

Chapter 7

- 7.1 Measures of predictive accuracy
- 7.2 Information criteria and cross-validation
 - Instead of 7.2, read:
Vehtari, A., Gelman, A., Gabry, J. (2017). Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC. *Statistics and Computing*. 27(5):1413–1432. [arXiv preprint](#).
- 7.3 Model comparison based on predictive performance
- 7.4 Model comparison using Bayes factors
- 7.5 Continuous model expansion / sensitivity analysis
- 7.5 Example (may be skipped)

Model assesment, selection and inference after selection

- Extra material at <https://avehtari.github.io/modelselection/>
 - Videos, Slides, Notebooks, References
 - The most relevant for the course is the first part of the talk “Model assesment, comparison and selection at Master class in Bayesian statistics, CIRM, Marseille”

Predicting concrete quality



Predicting cancer recurrence

GIST Risk calculator

Tumor size (cm)

Mitotic count (per 50 HPFs*)

Tumor site

Tumor rupture

CALCULATE!

*HPF = high-power field of the microscope

[Show risk tables](#)

Made by

kaiku
HEALTH

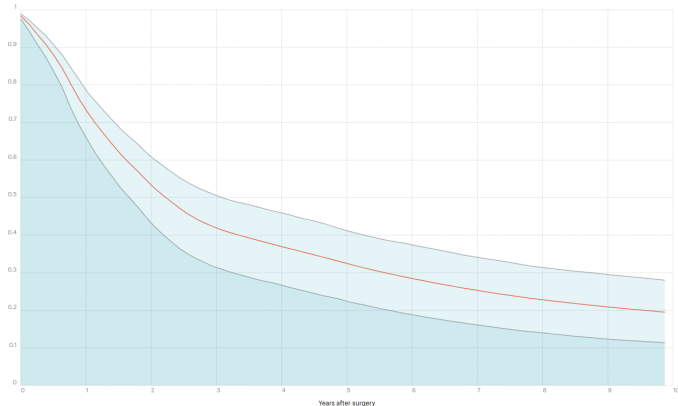
Online platform for the future of data-driven
and personalized cancer care

Reaktor

Patients alive without recurrence [Show hazard](#)

90 % credible interval

10 year risk of GIST recurrence: 80%



Predictive performance

- True predictive performance is found out by using it to make predictions and comparing predictions to true observations
 - external validation

Predictive performance

- 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

Predictive performance

- We need to choose the utility/cost function
- Application specific utility/cost functions are important
 - eg. money, life years, quality adjusted life years, etc.

Predictive performance

- We need to choose the utility/cost function
- Application specific utility/cost functions are important
 - eg. money, life years, quality adjusted life years, etc.
- If are interested overall in the goodness of the predictive distribution, or we don't know (yet) the application specific utility, then good information theoretically justified choice is log-score

$$\log p(y^{\text{rep}}|y, M),$$

Outline

- What is cross-validation
 - Leave-one-out cross-validation (`elpd_loo`, `p_loo`)
 - Uncertainty in LOO (SE)
- When is cross-validation applicable?
 - data generating mechanisms and prediction tasks
 - leave-many-out cross-validation
- Fast cross-validation
 - PSIS and diagnostics in `loo` package (Pareto k , n_{eff} , Monte Carlo SE)
 - K-fold cross-validation
- Related methods (WAIC, \ast IC, BF)
- Model comparison and selection (`elpd_diff`, `se`)
- Model averaging with Bayesian stacking

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 ($k < 0.7$).

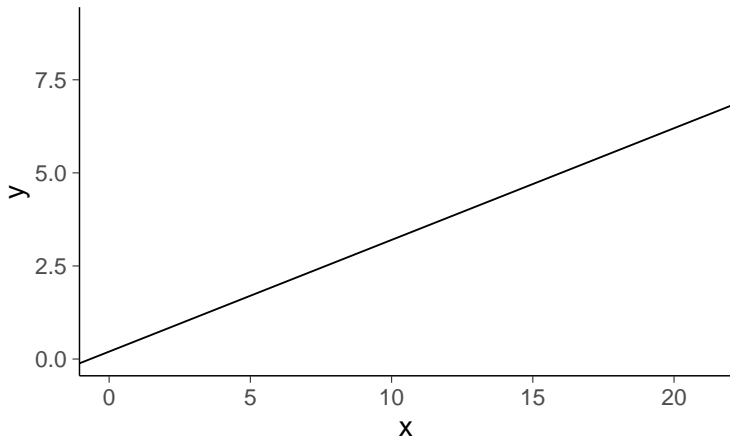
See `help('pareto-k-diagnostic')` for details.

Model comparison:

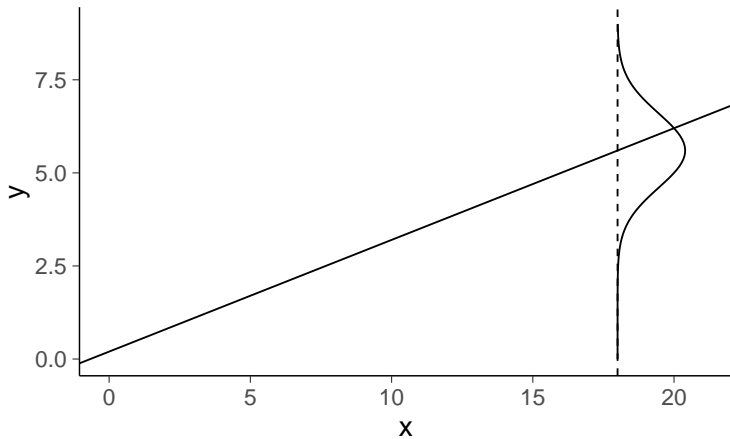
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff	se
-0.2	0.1

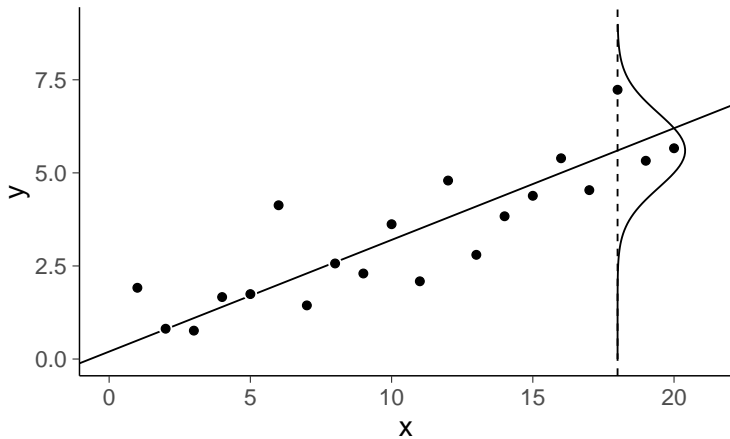
True mean $y = a + bx$



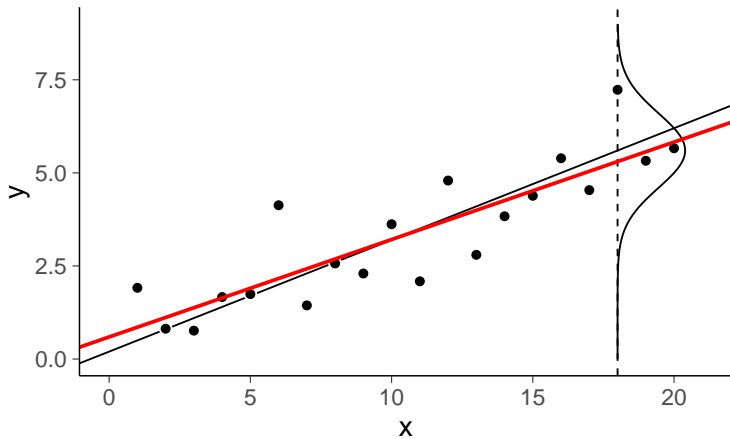
True mean and sigma



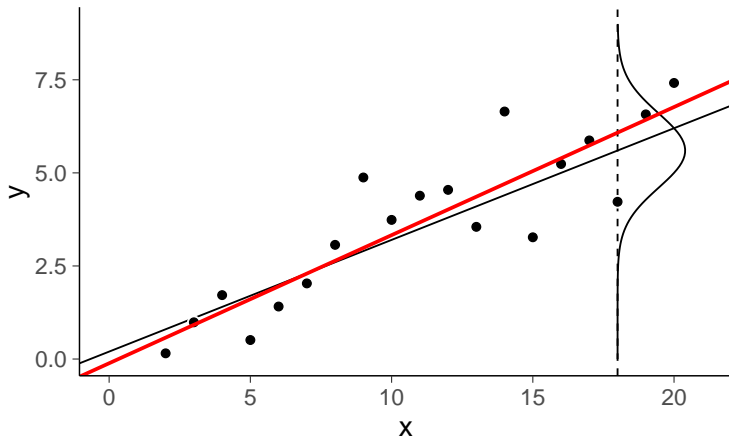
Data



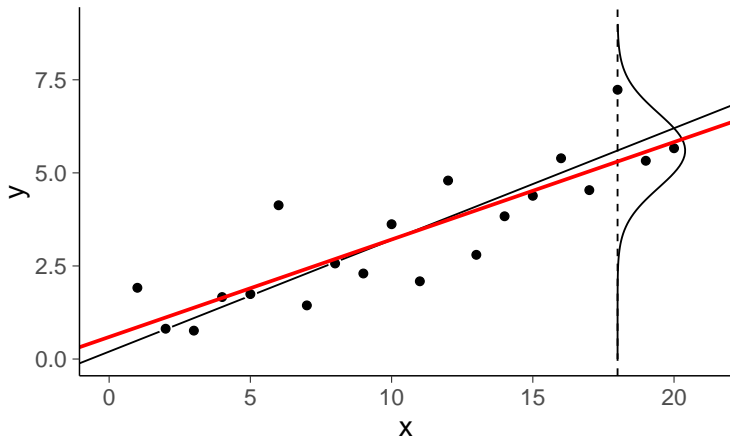
Posterior mean



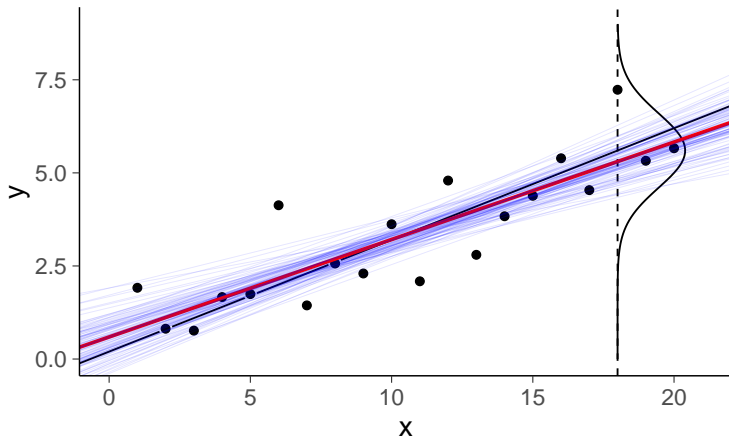
Posterior mean, alternative data realisation



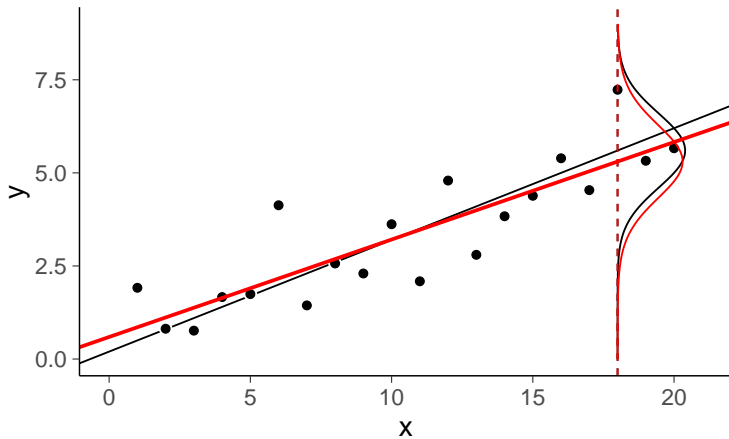
Posterior mean



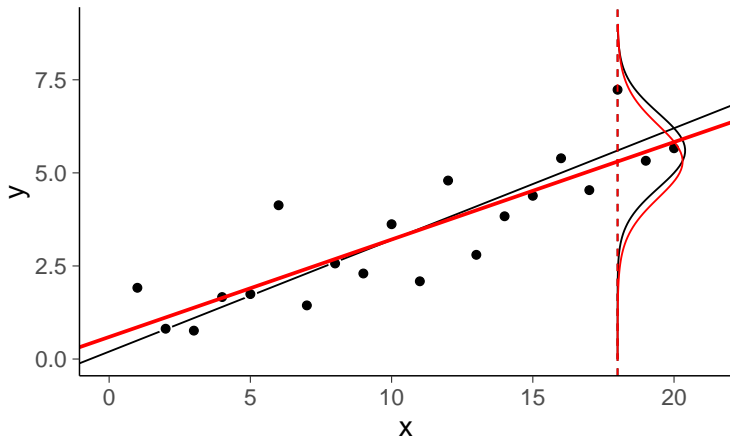
Posterior draws



Posterior predictive distribution

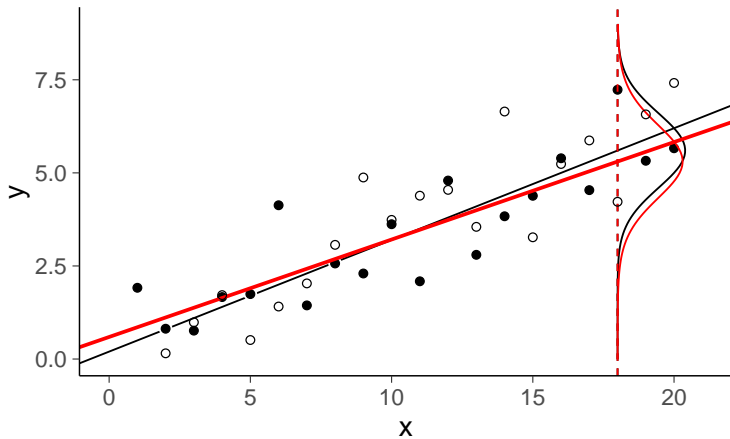


Posterior predictive distribution

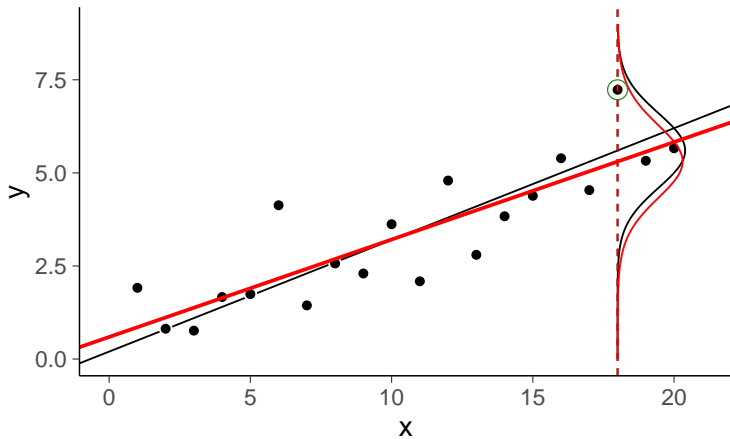


$$p(\tilde{y}|\tilde{x} = 18, x, y) = \int p(\tilde{y}|\tilde{x} = 18, \theta)p(\theta|x, y)d\theta$$

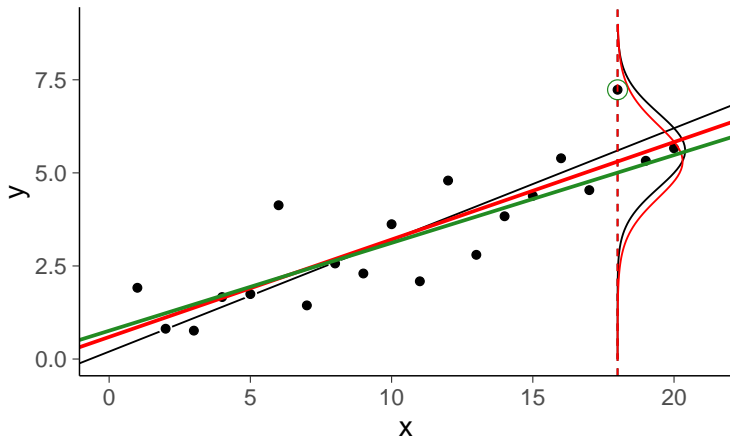
New data



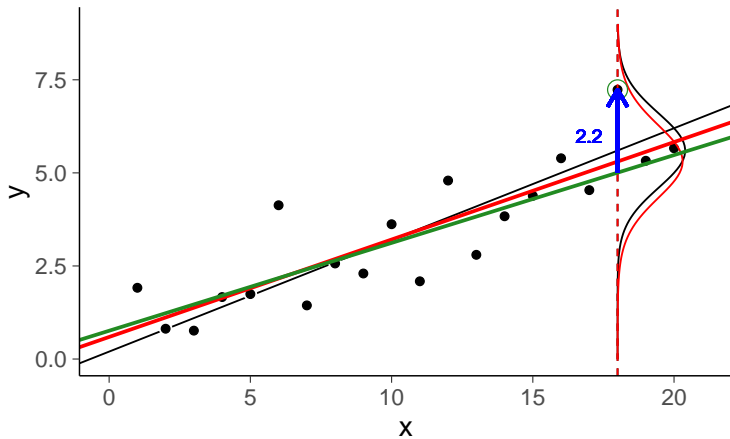
Posterior predictive distribution



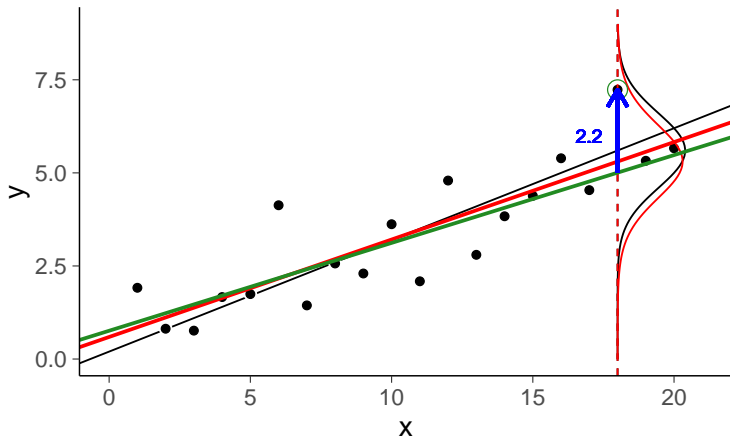
Leave-one-out mean



Leave-one-out residual

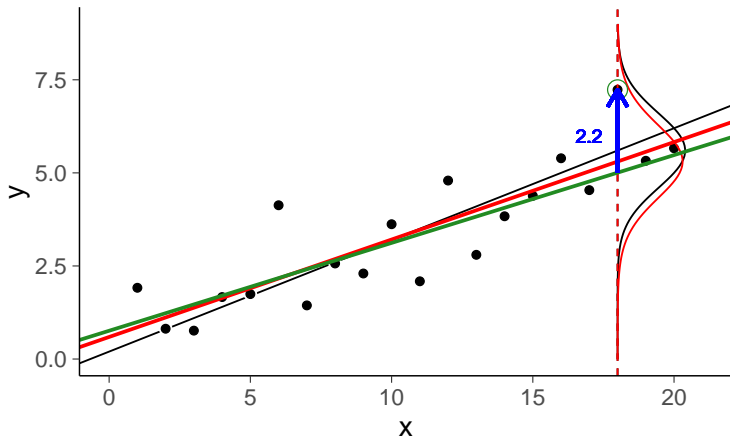


Leave-one-out residual



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

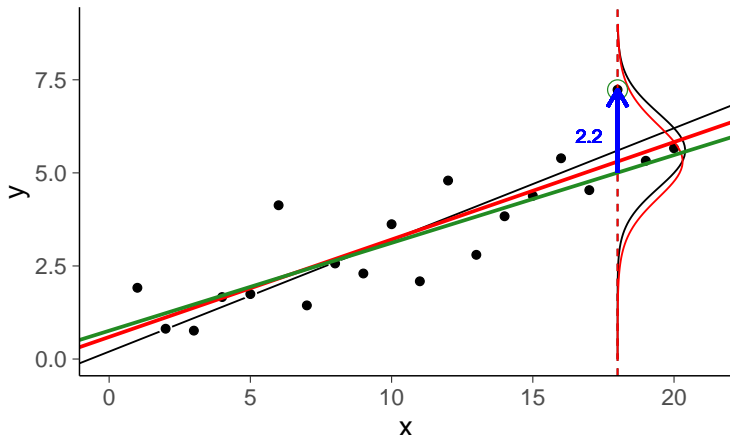
Leave-one-out residual



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

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

Leave-one-out residual

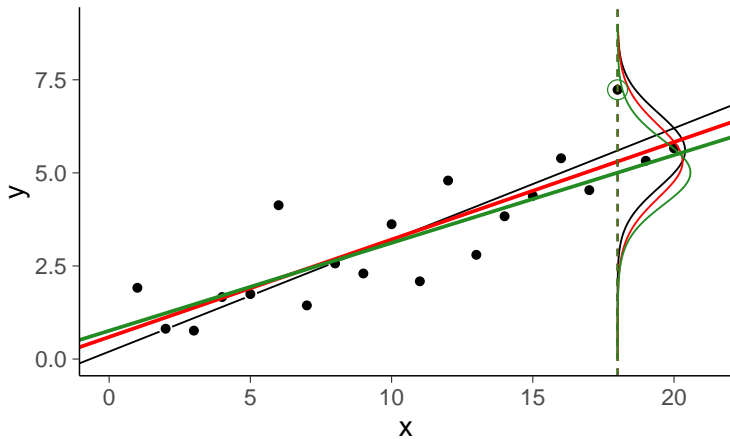


$$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$$

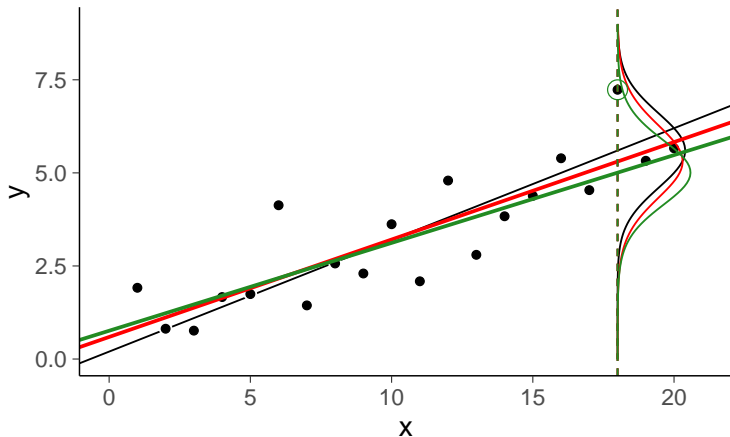
Can be used to compute, e.g., RMSE, R^2 , 90% error

See LOO- R^2 at avehtari.github.io/bayes_R2/bayes_R2.html

Leave-one-out predictive distribution

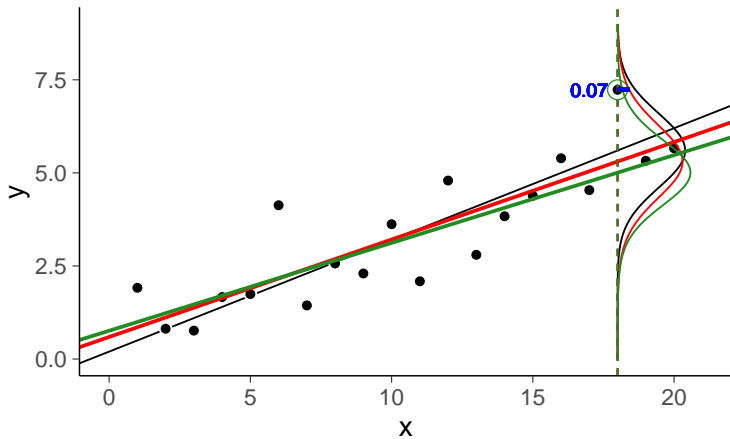


Leave-one-out predictive distribution

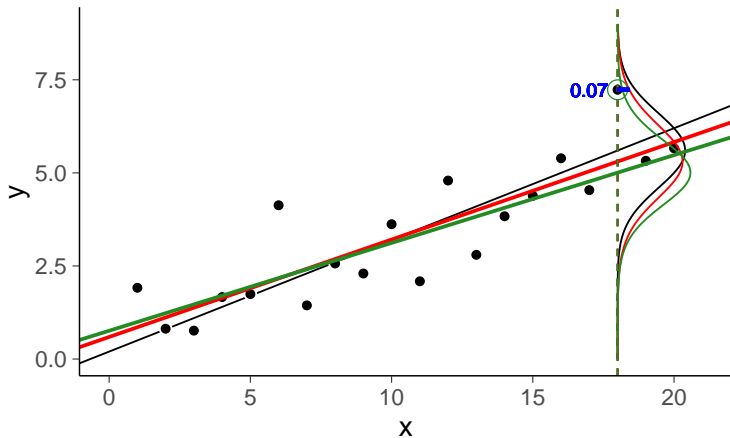


$$p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18}) = \int p(\tilde{y}|\tilde{x} = 18, \theta)p(\theta|x_{-18}, y_{-18})d\theta$$

Posterior predictive density

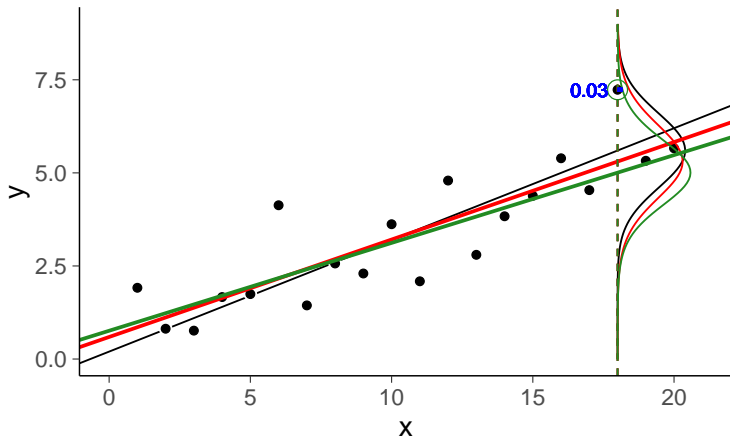


Posterior predictive density



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

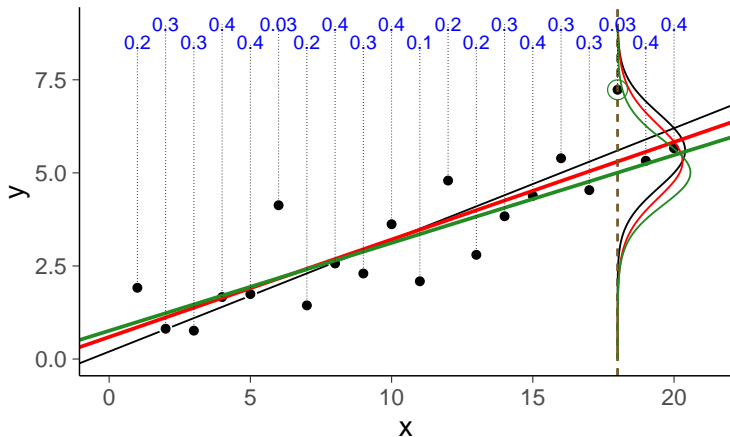
Leave-one-out predictive density



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

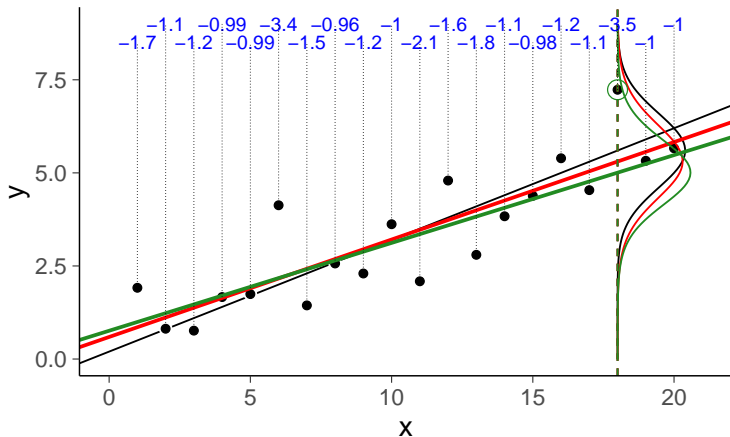
$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$$

Leave-one-out predictive densities



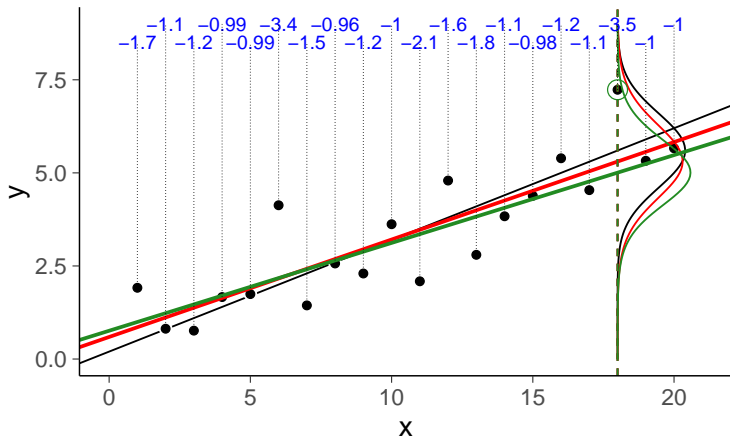
$$p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \dots, 20$$

Leave-one-out log predictive densities



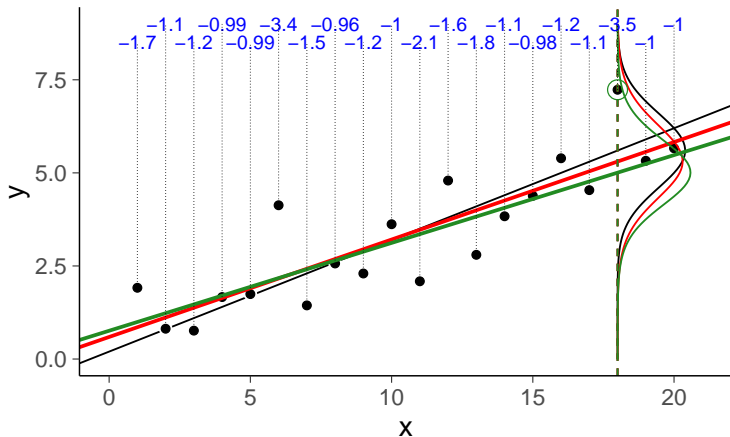
$$\log p(y_i | x_i, x_{-i}, y_{-i}), \quad i = 1, \dots, 20$$

Leave-one-out log predictive densities



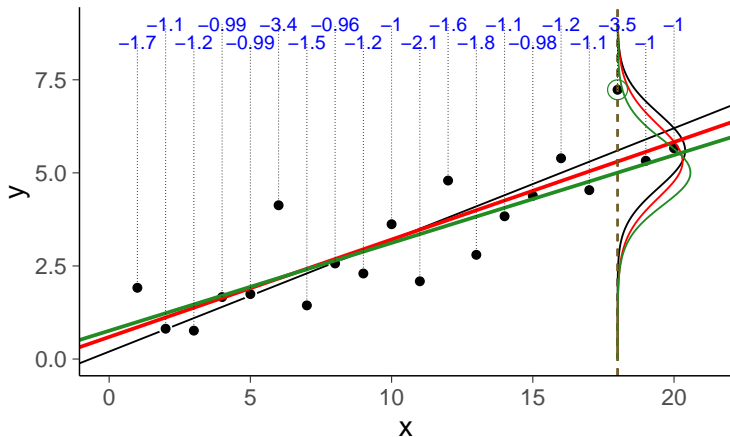
$$\sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

Leave-one-out log predictive densities



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

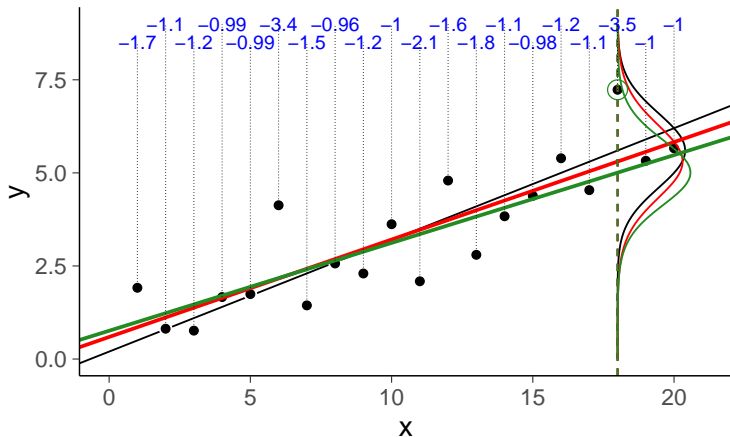
Leave-one-out log predictive densities



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

unbiased estimate of log posterior pred. density for new data

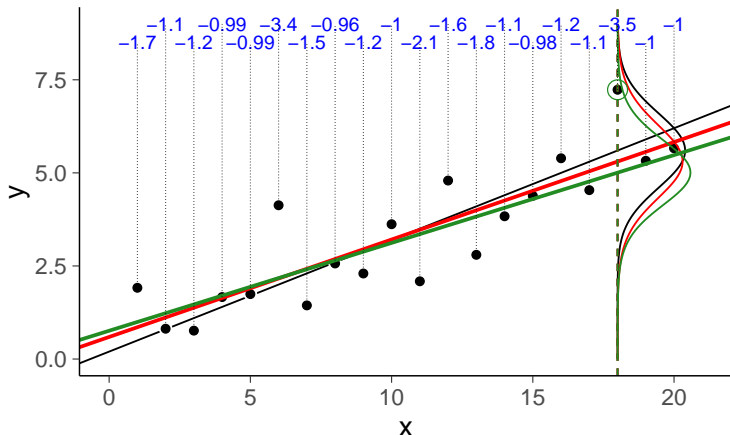
Leave-one-out log predictive densities



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

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

Leave-one-out log predictive densities

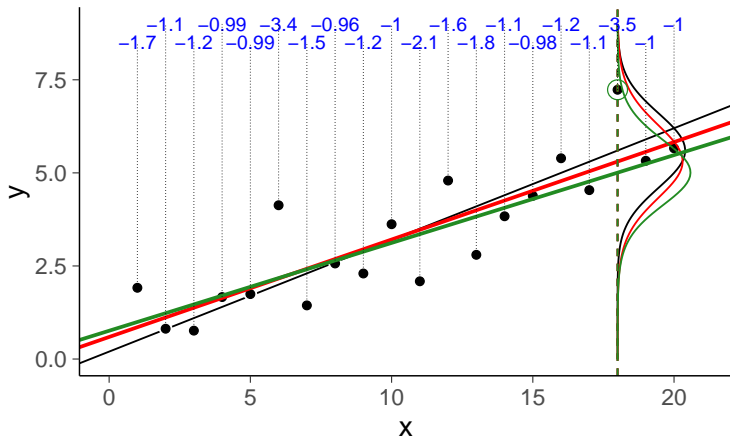


$$\text{elpd_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

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

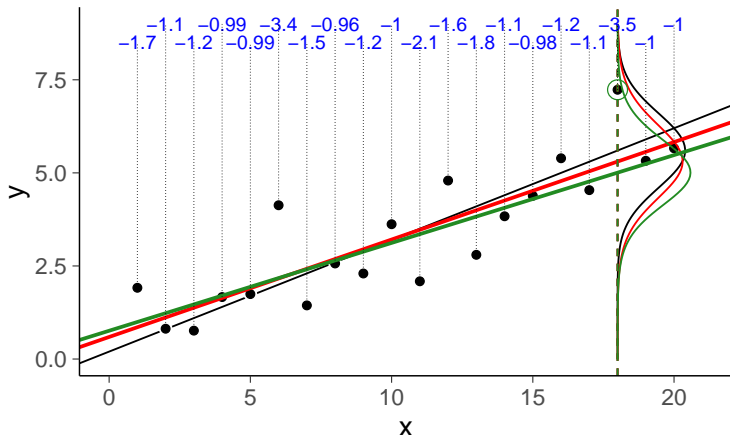
Leave-one-out log predictive densities



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

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

Leave-one-out log predictive densities

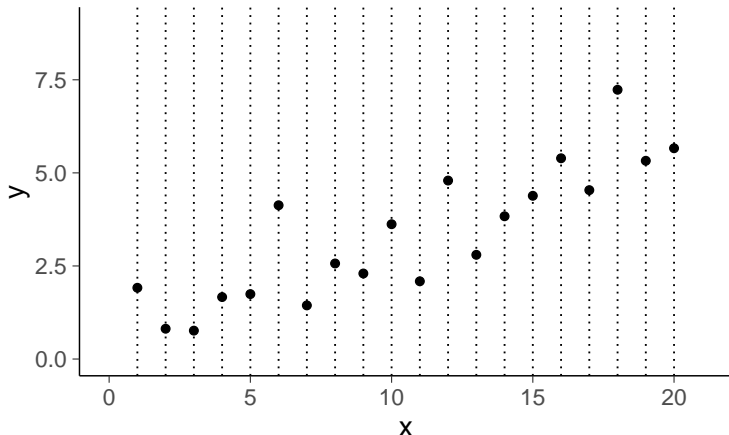


$$\text{elpd_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

see Vehtari, Gelman & Gabry (2017a) and Vehtari & Ojanen (2012) for more

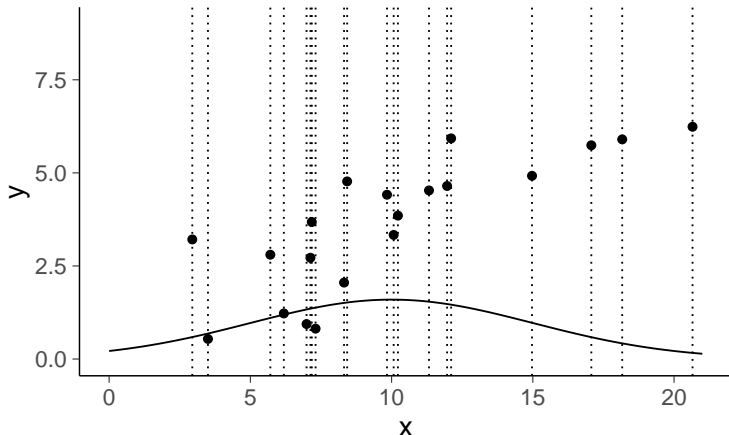
Fixed / designed x



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

see [Vehtari & Ojanen \(2012\)](#) and andrewgelman.com/2018/08/03/loo-cross-validation-approaches-valid/

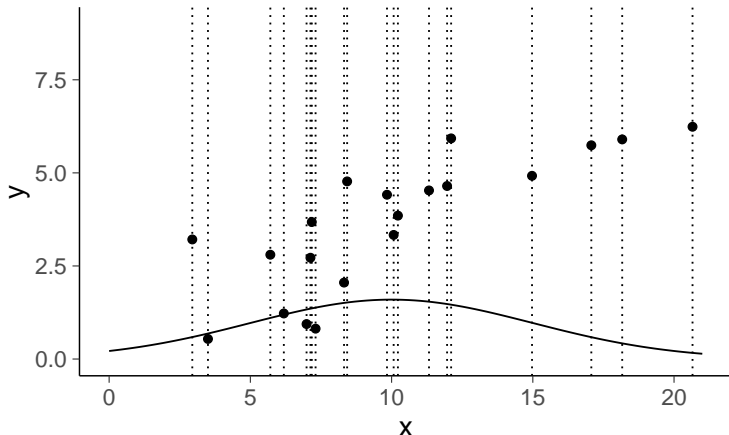
Distribution for x



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

see [Vehtari & Ojanen \(2012\)](#) and andrewgelman.com/2018/08/03/loo-cross-validation-approaches-valid/

Distribution for x



LOO is ok for random x . SE is uncertainty about $y|x$ and x .
Covariate shift can be handled with importance weighting or modelling
see [Vehtari & Ojanen \(2012\)](#) and andrewgelman.com/2018/08/03/loo-cross-validation-approaches-valid/

loo package

Computed from 4000 by 20 log-likelihood matrix

	Estimate	SE
elpd_loo	-29.5	3.3
p_loo	2.7	1.0

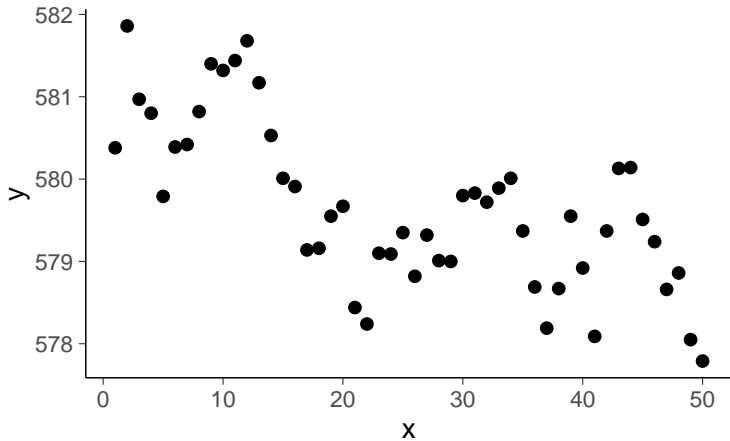
Monte Carlo SE of elpd_loo is 0.1.

Pareto k diagnostic values:

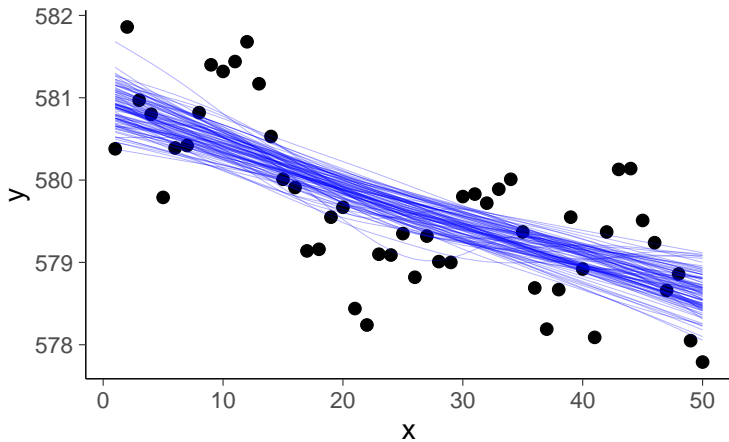
		Count	Pct.	Min.	n_eff
(-Inf, 0.5]	(good)	18	90.0%	899	
(0.5, 0.7]	(ok)	2	10.0%	459	
(0.7, 1]	(bad)	0	0.0%	<NA>	
(1, Inf)	(very bad)	0	0.0%	<NA>	

All Pareto k estimates are ok ($k < 0.7$).

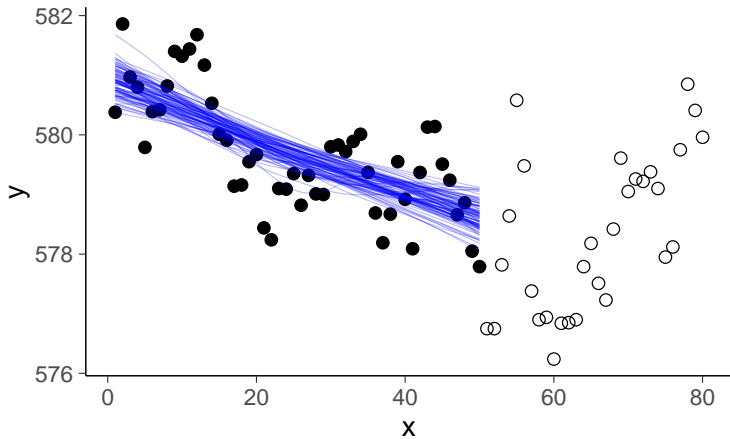
See `help('pareto-k-diagnostic')` for details.



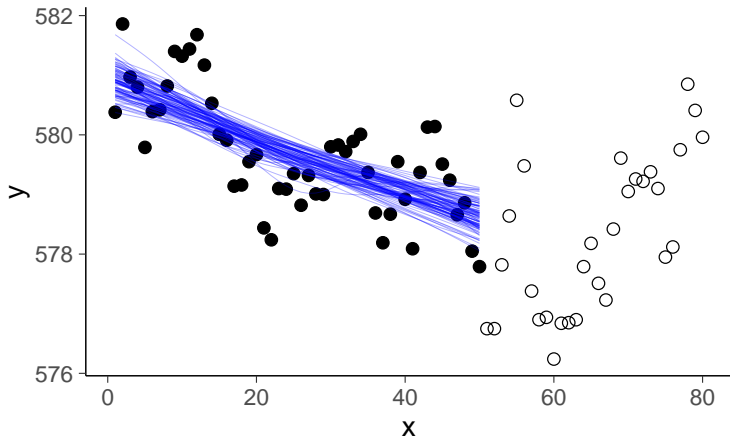
Nonlinear model fit



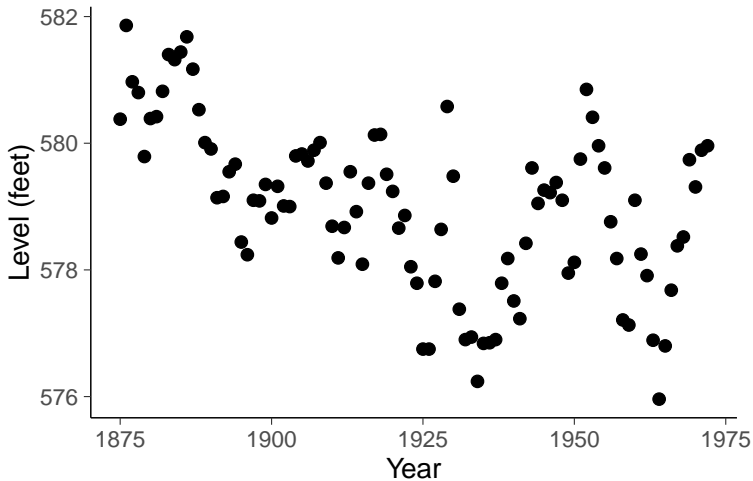
Nonlinear model fit + new data



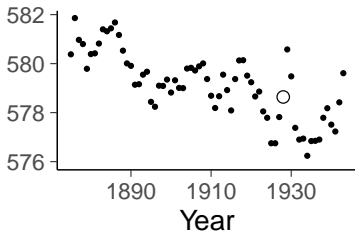
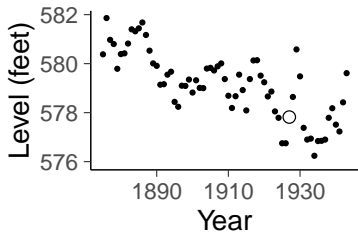
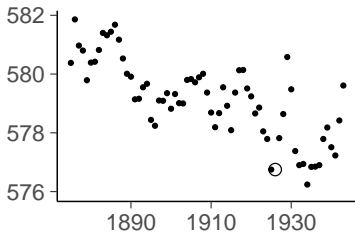
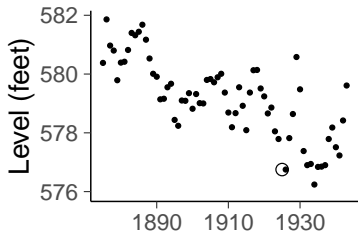
Nonlinear model fit + new data



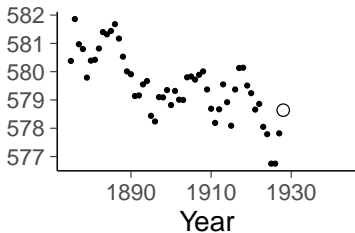
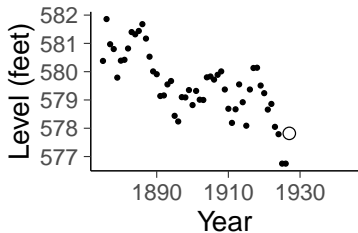
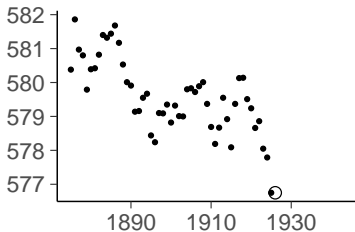
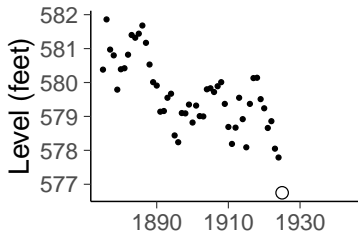
Extrapolation is more difficult



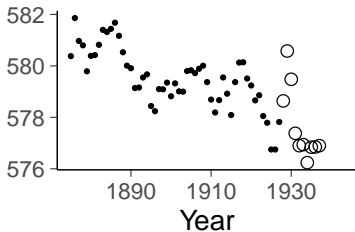
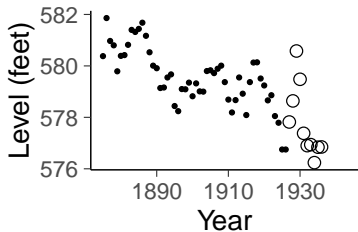
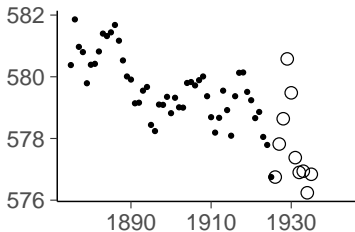
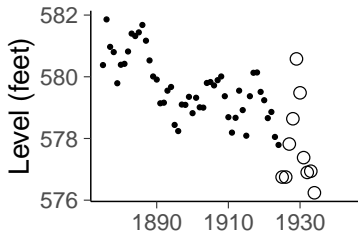
Can LOO or other cross-validation be used with time series?



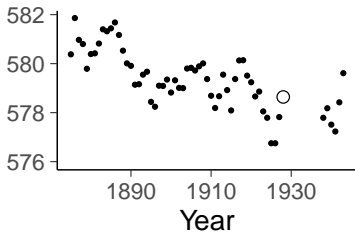
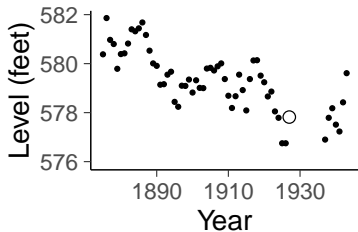
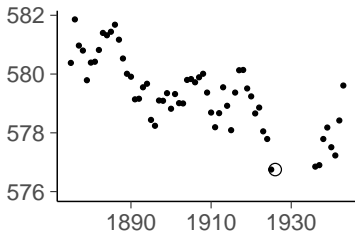
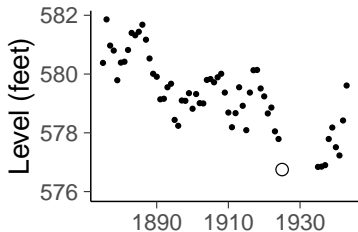
Leave-one-out cross-validation is ok for assessing conditional model



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

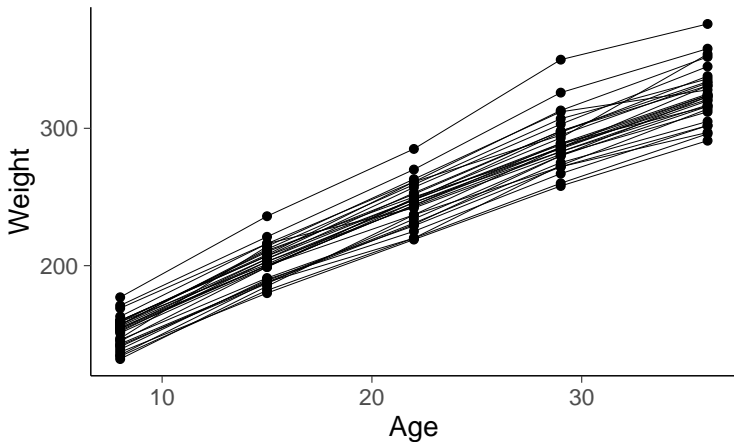


m-step-ahead cross-validation is better for predicting further future



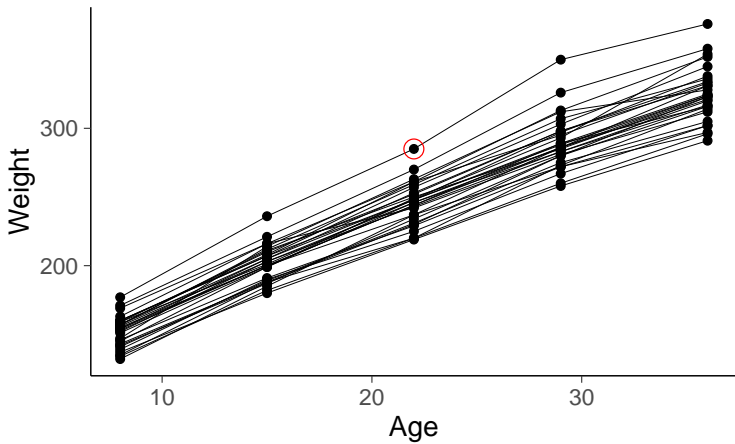
m-step-ahead leave-a-block-out cross-validation

Rats data



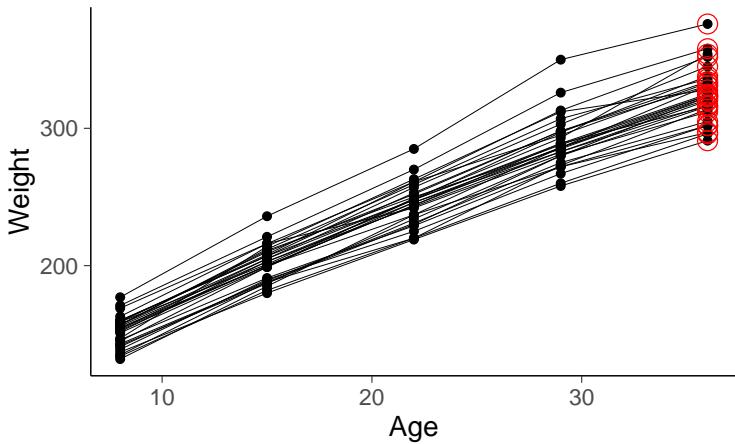
Can LOO or other cross-validation be used with hierarchical data?

Leave-one-out?



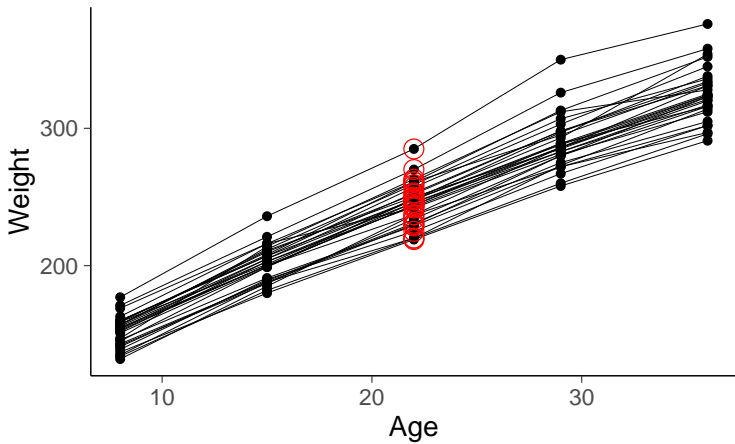
Yes!

1-step-ahead?



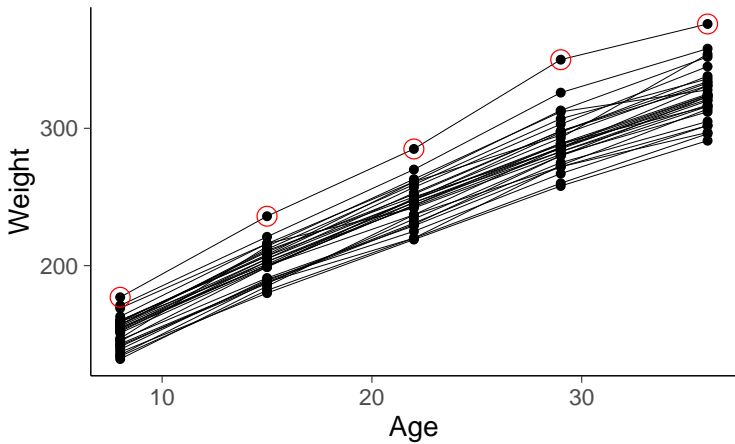
Yes!

Leave-one-time-point-out?



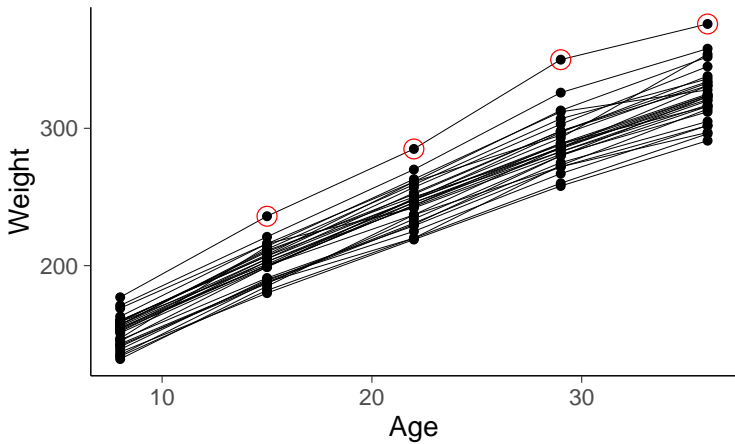
Yes!

Leave-one-rat-out?



Yes!

Predict given initial weight?



Yes!

Summary of data generating mechanisms and prediction tasks

- You have to make some assumptions on data generating mechanism
- Use the knowledge of the prediction task if available
- Cross-validation can be used to analyse different parts, even if there is no clear prediction task

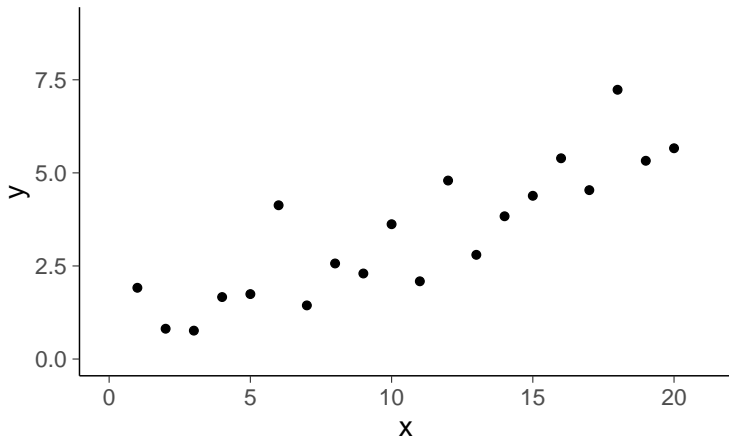
see [Vehtari & Ojanen \(2012\)](#) and andrewgelman.com/2018/08/03/loo-cross-validation-approaches-valid/

Fast cross-validation

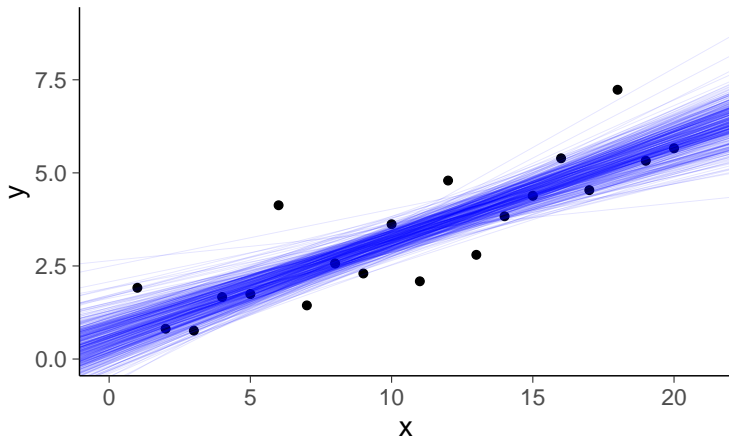
- Pareto smoothed importance sampling LOO (PSIS-LOO)
- K-fold cross-validation

see [Vehtari, Gelman & Gabry \(2017a\)](#) and mc-stan.org/loo/

Data

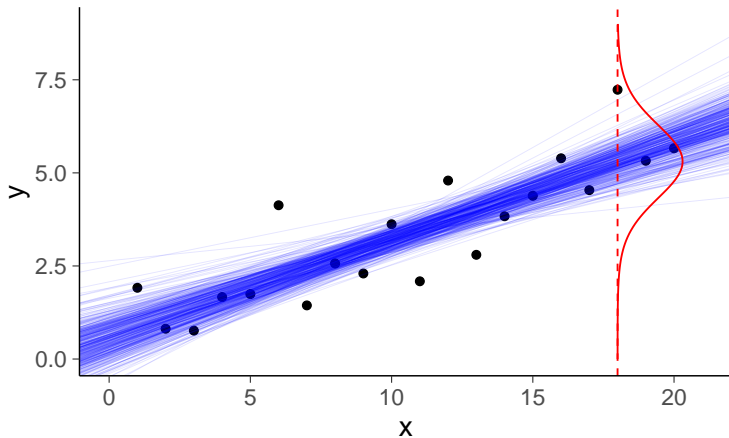


Posterior draws



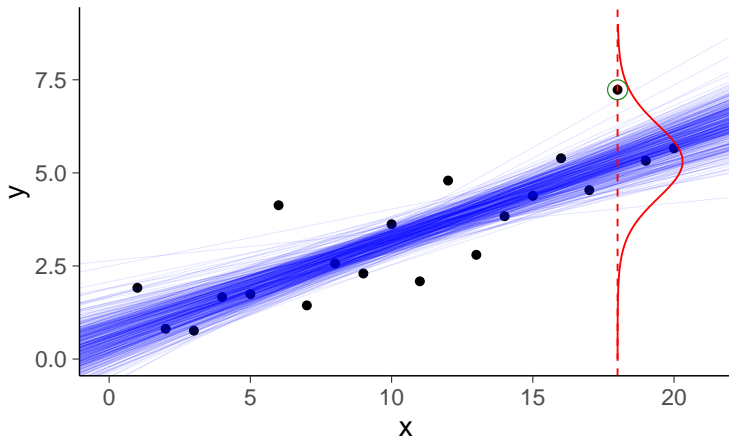
$$\theta^{(s)} \sim p(\theta|x, y)$$

Posterior predictive distribution



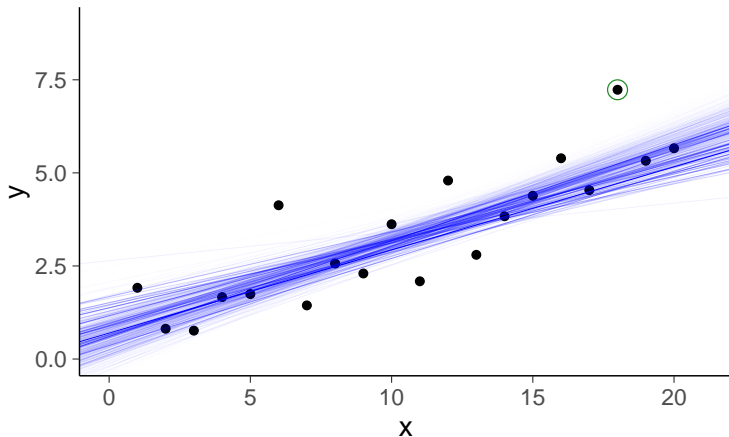
$$\theta^{(s)} \sim p(\theta|x, y), \quad p(\tilde{y}|\tilde{x}, x, y) \approx \frac{1}{S} \sum_{s=1}^S p(\tilde{y}|\tilde{x}, \theta^{(s)})$$

Posterior predictive distribution



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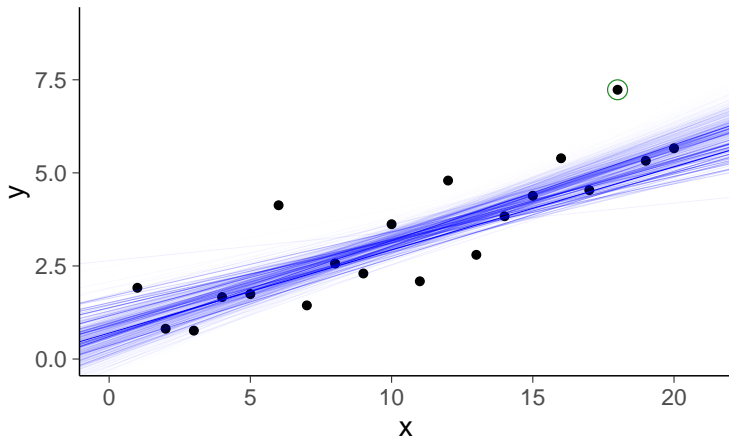
PSIS-LOO weighted draws



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

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

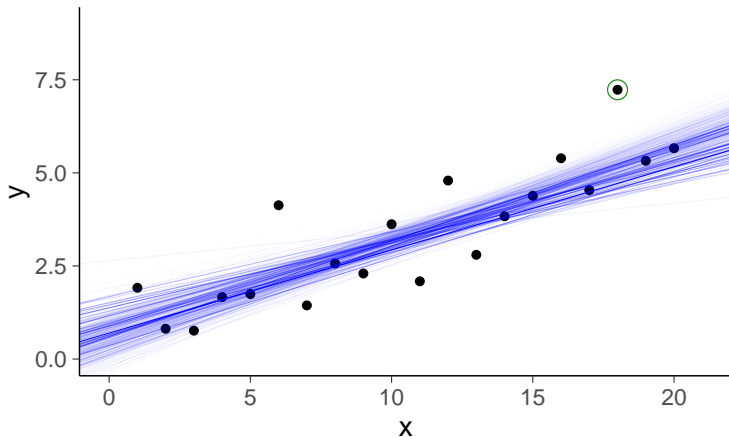
PSIS-LOO weighted draws



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

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

PSIS-LOO weighted draws

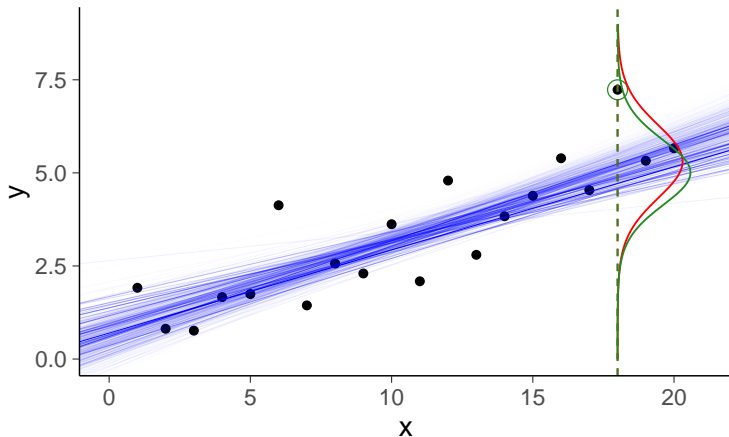


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$$\log(1/p(y_i|x_i, \theta^{(s)})) = -\log_lik[i]$$

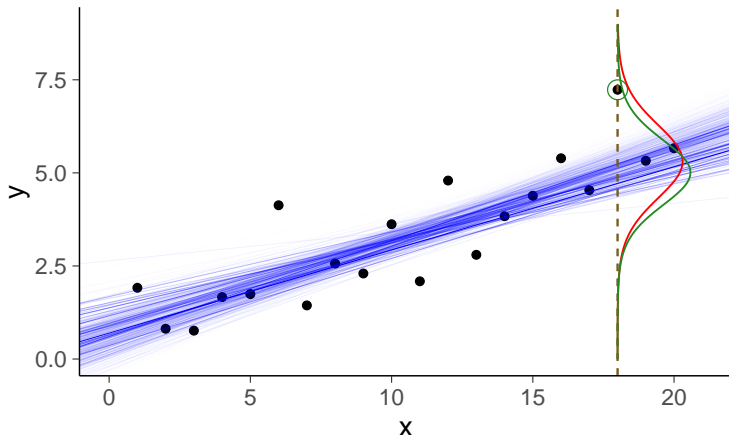
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PSIS-LOO weighted predictive distribution

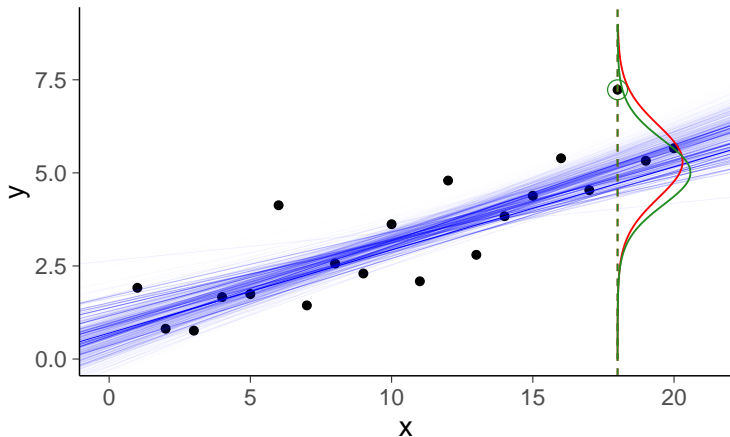


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$$p(y_i|x_i, x_{-i}, y_{-i}) \approx \sum_{s=1}^S [w_i^{(s)} p(y_i|x_i, \theta^{(s)})]$$

PSIS-LOO weighted predictive distribution

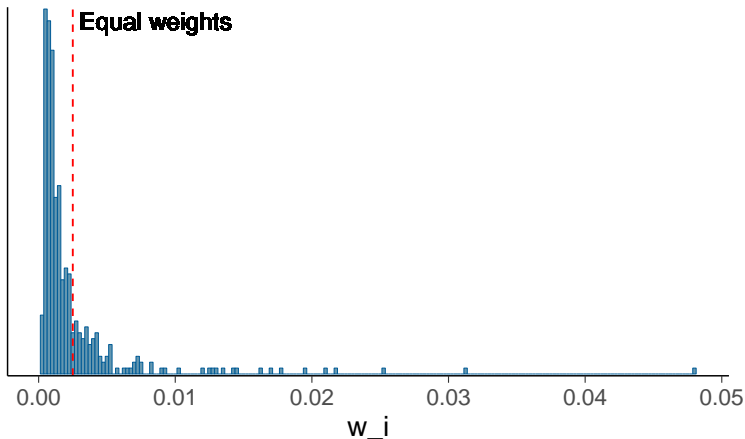


$$\theta^{(s)} \sim p(\theta|x, y)$$

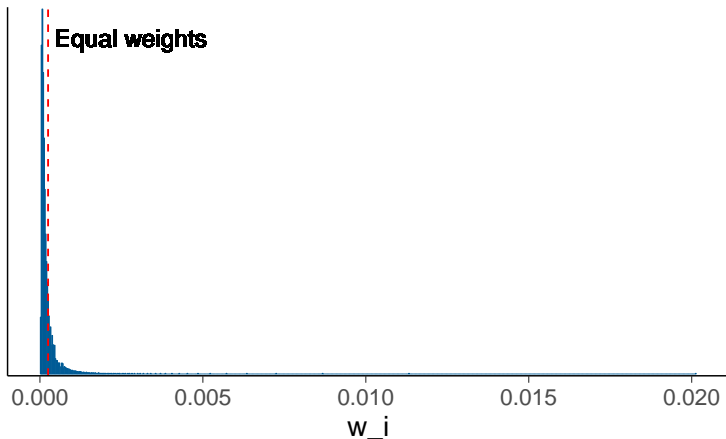
$$r_i^{(s)} = p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y) \propto 1/p(y_i|x_i, \theta^{(s)})$$

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

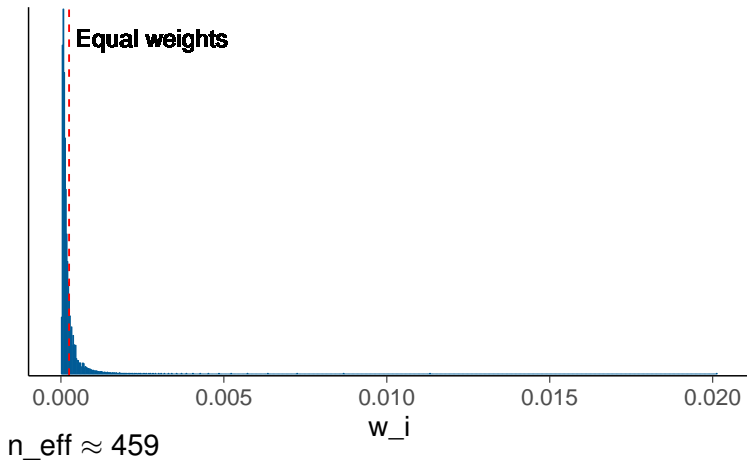
400 importance weights for leave-18th-out



4000 importance weights for leave-18th-out

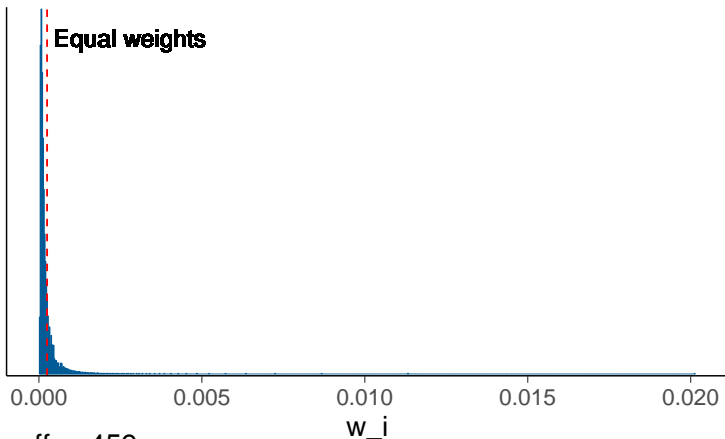


4000 importance weights for leave-18th-out



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

4000 importance weights for leave-18th-out



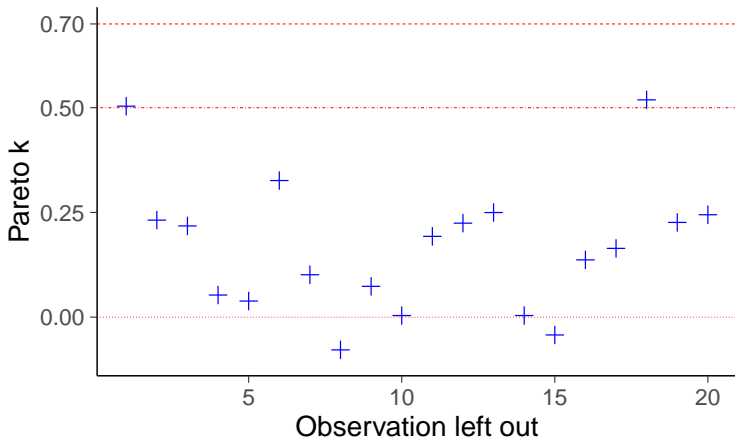
$n_{\text{eff}} \approx 459$

Pareto $\hat{k} \approx 0.52$

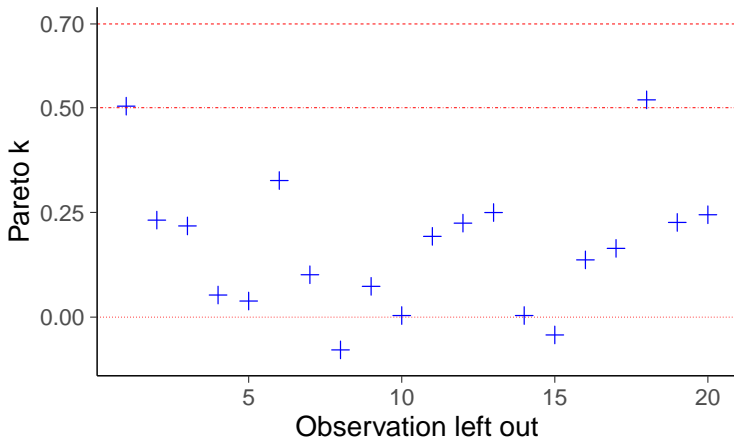
- Pareto \hat{k} estimates the tail shape which determines the convergence rate of PSIS. Less than 0.7 is ok.

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

PSIS-LOO diagnostics



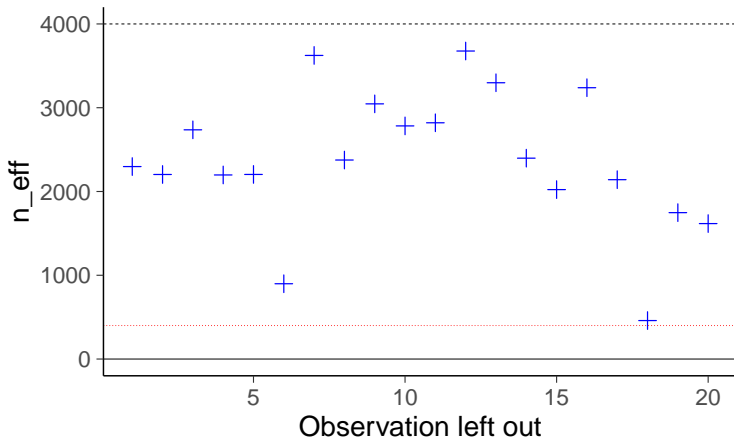
PSIS-LOO diagnostics



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>

PSIS-LOO diagnostics



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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.

Pareto k diagnostic values:

		Count	Pct.	Min.	n_eff
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(1, Inf)	(very bad)	0	0.0%	<NA>	

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

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

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);  
}
```

Stan code

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}
```

- RStanARM and BRMS compute log_lik by default

Pareto smoothed importance sampling LOO

- PSIS-LOO for hierarchical models
 - leave-one-group out is challenging for PSIS-LOO
see Merkel, Furr and Rabe-Hesketh (2018) for an approach
using quadrature integration

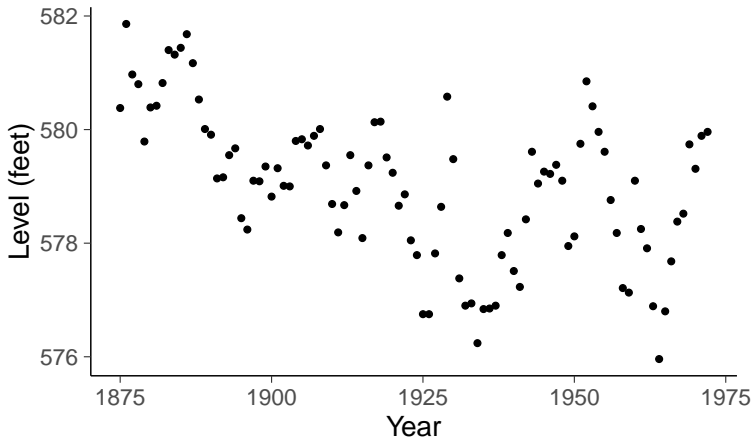
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- PSIS-LOO for non-factorizable models
 - mc-stan.org/loo/articles/loo2-non-factorizable.html

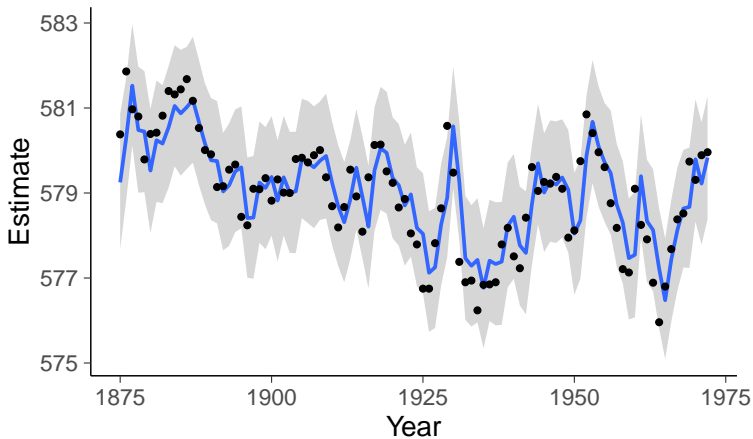
Pareto smoothed importance sampling LOO

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 - mc-stan.org/loo/articles/loo2-non-factorizable.html
- PSIS-LOO for time series
 - Approximate leave-future-out cross-validation
mc-stan.org/loo/articles/loo2-lfo.html

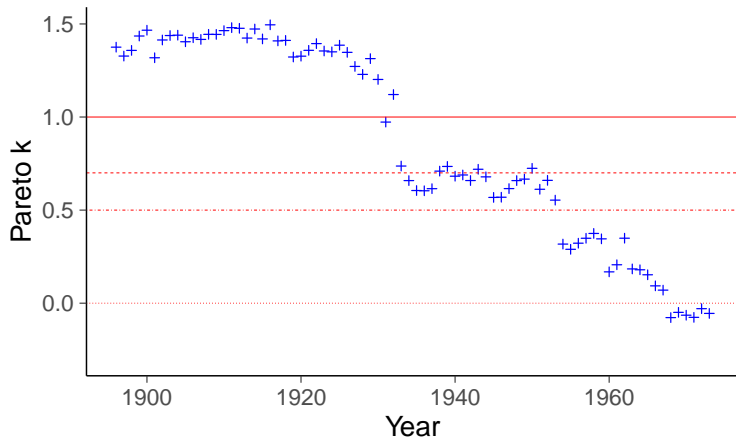
Data



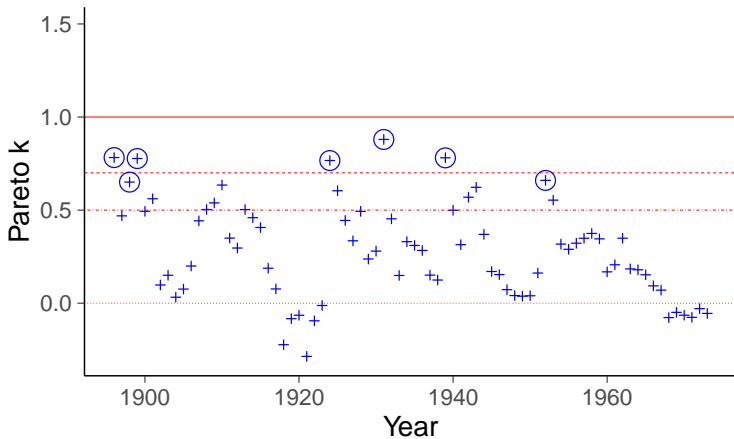
AR-2 prediction with 95% interval



PSIS-1-step-ahead



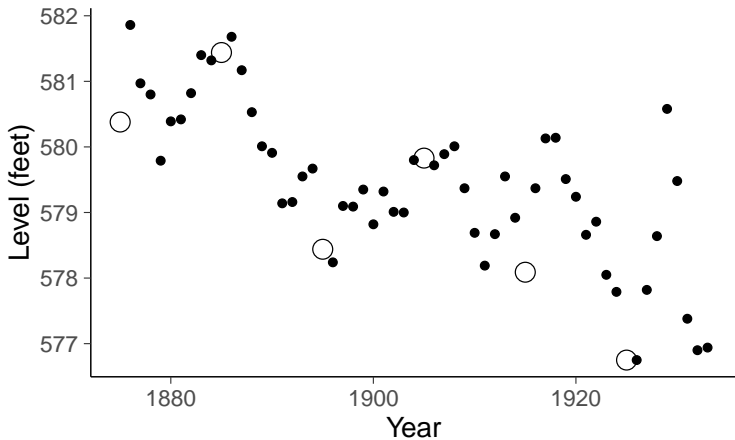
PSIS-1-step-ahead with refits



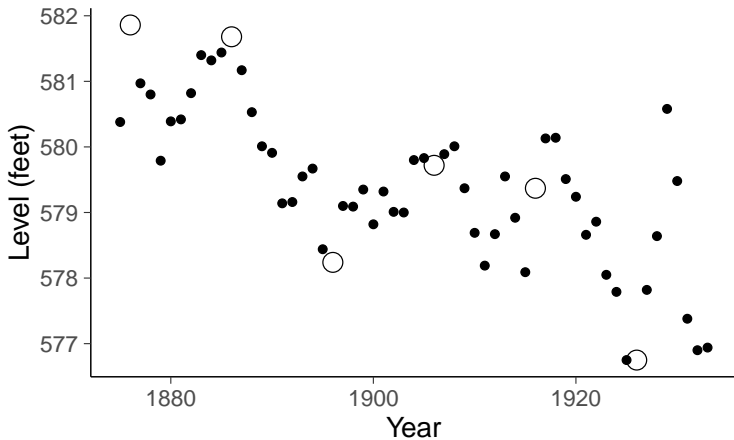
K-fold cross-validation

- K-fold cross-validation can approximate LOO
 - all uses for LOO
- K-fold cross-validation can be used for hierarchical models
 - good for leave-one-group-out
- K-fold cross-validation can be used for time series
 - with leave-block-out

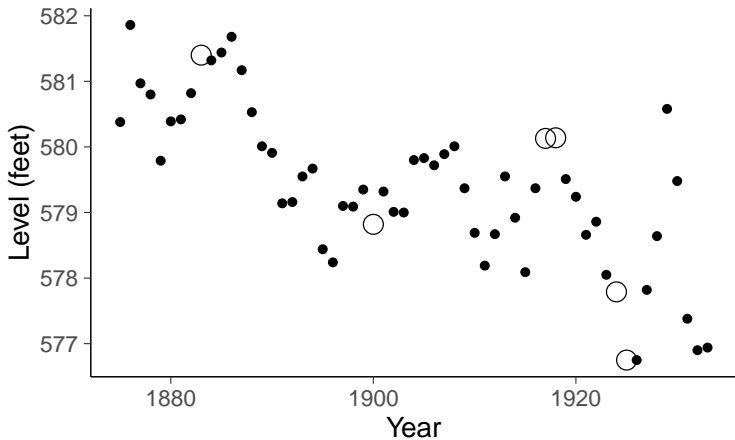
Balance k-fold approximation of LOO



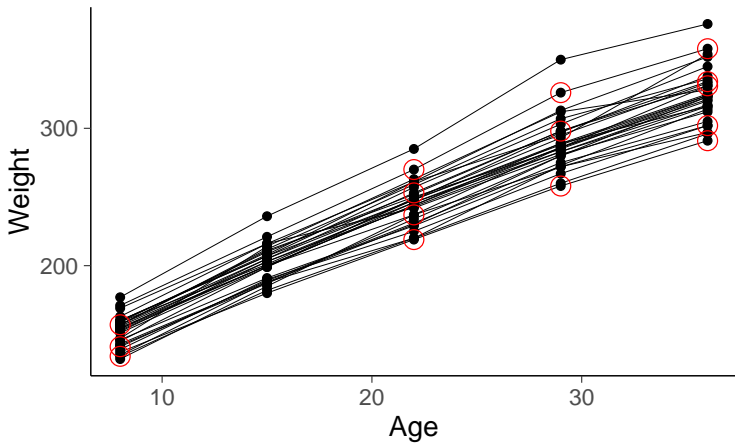
Balance k-fold approximation of LOO



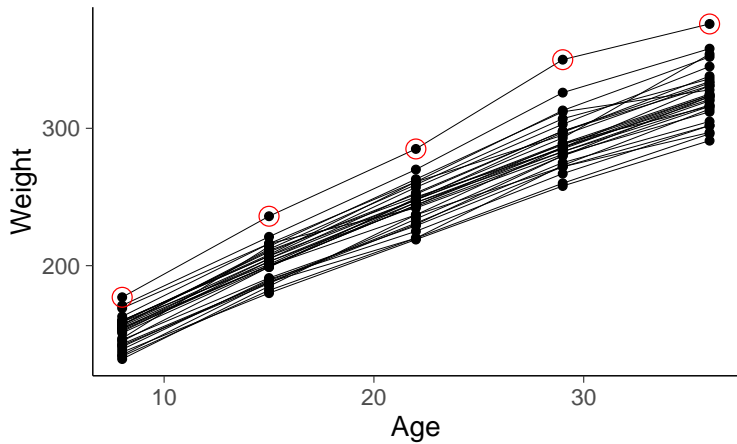
Random k-fold approximation of LOO



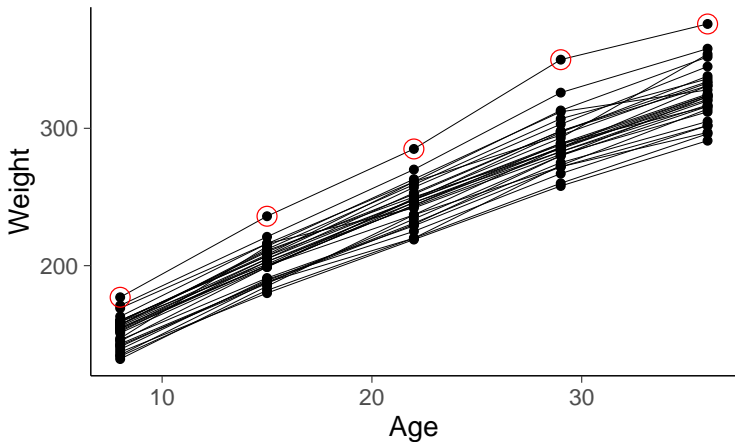
Random kfold approximation of LOO



Leave-one-rat-out



Leave-one-rat-out



`kfold_split_random()`

`kfold_split_balanced()`

`kfold_split_stratified()`

WAIC vs PSIS-LOO

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

WAIC vs PSIS-LOO

- WAIC has same assumptions as LOO

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

WAIC vs PSIS-LOO

- WAIC has same assumptions as LOO
- PSIS-LOO is more accurate

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

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

WAIC vs PSIS-LOO

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

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

WAIC vs PSIS-LOO

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

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

*IC

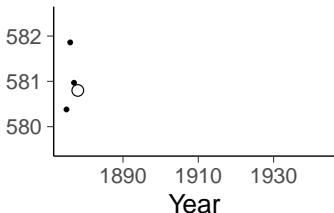
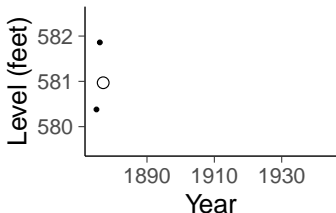
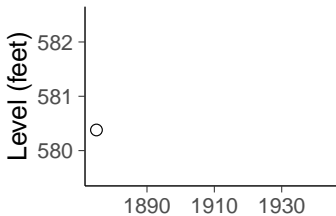
- AIC uses maximum likelihood estimate for prediction
- DIC uses posterior mean for prediction
- BIC is an approximation for marginal likelihood
- TIC, NIC, RIC, PIC, BPIC, QIC, AICc, ...

Marginal likelihood / Bayes factor

- Like leave-future-out 1-step-ahead corss-validation but starting with 0 observations

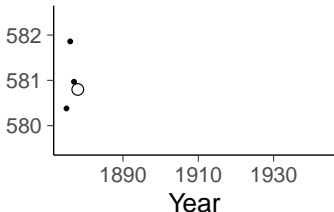
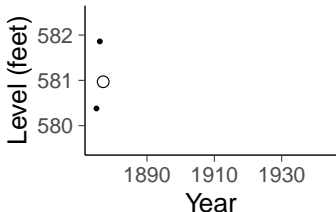
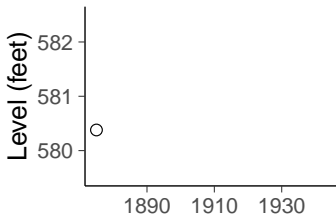
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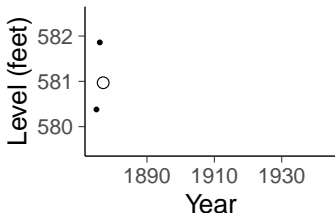
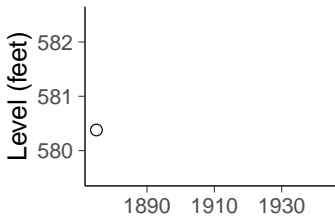
Marginal likelihood / Bayes factor

- Like leave-future-out 1-step-ahead corss-validation but starting with 0 observations
 - which makes it very sensitive to prior



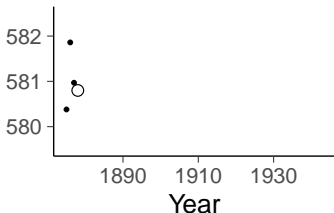
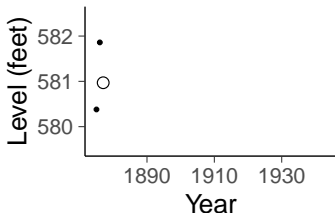
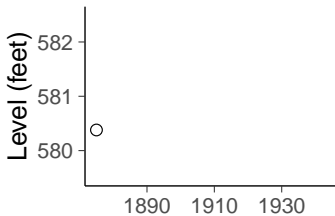
Marginal likelihood / Bayes factor

- Like leave-future-out 1-step-ahead cross-validation but starting with 0 observations
 - which makes it very sensitive to prior and
 - unstable in case of misspecified models



Marginal likelihood / Bayes factor

- Like leave-future-out 1-step-ahead cross-validation but starting with 0 observations
 - which makes it very sensitive to prior and
 - unstable in case of misspecified models also asymptotically



Cross-validation for model assessment

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

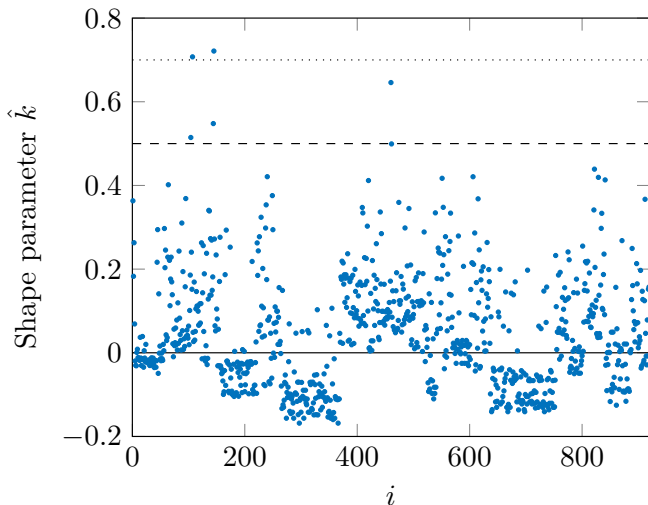
Cross-validation for model assessment

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

see demos avehtari.github.io/modelselection/

Radon example

PSIS-LOO diagnostics

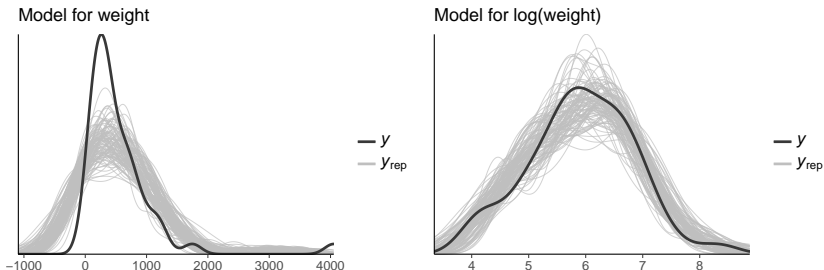


see [Vehtari, Gelman & Gabry \(2017a\)](#)

Sometimes cross-validation is not needed

Sometimes cross-validation is not needed

- Posterior predictive checking is often sufficient

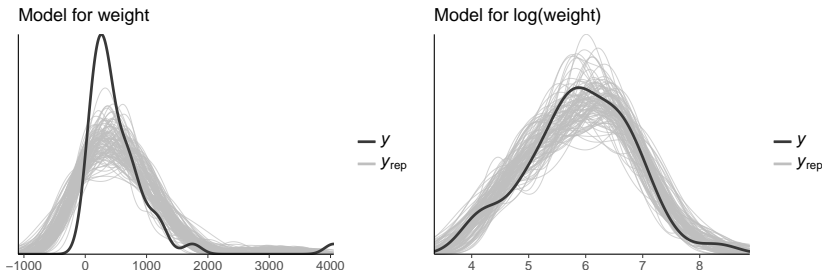


Predicting the yields of mesquite bushes.

Gelman, Hill & Vehtari (2019): Regression and Other Stories, Chapter 11.

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Predicting the yields of mesquite bushes.

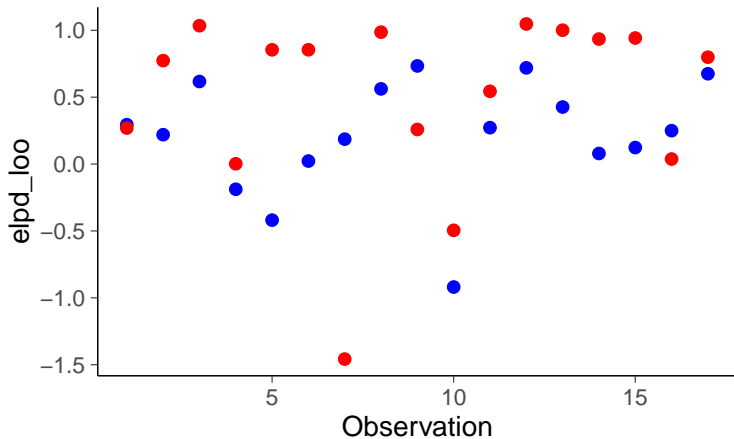
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- BDA3, Chapter 6
- Gabry, Simpson, Vehtari, Betancourt, Gelman (2018). Visualization in Bayesian workflow. JRSS A, [preprint arXiv:1709.01449](https://arxiv.org/abs/1709.01449)
- mc-stan.org/bayesplot/articles/graphical-ppcs.html
- betanalpha.github.io/assets/case_studies/principled_bayesian_workflow.html

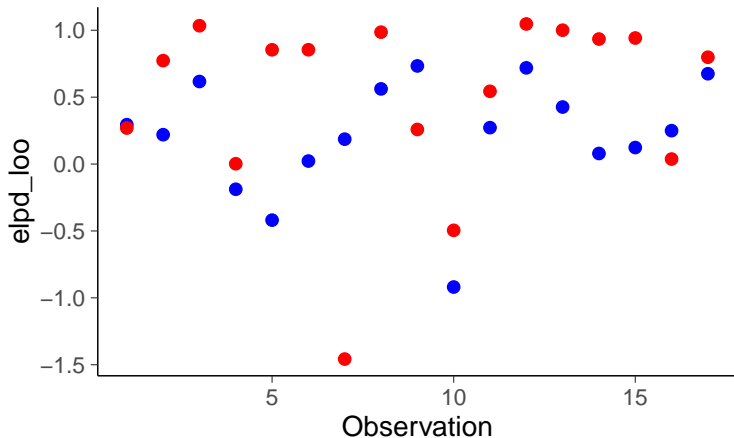
Model comparison

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

Pointwise comparison LOO models: Model 1



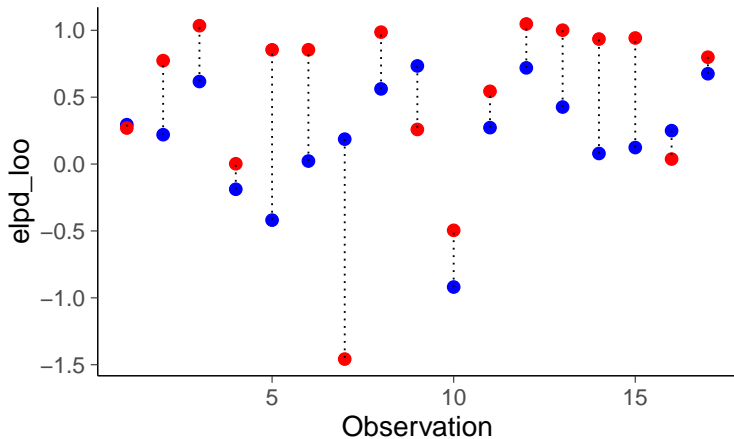
Pointwise comparison LOO models: Model 1



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

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

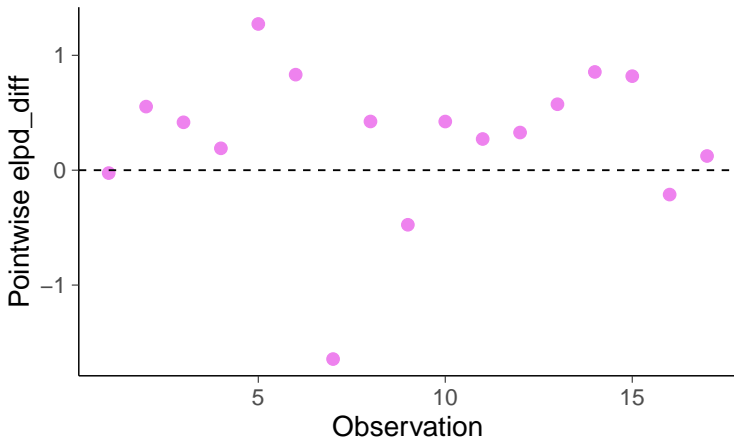
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Pointwise comparison LOO models

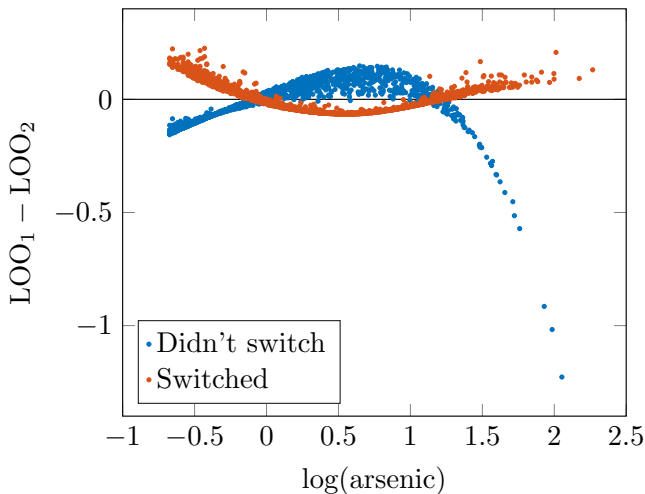


Model comparison:

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

elpd_diff	se
4.7	2.7

Arsenic well example – Model comparison

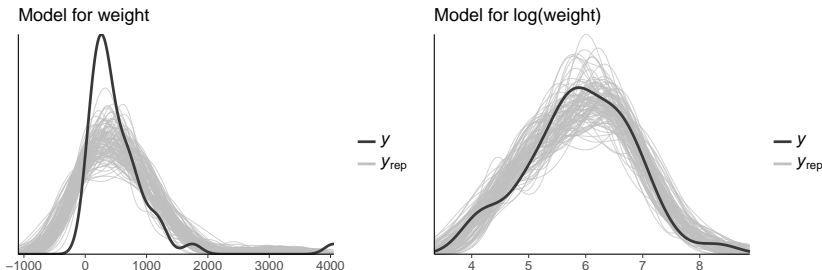


An estimated difference in elpd_{loo} of 16.4 with SE of 4.4.

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

Sometimes cross-validation is not needed

- Posterior predictive checking is often sufficient



Predicting the yields of mesquite bushes.

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- For some very simple cases you may assume that true model is included in the list of models considered (M -closed)

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 - see predictive model selection in M -closed case by San Martini and Spezzaferri (1984)

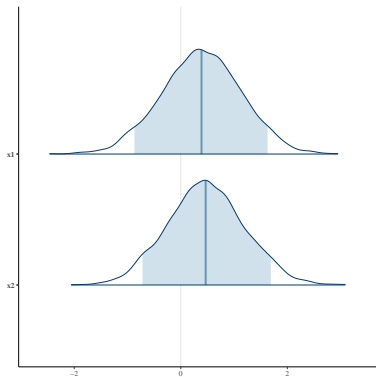
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avehtari.github.io/modelselection/betablockers.html

Sometimes predictive model comparison can be useful

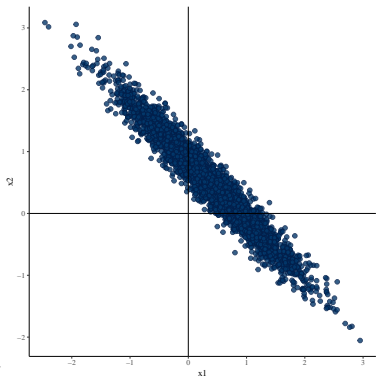


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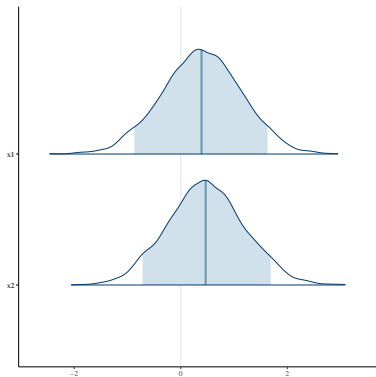
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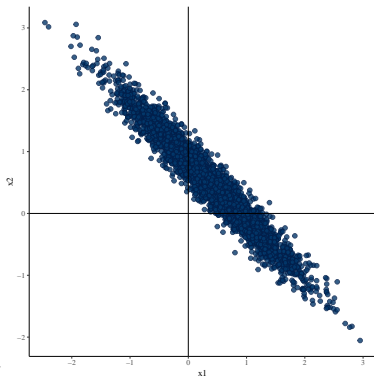
Joint posterior density

`rstanarm` + `bayesplot`

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see also [Collinear demo](#)

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- Bayesian stacking may work better than BMA
 - Yao, Vehtari, Simpson, & Gelman (2018)

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Selection induced bias and overfitting

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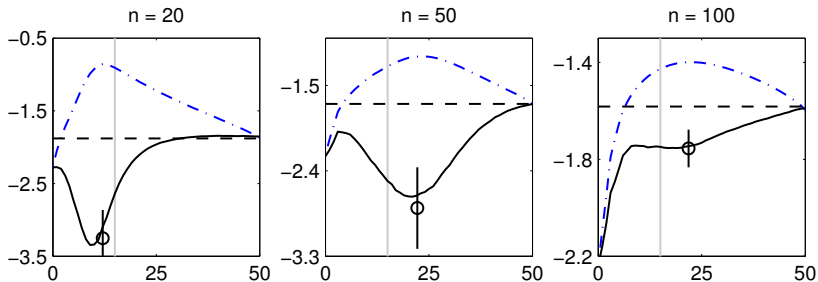
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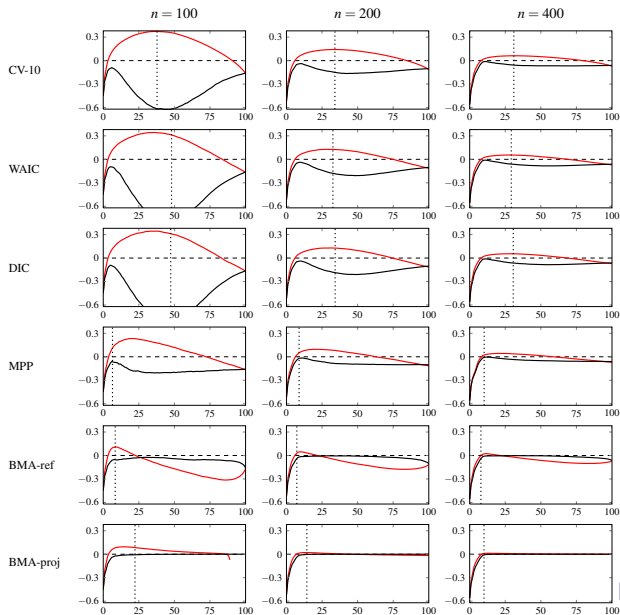
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- Bigger problem if there is a large number of models as in covariate selection

Selection induced bias in variable selection

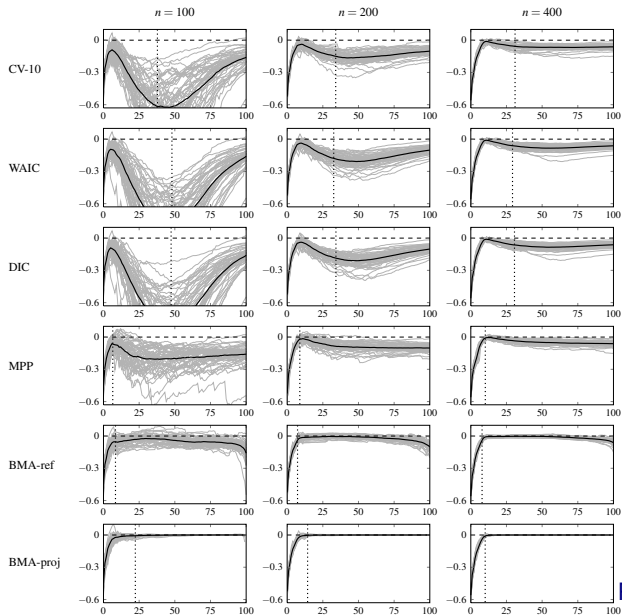


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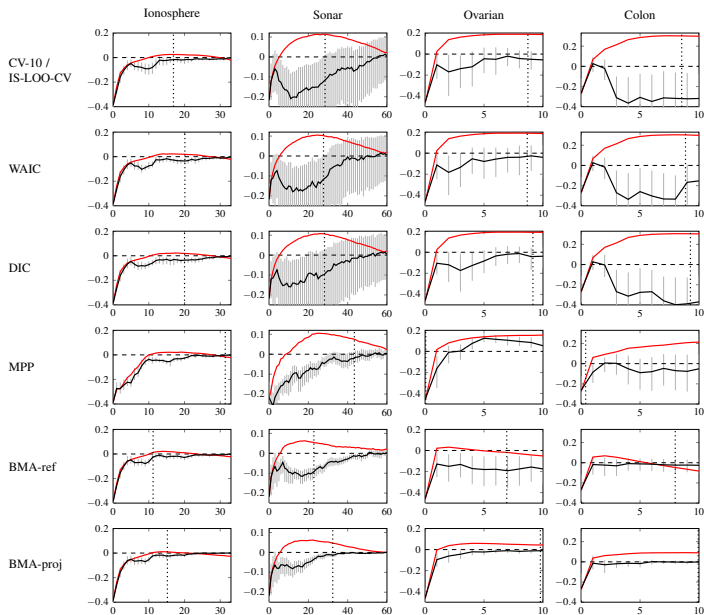
Piironen & Vehtari (2017)

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Take-home messages

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- Cross-validation can simulate predicting and observing new data
- Cross-validation is good if you don't trust your model
- Different variants of cross-validation are useful in different scenarios
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