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Bayesian Statistics and Data Analysis

Lecture 8b

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Thanks to Aki Vehtari, Aalto University

- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
 - When is LOO applicable
 - Fast LOO-CV
 - K-fold cross-validation
 - Comparison and selection
 - Additional reading
- Information criteria
- Model averaging
- Summary



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Section 1

Model assessment and selection

- Model assessment and selection
 - Measures of predictive accuracy
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Predictive performance

- Model assessment and selection

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- Modeling complex phenomena with models that are simplified

All models are wrong... but some are useful.



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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



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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 assessment and selection**

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- **Summary**

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



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

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



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 - eg. money, life years, quality adjusted life years, etc.
- General utility: overall in the goodness of the predictive distribution
 - we don't know (yet) the application specific utility then good information theoretically justified choice is log-score for model M

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



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

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



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Subsection 1

Measures of predictive accuracy



- Point residuals

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

where

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

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

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

- The log predictive density (lpd)

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



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

- 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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- 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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- The expectation is with respect to p_{true}



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- The expectation is with respect to p_{true}
- 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



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

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

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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 $p_{\text{true}}(\tilde{y}_i)$?



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

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

- Model assessment and selection

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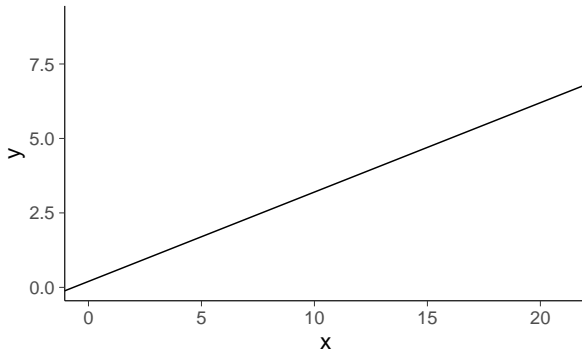
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- **Analogy:** Monte Carlo approximation using our data
- Similar to **jack-knife resampling**
- The elpd, lpd and efficient number of parameters (p_{loo})

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



True mean $y = a + bx$

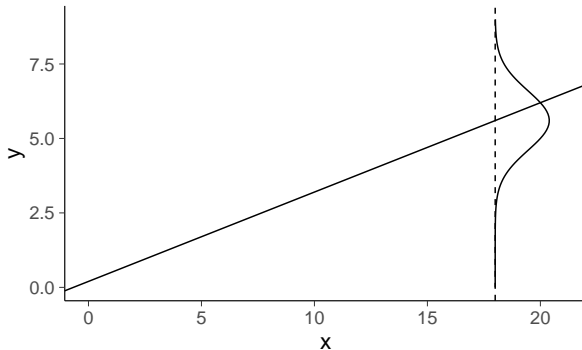


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True mean and sigma





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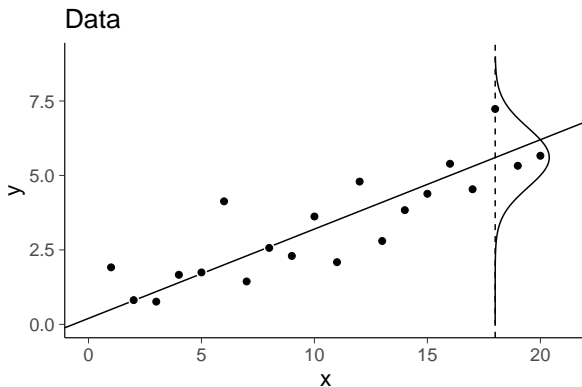
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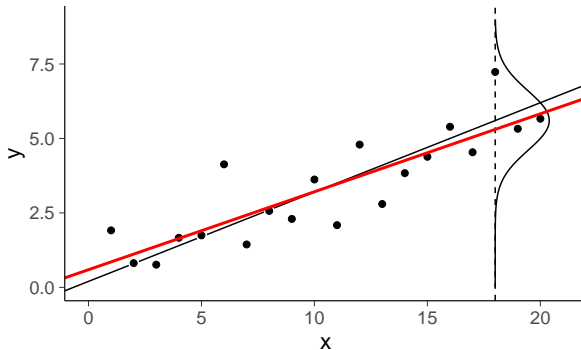
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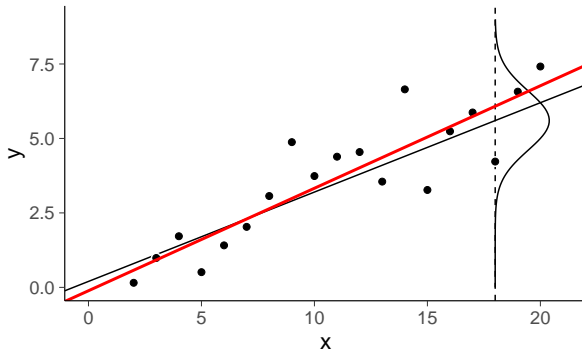
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Posterior mean





Posterior mean, alternative data realisation



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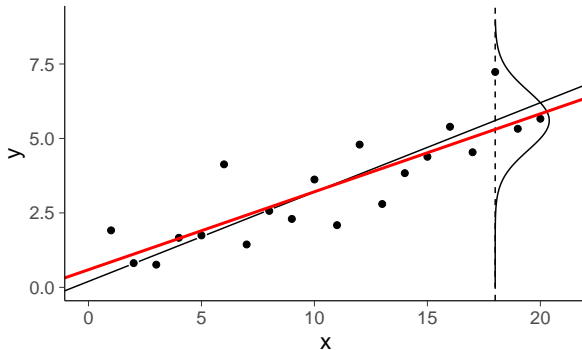
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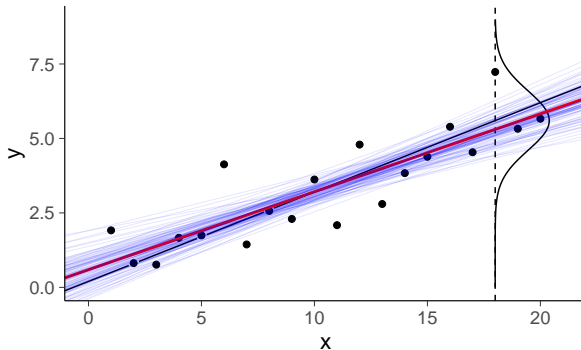
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Posterior draws





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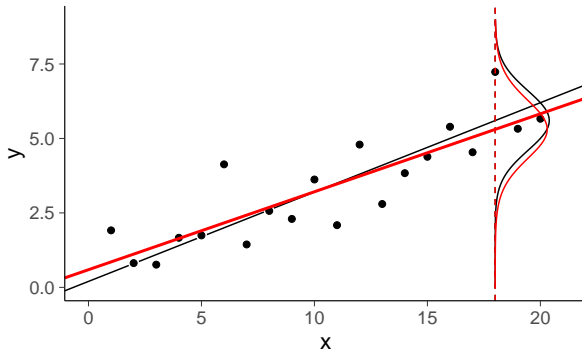
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Posterior predictive distribution





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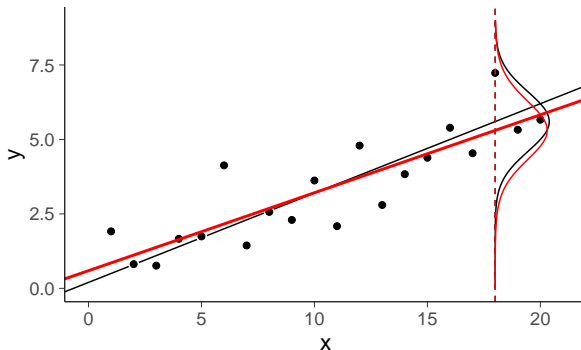
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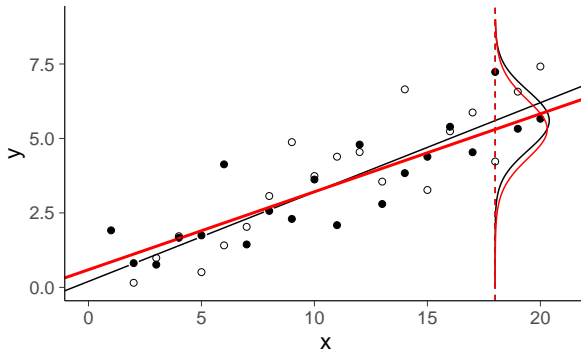
Posterior predictive distribution



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



New data



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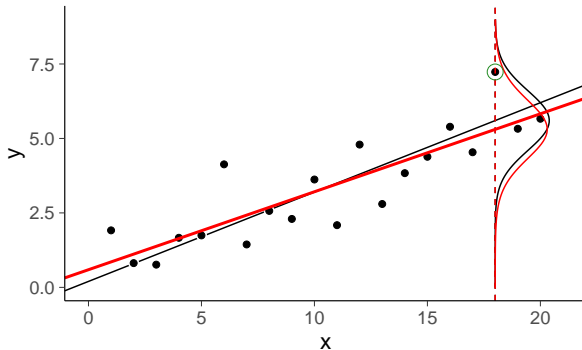
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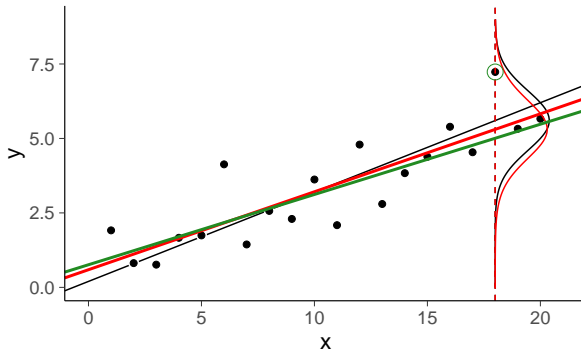
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Leave-one-out mean





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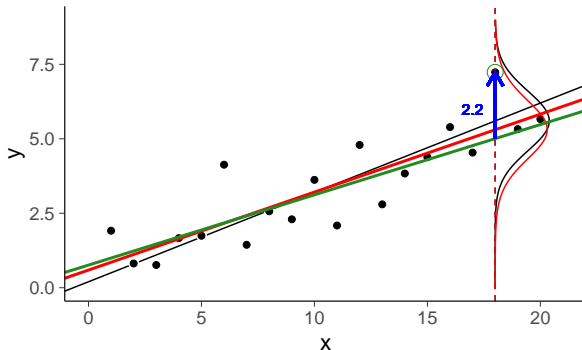
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Leave-one-out residual





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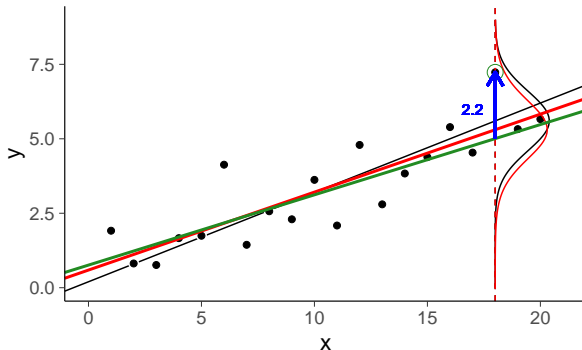
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Leave-one-out residual



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



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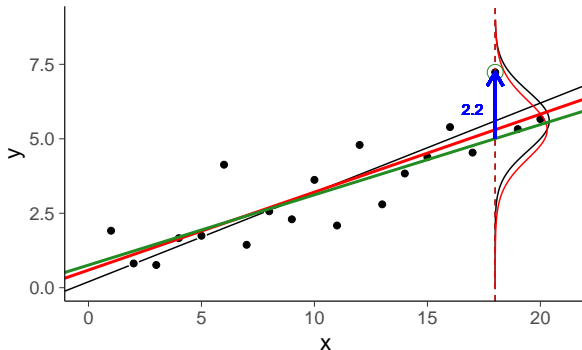
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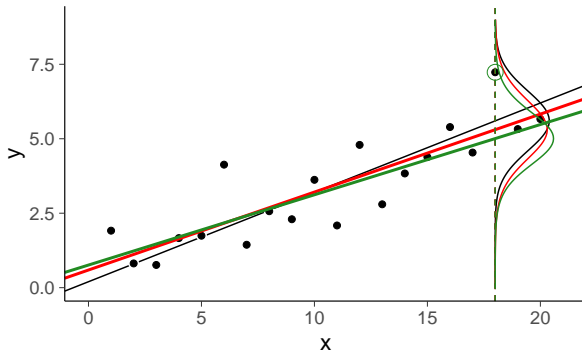


$$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$$

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



Leave-one-out predictive distribution



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- Additional reading

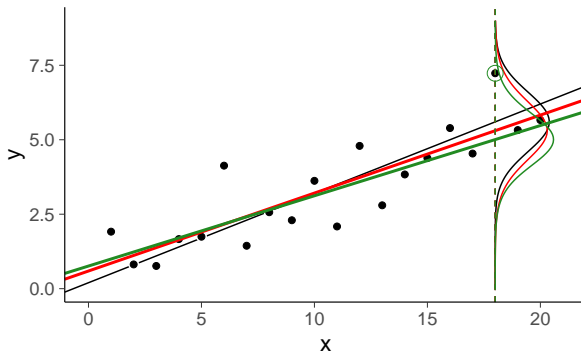
- Information criteria

- Model averaging

- Summary



Leave-one-out predictive distribution



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

- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
 - When is LOO applicable
 - Fast LOO-CV
 - K-fold cross-validation
 - Comparison and selection
 - Additional reading
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- Model averaging
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- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

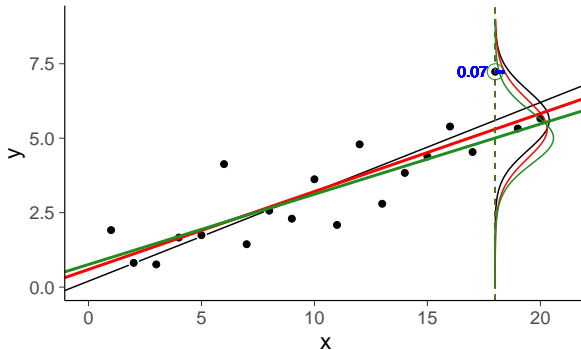
- When is LOO applicable
- Fast LOO-CV
- K-fold cross-validation
- Comparison and selection
- Additional reading

- Information criteria

- Model averaging

- Summary

Posterior predictive density





- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

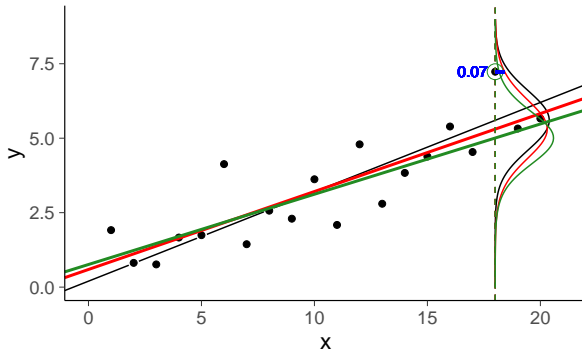
- When is LOO applicable
- Fast LOO-CV
- K-fold cross-validation
- Comparison and selection
- Additional reading

- Information criteria

- Model averaging

- Summary

Posterior predictive density

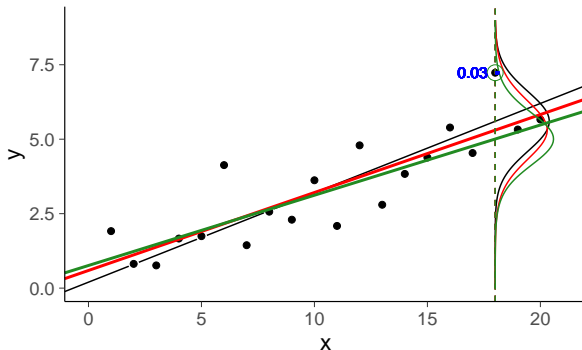


$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$$



- Model assessment and selection
 - Measures of predictive accuracy
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- Cross-validation
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 - Fast LOO-CV
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 - Comparison and selection
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- Information criteria
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Leave-one-out predictive density

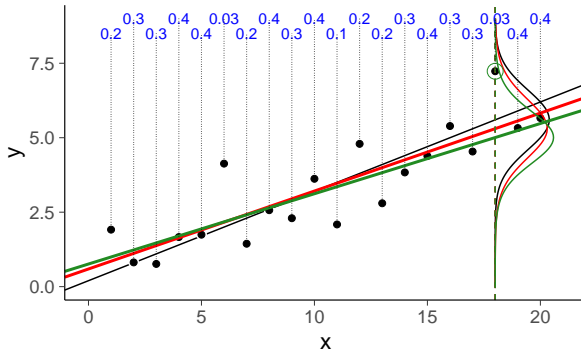


$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$$

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



Leave-one-out predictive densities



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

- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
 - When is LOO applicable
 - Fast LOO-CV
 - K-fold cross-validation
 - Comparison and selection
 - Additional reading
- Information criteria
- Model averaging
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- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

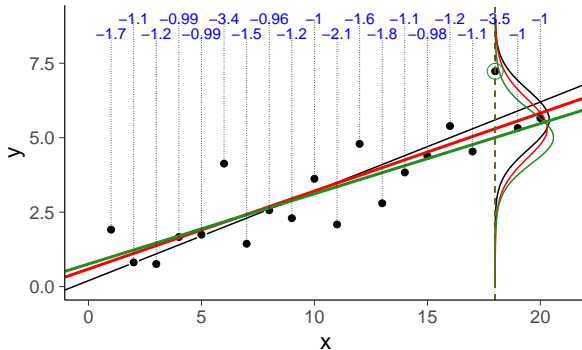
- When is LOO applicable
- Fast LOO-CV
- K-fold cross-validation
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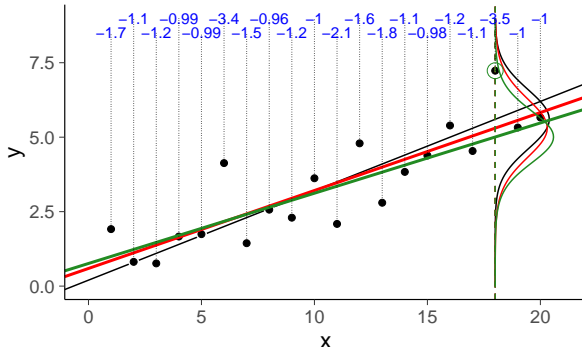
Leave-one-out log predictive densities



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



Leave-one-out log predictive densities



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

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

- When is LOO applicable
- Fast LOO-CV
- K-fold cross-validation
- Comparison and selection
- Additional reading

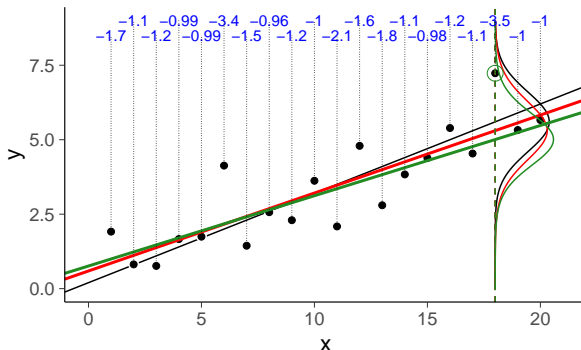
- Information criteria

- Model averaging

- Summary



Leave-one-out log predictive densities



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

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

- When is LOO applicable
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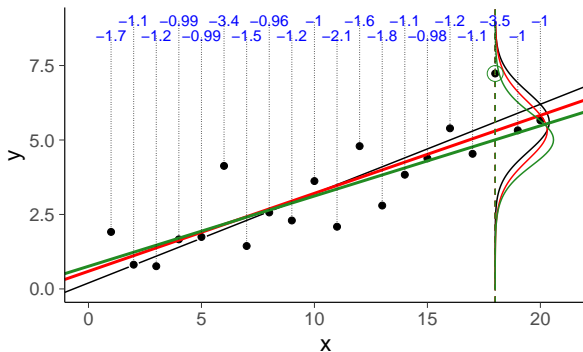
- Information criteria

- Model averaging

- Summary



Leave-one-out log predictive densities



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

unbiased estimate of log posterior pred. density for new data

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

- When is LOO applicable
- Fast LOO-CV
- K-fold cross-validation
- Comparison and selection
- Additional reading

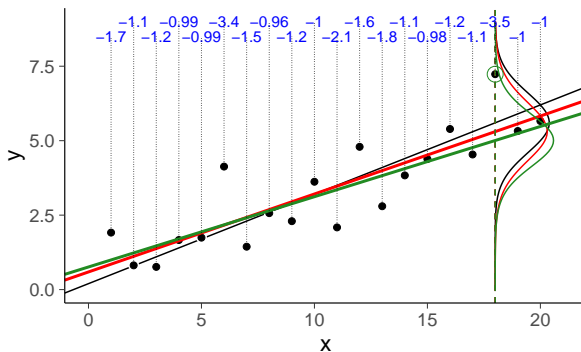
- Information criteria

- Model averaging

- Summary



Leave-one-out log predictive densities



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

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

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

- When is LOO applicable
- Fast LOO-CV
- K-fold cross-validation
- Comparison and selection
- Additional reading

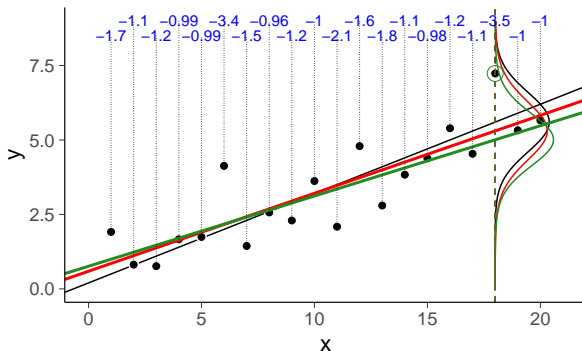
- Information criteria

- Model averaging

- Summary



Leave-one-out log predictive densities



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

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

$$\text{p_loo} = \text{lpd} - \text{elpd_loo} \approx 2.7$$

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

- When is LOO applicable
- Fast LOO-CV
- K-fold cross-validation
- Comparison and selection
- Additional reading

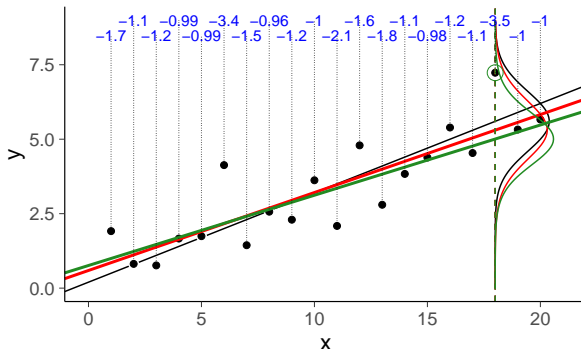
- Information criteria

- Model averaging

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Leave-one-out log predictive densities



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

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

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

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- When is LOO applicable
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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.

- Model assessment and selection
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- Model assessment and selection
 - Measures of predictive accuracy
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Subsection 1

When is LOO applicable



- Model assessment and selection
 - Measures of predictive accuracy
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 - When is LOO applicable
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- Summary

- + Intuitive
- + Robust
- + Good theoretical properties



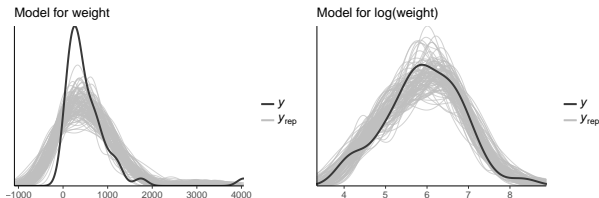
- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
 - When is LOO applicable
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- + Intuitive
- + Robust
- + Good theoretical properties
 - Can be costly (naive LOO-CV mean n posterior computations)



Sometimes cross-validation is not needed

- Posterior predictive checking can be sufficient



Predicting the yields of mesquite bushes.

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

- Model assessment and selection
 - Measures of predictive accuracy
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Sometimes cross-validation is not needed

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

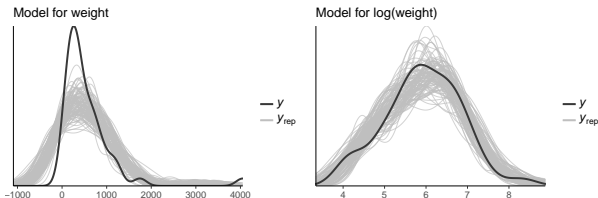
- When is LOO applicable
- Fast LOO-CV
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- Additional reading

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- Summary

- Posterior predictive checking can be sufficient



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



Data generating mechanisms and prediction tasks

- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
 - When is LOO applicable
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 - K-fold cross-validation
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- Information criteria
- Model averaging
- Summary

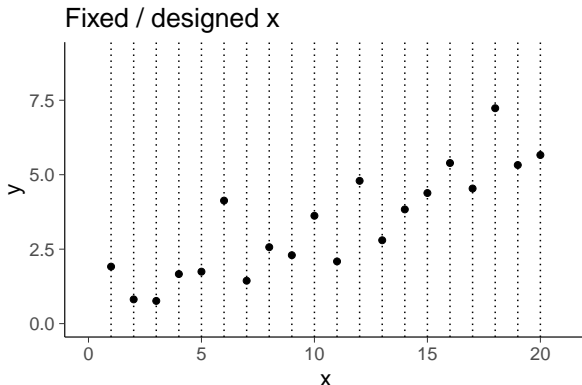
1. You have to make some assumptions on data generating mechanism p_{true}

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

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



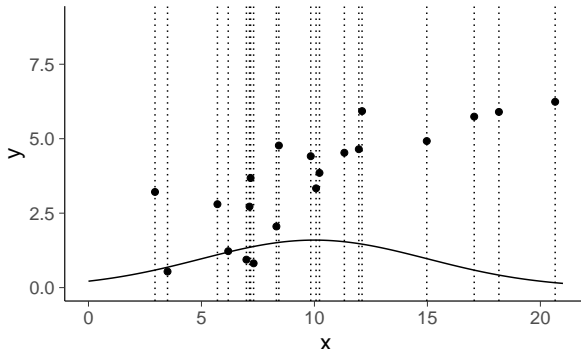
- Model assessment and selection
 - Measures of predictive accuracy
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LOO is ok for fixed / designed x : $p_{\text{true}}(y|x)$



Distribution for x



LOO is ok for random x . $p_{\text{true}}(y, x)$

- Model assessment and selection
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p_{true} extrapolation

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

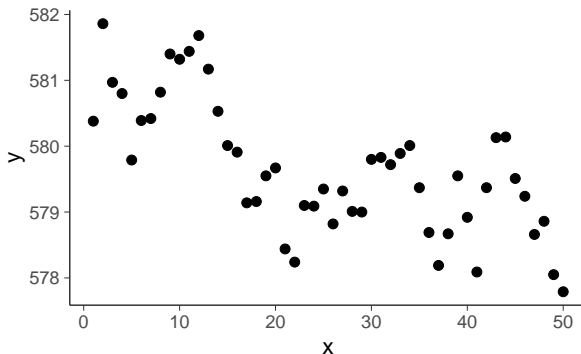
- Cross-validation

- When is LOO applicable
- Fast LOO-CV
- K-fold cross-validation
- Comparison and selection
- Additional reading

- Information criteria

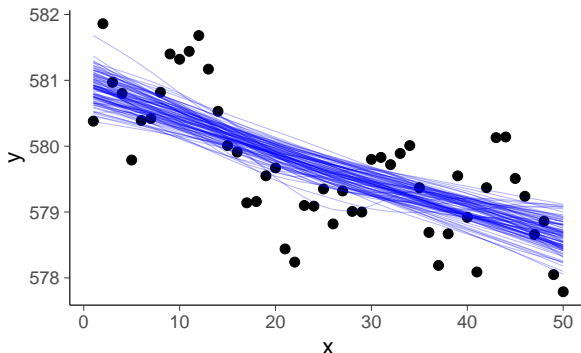
- Model averaging

- Summary





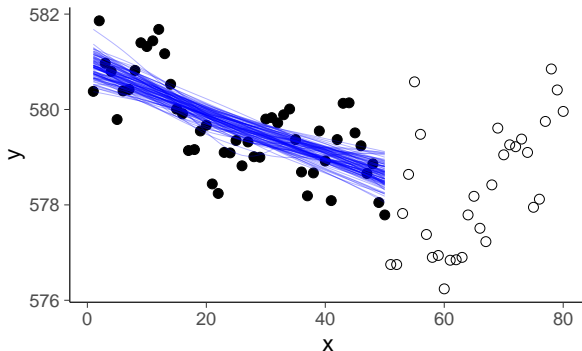
Nonlinear model fit



- Model assessment and selection
 - Measures of predictive accuracy
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Nonlinear model fit + new data



Extrapolation is more difficult

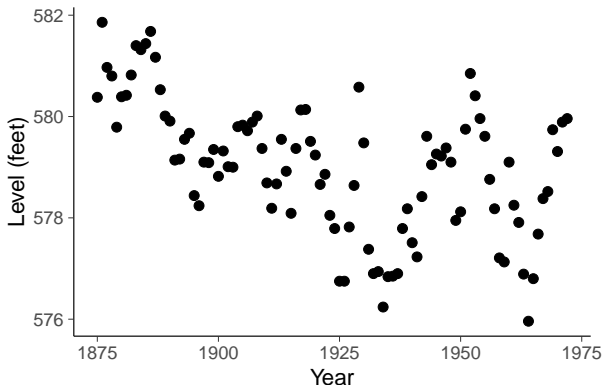
- Model assessment and selection
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- Model assessment and selection
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LOO for time series data



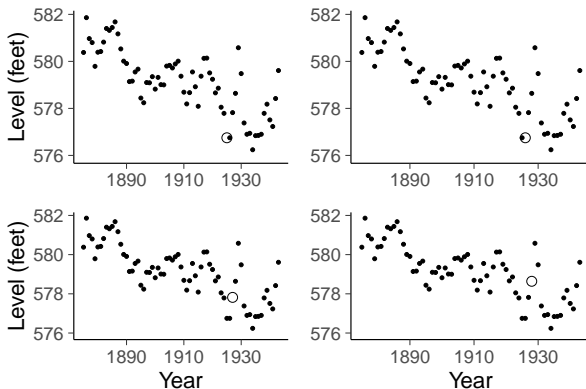
p_{true} for time series?



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LOO for time series

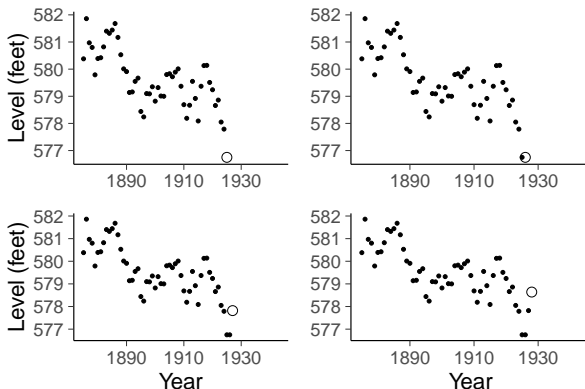


Leave-one-out cross-validation is ok for assessing conditional model



- Model assessment and selection
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LOO for time series



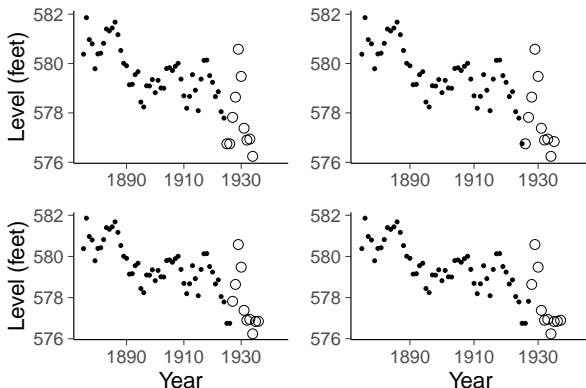
Leave-future-out cross-validation is better for predicting future



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- Model assessment and selection
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 - When is LOO applicable
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LOO for time series

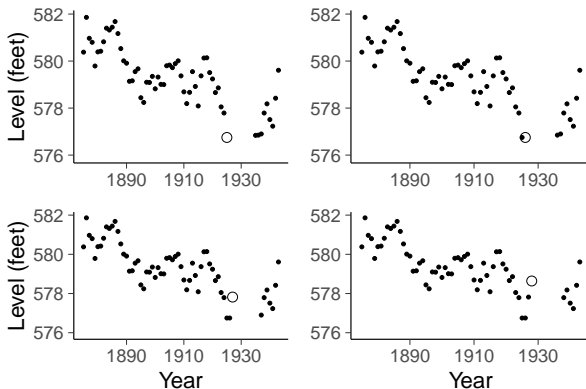


m-step-ahead cross-validation is better for predicting further future



- Model assessment and selection
 - Measures of predictive accuracy
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 - When is LOO applicable
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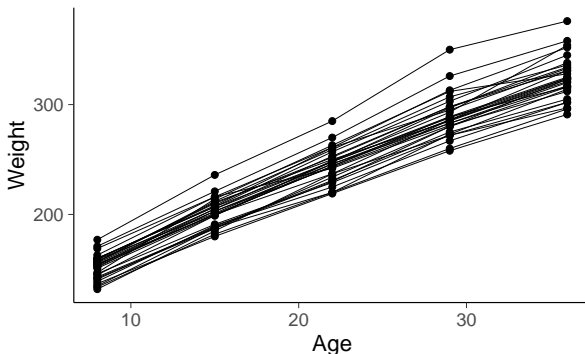
LOO for time series



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



Rats data

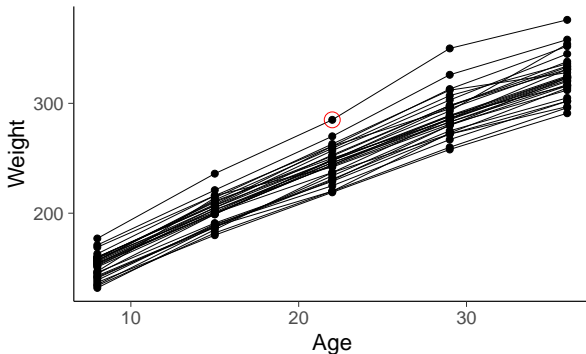


Can LOO or other cross-validation be used with hierarchical data?

- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
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Leave-one-out?

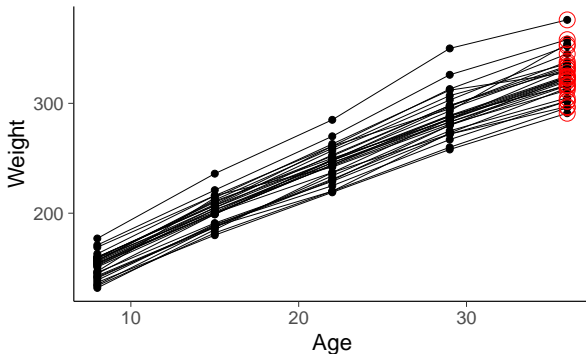


Yes!

- Model assessment and selection
 - Measures of predictive accuracy
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1-step-ahead?

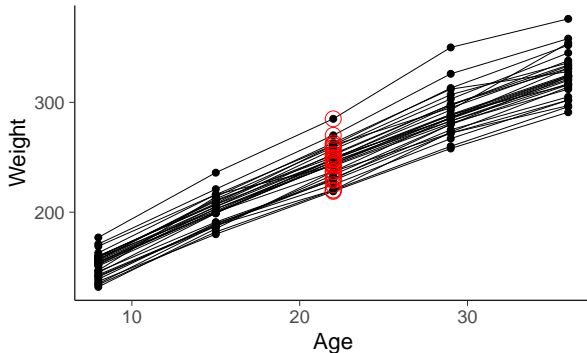


Yes!

- Model assessment and selection
 - Measures of predictive accuracy
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Leave-one-time-point-out?

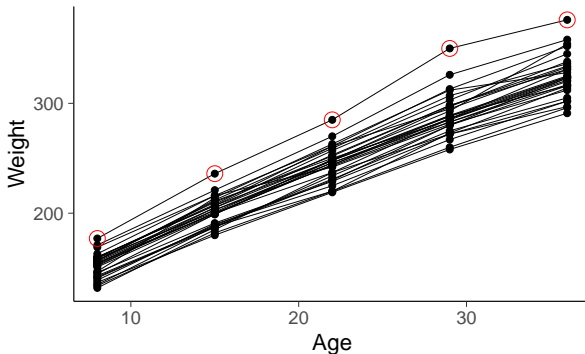


Yes!

- Model assessment and selection
 - Measures of predictive accuracy
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Leave-one-rat-out?

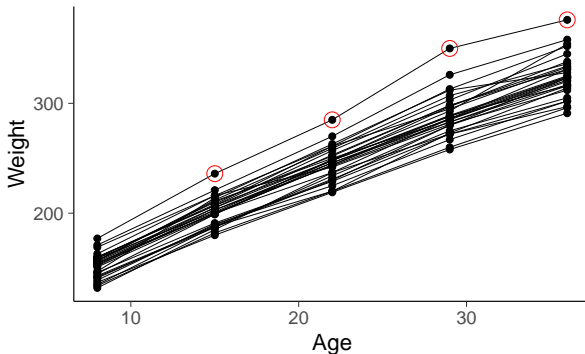


Yes!

- Model assessment and selection
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Predict given initial weight?



Yes!

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- Model assessment and selection
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Subsection 2

Fast LOO-CV



1. Pareto smoothed importance sampling LOO (PSIS-LOO)

- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
 - When is LOO applicable
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1. Pareto smoothed importance sampling LOO (PSIS-LOO)
2. K-fold cross-validation

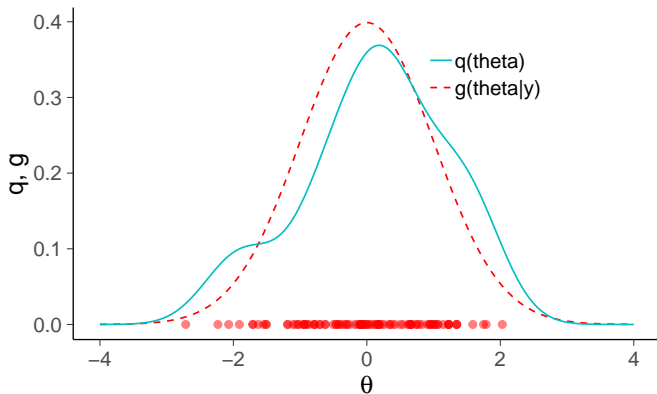
- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
 - When is LOO applicable
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- Model assessment and selection
 - Measures of predictive accuracy
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Recap: Importance sampling

Target, proposal, and draws

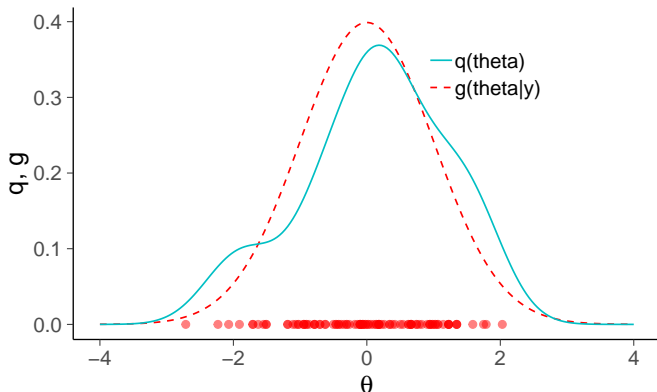




- Model assessment and selection
 - Measures of predictive accuracy
 - Model selection
- Cross-validation
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Recap: Importance sampling

Target, proposal, and draws



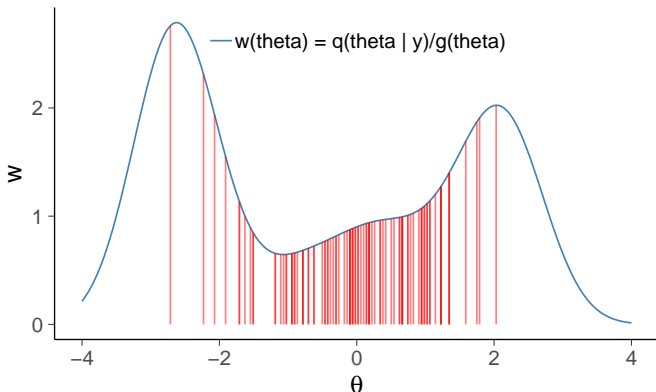
$$E[f(\theta)] \approx \frac{\sum_s w_s f(\theta^{(s)})}{\sum_s w_s}, \quad \text{where} \quad w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$



- Model assessment and selection
 - Measures of predictive accuracy
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Recap: Importance sampling

Draws and importance weights



$$E[f(\theta)] \approx \frac{\sum_s w_s f(\theta^{(s)})}{\sum_s w_s}, \quad \text{where } w_s = \frac{q(\theta^{(s)})}{g(\theta^{(s)})}$$



- 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

$$w_i^s = \frac{p(\theta^s|x_i, D_{-i})}{p(\theta^s|D)} \propto \frac{1}{p(y_i|\theta^s)}.$$

- Model assessment and selection
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- 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

$$w_i^s = \frac{p(\theta^s|x_i, D_{-i})}{p(\theta^s|D)} \propto \frac{1}{p(y_i|\theta^s)}.$$

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

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

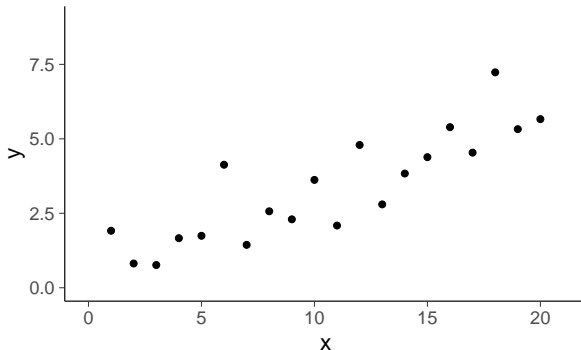
- Model assessment and selection
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 - K-fold cross-validation
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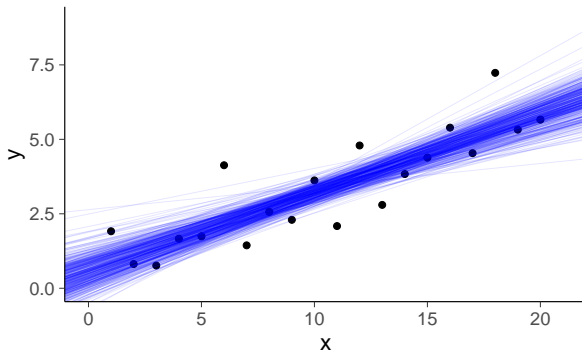
Data





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Posterior draws

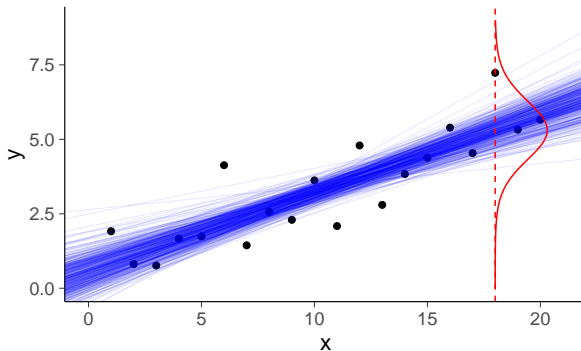


$$\theta^{(s)} \sim p(\theta|x, y)$$



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Posterior predictive distribution

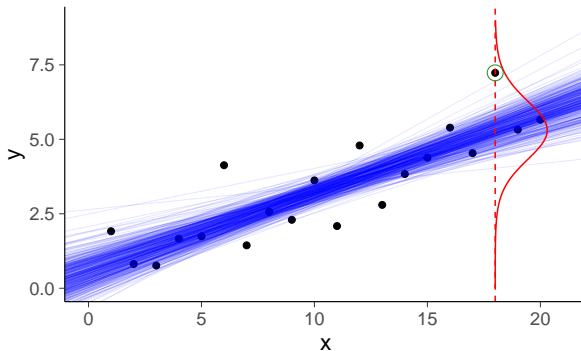


$$\theta^{(s)} \sim p(\theta|x, y), \quad p(\tilde{y}|\tilde{x}, x, y) \approx \frac{1}{S} \sum_{s=1}^S p(\tilde{y}|\tilde{x}, \theta^{(s)})$$



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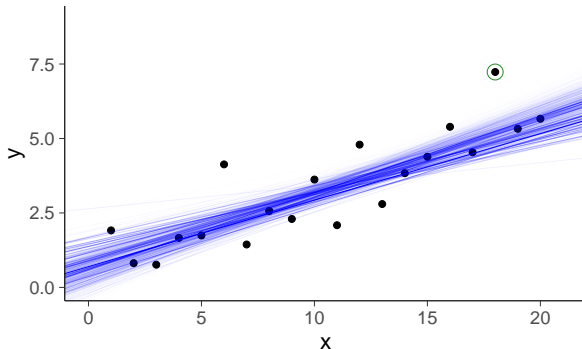
Posterior predictive distribution



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



PSIS-LOO weighted draws



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

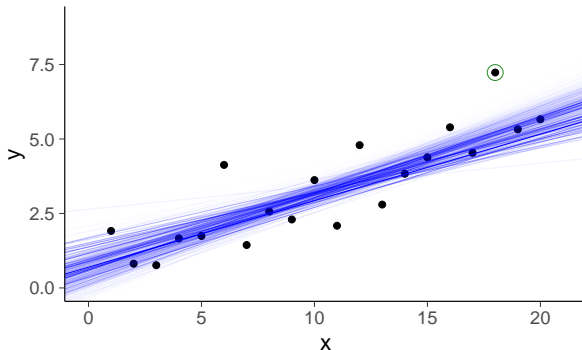
$$r_i^{(s)} = p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y)$$

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PSIS-LOO weighted draws



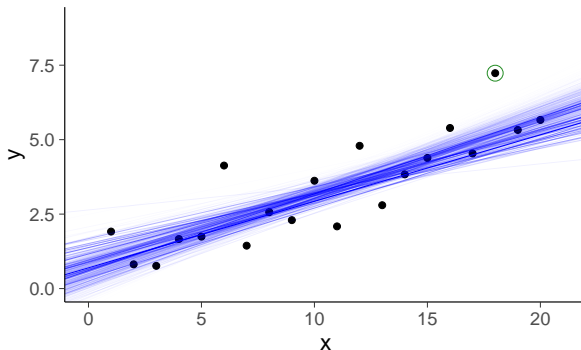
$$\theta^{(s)} \sim p(\theta|x, y)$$

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



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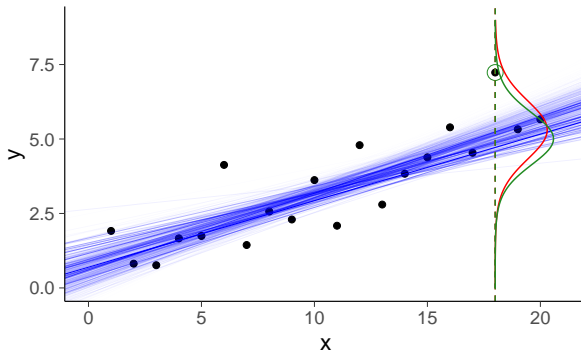
$$r_i^{(s)} = p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y) \propto 1/p(y_i|x_i, \theta^{(s)})$$

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



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PSIS-LOO weighted predictive distribution



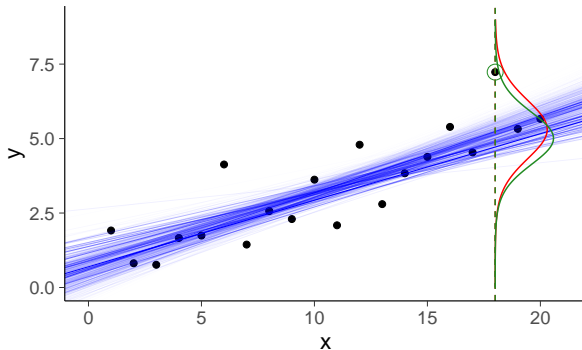
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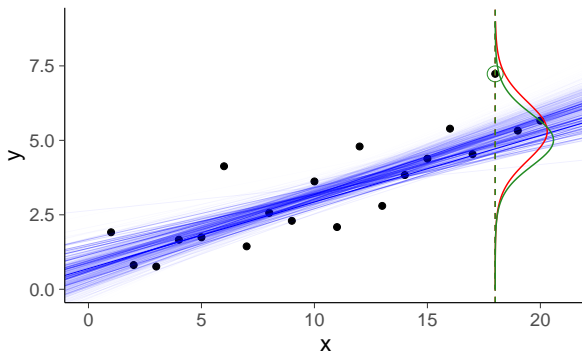
$$\theta^{(s)} \sim p(\theta|x, y)$$

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

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



PSIS-LOO weighted predictive distribution



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

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

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



- Model assessment and selection

- Measures of predictive accuracy
- Model selection

- Cross-validation

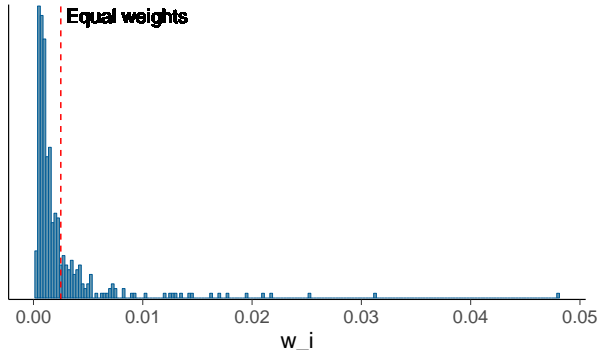
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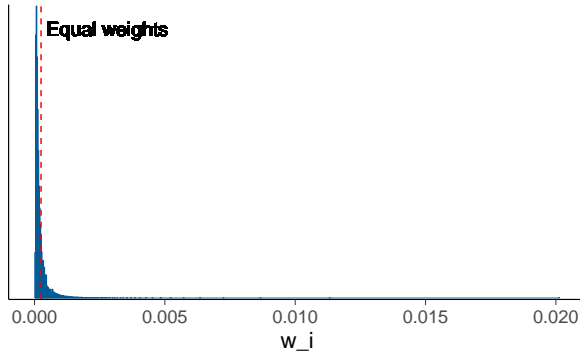
400 importance weights for leave-18th-out





- Model assessment and selection
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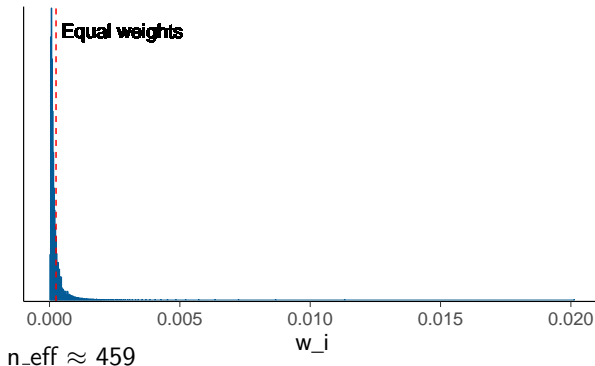
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4000 importance weights for leave-18th-out

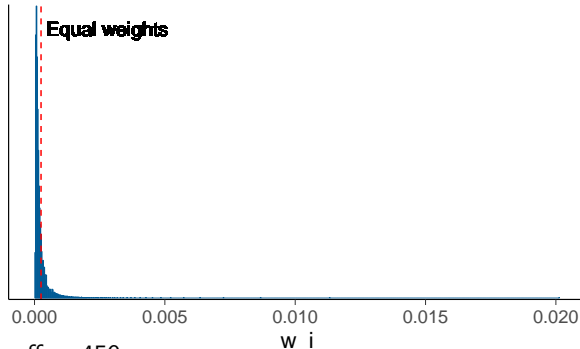


see [Vehtari, Gelman & Gabry \(2017b\)](#)



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4000 importance weights for leave-18th-out



$n_{\text{eff}} \approx 459$

Pareto $\hat{k} \approx 0.52$

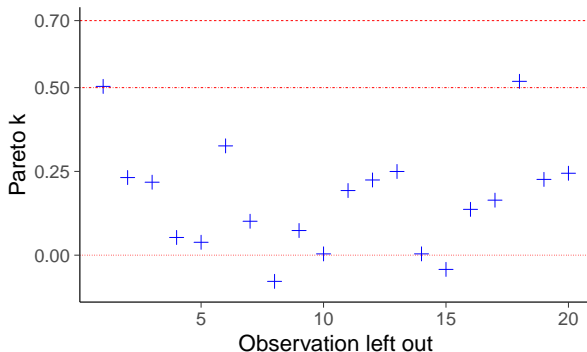
1. Pareto \hat{k} estimates the tail shape which determines the convergence rate of PSIS. Less than 0.7 is ok.

see [Vehtari, Gelman & Gabry \(2017b\)](#)



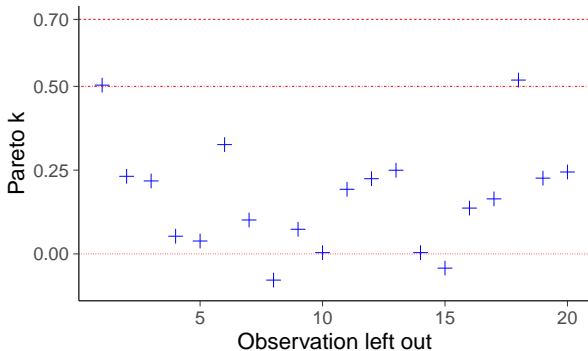
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PSIS-LOO diagnostics





PSIS-LOO diagnostics



Pareto k diagnostic values:

		Count	Pct.	Min. n_eff
$(-\infty, 0.5]$	(good)	18	90.0%	899
$(0.5, 0.7]$	(ok)	2	10.0%	459
$(0.7, 1]$	(bad)	0	0.0%	<NA>
$(1, \infty)$	(very bad)	0	0.0%	<NA>

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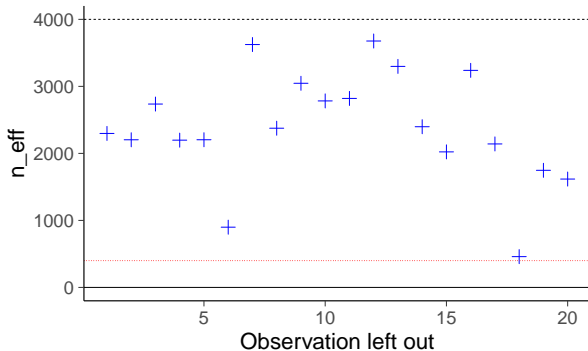
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Computed from 4000 by 20 log-likelihood matrix

	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 \(2017b\)](#)

- Model assessment and selection

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Model comparison:

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

elpd_diff	se
-0.2	0.1

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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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```
...  
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);  
}
```




Pareto smoothed importance sampling LOO

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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



Pareto smoothed importance sampling LOO

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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

2. PSIS-LOO for non-factorizable models

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



Pareto smoothed importance sampling LOO

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1. PSIS-LOO for hierarchical models

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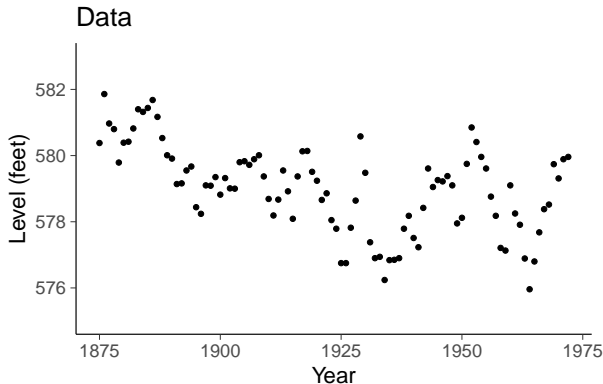
- 2.1 mc-stan.org/loo/articles/loo2-non-factorizable.html

3. PSIS-LOO for time series

- 3.1 Approximate leave-future-out cross-validation
mc-stan.org/loo/articles/loo2-lfo.html

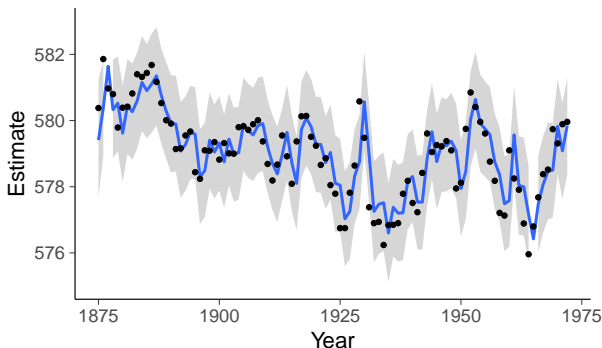


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AR-4 prediction with 95% interval



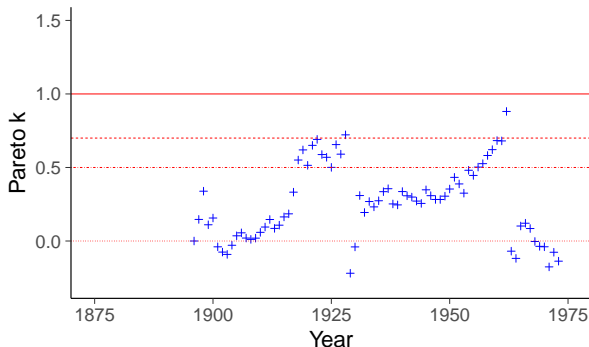
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PSIS-LOO for time series

PSIS-1-step-ahead with refits



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



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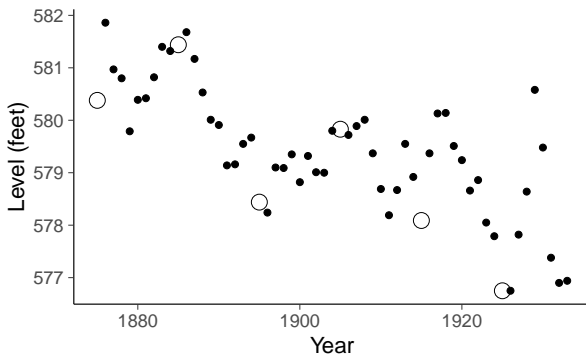
1. K-fold cross-validation can approximate LOO
 - 1.1 all uses for LOO
2. K-fold cross-validation can be used for hierarchical models
 - 2.1 good for leave-one-group-out
3. K-fold cross-validation can be used for time series
 - 3.1 with leave-block-out



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Balance k-fold approximation of LOO

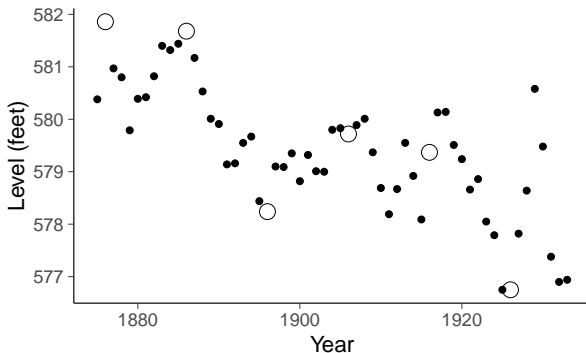




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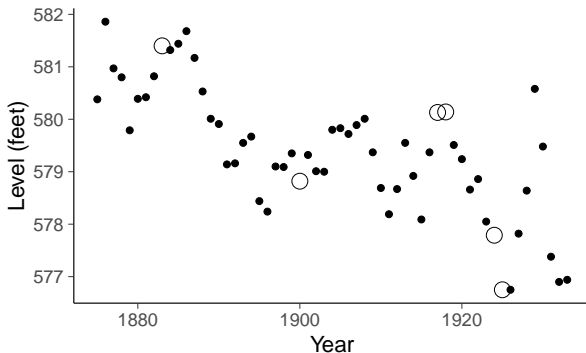




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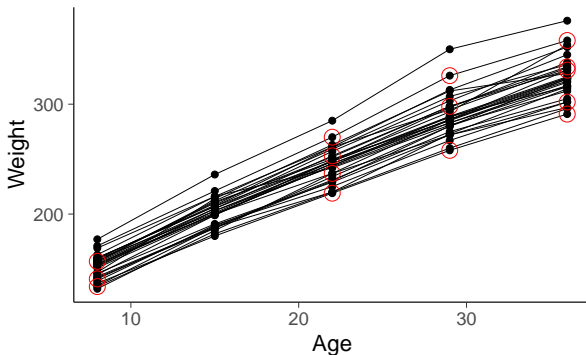
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Random k-fold approximation of LOO





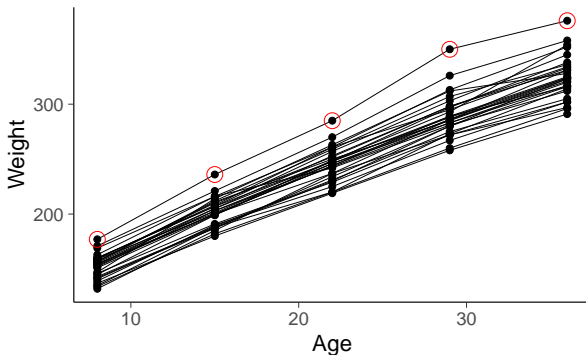
Random kfold approximation of LOO



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Leave-one-rat-out

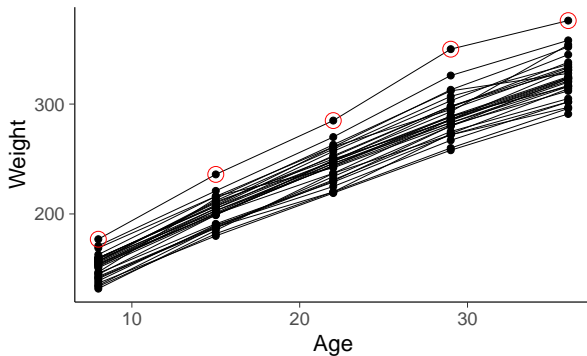


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Leave-one-rat-out



```
kfold_split_random()  
kfold_split_balanced()  
kfold_split_stratified()
```



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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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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/



- Model assessment and selection
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Model comparison

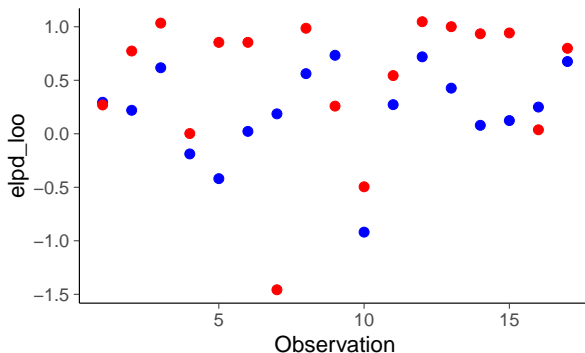
1. “A popular hypothesis has it that primates with larger brains produce more energetic milk, so that brains can grow quickly” (from Statistical Rethinking)
 - 1.1 Model 1: $\text{formula} = \text{kcal.per.g} \sim \text{neocortex}$
 - 1.2 Model 2: $\text{formula} = \text{kcal.per.g} \sim \text{neocortex}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

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



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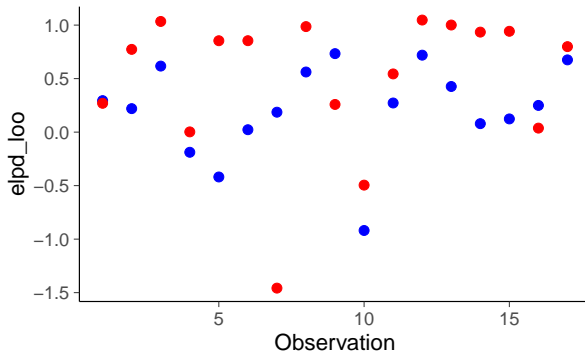
Pointwise comparison LOO models: Model 1





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Pointwise comparison LOO models: Model 1



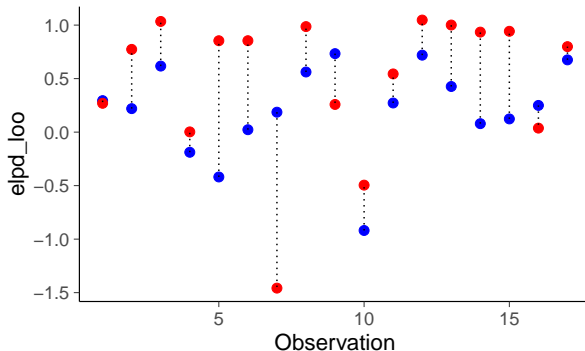
Model 1 $\text{elpd_loo} \approx 3.7$, $\text{SE}=1.8$

Model 2 $\text{elpd_loo} \approx 8.4$, $\text{SE}=2.8$



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Pointwise comparison LOO models: Model 1



Model 1 $\text{elpd_loo} \approx 3.7$, $\text{SE}=1.8$

Model 2 $\text{elpd_loo} \approx 8.4$, $\text{SE}=2.8$



- Model assessment and selection

- Measures of predictive accuracy
- Model selection

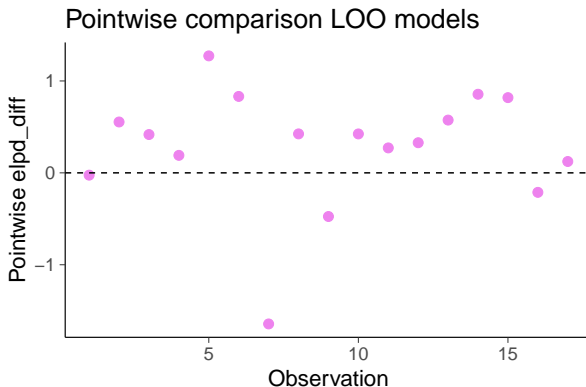
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Model comparison:

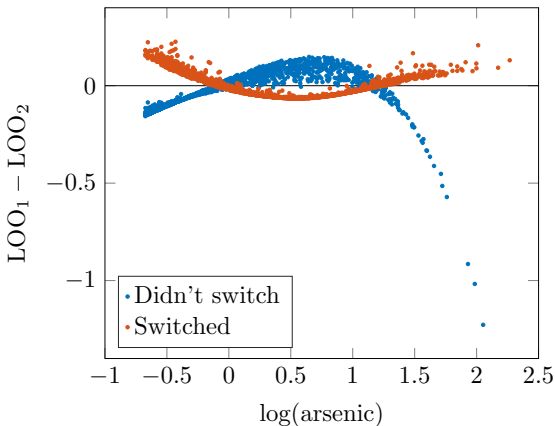
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff	se
4.7	2.7



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Arsenic well example – Model comparison



An estimated difference in elpd_{loo} of 16.4 with SE of 4.4.

see [Vehtari, Gelman & Gabry \(2017a\)](#)



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Arsenic well example – Model comparison

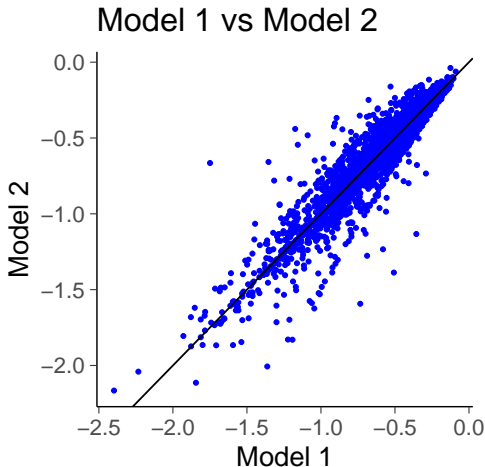
1. Probability of switching well with high arsenic level in rural Bangladesh
 - 1.1 Model 1 covariates: $\log(\text{arsenic})$ and distance
 - 1.2 Model 2 covariates: $\log(\text{arsenic})$, distance and education level

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



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Arsenic well example – Model comparison



Model 1 elpd_loo \approx -1952, SE=16

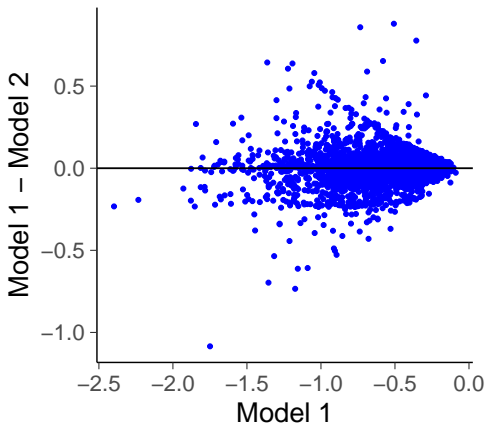
Model 2 elpd_loo \approx -1938, SE=17



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Arsenic well example – Model comparison

Model 1 vs Model 2



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

`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).



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
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2. Model averaging with BMA or Bayesian stacking?

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

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2. Model averaging with BMA or Bayesian stacking?

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

3. In a nested case choose simpler if assuming some cost for extra parts?

andrewgelman.com/2018/07/26/

[parsimonious-principle-vs-integration-uncertainties/](https://andrewgelman.com/2018/07/26/parsimonious-principle-vs-integration-uncertainties/)



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andrewgelman.com/2018/07/26/parsimonious-principle-vs-integration-uncertainties/
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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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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1. Cross-validation can be used for model selection if
 - 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



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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 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)



Selection induced bias and overfitting

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 - same data is used to assess the performance and make the selection
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 - 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



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- 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)
- 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



Selection induced bias in variable selection

- Model assessment and selection

- Measures of predictive accuracy
- Model selection

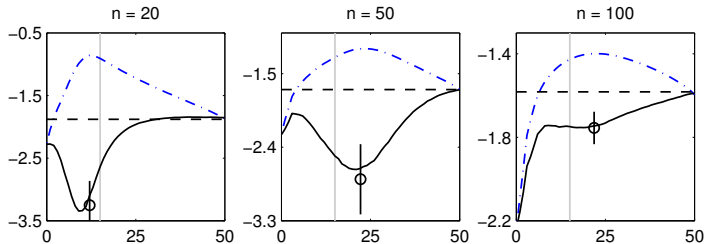
- Cross-validation

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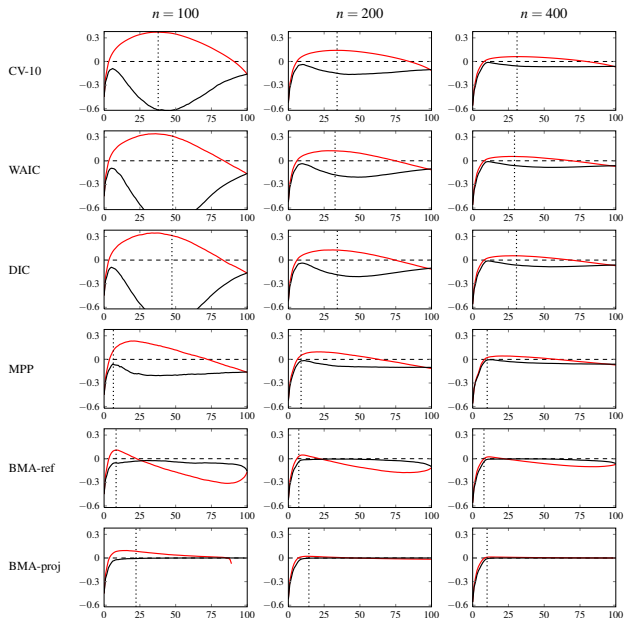
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Selection induced bias in variable selection



- Model assessment and selection

- Measures of predictive accuracy
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Section 3

Information criteria



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WAIC vs PSIS-LOO

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see [Vehtari, Gelman & Gabry \(2017a\)](#)



1. WAIC has same assumptions as LOO

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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

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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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WAIC vs PSIS-LOO

1. WAIC has same assumptions as LOO
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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 \(2017a\)](#)



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

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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



Take-home messages

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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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