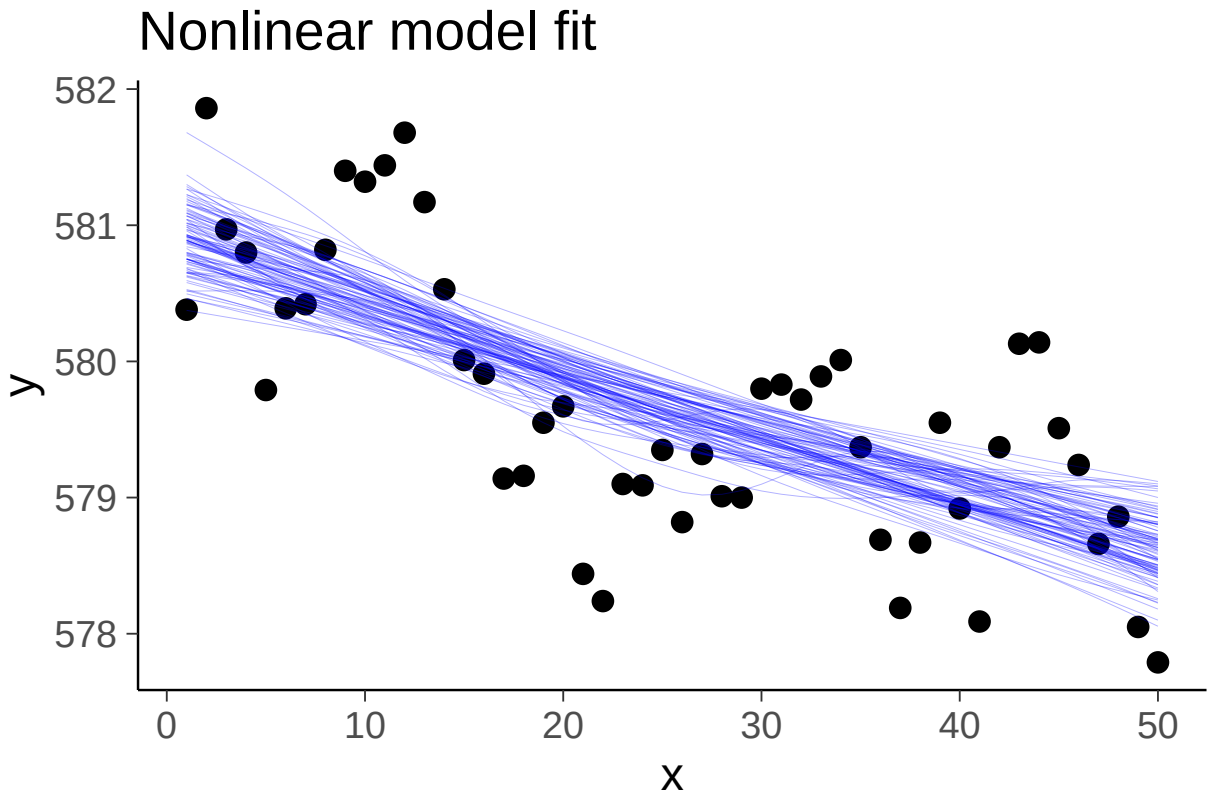

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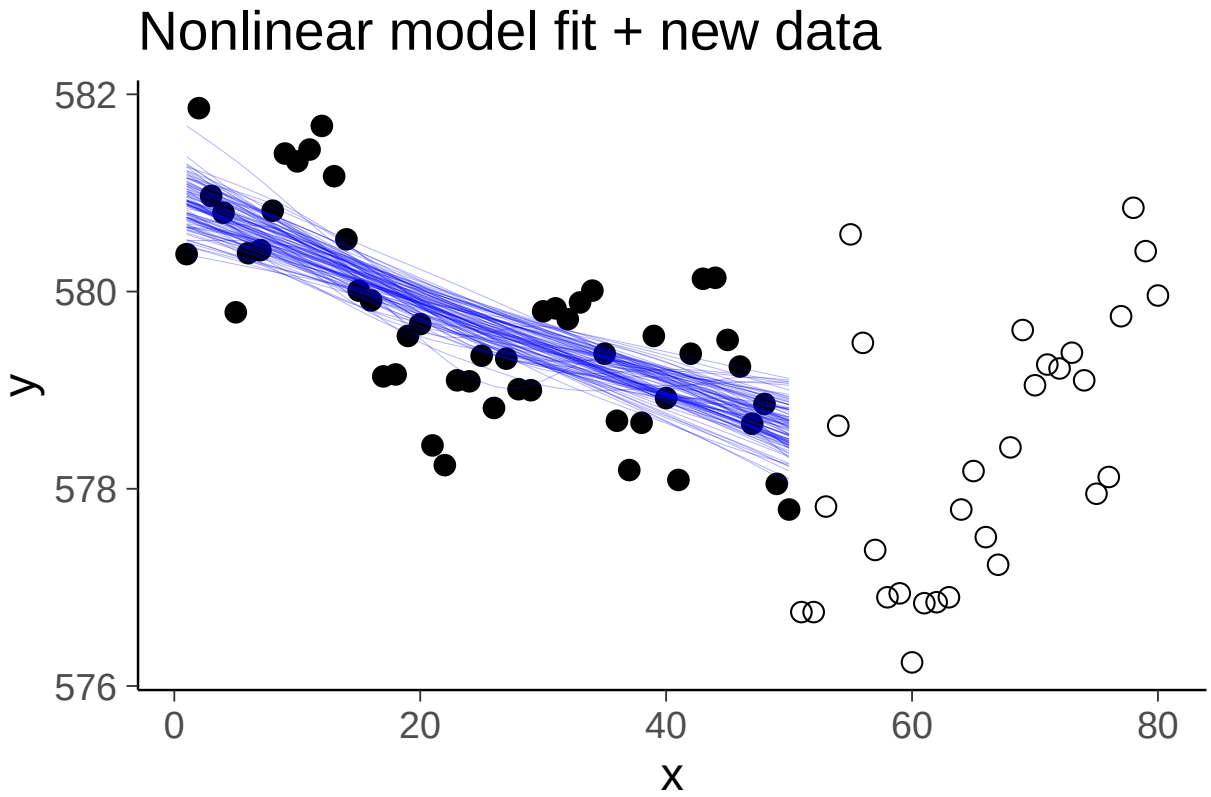

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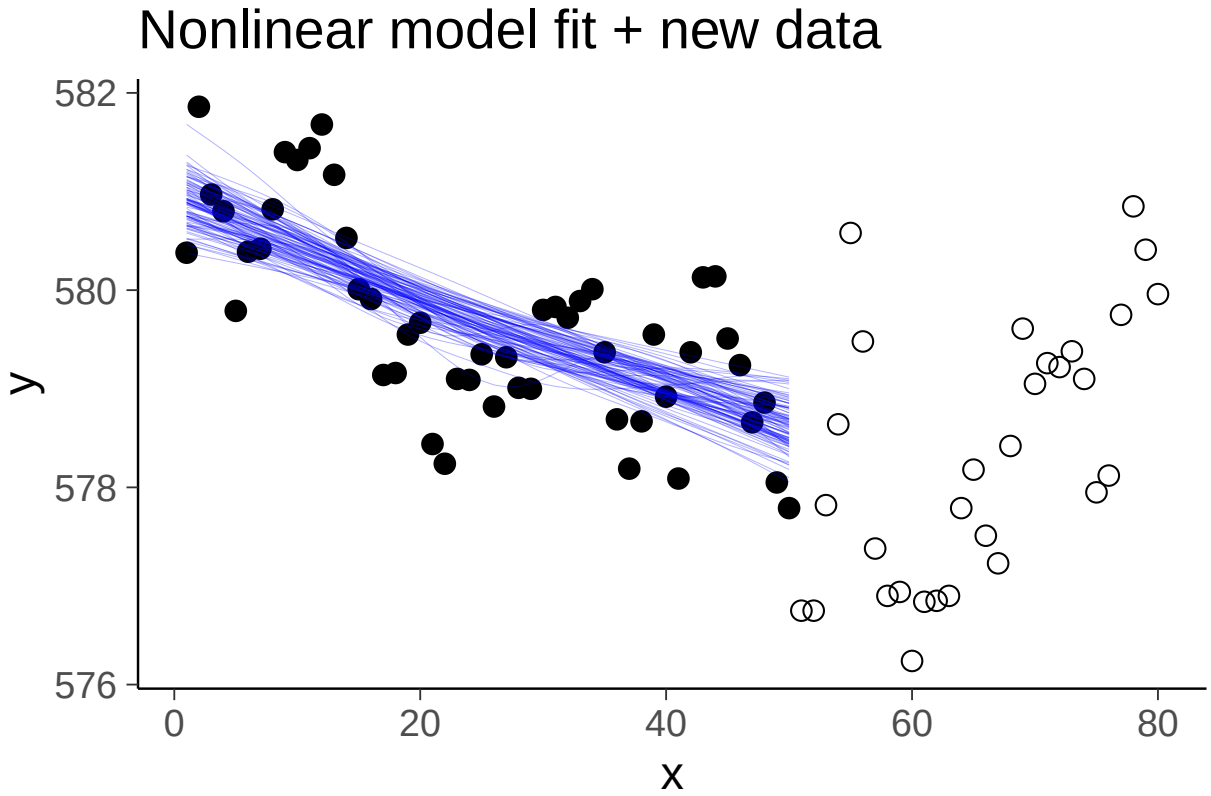

Extrapolation is more difficult

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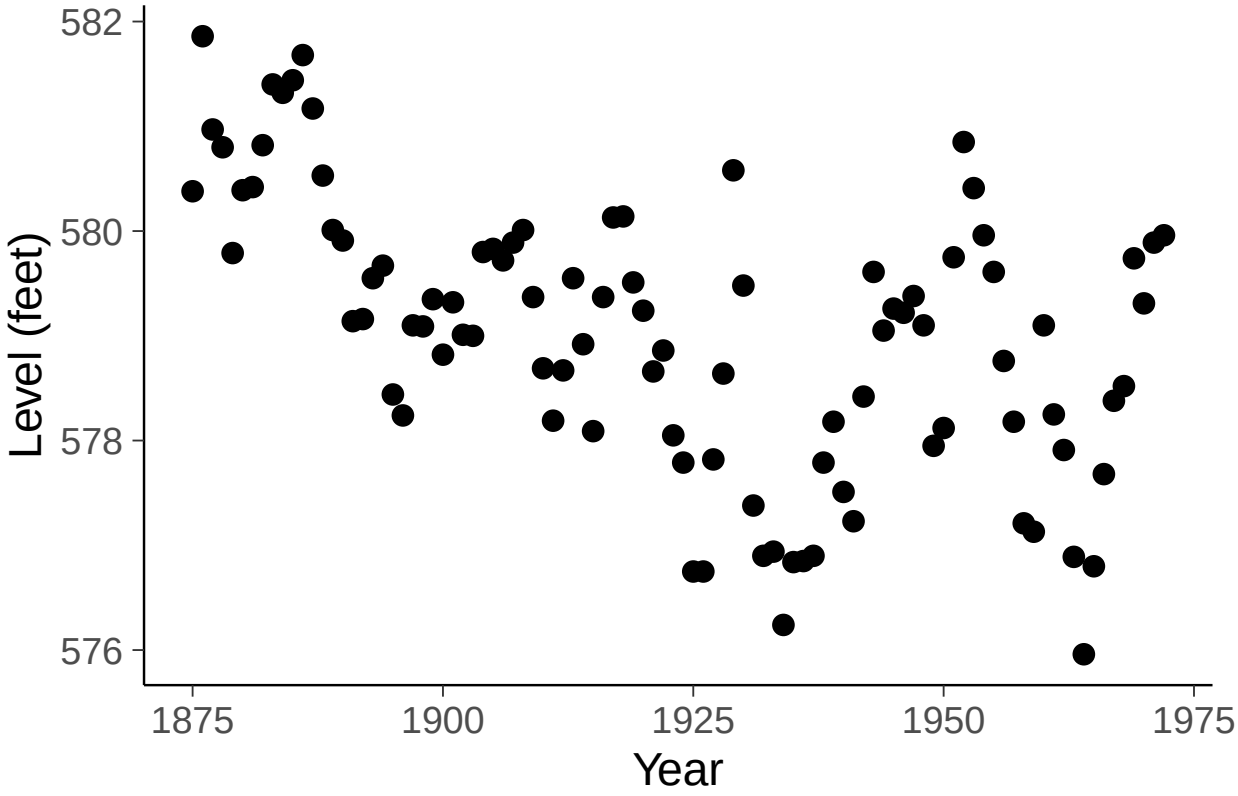

Can LOO or other cross-validation be used with time series?

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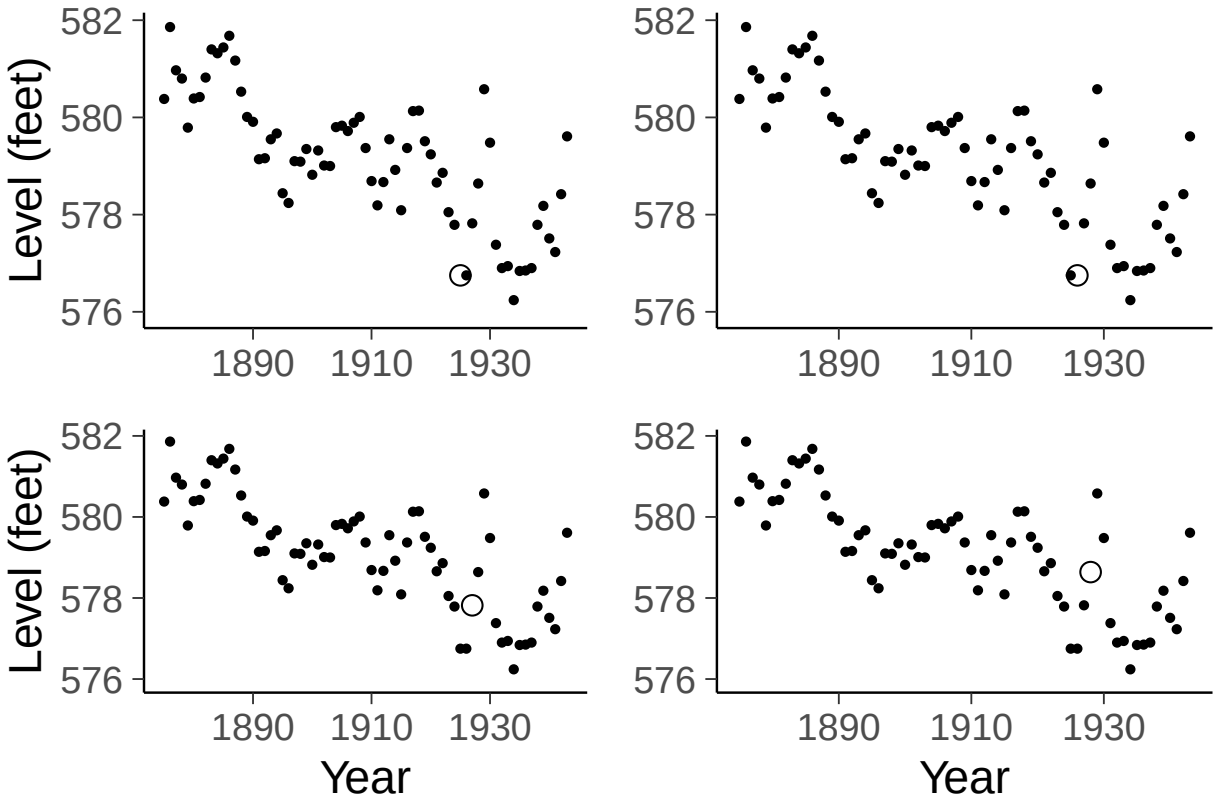

Leave-one-out cross-validation is ok for assessing conditional model

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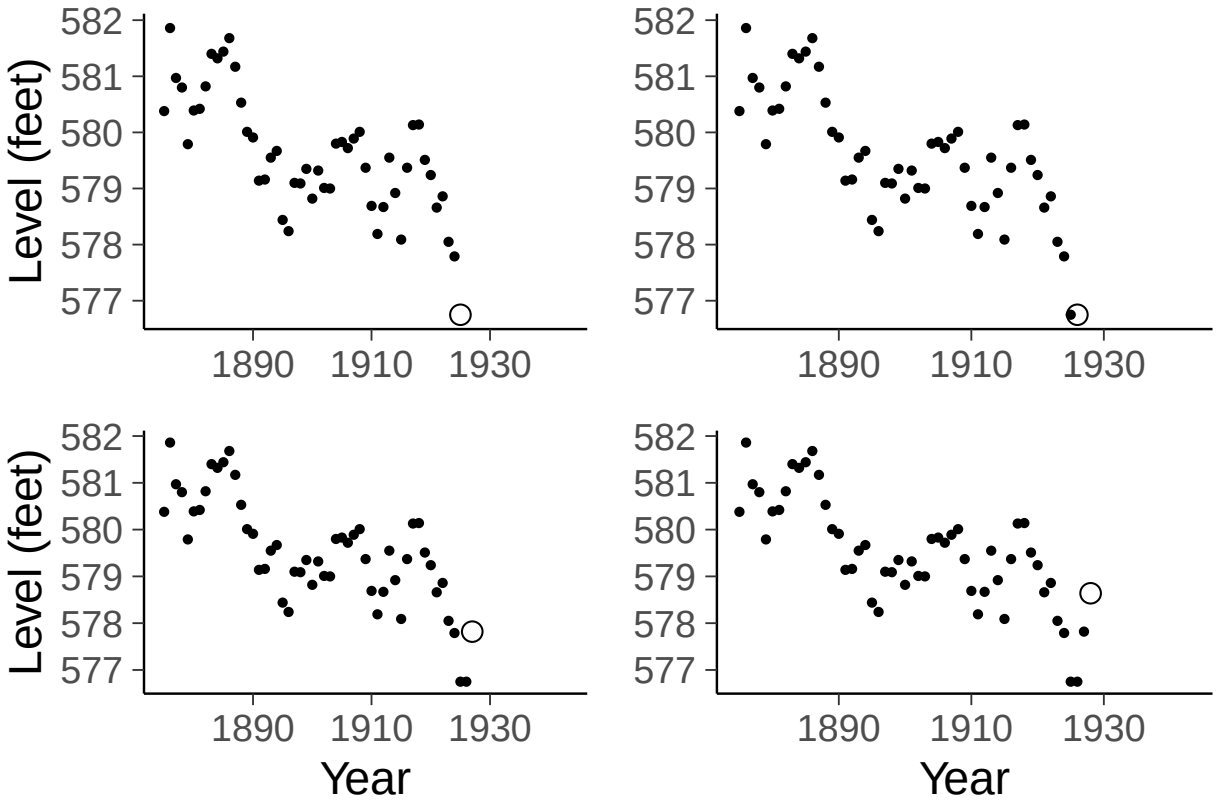

Leave-future-out cross-validation is better for predicting future

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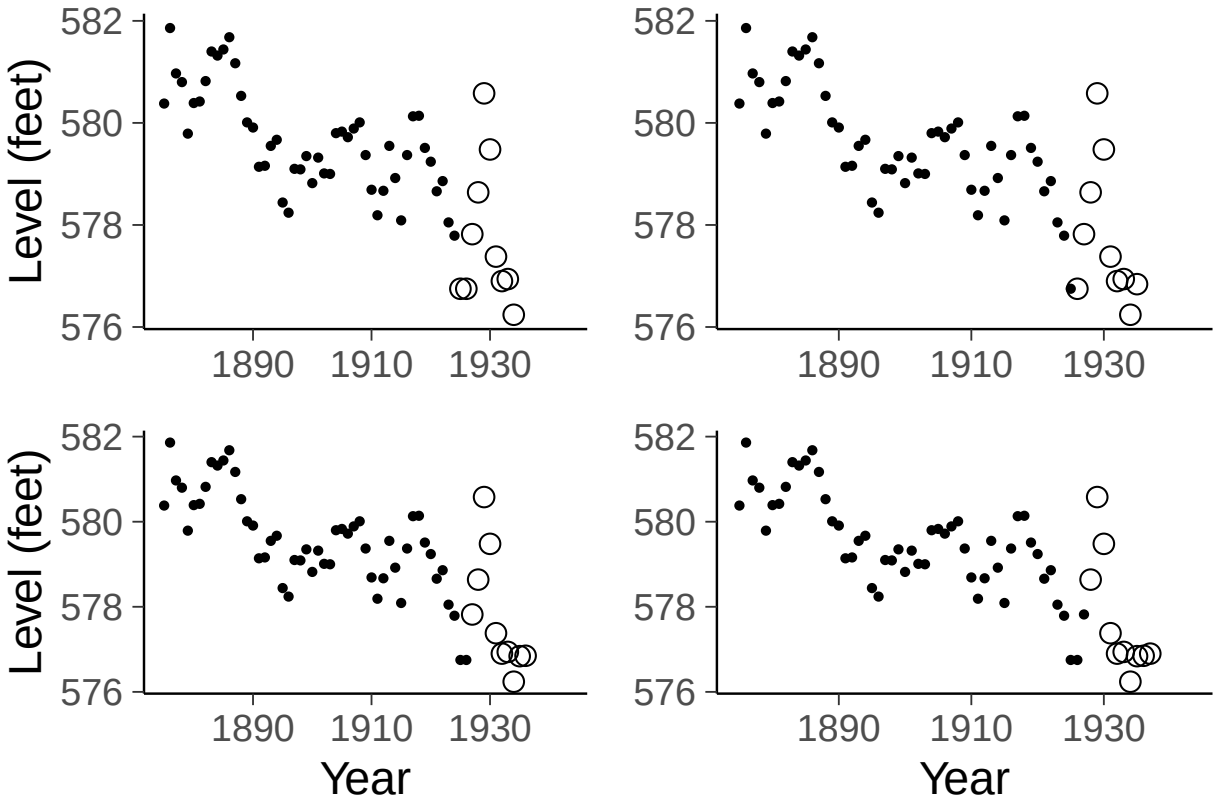

m-step-ahead cross-validation is better for predicting further future

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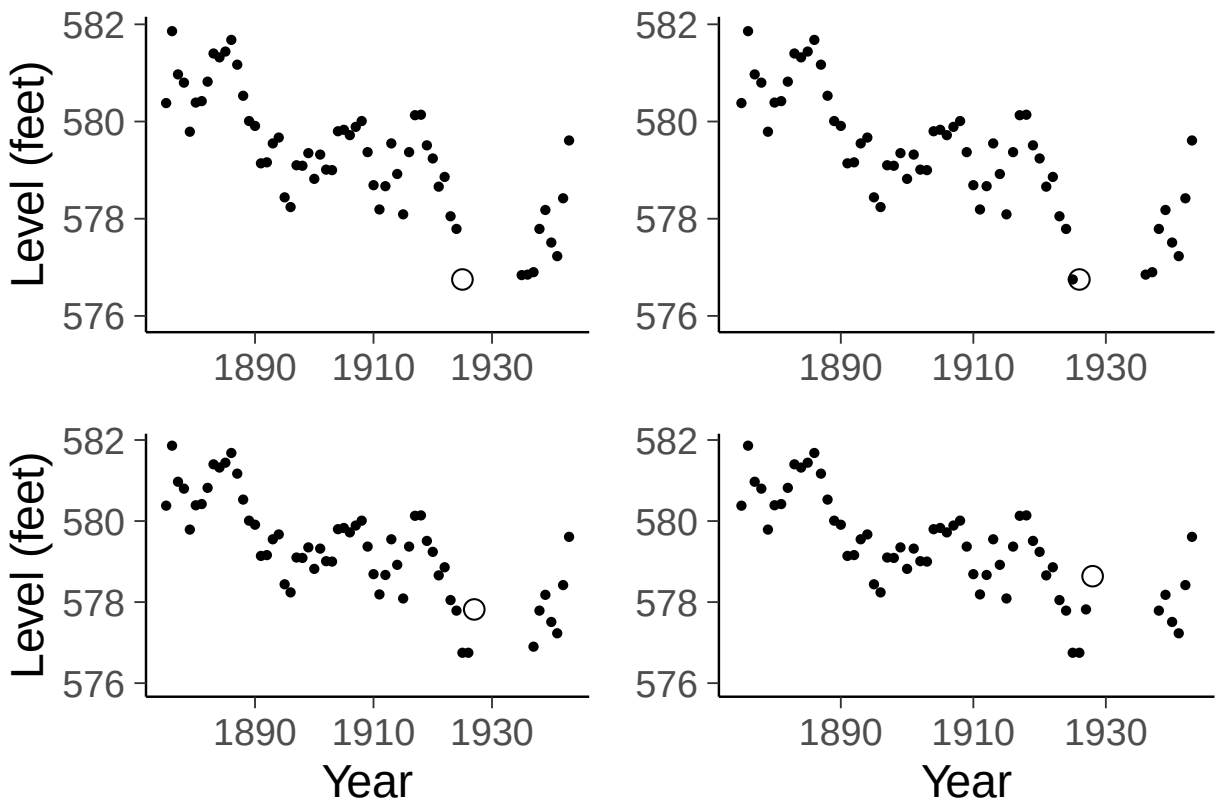

m-step-ahead leave-a-block-out cross-validation

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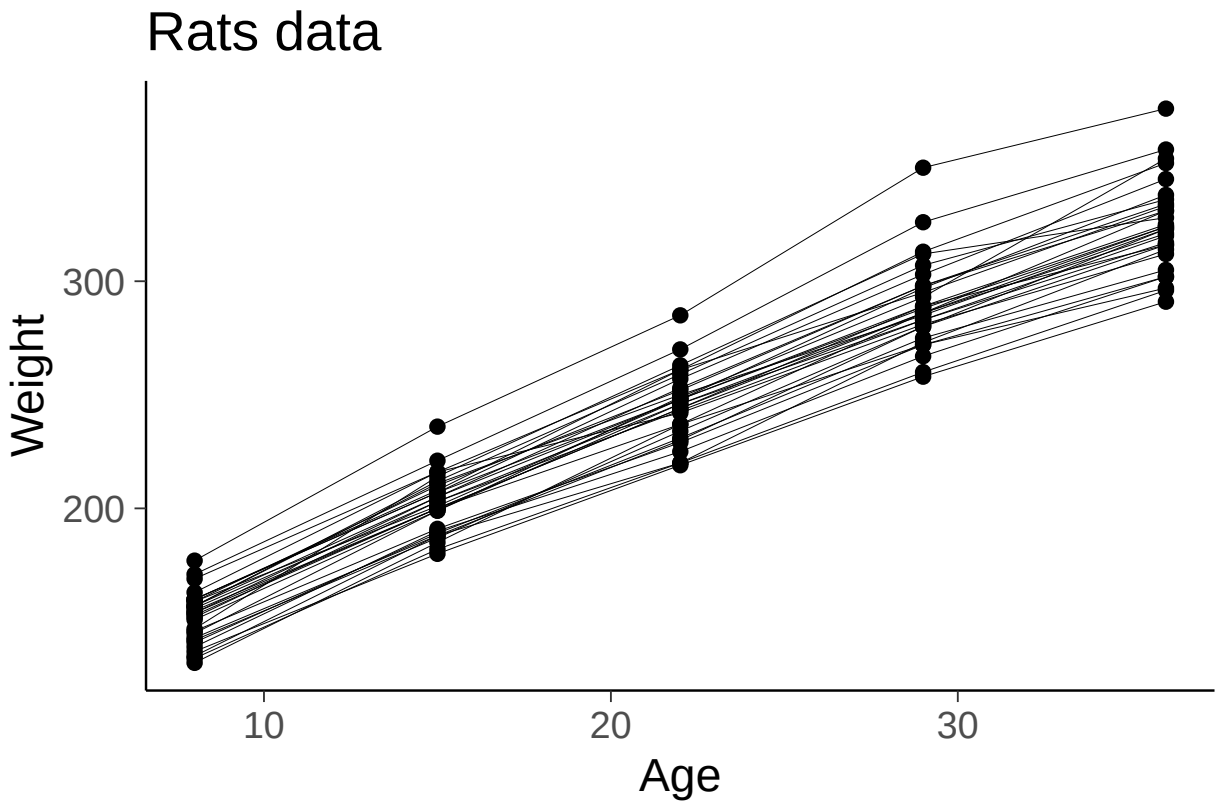

Can LOO or other cross-validation be used with hierarchical data?

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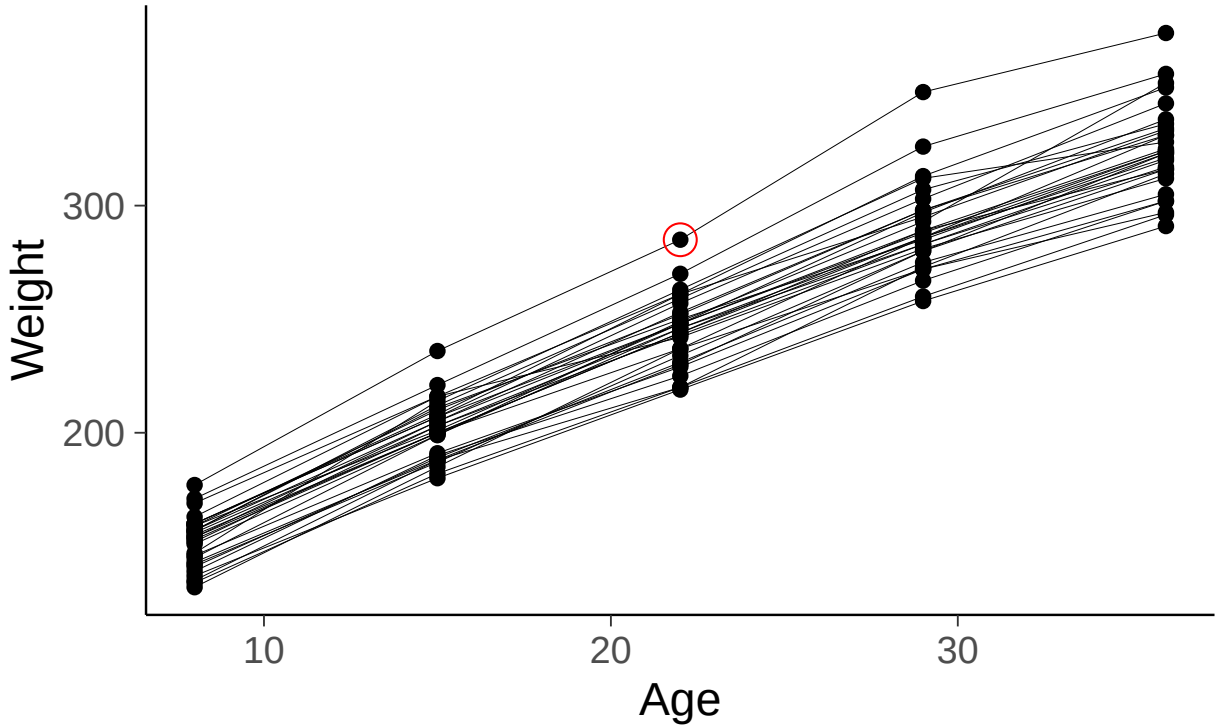
Leave−one−out?



Yes!

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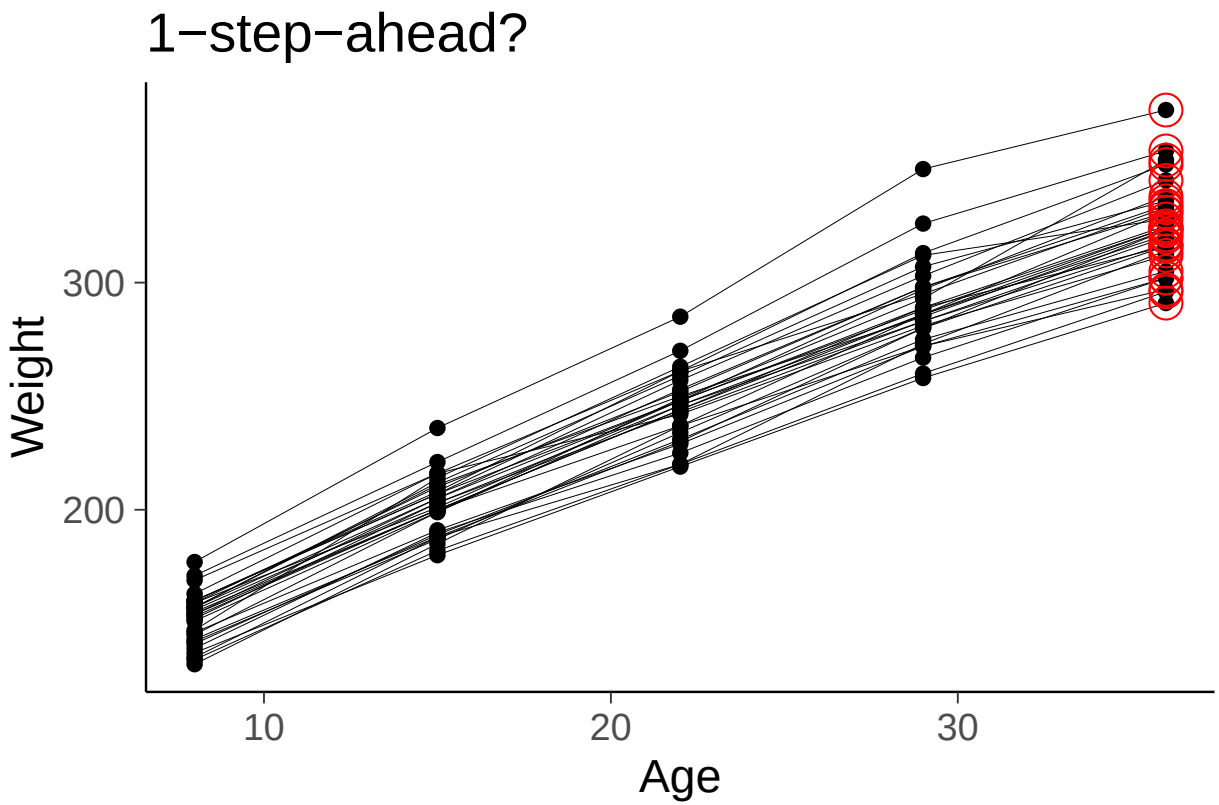

Yes!

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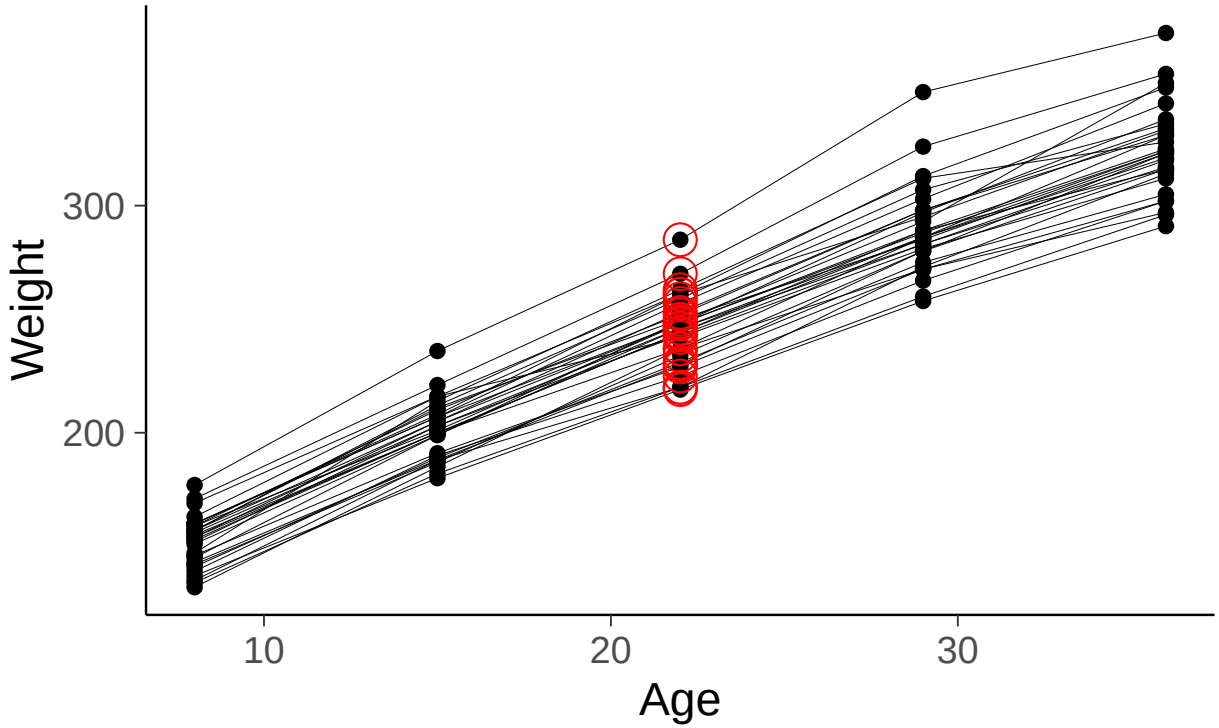
Leave−one−time−point−out?



Yes!

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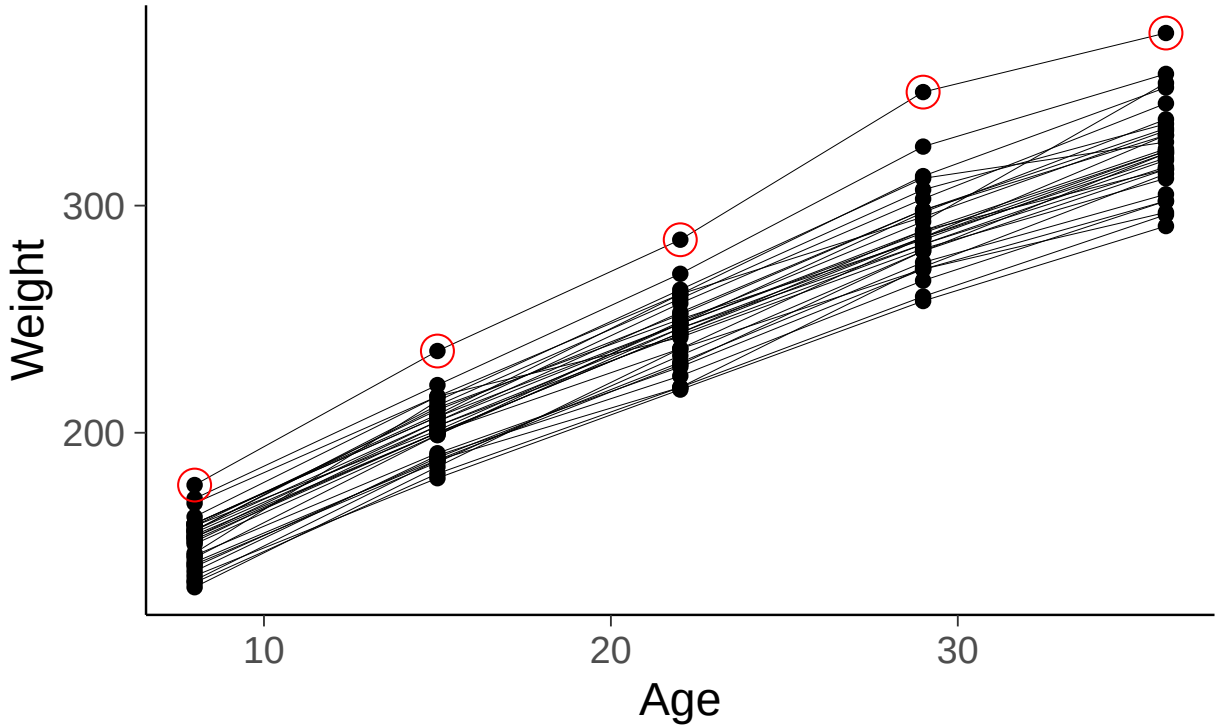
Leave−one−rat−out?



Yes!

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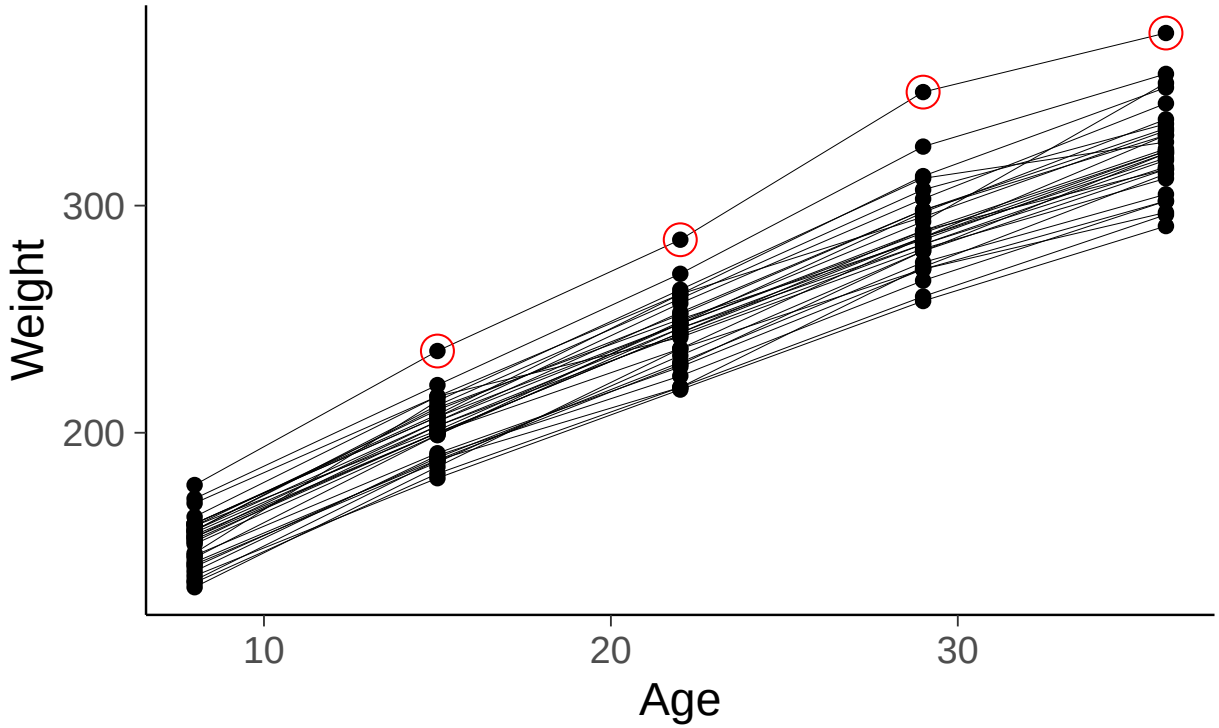
Predict given initial weight?



Yes!

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Fast cross-validation

1. Pareto smoothed importance sampling LOO (PSIS-LOO)
2. K-fold cross-validation

see Vehtari, Gelman & Gabry (2017a) and `mc-stan.org/loo/`

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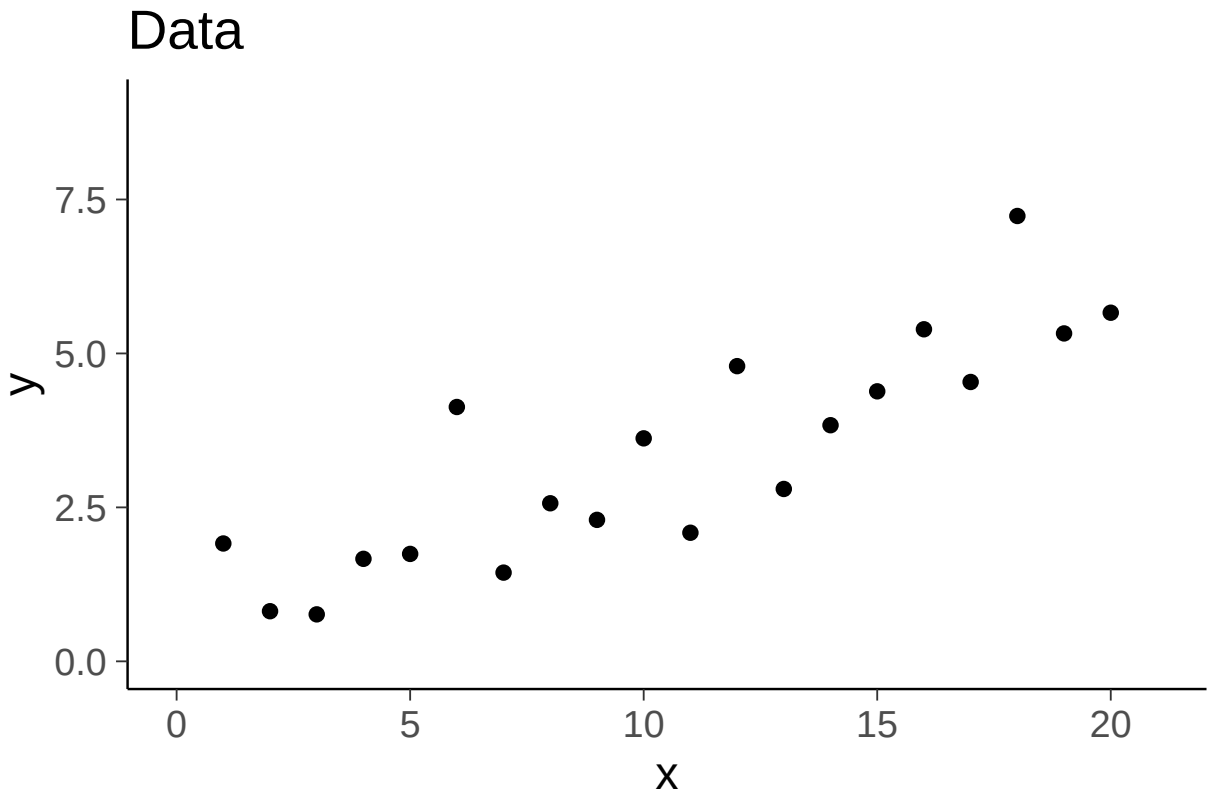

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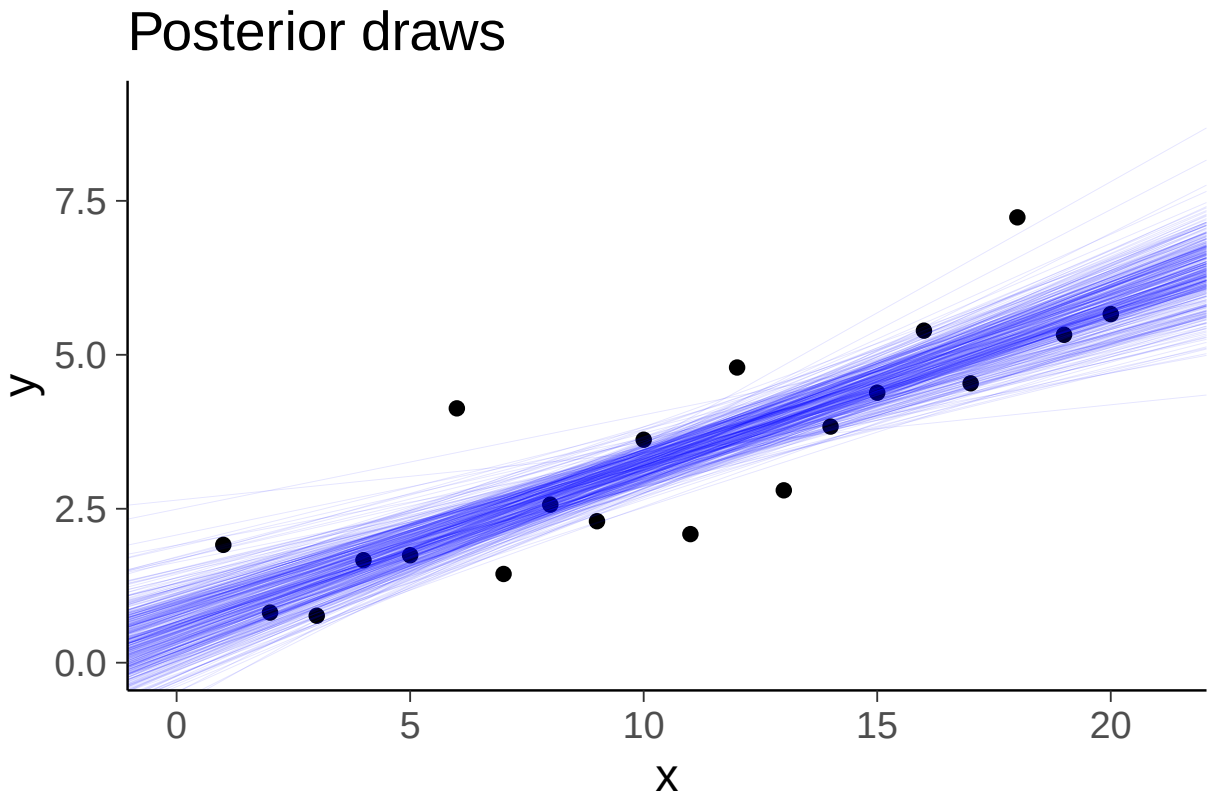

$$\theta^{(s)} \sim p(\theta|x, y)$$

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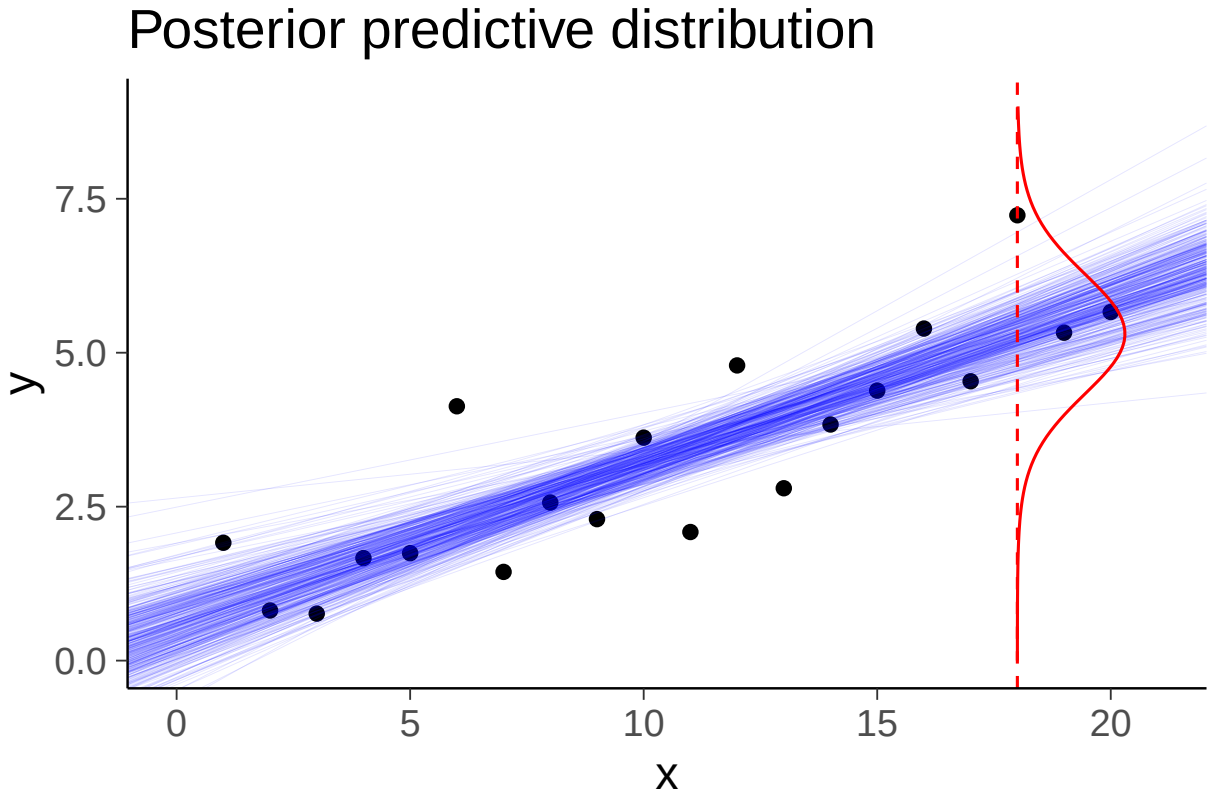

$$\theta^{(s)} \sim p(\theta|x,y), \quad p(\tilde{y}|\tilde{x},x,y) \approx \frac{1}{S}\sum_{s=1}^{S} p(\tilde{y}|\tilde{x},\theta^{(s)})$$

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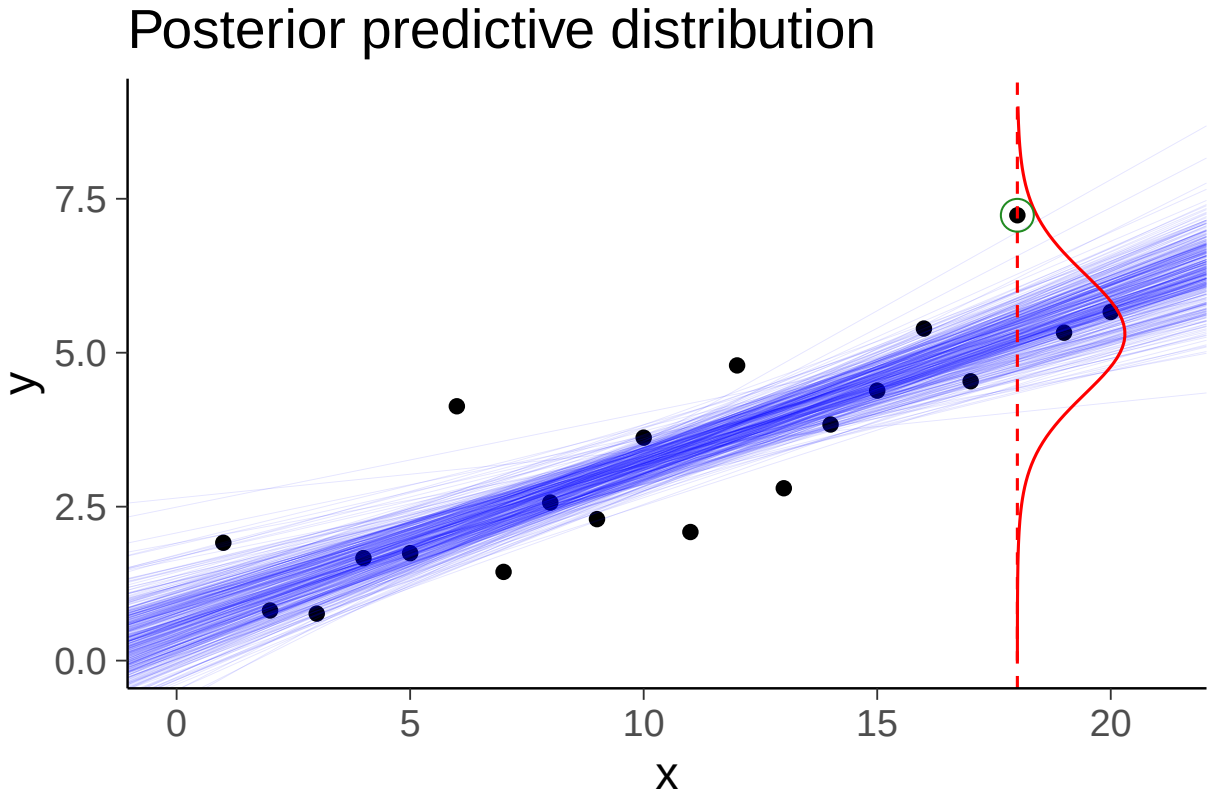

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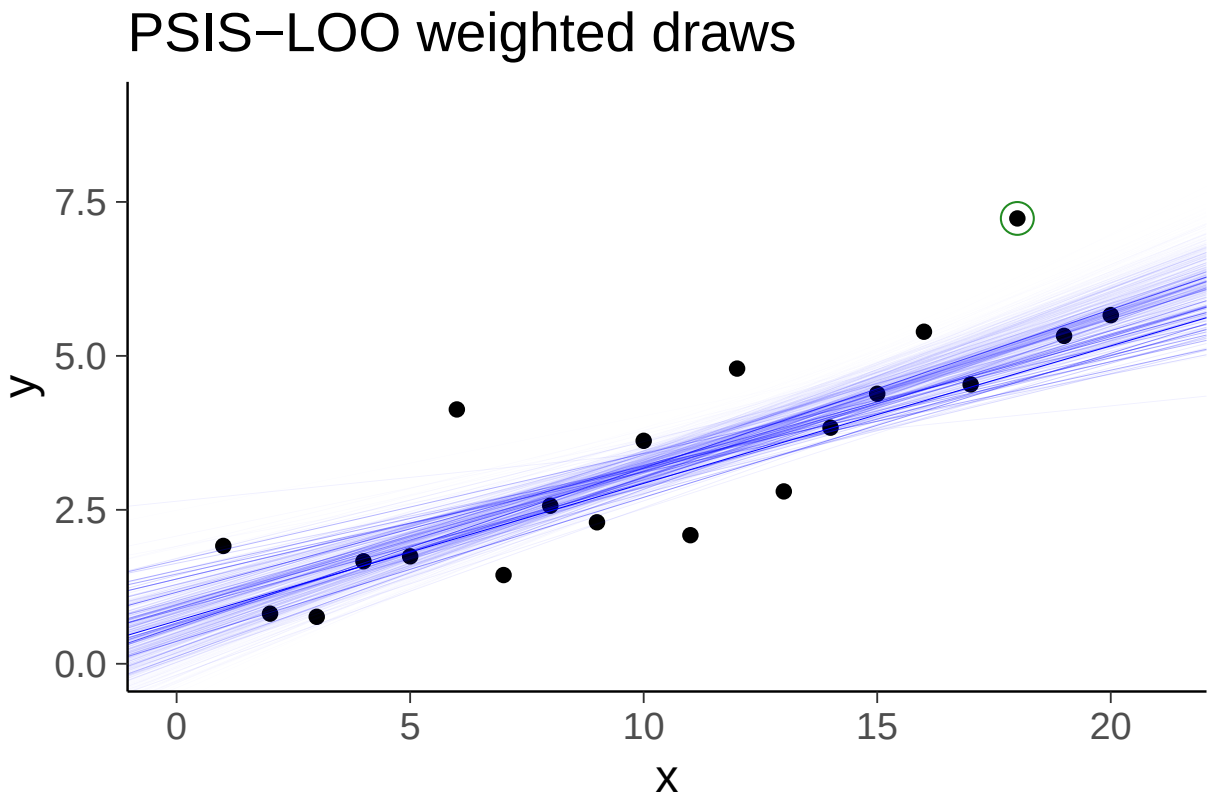

$$\theta^{(s)} \sim p(\theta|x,y)$$

$$r_i^{(s)} = p(\theta^{(s)}|x_{-i},y_{-i})/p(\theta^{(s)}|x,y)$$

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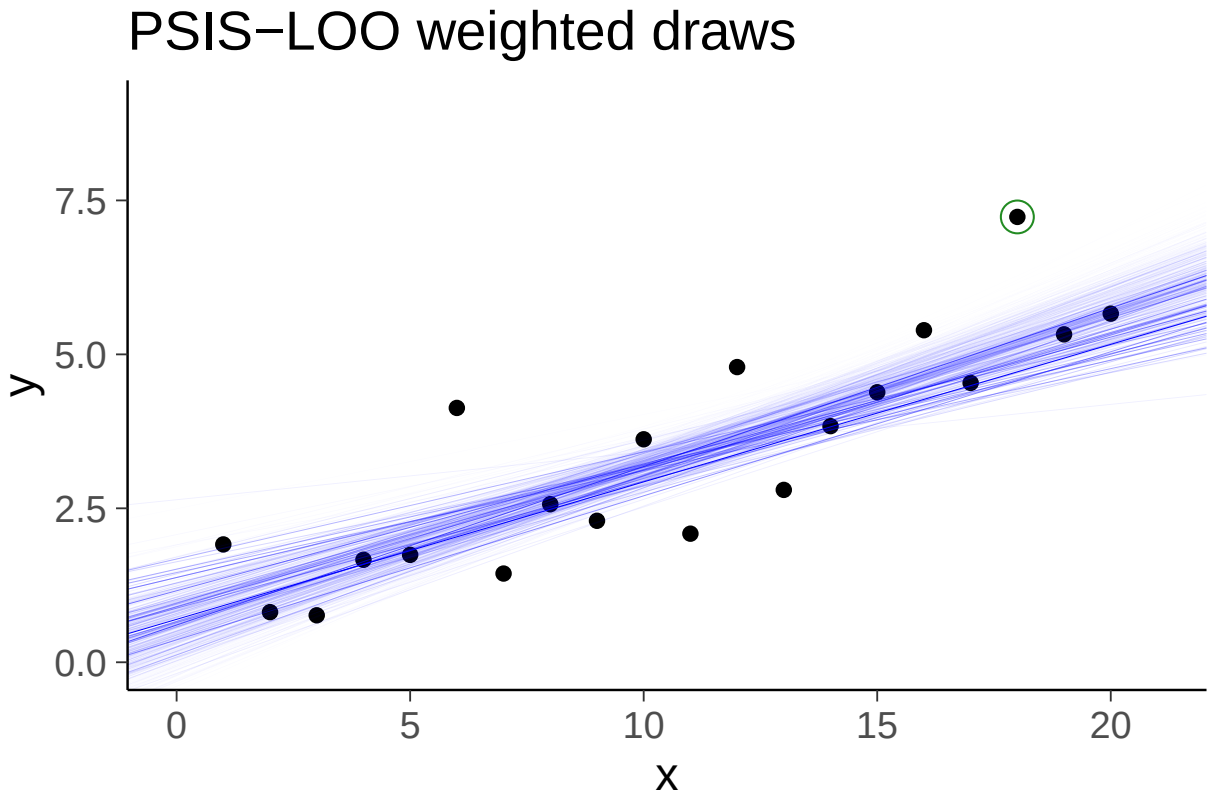

$$\theta^{(s)} \sim p(\theta|x,y)$$

$$r_i^{(s)} = p(\theta^{(s)}|x_{-i},y_{-i})/p(\theta^{(s)}|x,y) \propto 1/p(y_i|x_i,\theta^{(s)})$$

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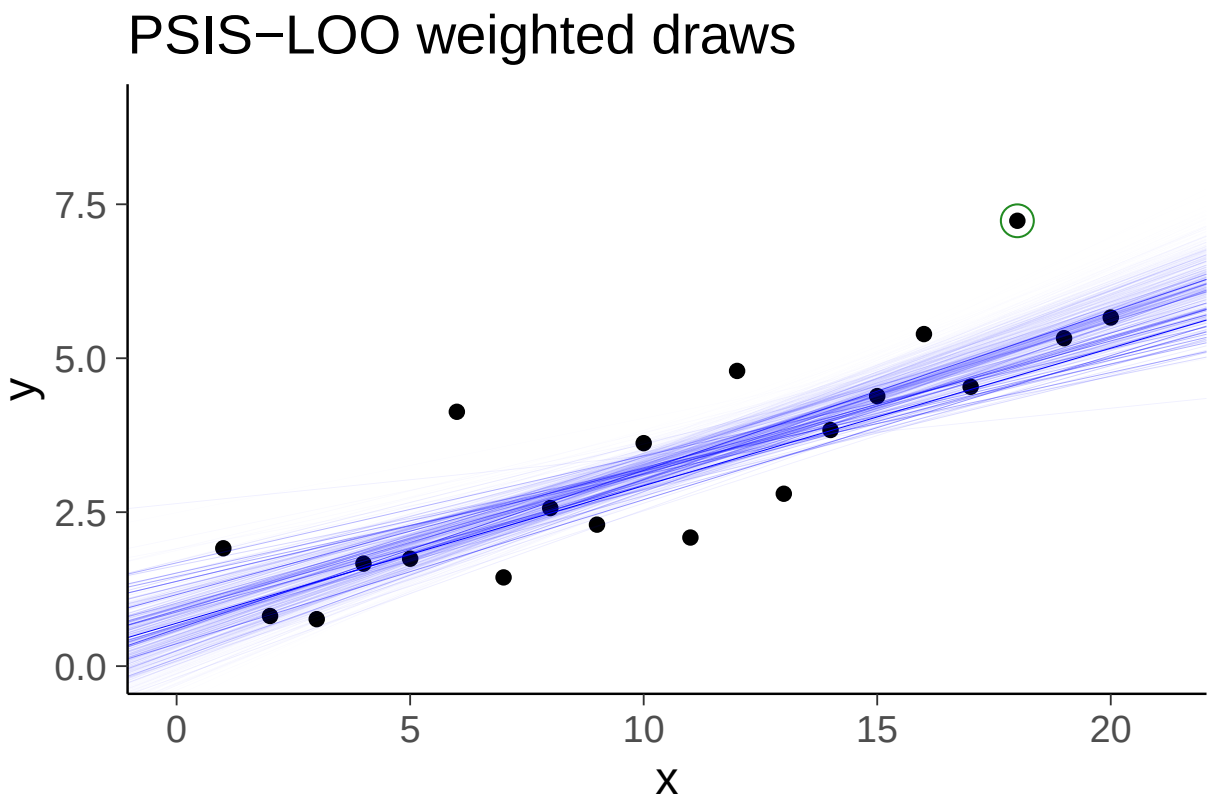

$$\theta^{(s)} \sim p(\theta|x,y)$$

$$r_i^{(s)} = p(\theta^{(s)}|x_{-i},y_{-i})/p(\theta^{(s)}|x,y) \propto 1/p(y_i|x_i,\theta^{(s)})$$

$$\log(1/p(y_i|x_i,\theta^{(s)})) = -\text{log\_lik}[i]$$

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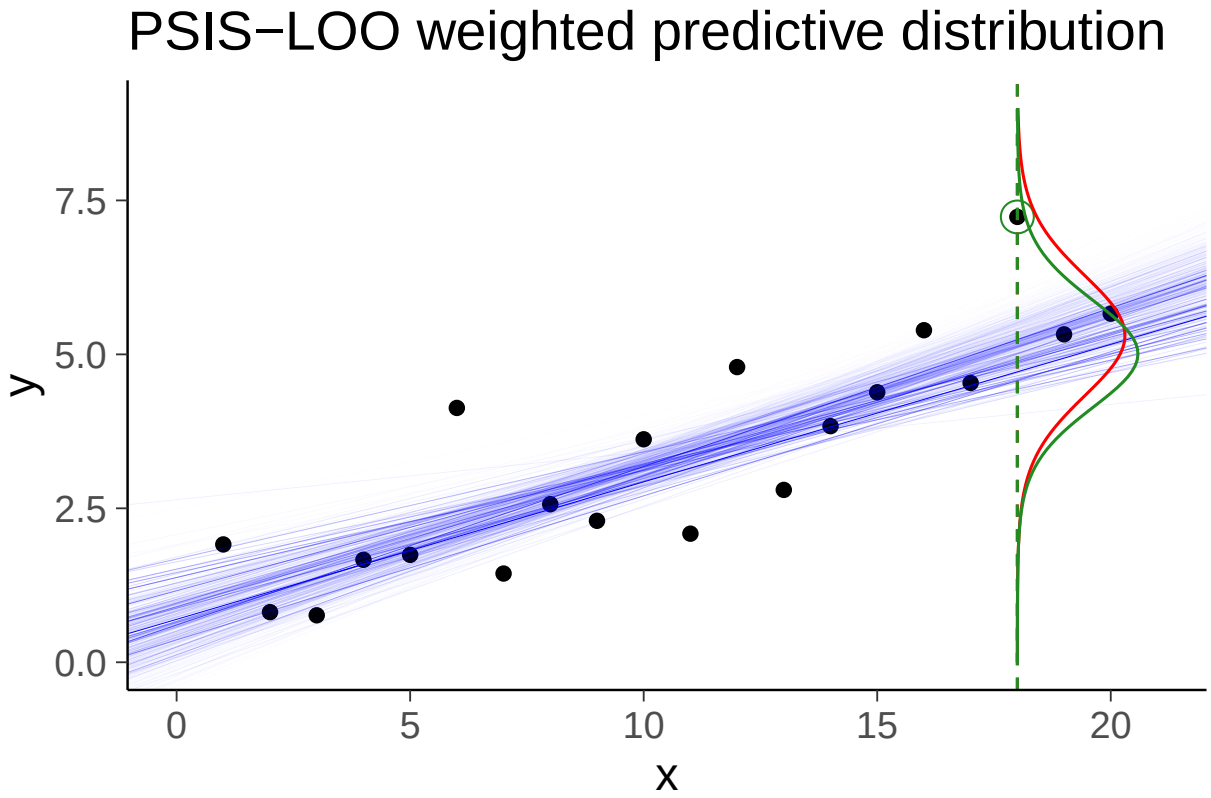

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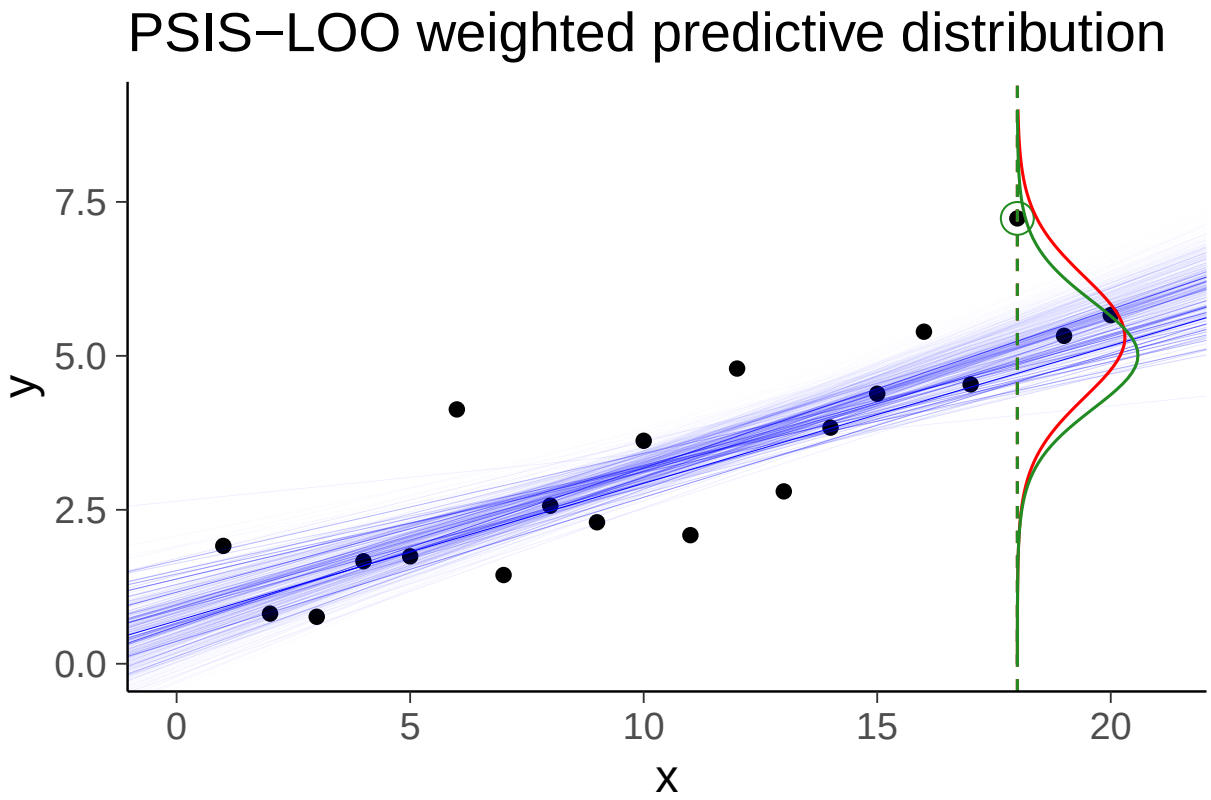

$$\theta^{(s)} \sim p(\theta|x,y)$$

$$r_i^{(s)} = p(\theta^{(s)}|x_{-i},y_{-i})/p(\theta^{(s)}|x,y) \propto 1/p(y_i|x_i,\theta^{(s)})$$

$$p(y_i|x_i,x_{-i},y_{-i}) \approx \sum_{s=1}^{S}[w_i^{(s)}p(y_i|x_i,\theta^{(s)})]$$

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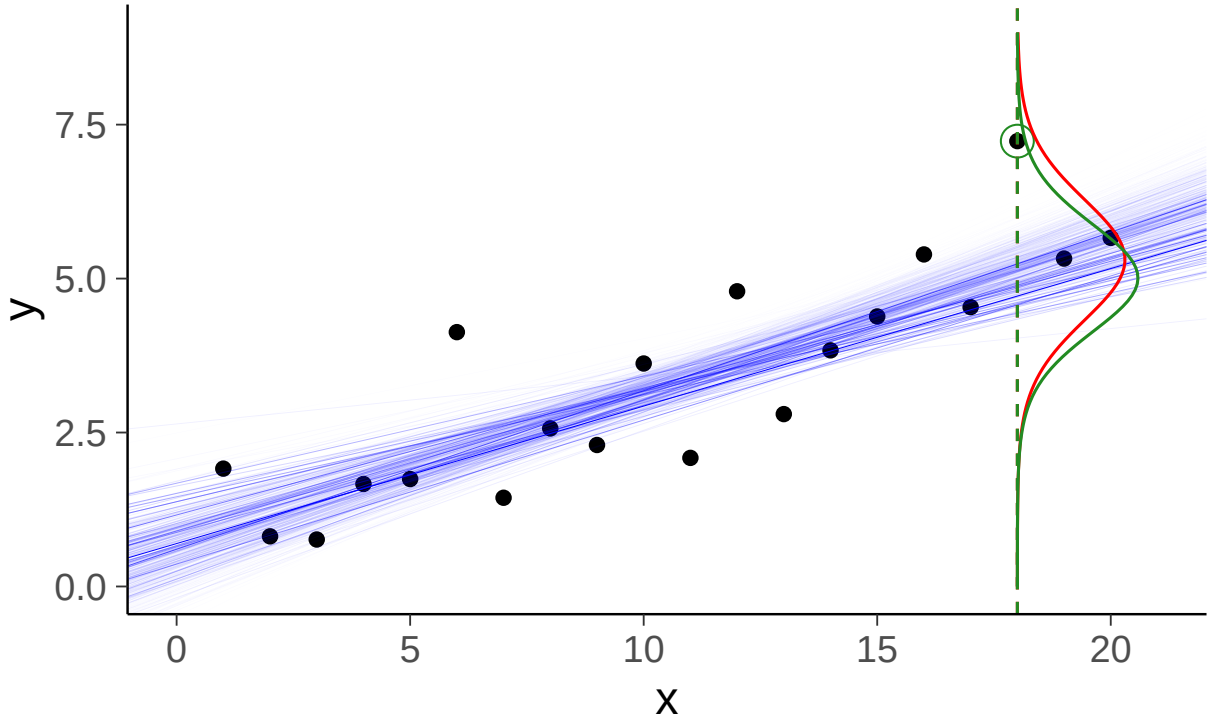
PSIS−LOO weighted predictive distribution



$\theta^{(s)} \sim p(\theta|x,y)$

$r_i^{(s)} = p(\theta^{(s)}|x_{-i},y_{-i})/p(\theta^{(s)}|x,y) \propto 1/p(y_i|x_i,\theta^{(s)})$

$p(y_i|x_i,x_{-i},y_{-i}) \approx \sum_{s=1}^{S}[w_i^{(s)}p(y_i|x_i,\theta^{(s)})]$, where $w \leftarrow \mathrm{PSIS}(r)$

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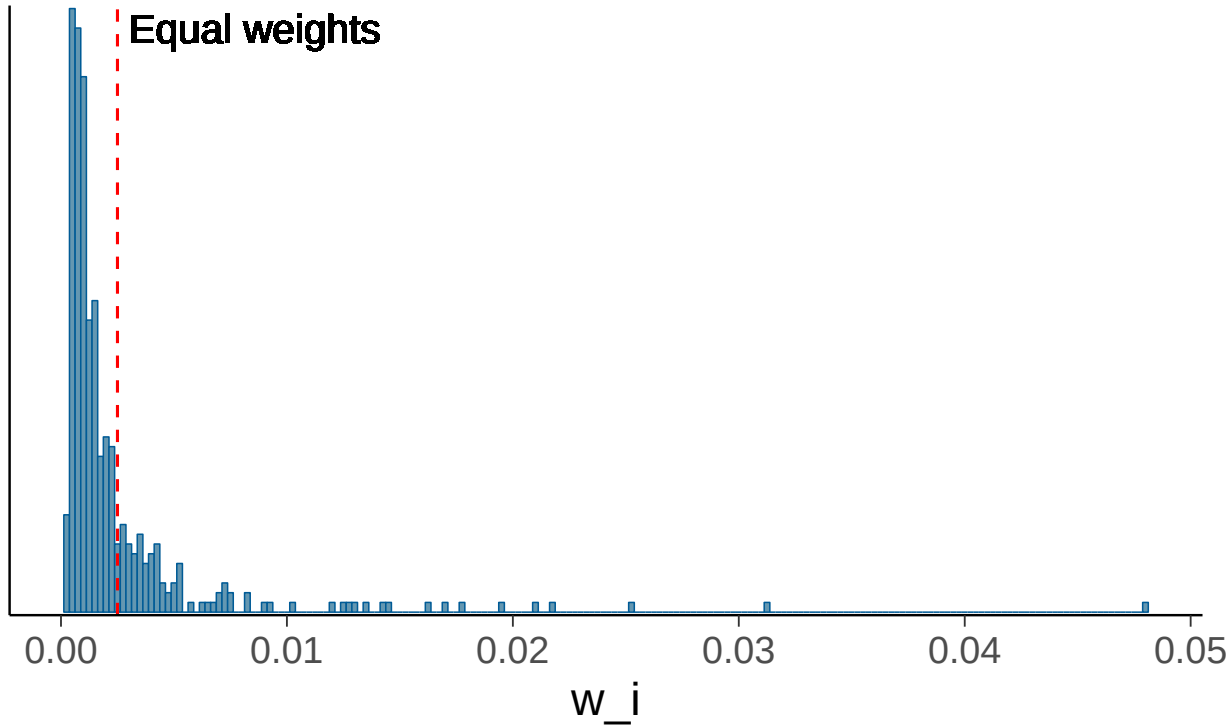
400 importance weights for leave−18th−out



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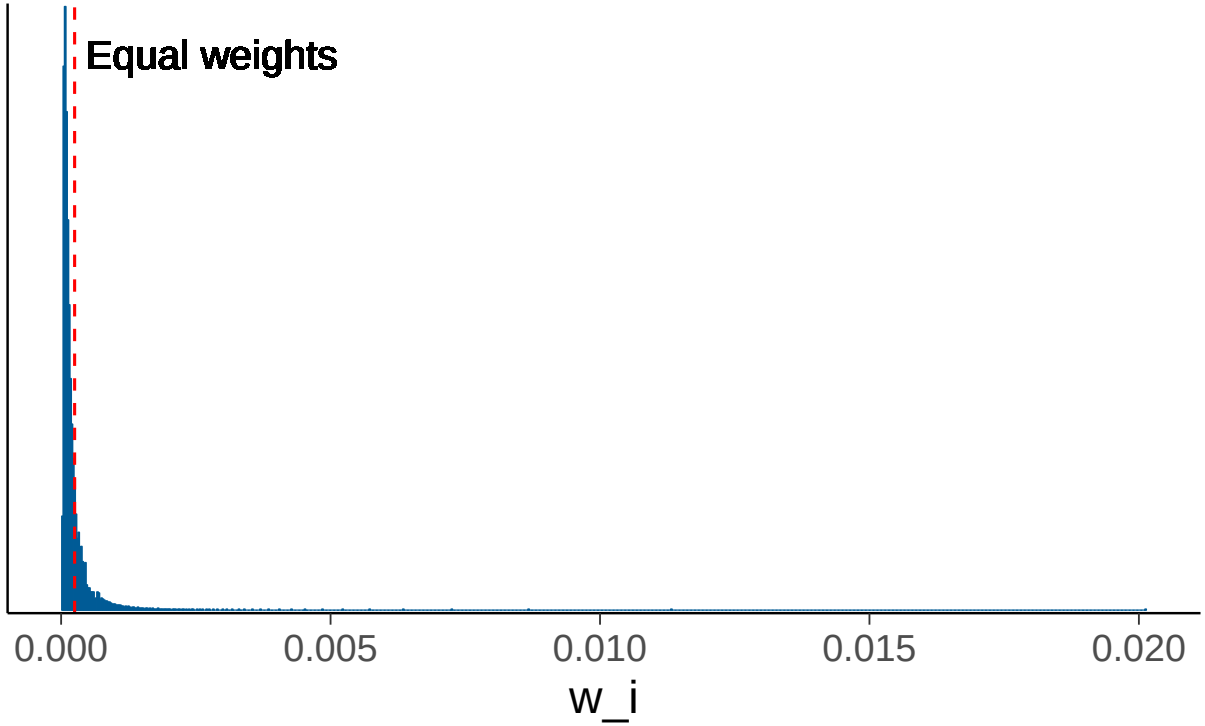
4000 importance weights for leave−18th−out



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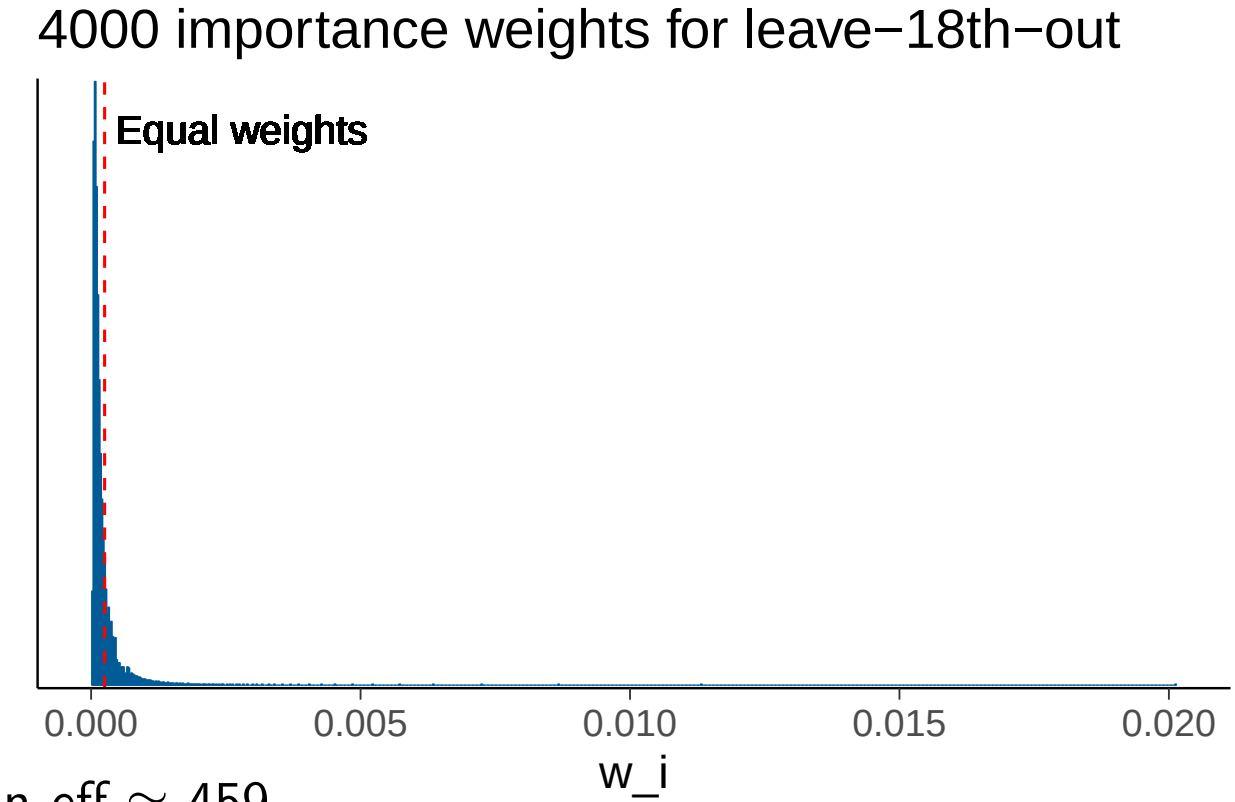

see Vehtari, Gelman & Gabry (2017b)

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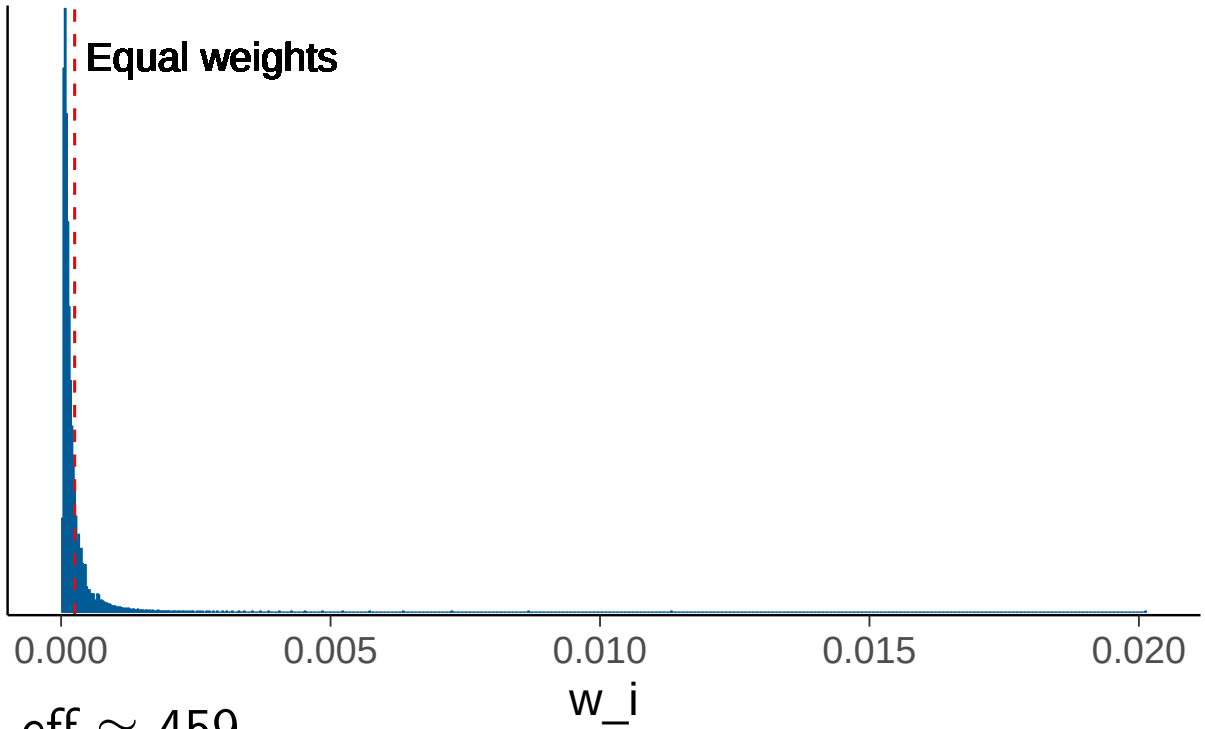

n_eff $\approx$ 459

Pareto $\hat{k} \approx 0.52$

1. Pareto $\hat{k}$ estimates the tail shape which determines the convergence rate of PSIS. Less than 0.7 is ok.

see Vehtari, Gelman & Gabry (2017b)

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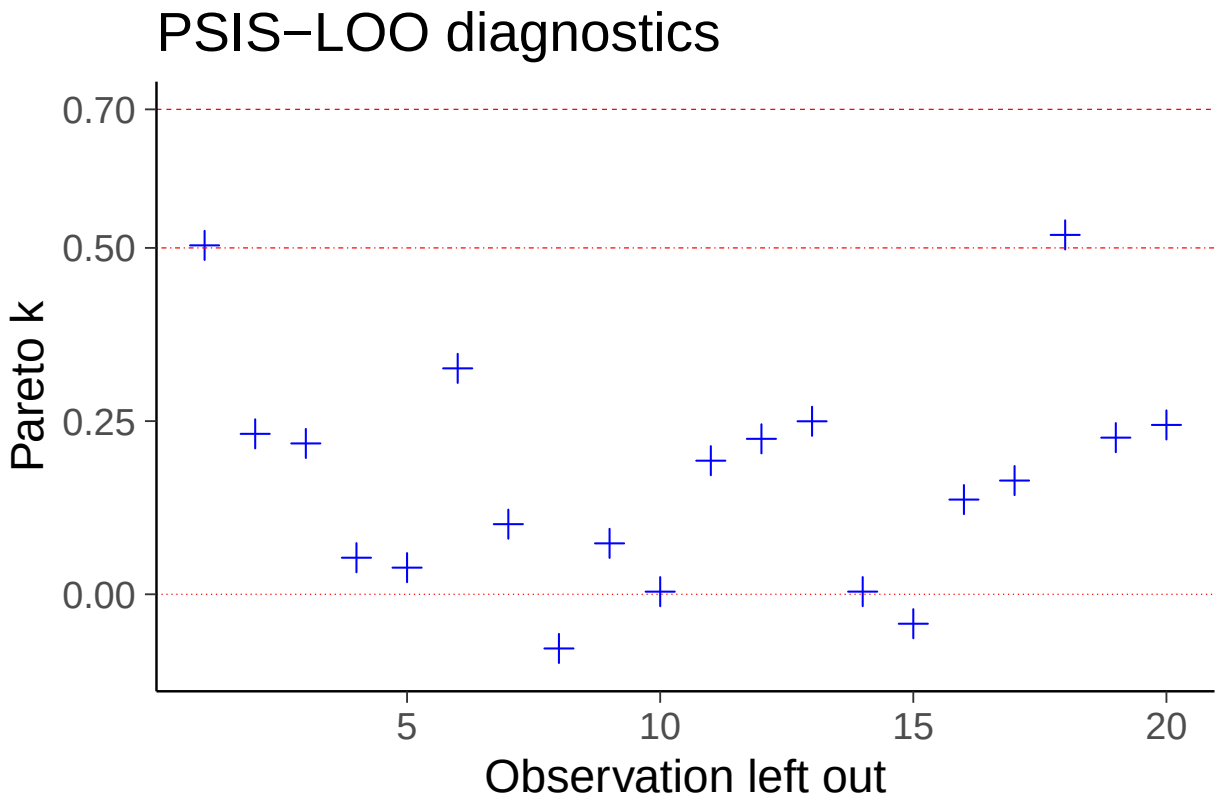

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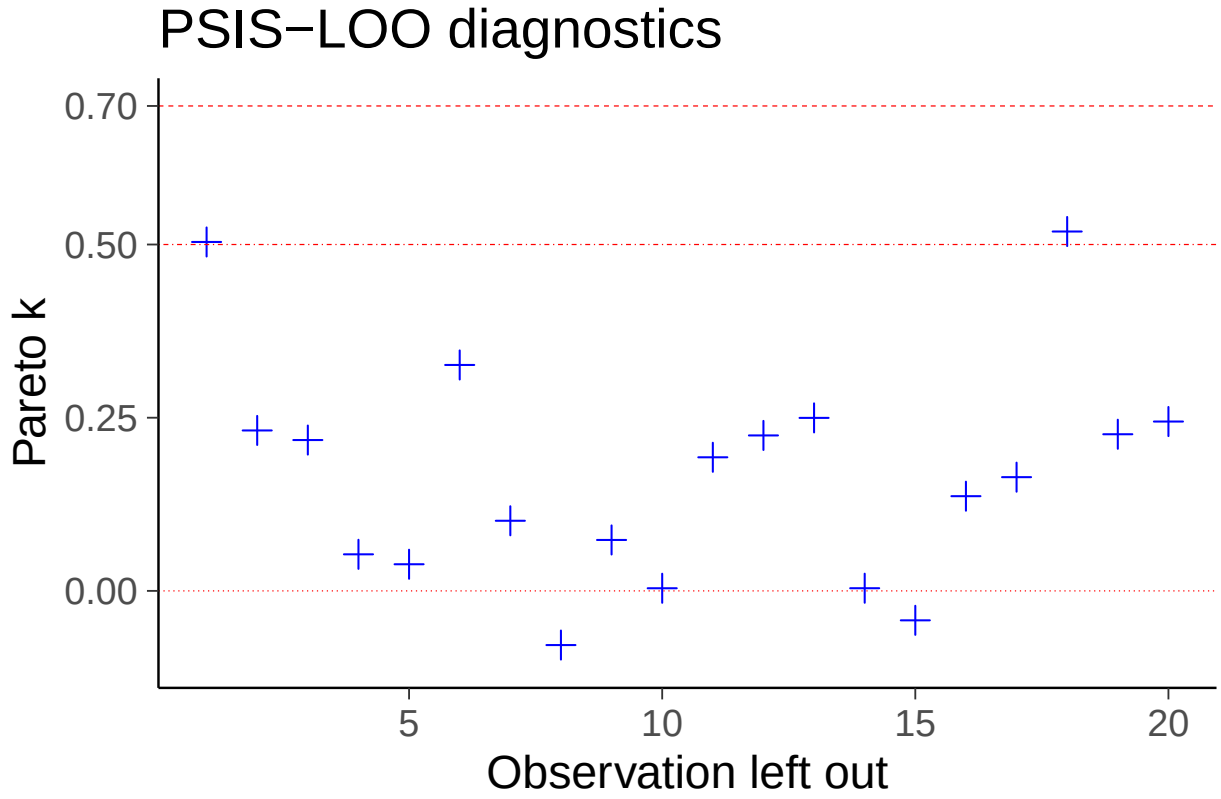


```
Pareto k diagnostic values:
                         Count Pct.    Min. n_eff
(-Inf, 0.5]   (good)     18    90.0%   899
 (0.5, 0.7]   (ok)        2    10.0%   459
   (0.7, 1]   (bad)       0     0.0%   <NA>
   (1, Inf)   (very bad)  0     0.0%   <NA>
```

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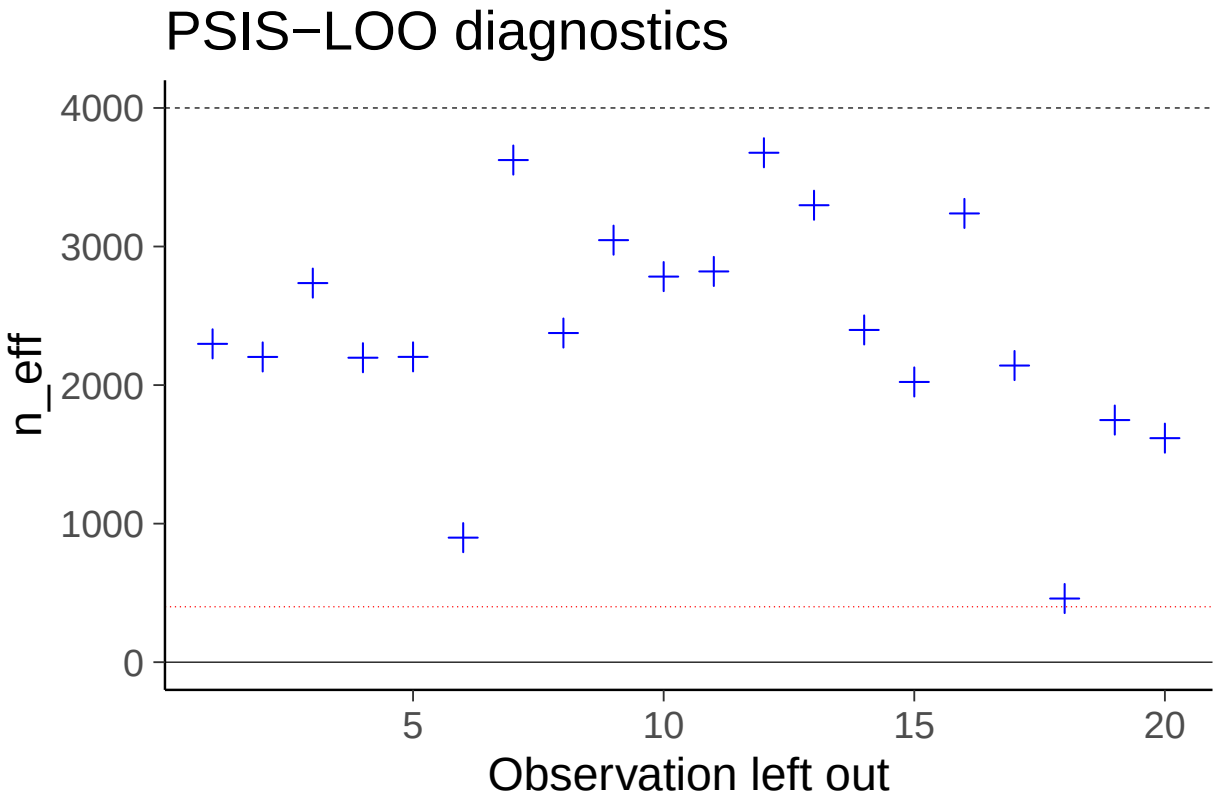


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```

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loo package

```
Computed from 4000 by 20 log-likelihood matrix

          Estimate  SE
elpd_loo    -29.5 3.3
p_loo         2.7 1.0

------

Monte Carlo SE of elpd_loo is 0.1.

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All Pareto k estimates are ok (k < 0.7).
See help('pareto-k-diagnostic') for details.
```

see more in Vehtari, Gelman & Gabry (2017b)

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Stan and loo package

```
 Computed from 4000 by 20 log-likelihood matrix

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See help('pareto-k-diagnostic') for details.

Model comparison:
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff        se
     -0.2       0.1
```

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loo package

```
Computed from 4000 by 20 log-likelihood matrix

          Estimate  SE
elpd_loo    -29.5 3.3
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Importance sampling

- Having samples θ^s from $p(\theta^s|D)$

$$p(\tilde{y}_i|x_i, D_{-i}) \approx \frac{\sum_{s=1}^{S} p(\tilde{y}_i|\theta^s) w_i^s}{\sum_{s=1}^{S} w_i^s},$$

where w_i^s are importance weights and

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- If evaluated with $\tilde{y}_i = y_i$

$$p(y_i|x_i, D_{-i}) \approx \frac{1}{\sum_{s=1}^{S} \frac{1}{p(y_i|\theta^s)}},$$

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Stan code

$$\log(r_i^{(s)}) = \log(1/p(y_i|x_i, \theta^{(s)})) = -\text{log\_lik}[i]$$

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Stan code

$$\log(r_i^{(s)}) = \log(1/p(y_i|x_i, \theta^{(s)})) = -\text{log\_lik}[i]$$

```
...
model {
  alpha ~ normal(pmualpha, psalpha);
  beta ~ normal(pmubeta, psbeta);
  y ~ normal(mu, sigma);
}
generated quantities {
  vector[N] log_lik;
  for (i in 1:N)
    log_lik[i] = normal_lpdf(y[i] | mu[i], sigma);
}
```

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Pareto smoothed importance sampling LOO

1. PSIS-LOO for hierarchical models
   1.1 leave-one-group out is challenging for PSIS-LOO

   see Merkel, Furr and Rabe-Hesketh (2018) for an approach using quadrature integration

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   2.1 `mc-stan.org/loo/articles/loo2-non-factorizable.html`

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Pareto smoothed importance sampling LOO

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2. PSIS-LOO for non-factorizable models
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3. PSIS-LOO for time series
   - 3.1 Approximate leave-future-out cross-validation

     mc-stan.org/loo/articles/loo2-lfo.html

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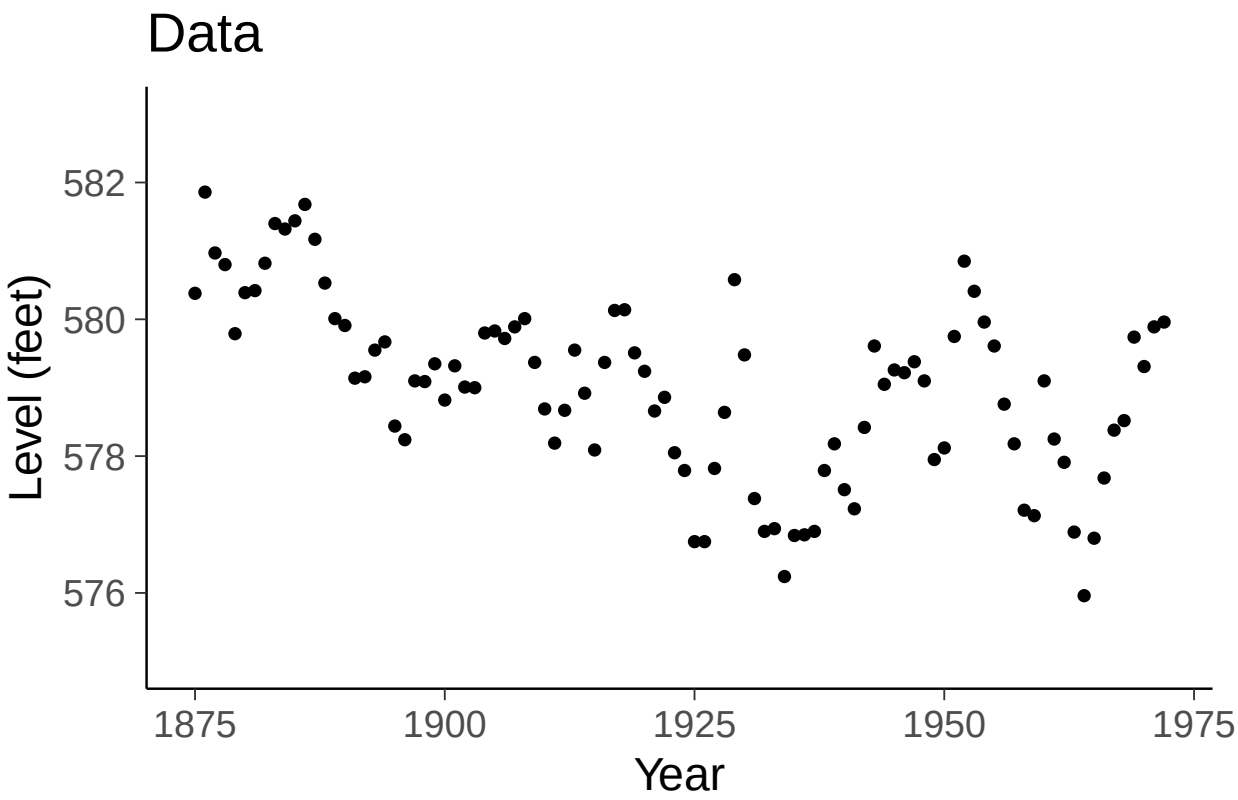
PSIS-LOO for time series



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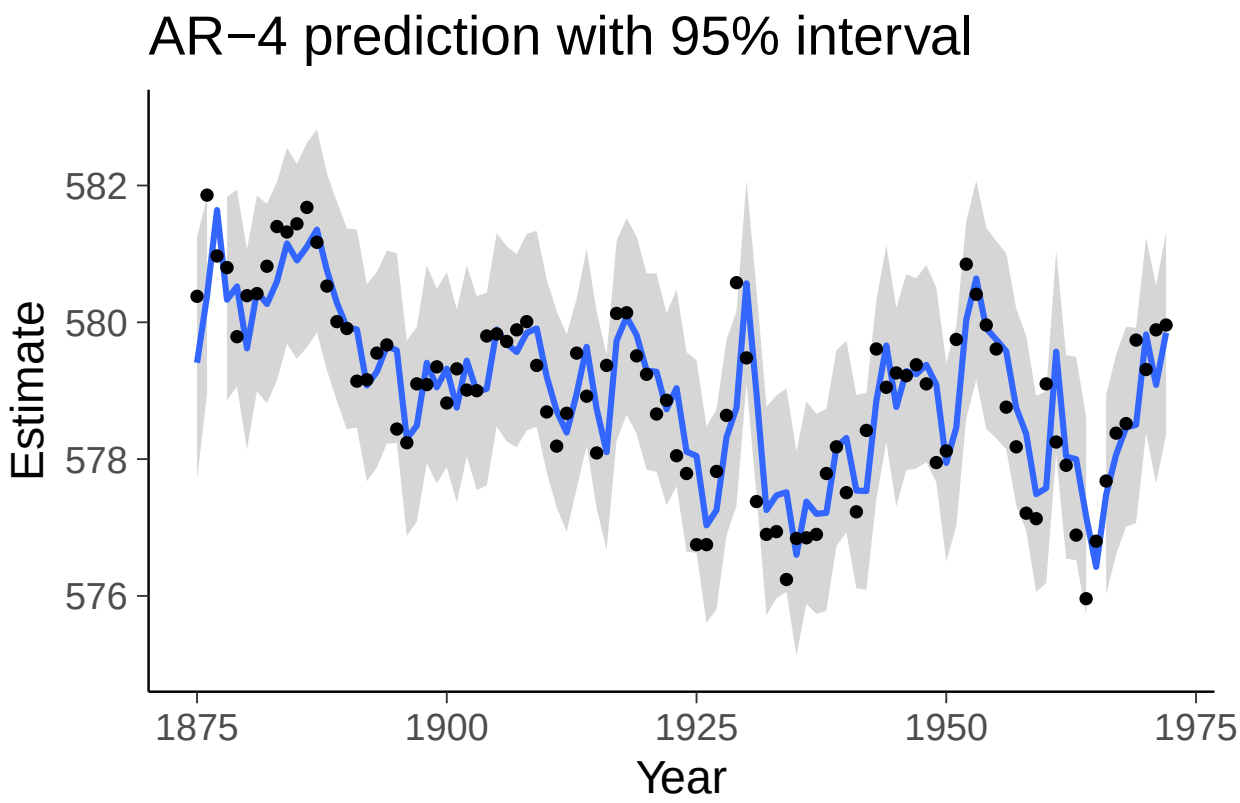
PSIS-LOO for time series



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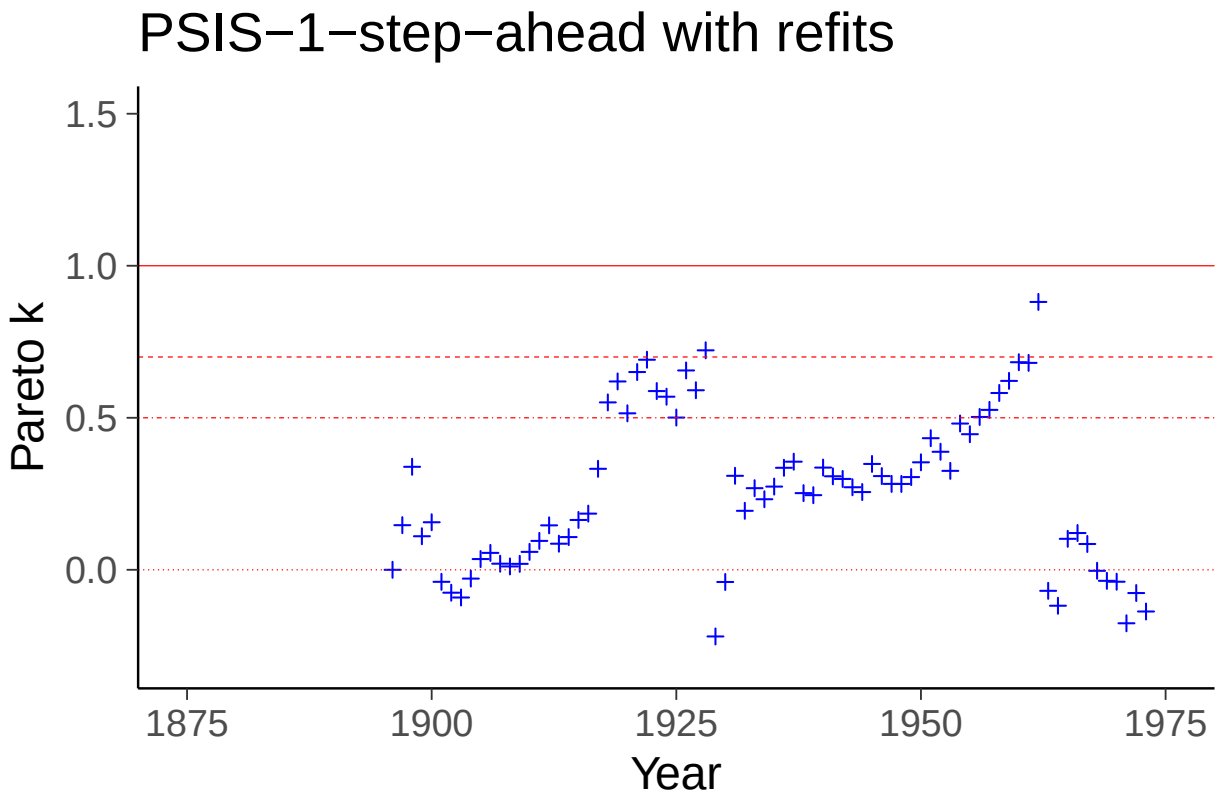
PSIS-LOO for time series



mc-stan.org/loo/articles/loo2-lfo.html

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K-fold cross-validation

1. K-fold cross-validation can approximate LOO
   1.1 all uses for LOO
2. K-fold cross-validation can be used for hierarchical models
   2.1 good for leave-one-group-out
3. K-fold cross-validation can be used for time series
   3.1 with leave-block-out

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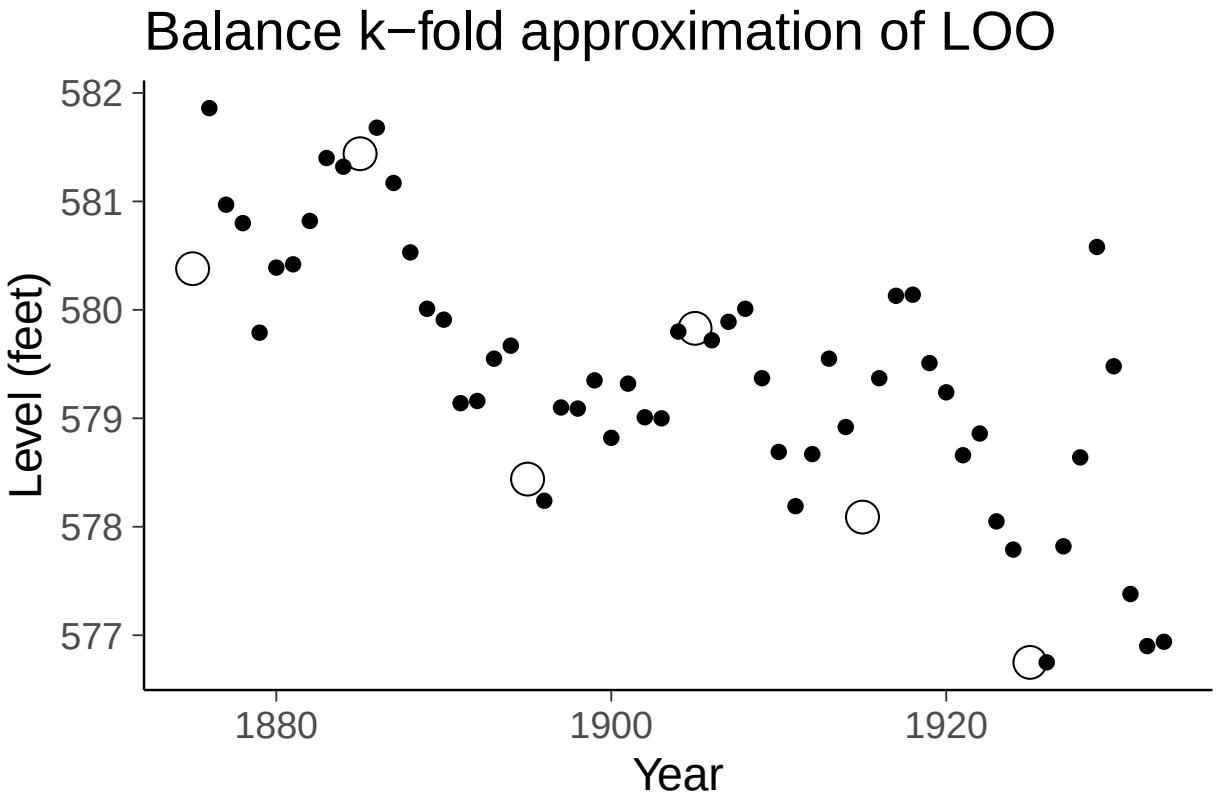

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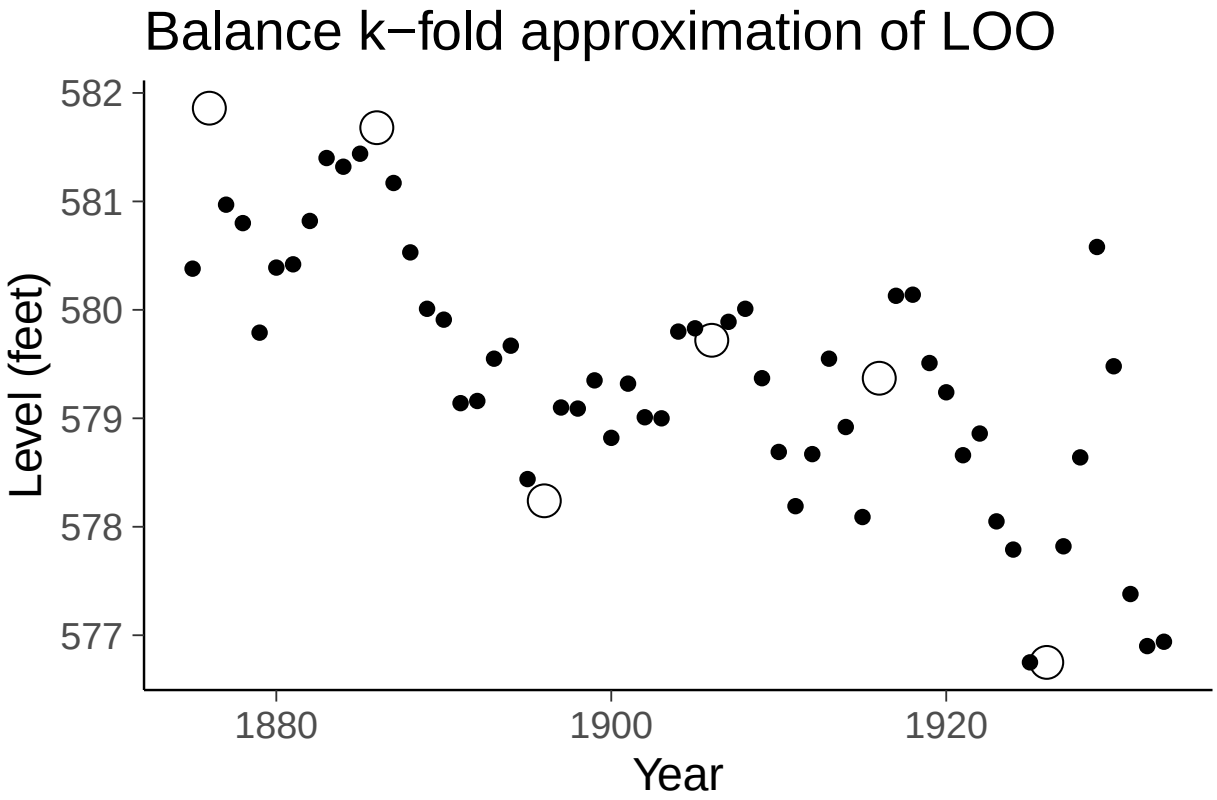

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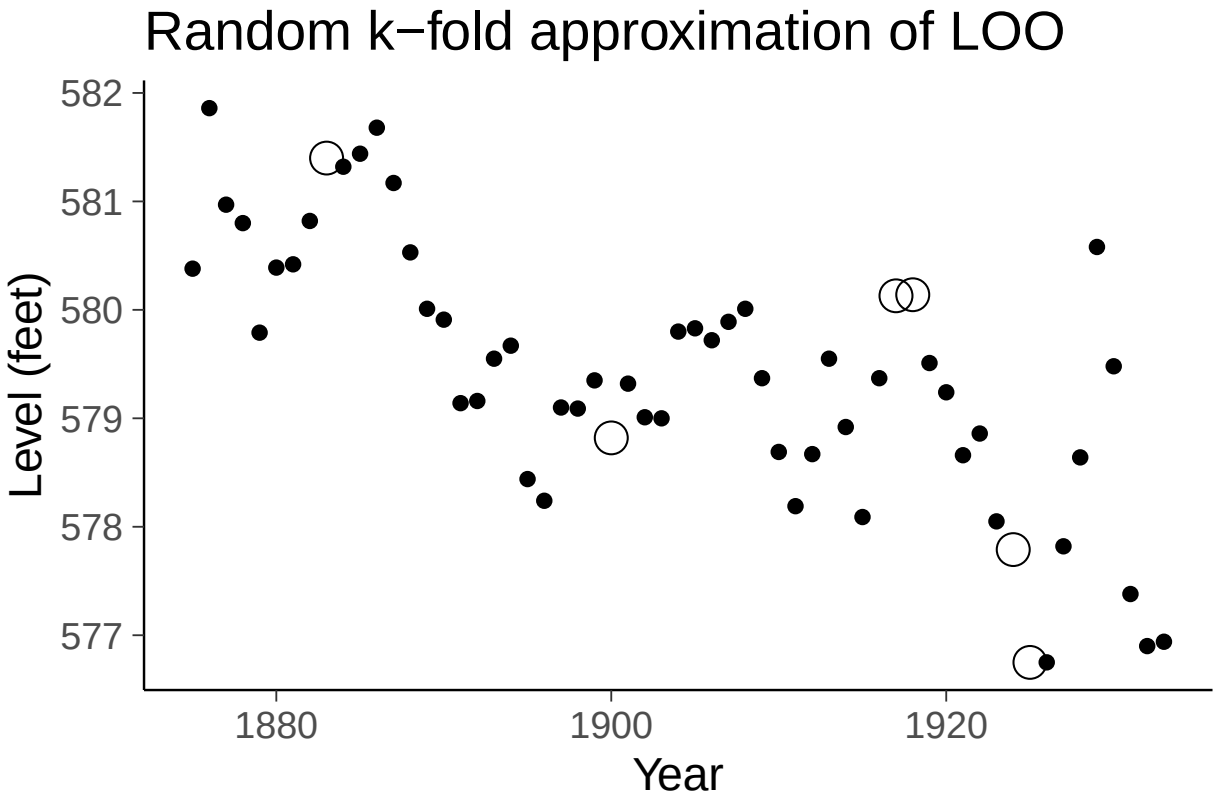

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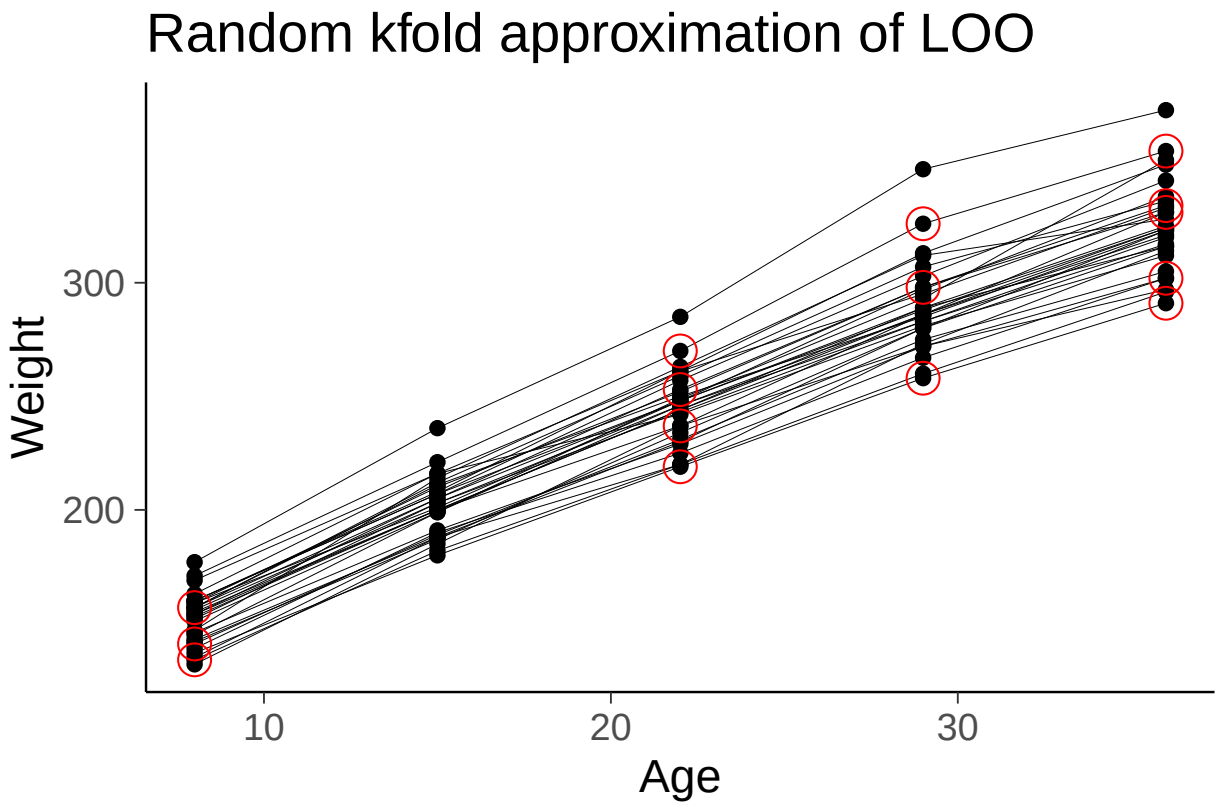

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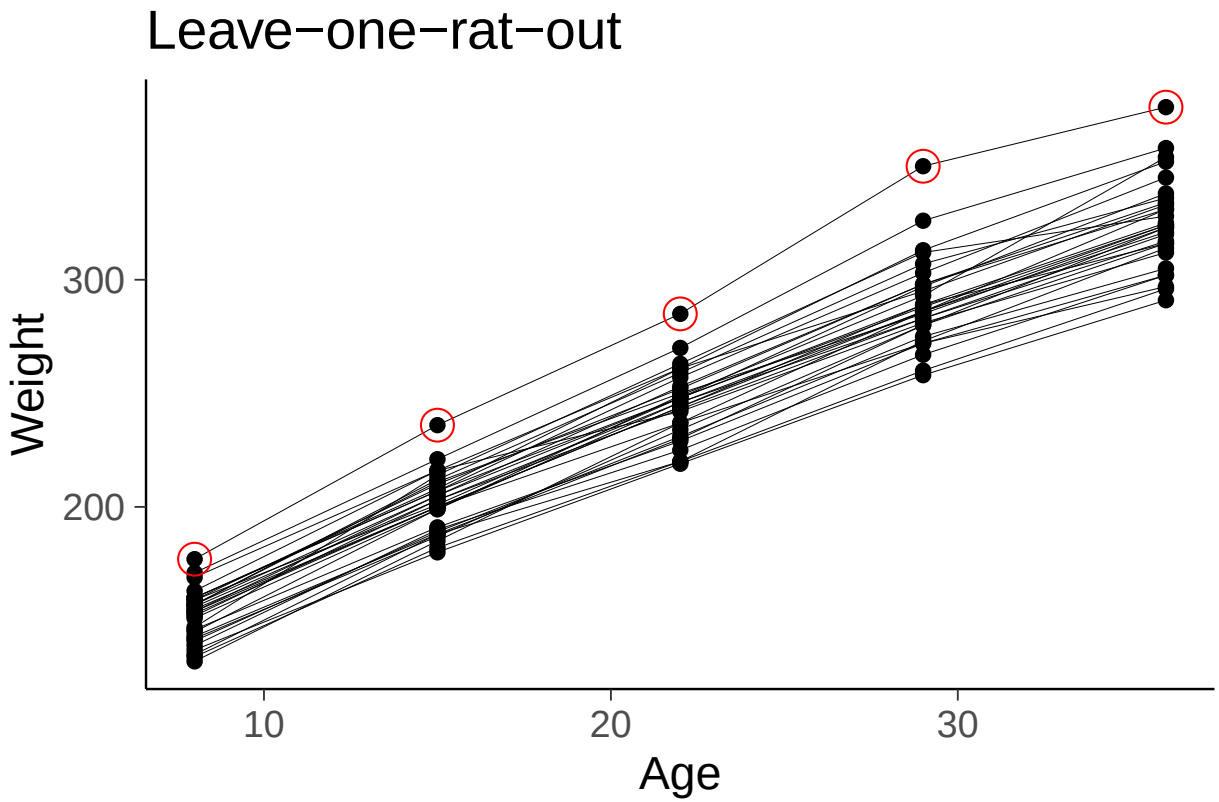

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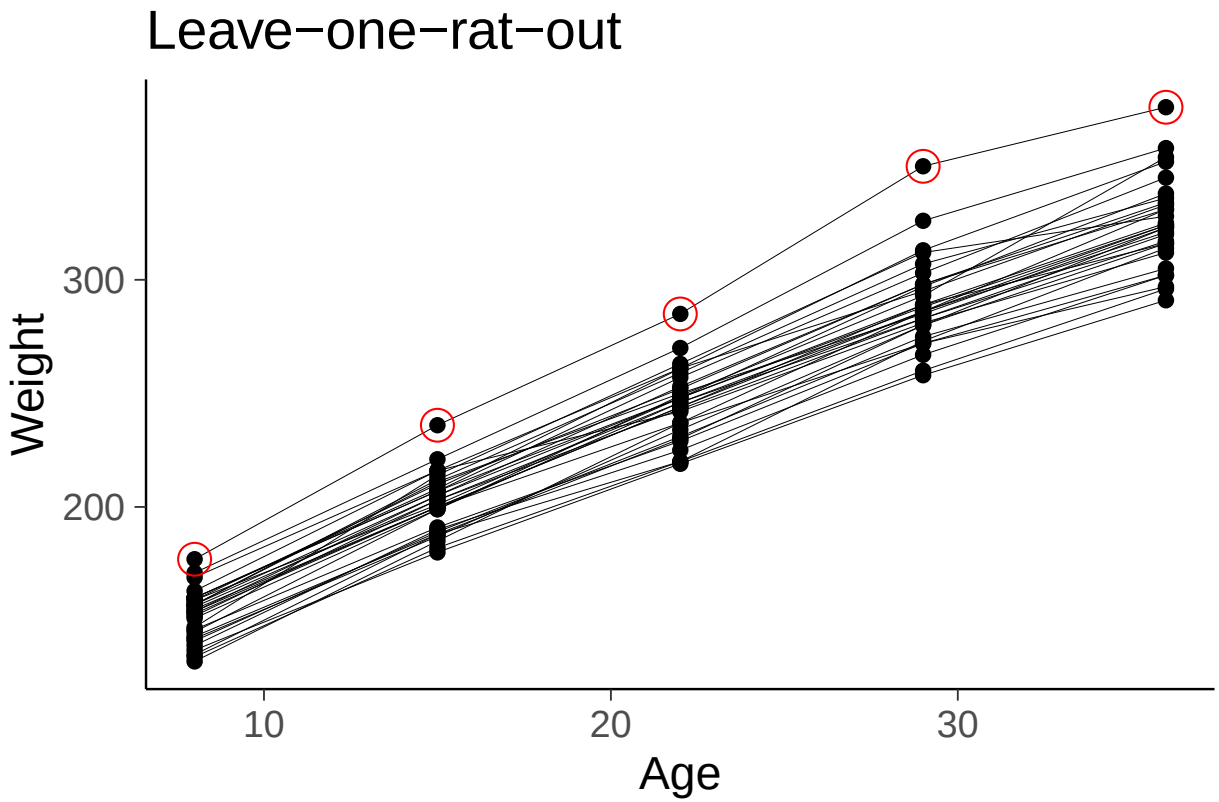

kfold_split_random()

kfold_split_balanced()

kfold_split_stratified()

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Cross-validation for model assessment

1. CV is good for model assessment when application specific utility/cost functions are used
   1.1 e.g. 90% absolute error

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Cross-validation for model assessment

1. CV is good for model assessment when application specific utility/cost functions are used
   - 1.1 e.g. 90% absolute error
2. Also useful in model checking in similar way as posterior predictive checking (PPC)
   - 2.1 model misspecification diagnostics (e.g. Pareto-k and p_loo)
   - 2.2 checking calibration of leave-one-out predictive posteriors (ppc_loo_pit in bayesplot)

see demos avehtari.github.io/modelselection/

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Model comparison

1. "A popular hypothesis has it that primates with larger brains produce more energetic milk, so that brains can grow quickly" (from Statistical Rethinking)
   - 1.1 Model 1: formula = kcal.per.g $\sim$ neocortex
   - 1.2 Model 2: formula = kcal.per.g $\sim$ neocortex + log(mass)

mc-stan.org/loo/articles/loo2-example.html

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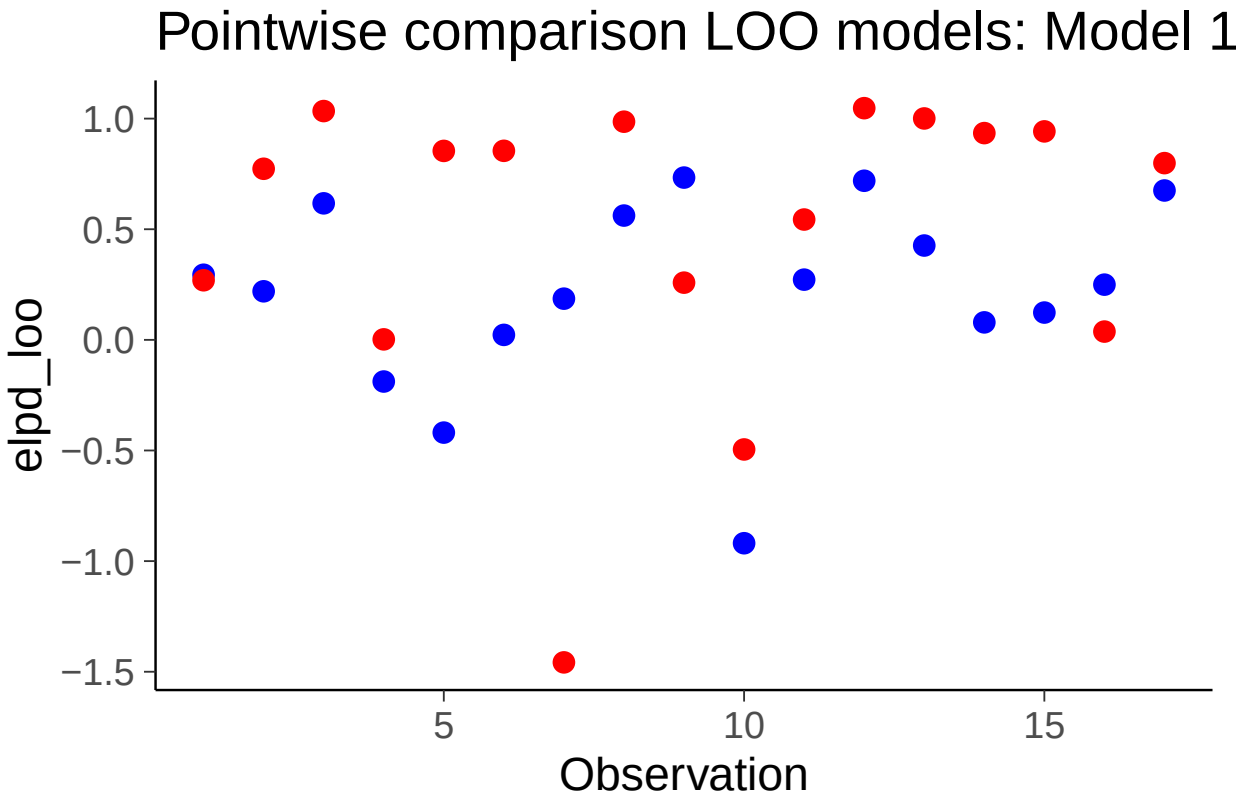

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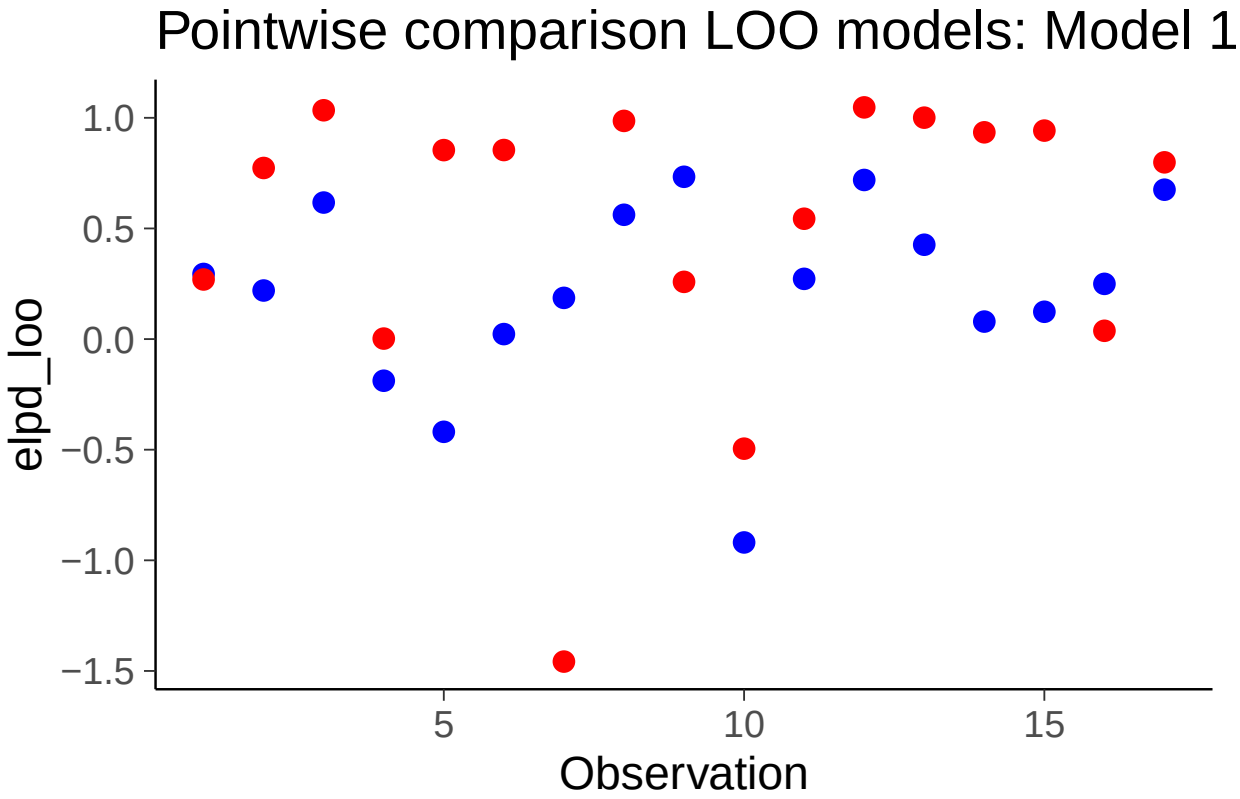

Model 1 elpd_loo $\approx$ 3.7, SE=1.8
Model 2 elpd_loo $\approx$ 8.4, SE=2.8

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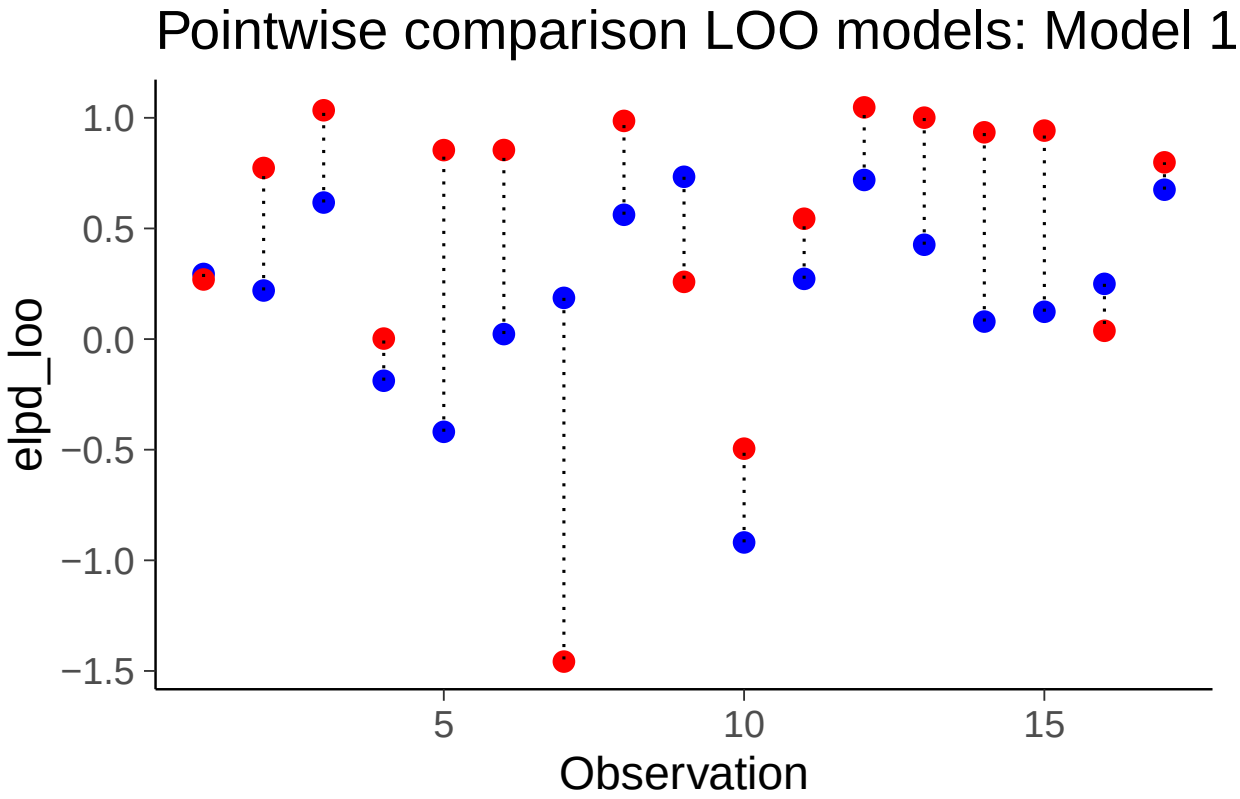

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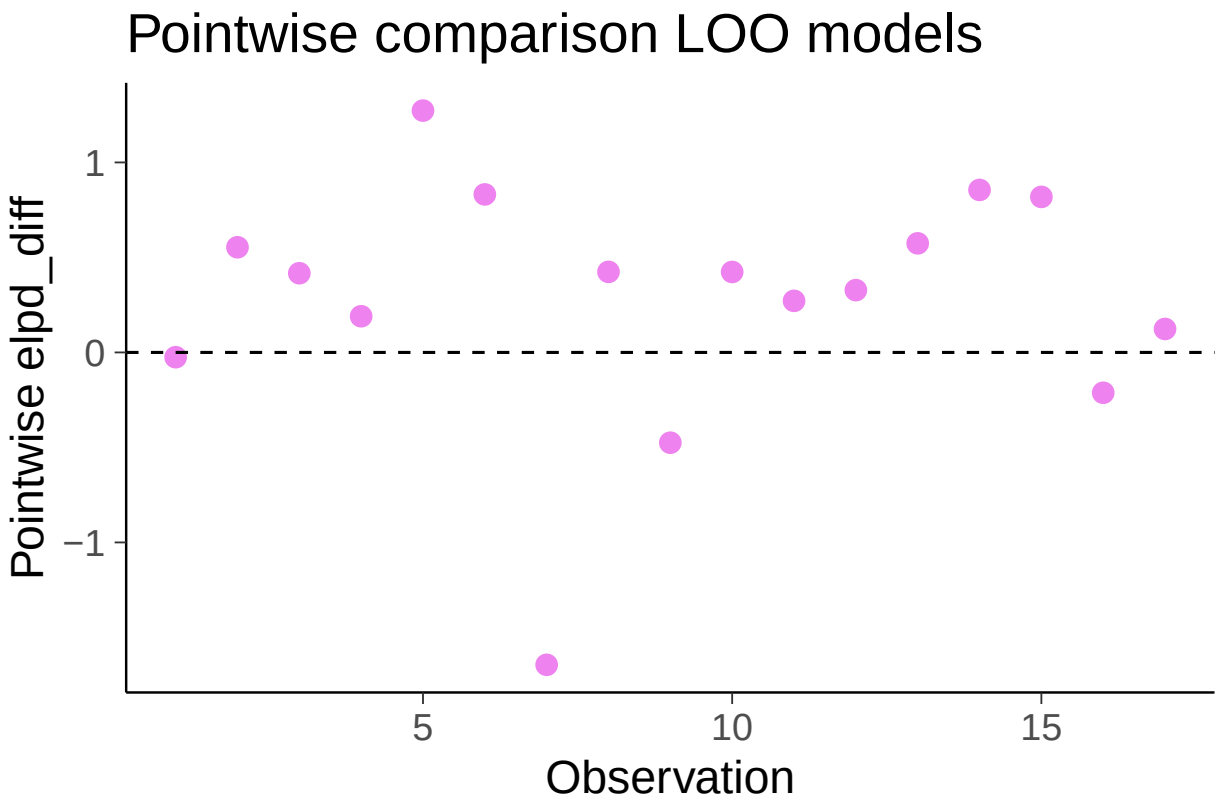


```
Model comparison:
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff         se
      4.7        2.7
```

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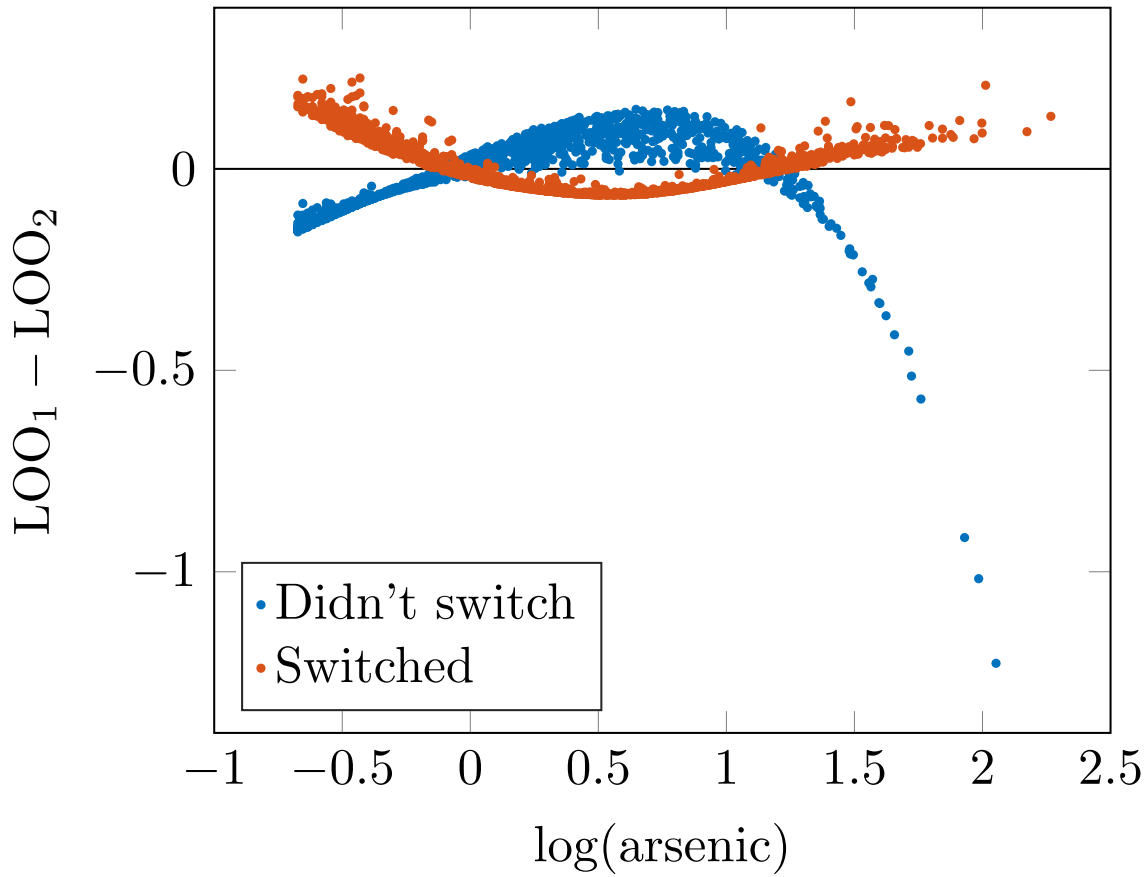
Arsenic well example – Model comparison



An estimated difference in $\mathrm{elpd}_{\mathrm{loo}}$ of 16.4 with SE of 4.4.

see Vehtari, Gelman & Gabry (2017a)

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Arsenic well example – Model comparison

1. Probability of switching well with high arsenic level in rural Bangladesh
   - 1.1 Model 1 covariates: log(arsenic) and distance
   - 1.2 Model 2 covariates: log(arsenic), distance and education level

Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 13.

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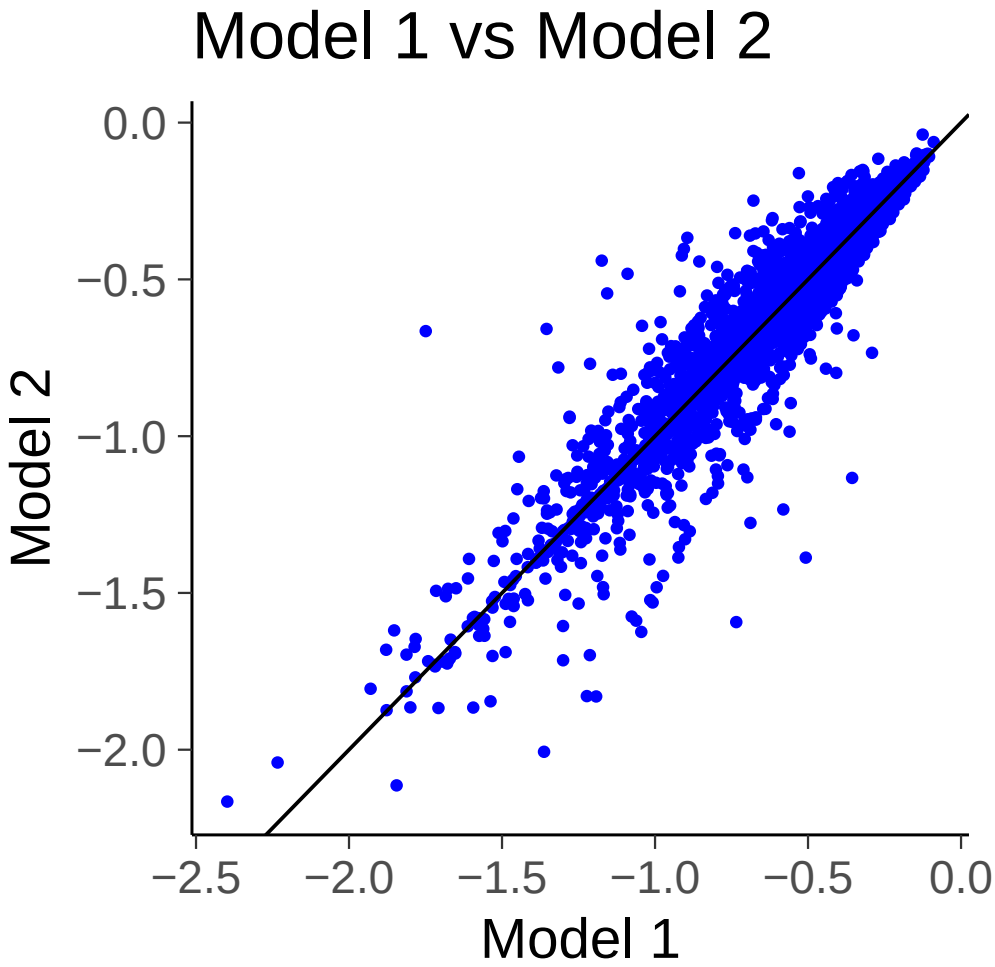
Arsenic well example – Model comparison



Model 1 elpd_loo ≈ -1952, SE=16
Model 2 elpd_loo ≈ -1938, SE=17

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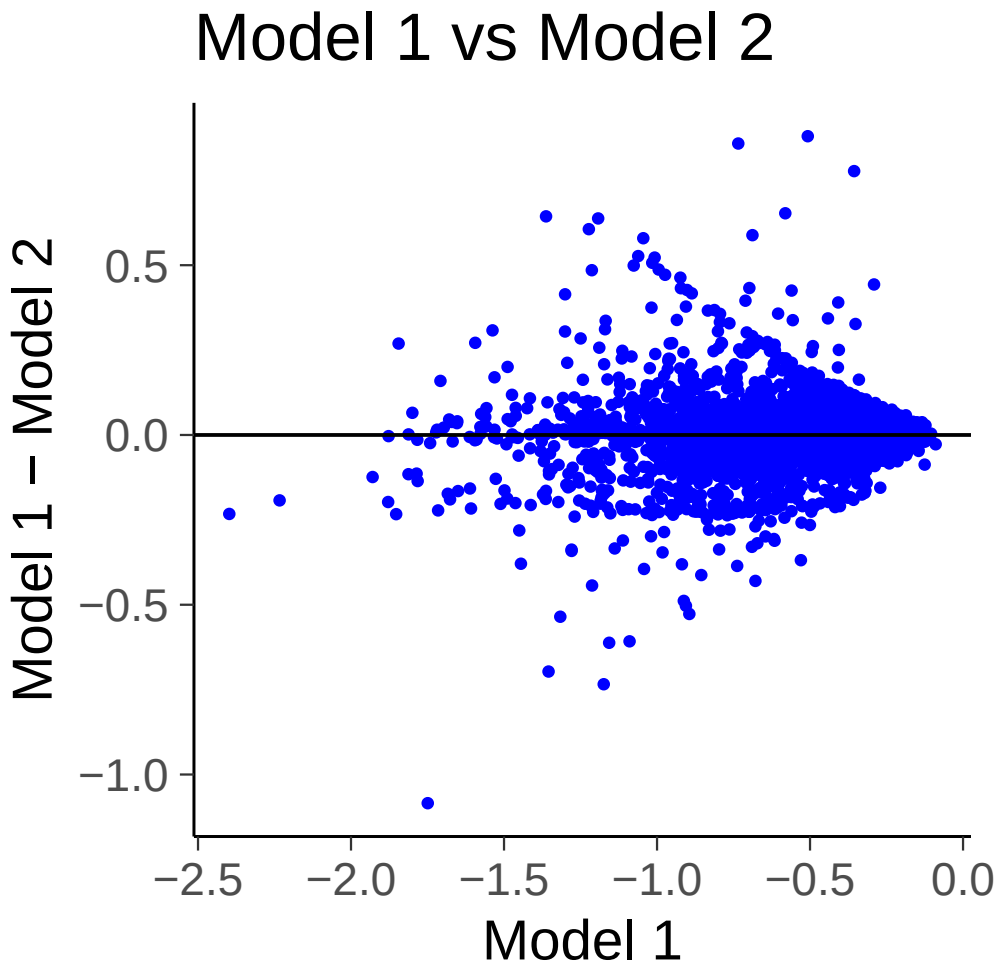
Arsenic well example – Model comparison




```
> loo_compare(model1, model2)
       elpd_diff se_diff
model2    0.0       0.0
model1  −14.4       6.1
```

see Vehtari, Gelman & Gabry (2017a)

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Arsenic well example – Model comparison

```
> loo_compare(model1, model2)
       elpd_diff se_diff
model2    0.0       0.0
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```

`se_diff` and normal approximation for the uncertainty in the difference is good only if models are well specified and the number of observations is relatively big (more details in a forthcoming article).

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What if one is not clearly better than others?

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What if one is not clearly better than others?

1. Continuous expansion including all models?
   - 1.1 and then analyse the posterior distribution directly
     avehtari.github.io/modelselection/betablockers.html
   - 1.2 sparse priors like regularized horseshoe prior instead of variable selection
     video, refs and demos at
     avehtari.github.io/modelselection/

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4. In a nested case choose more complex if you want to take into account all the uncertainties.
   andrewgelman.com/2018/07/26/parsimonious-principle-vs-integration-uncertainties/

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Cross-validation and model selection

1. Cross-validation can be used for model selection if
   1.1 small number of models
   1.2 the difference between models is clear

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   - 2.1 selection process leads to overfitting

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   - 1.1 small number of models
   - 1.2 the difference between models is clear
2. Do not use cross-validation to choose from a large set of models
   - 2.1 selection process leads to overfitting
3. Overfitting in selection process is not unique for cross-validation

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Selection induced bias and overfitting

- Selection induced bias in cross-validation
  - same data is used to assess the performance and make the selection
  - the selected model fits more to the data
  - the CV estimate for the selected model is biased
  - recognized already, e.g., by Stone (1974)

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  - the selected model fits more to the data
  - the CV estimate for the selected model is biased
  - recognized already, e.g., by Stone (1974)
- Performance of the selection process itself can be assessed using two level cross-validation, but it does not help choosing better models
- Bigger problem if there is a large number of models as in covariate selection

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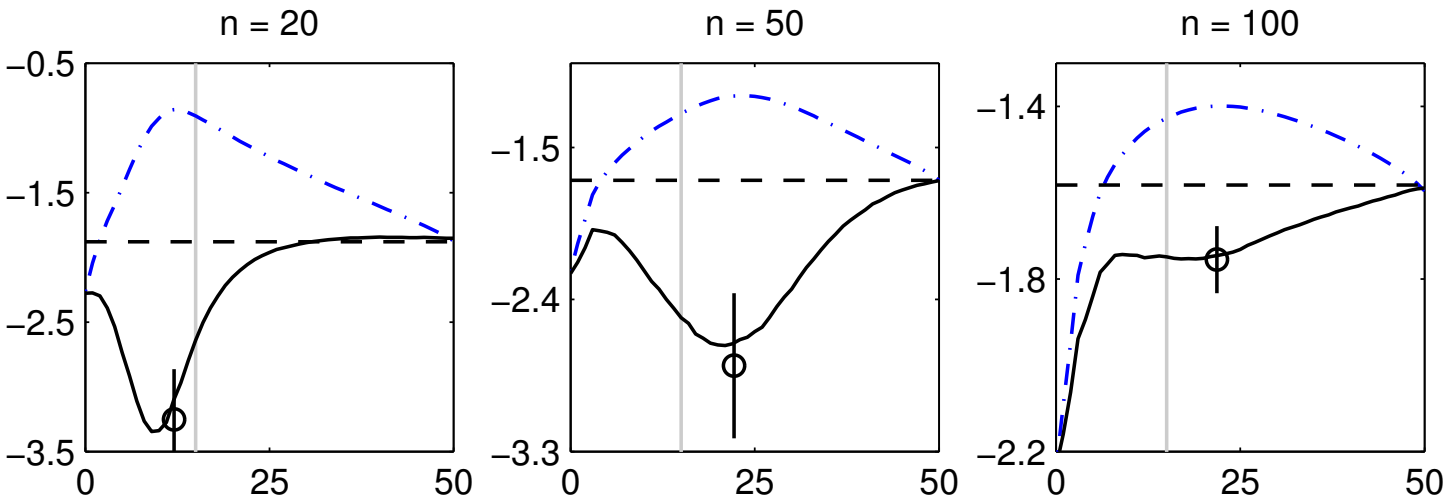
Selection induced bias in variable selection



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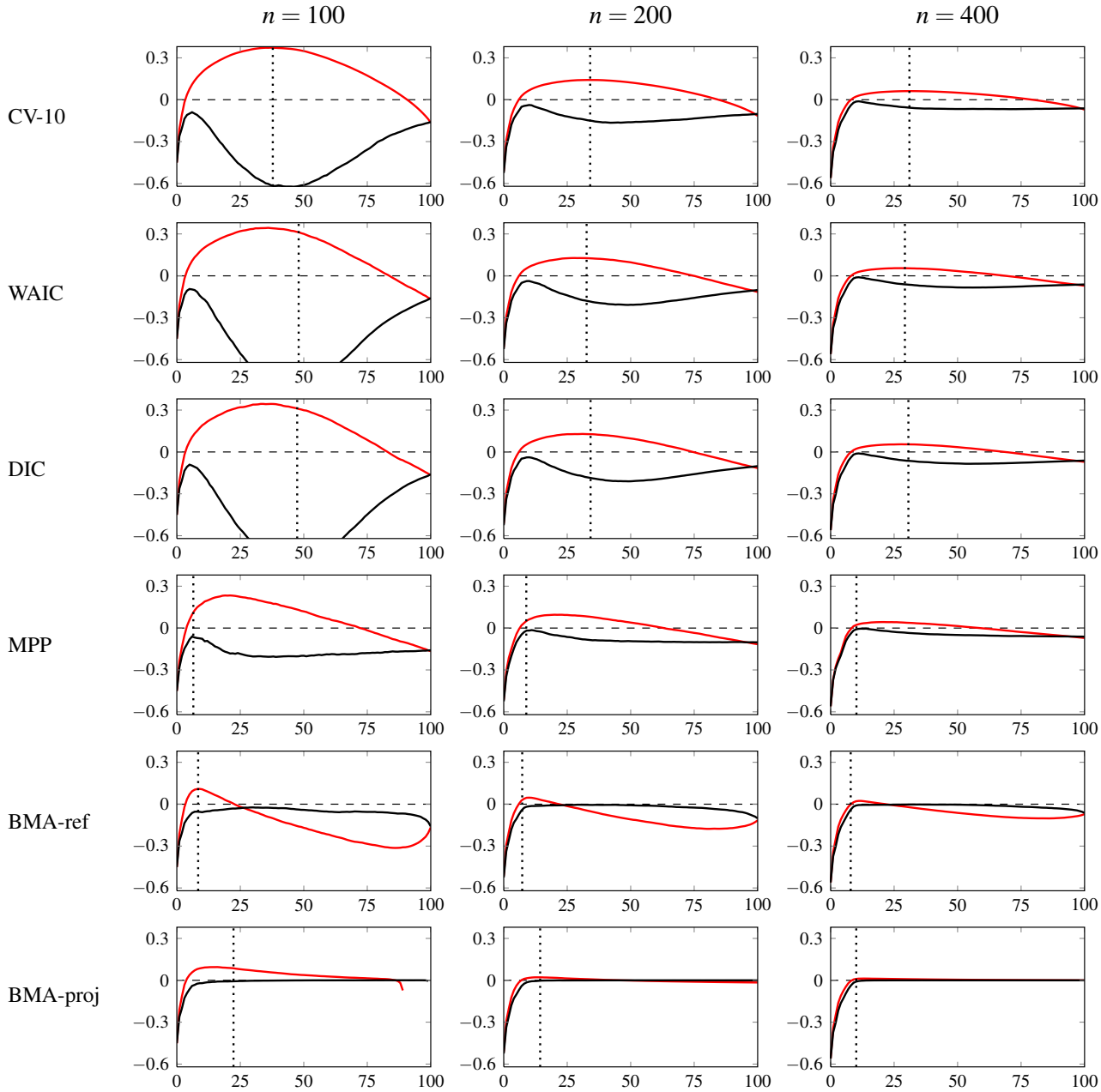
Selection induced bias in variable selection



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Section 3

Information criteria

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WAIC vs PSIS-LOO

see Vehtari, Gelman & Gabry (2017a)

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WAIC vs PSIS-LOO

1. WAIC has same assumptions as LOO

see Vehtari, Gelman & Gabry (2017a)

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WAIC vs PSIS-LOO

1. WAIC has same assumptions as LOO
2. PSIS-LOO is more accurate

see Vehtari, Gelman & Gabry (2017a)

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WAIC vs PSIS-LOO

1. WAIC has same assumptions as LOO
2. PSIS-LOO is more accurate
3. PSIS-LOO has much better diagnostics

see Vehtari, Gelman & Gabry (2017a)

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4. LOO makes the prediction assumption more clear, which helps if K-fold-CV is needed instead

see Vehtari, Gelman & Gabry (2017a)

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WAIC vs PSIS-LOO

1. WAIC has same assumptions as LOO
2. PSIS-LOO is more accurate
3. PSIS-LOO has much better diagnostics
4. LOO makes the prediction assumption more clear, which helps if K-fold-CV is needed instead
5. Multiplying by -2 doesn't give any benefit (Watanabe didn't multiply by -2)

see Vehtari, Gelman & Gabry (2017a)

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*IC

1. AIC uses maximum likelihood estimate for prediction
2. DIC uses posterior mean for prediction
3. BIC is an approximation for marginal likelihood
4. TIC, NIC, RIC, PIC, BPIC, QIC, AICc, ...

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Section 4

Model averaging

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Section 5

Summary

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Take-home messages

1. It's good to think predictions of observables, because observables are the only ones we can observe
2. Cross-validation can simulate predicting and observing new data
3. Cross-validation is good if you don't trust your model
4. Different variants of cross-validation are useful in different scenarios
5. Cross-validation has high variance, and **if** you trust your model you can beat cross-validation in accuracy

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