

# 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 assessment, selection and inference after selection

- Extra material at <https://avehtari.github.io/modelselection/>
  - Videos, Slides, Notebooks, References
- CV-FAQ  
<https://avehtari.github.io/modelselection/CV-FAQ.html>

## 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

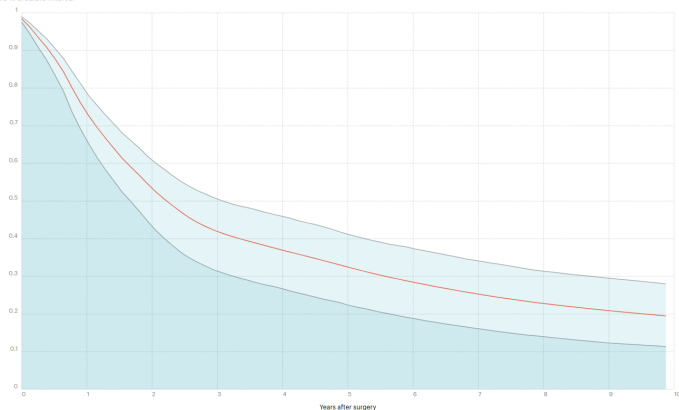
*kaiku*

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

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- ▶ 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

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



- 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, \*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>	

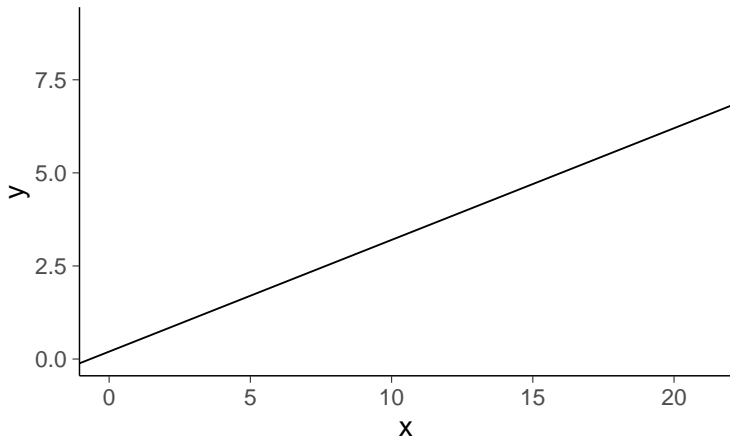
All Pareto k estimates are ok ( $k < 0.7$ ).  
See `help('pareto-k-diagnostic')` for details.

Model comparison:

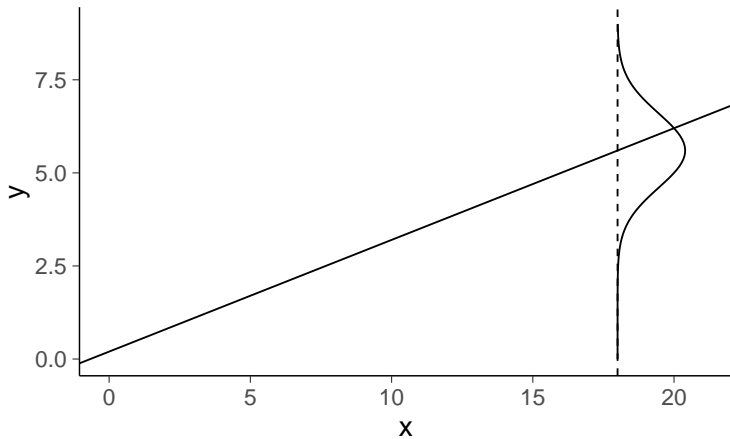
(negative 'elpd\_diff' favors 1st model, positive favors 2nd)

elpd_diff	se
-0.2	0.1

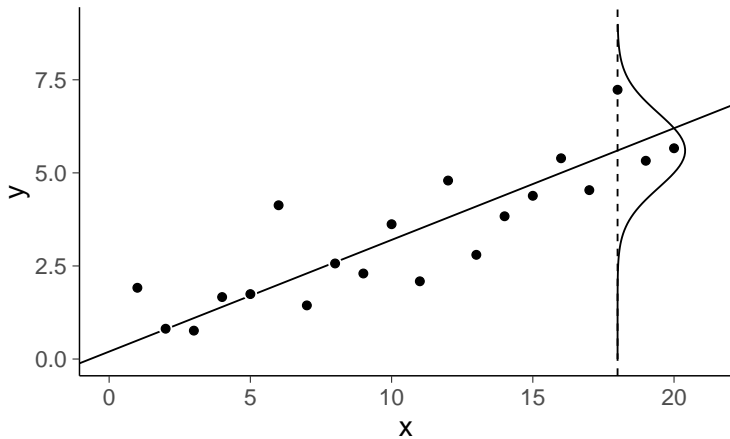
True mean  $y = a + bx$



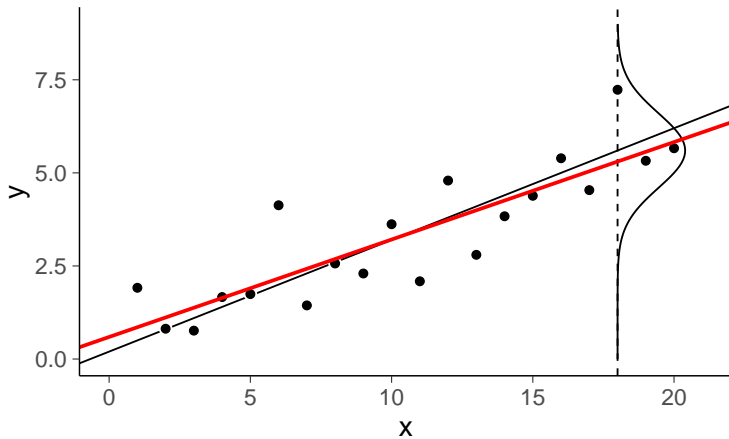
## True mean and sigma



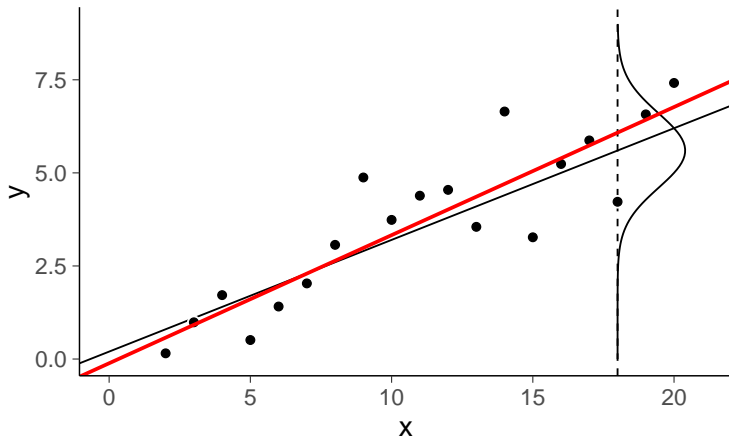
# Data



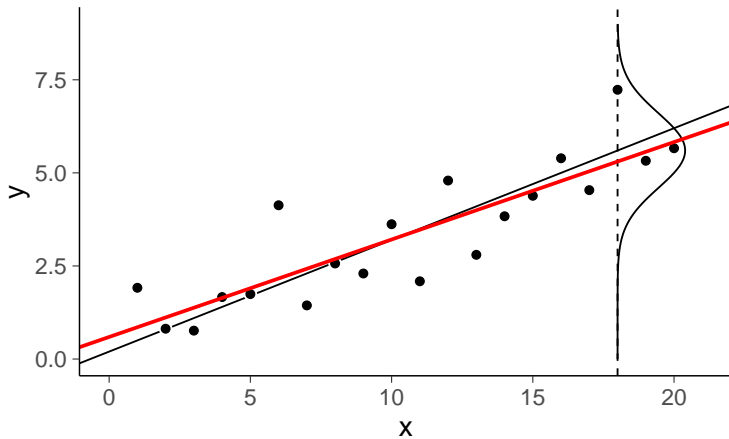
## Posterior mean



## Posterior mean, alternative data realisation

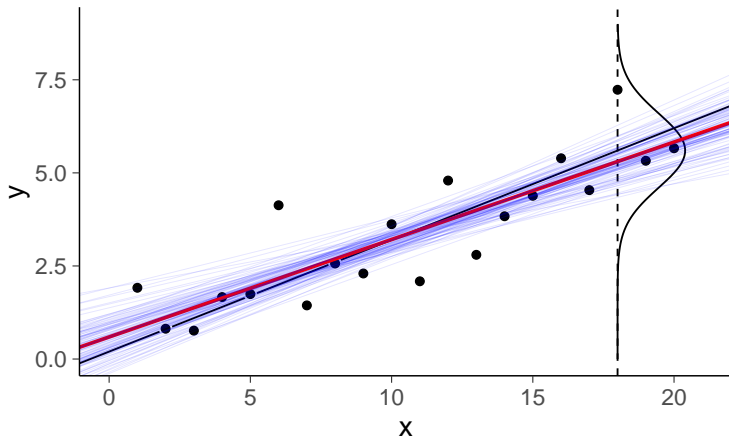


## Posterior mean

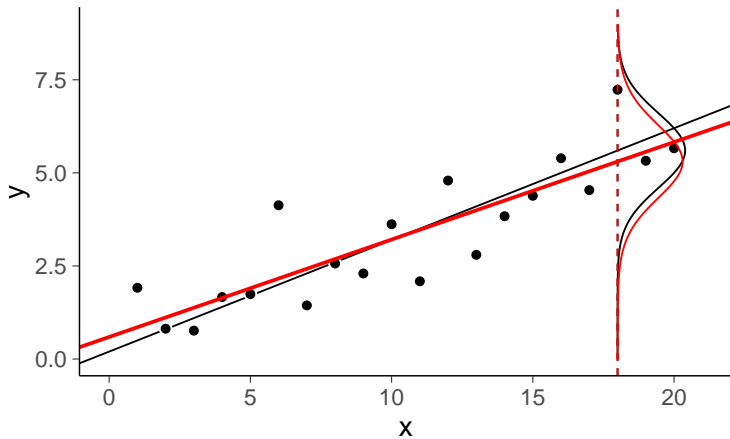




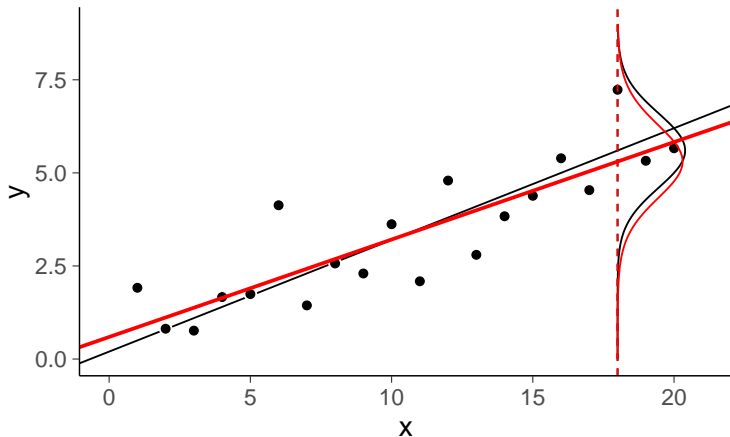
## Posterior draws



## Posterior predictive distribution

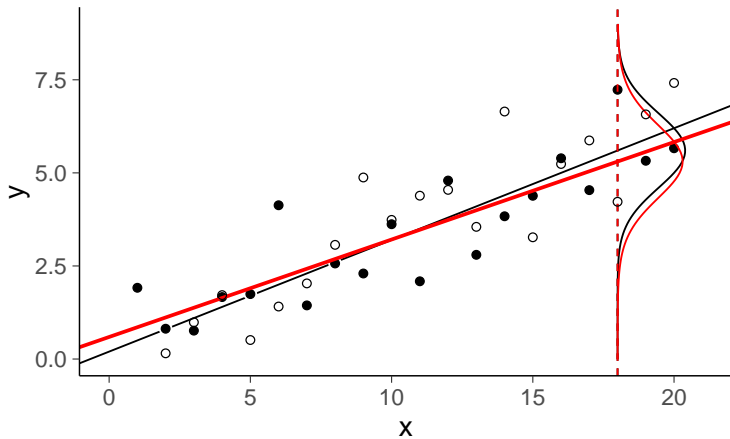


## Posterior predictive distribution

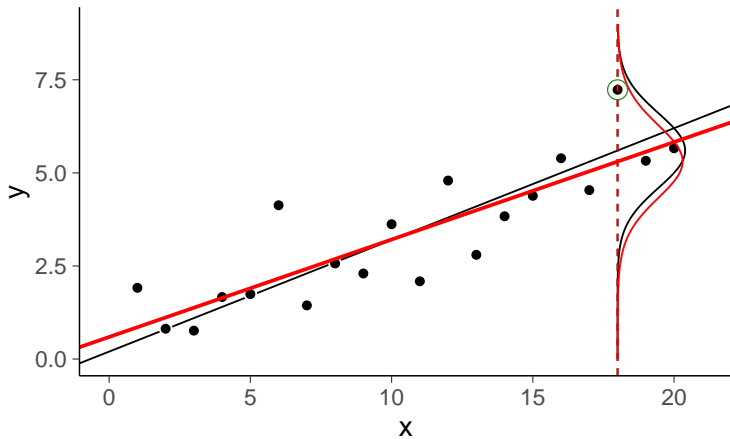


$$p(\tilde{y} \mid \tilde{x} = 18, x, y) = \int p(\tilde{y} \mid \tilde{x} = 18, \theta) p(\theta \mid x, y) d\theta$$

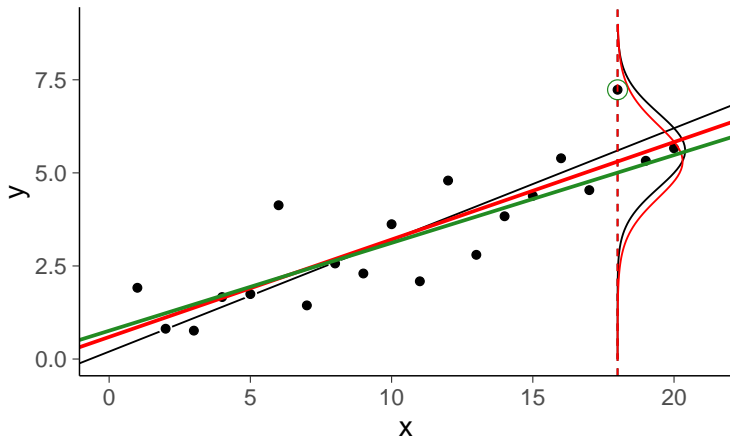
## New data



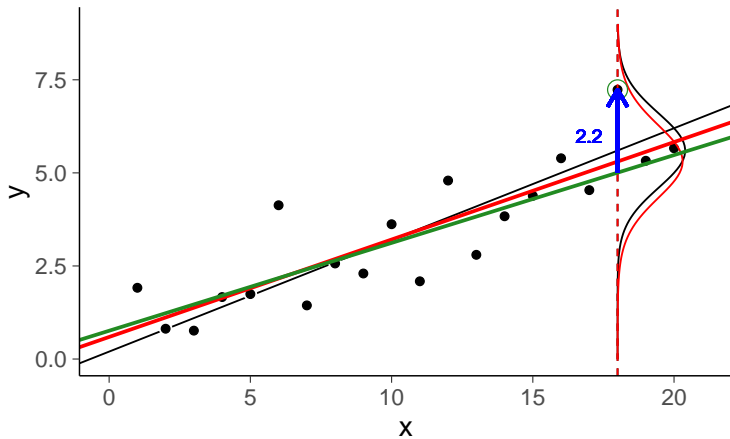
## Posterior predictive distribution



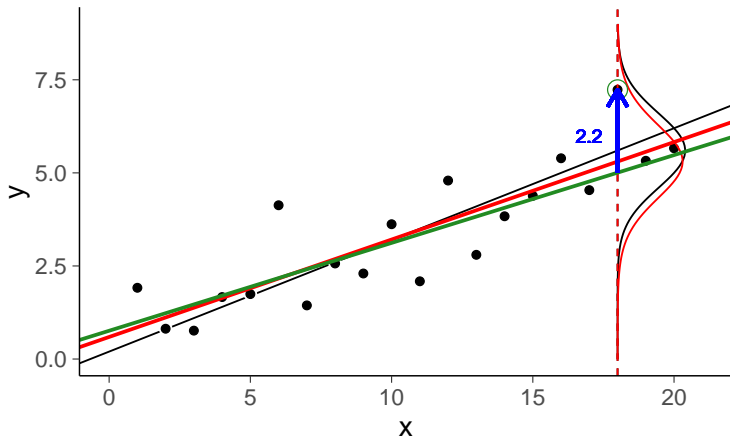
## Leave-one-out mean



## Leave-one-out residual



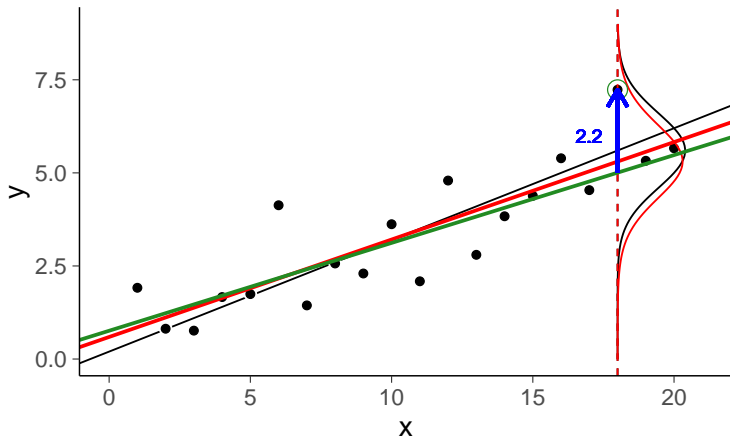
## Leave-one-out residual



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



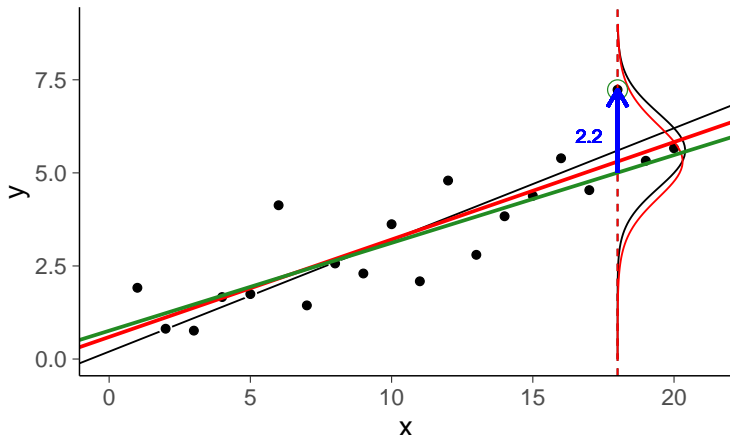
## Leave-one-out residual



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

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

## Leave-one-out residual

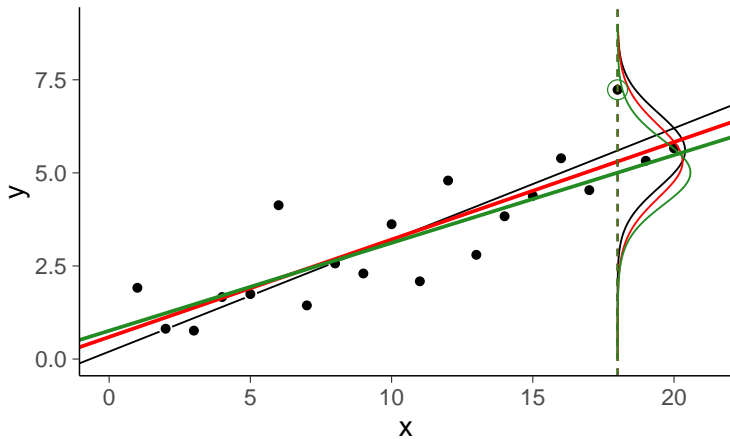


$$y_{18} - E[p(\tilde{y} \mid \tilde{x} = 18, x_{-18}, y_{-18})]$$

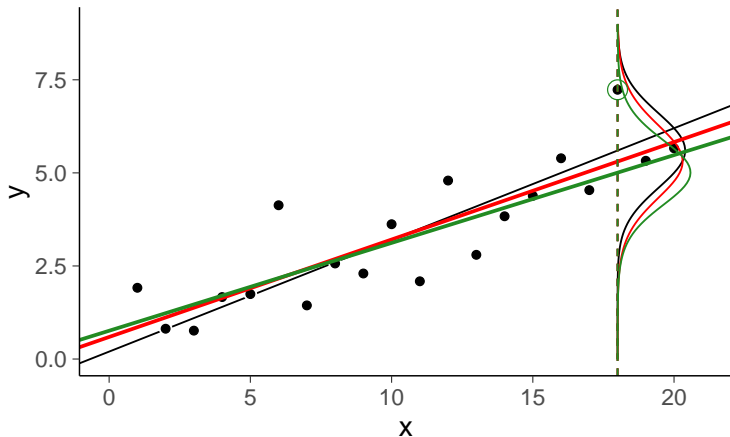
Can be use to compute, e.g., RMSE,  $R^2$ , 90% error

See LOO- $R^2$  at [avehtari.github.io/bayes\\_R2/bayes\\_R2.html](https://avehtari.github.io/bayes_R2/bayes_R2.html)

## Leave-one-out predictive distribution

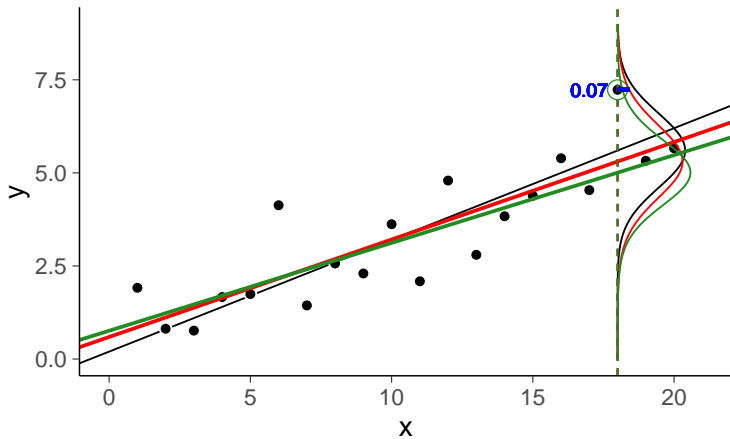


## Leave-one-out predictive distribution

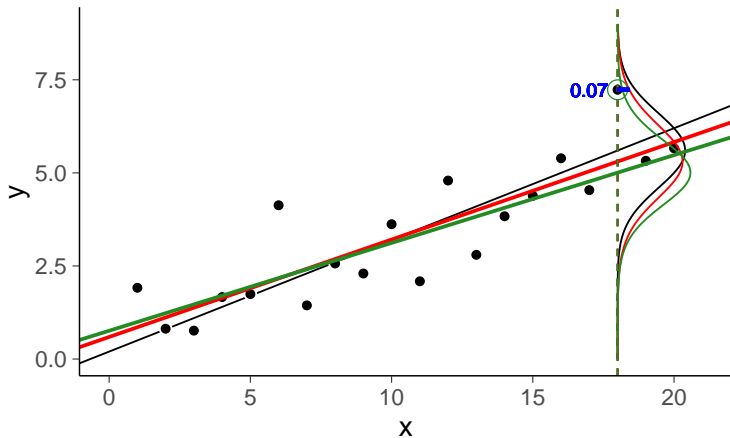


$$p(\tilde{y} \mid \tilde{x} = 18, x_{-18}, y_{-18}) = \int p(\tilde{y} \mid \tilde{x} = 18, \theta) p(\theta \mid x_{-18}, y_{-18}) d\theta$$

## Posterior predictive density

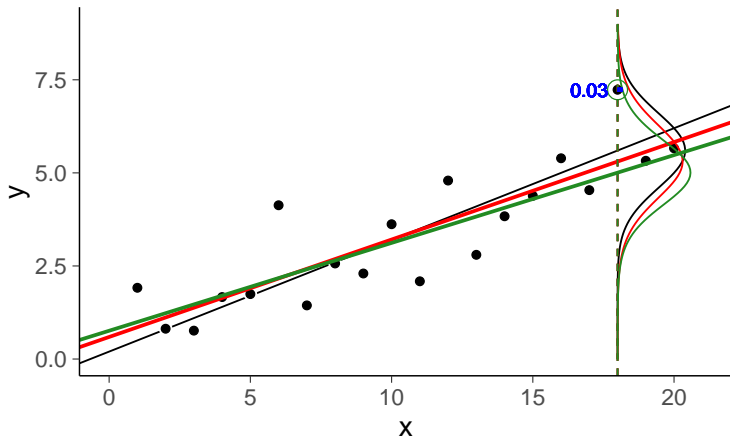


## Posterior predictive density



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

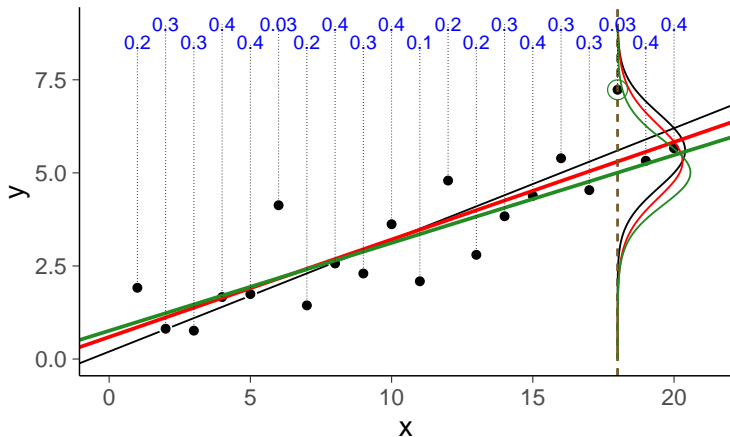
## Leave-one-out predictive density



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

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

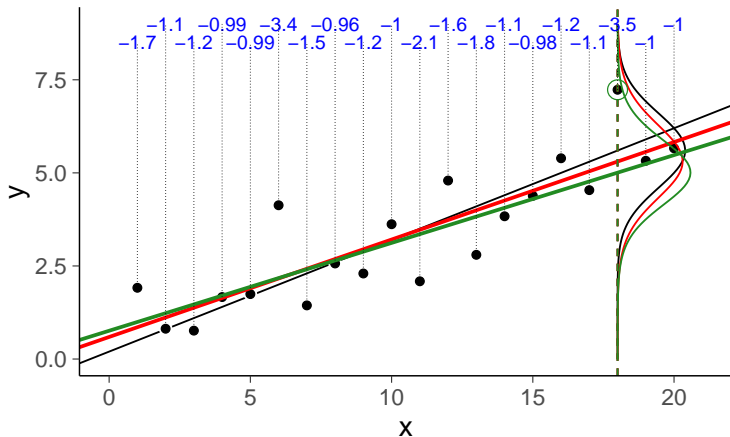
# Leave-one-out predictive densities



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

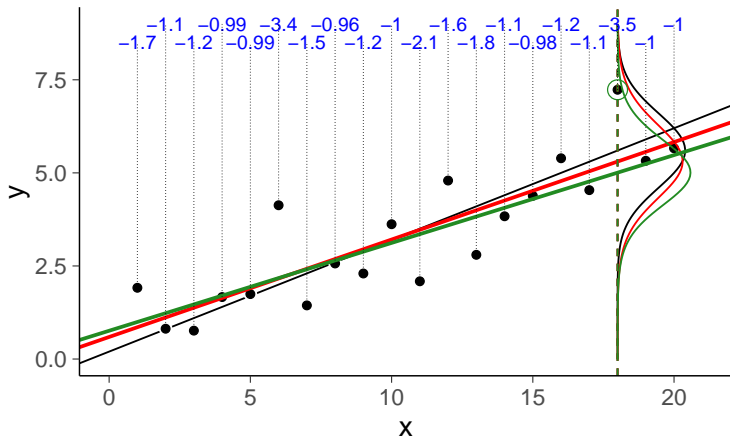


# Leave-one-out log predictive densities



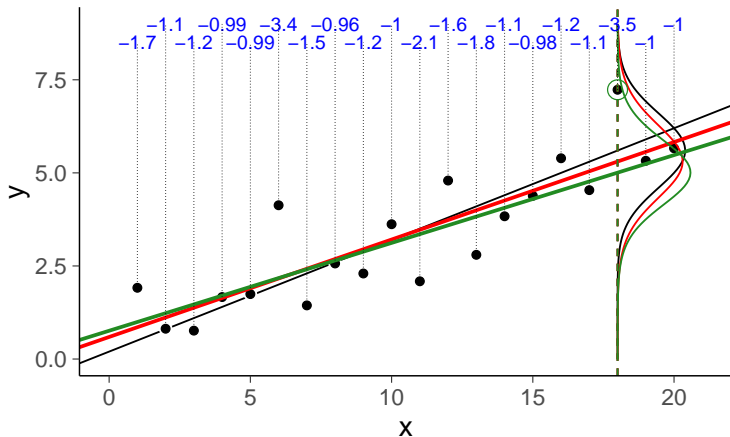
$$\log p(y_i | x_i, x_{-i}, y_{-i}), \quad i = 1, \dots, 20$$

# Leave-one-out log predictive densities



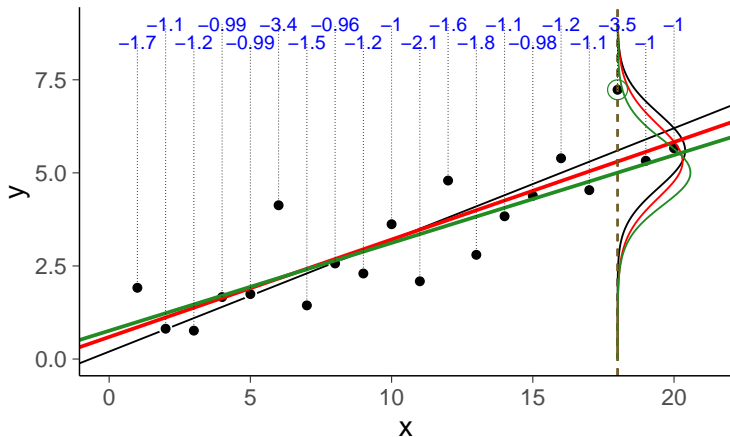
$$\sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

# Leave-one-out log predictive densities



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

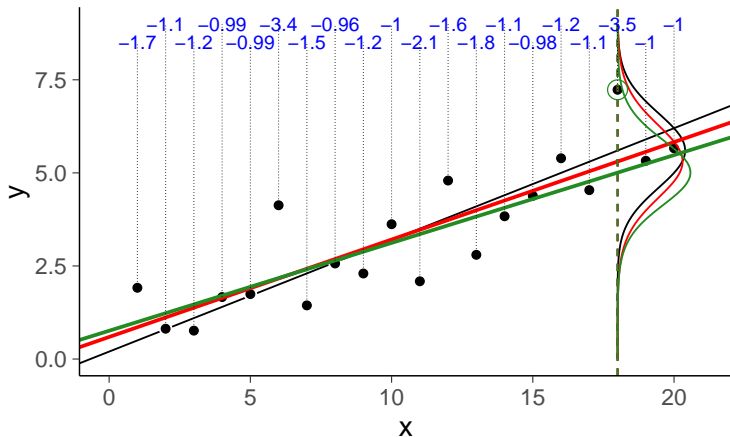
## Leave-one-out log predictive densities



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

an estimate of log posterior pred. density for new data

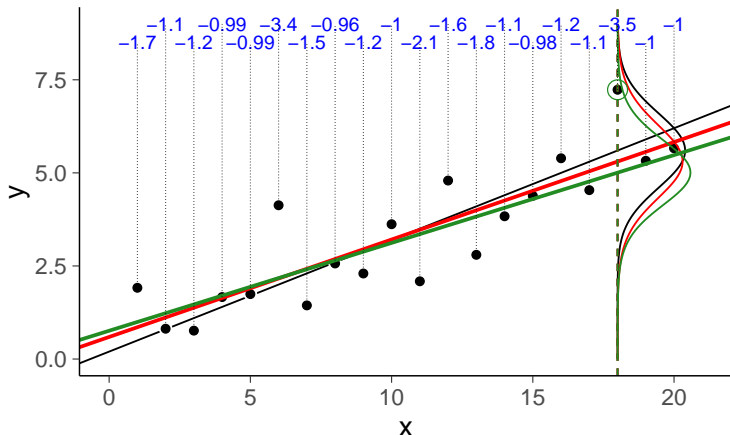
## Leave-one-out log predictive densities



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

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

## Leave-one-out log predictive densities

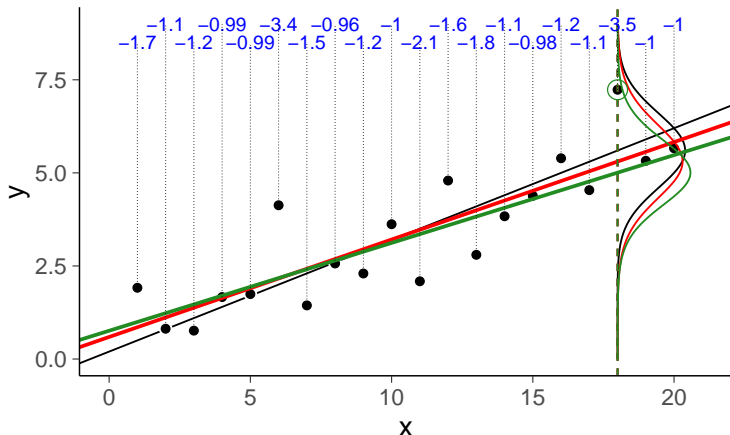


$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

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

## Leave-one-out log predictive densities

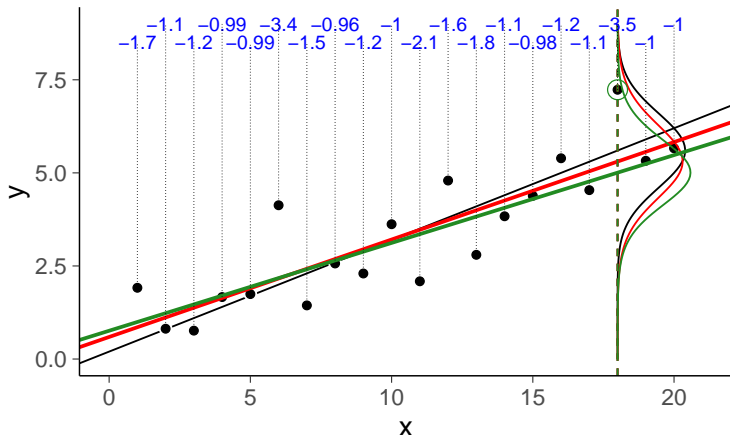


$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

asymptotically approaches  $p$  in case of regular faithful model

## Leave-one-out log predictive densities



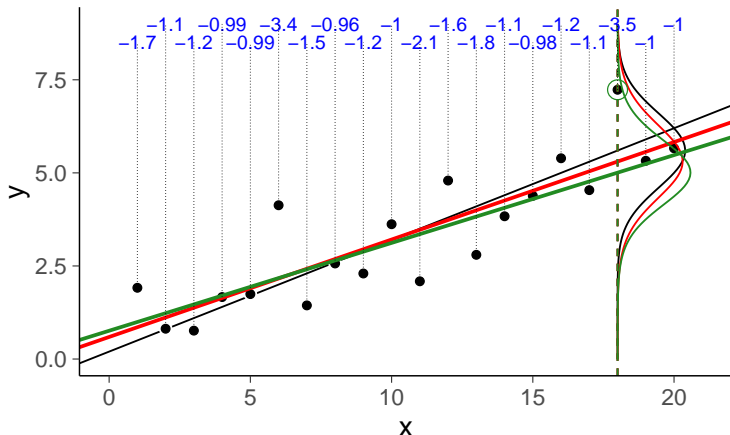
$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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asymptotically approaches  $p$  in case of regular faithful model



## Leave-one-out log predictive densities

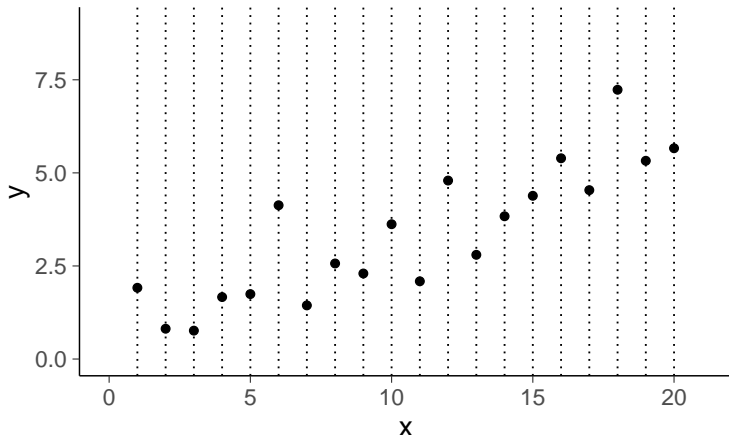


$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

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

## Fixed / designed x

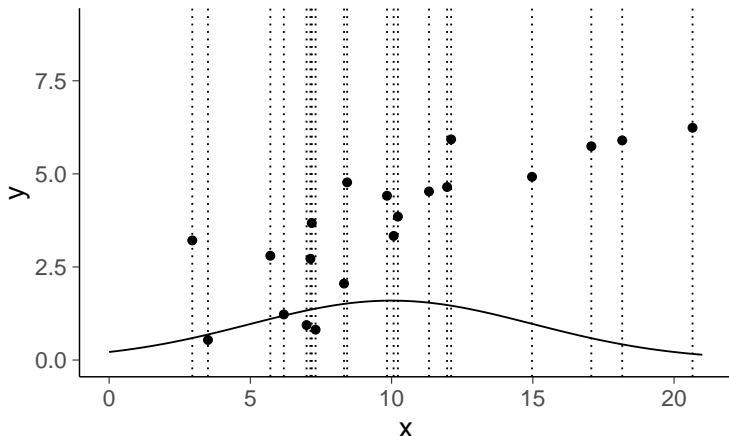


$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

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

## Distribution for x

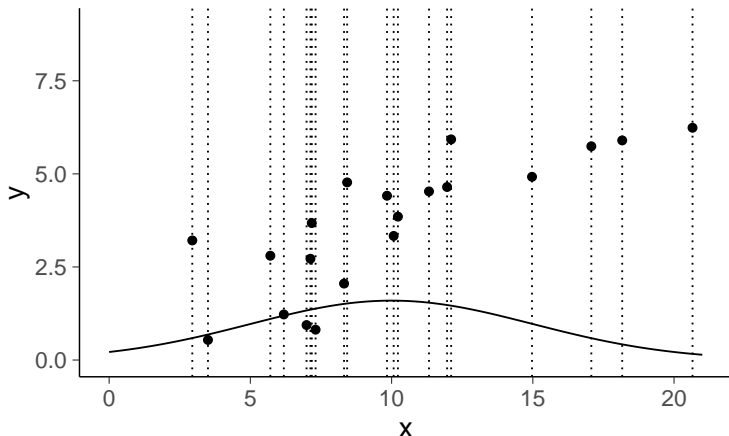


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LOO is ok for random x. SE is uncertainty about  $y | x$  and  $x$ .

## Distribution for x



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

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

LOO is ok for random x. SE is uncertainty about  $y | x$  and  $x$ .  
Covariate shift can be handled with importance weighting or modelling

## loo package

Computed from 4000 by 20 log-likelihood matrix

	Estimate	SE
elpd_loo	-29.5	3.3
p_loo	2.7	1.0

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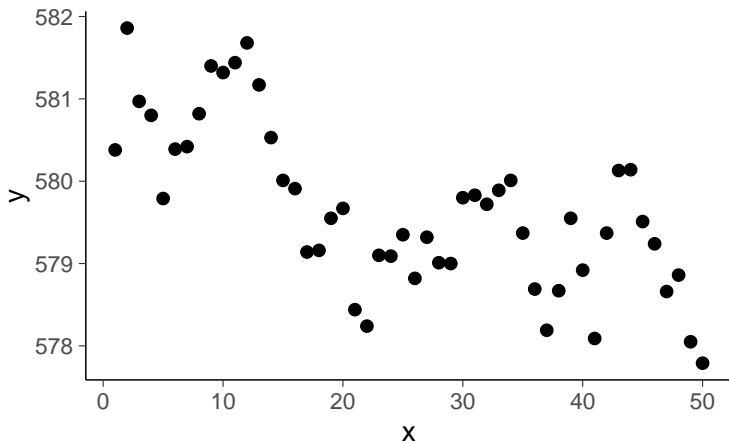
Monte Carlo SE of elpd\_loo is 0.1.

Pareto k diagnostic values:

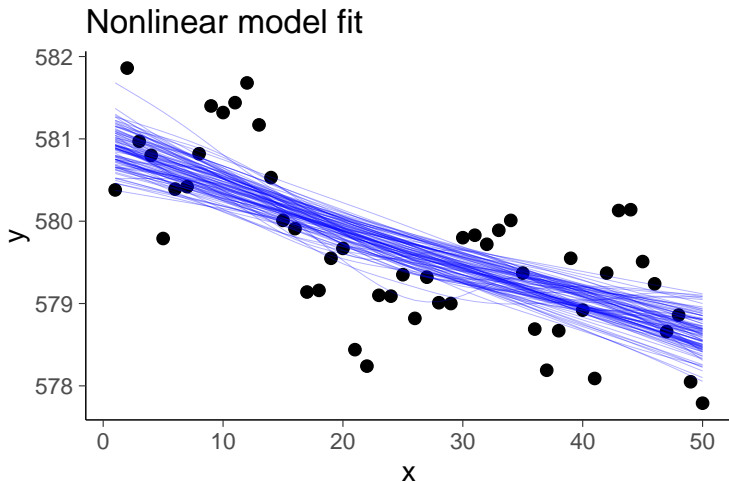
		Count	Pct.	Min.	n_eff
(-Inf, 0.5]	(good)	18	90.0%	899	
(0.5, 0.7]	(ok)	2	10.0%	459	
(0.7, 1]	(bad)	0	0.0%	<NA>	
(1, Inf)	(very bad)	0	0.0%	<NA>	

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

# Interpolation vs extrapolation

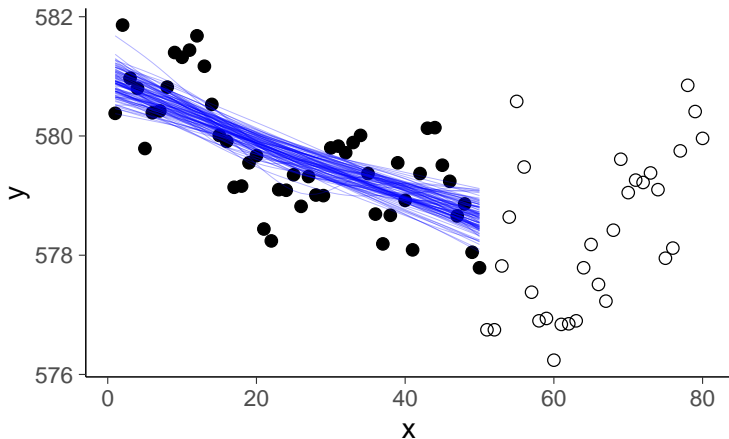


# Interpolation vs extrapolation



# Interpolation vs extrapolation

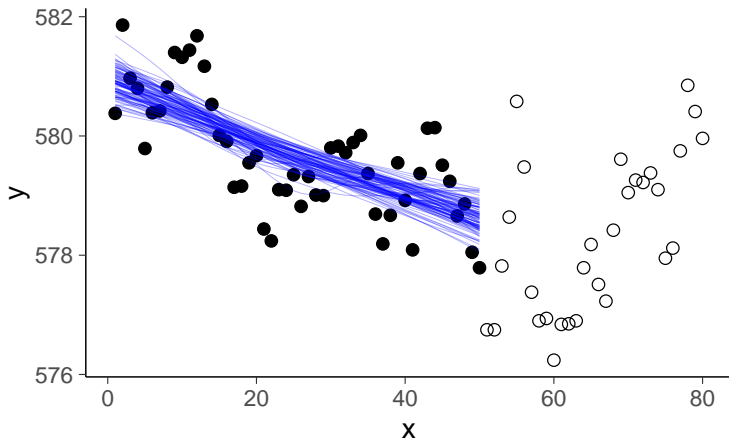
Nonlinear model fit + new data





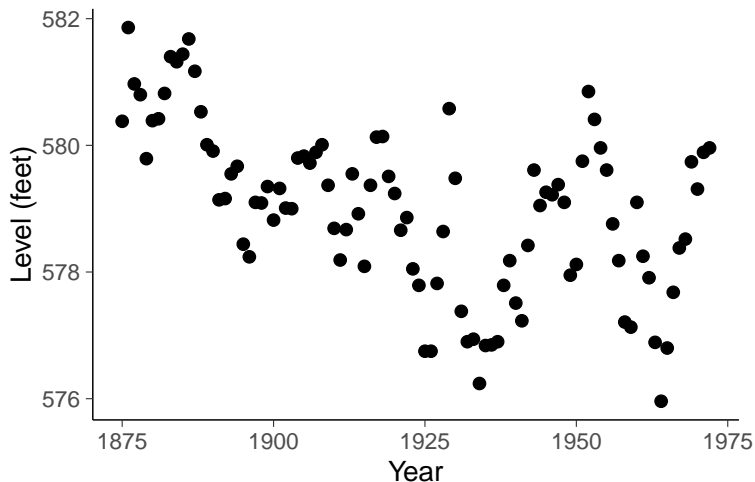
# Interpolation vs extrapolation

Nonlinear model fit + new data



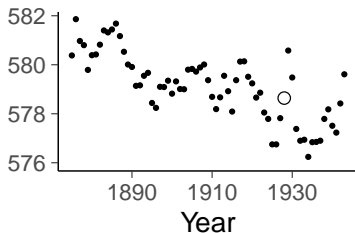
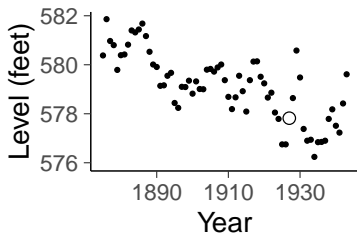
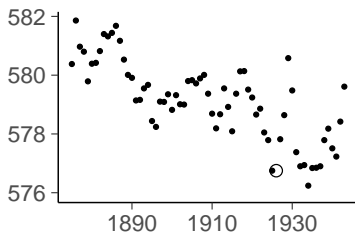
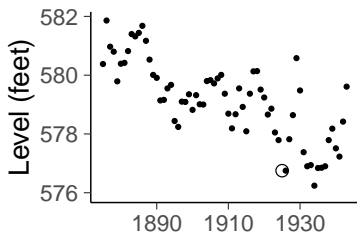
Extrapolation is more difficult

## Cross-validation for time series?



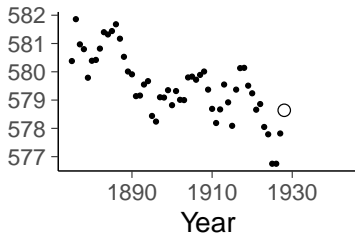
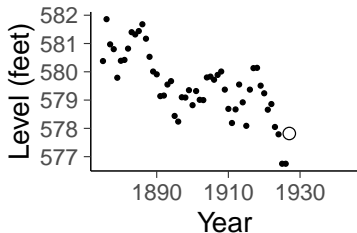
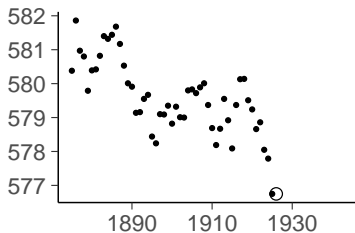
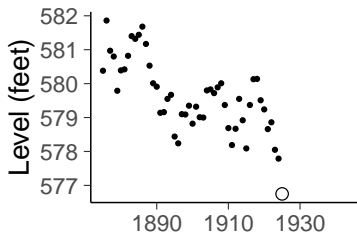
Can LOO or other cross-validation be used with time series?

## Cross-validation for time series



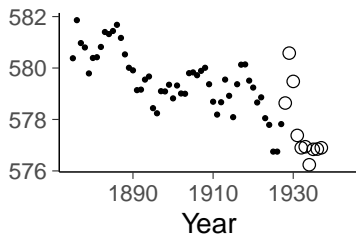
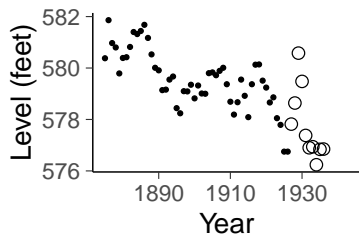
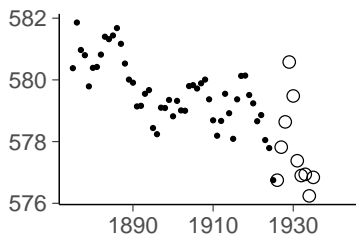
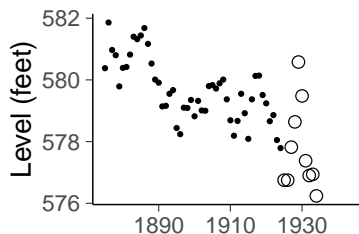
Leave-one-out cross-validation is ok for assessing conditional model

## Cross-validation for time series



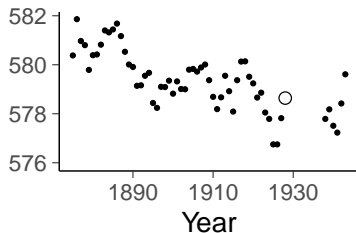
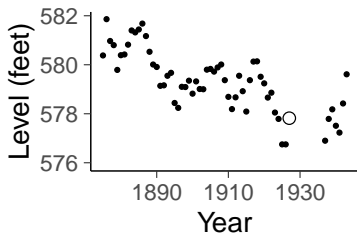
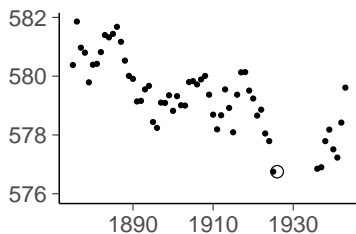
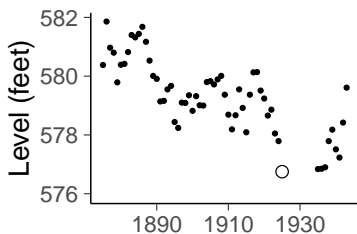
Leave-future-out cross-validation is better for predicting future

# Cross-validation for time series



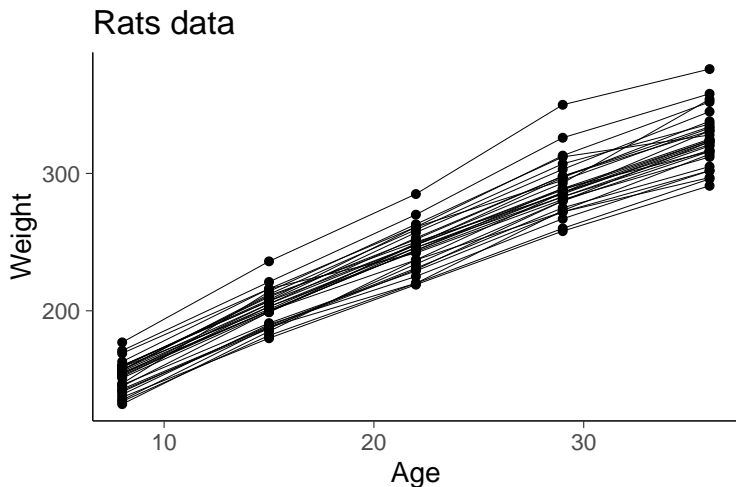
*m*-step-ahead cross-validation is better for predicting further future

# Cross-validation for time series



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

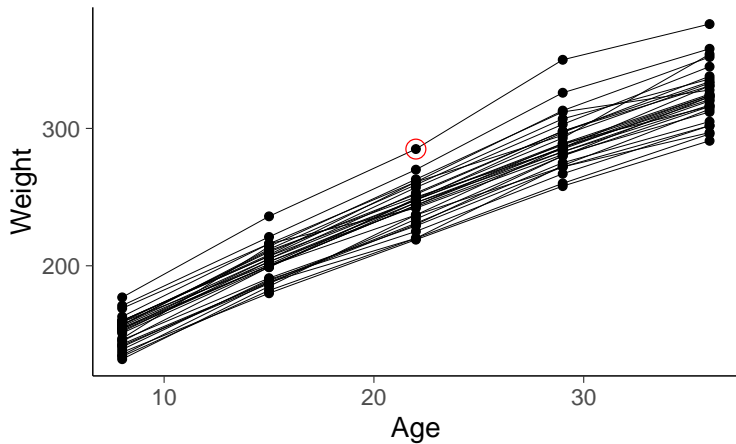
# Cross-validation for hierarchical data



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

# Cross-validation for hierarchical data

Leave-one-out?

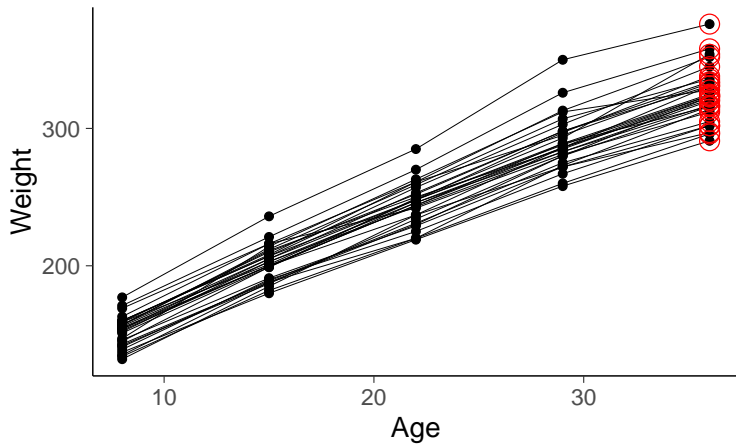


Yes!



# Cross-validation for hierarchical data

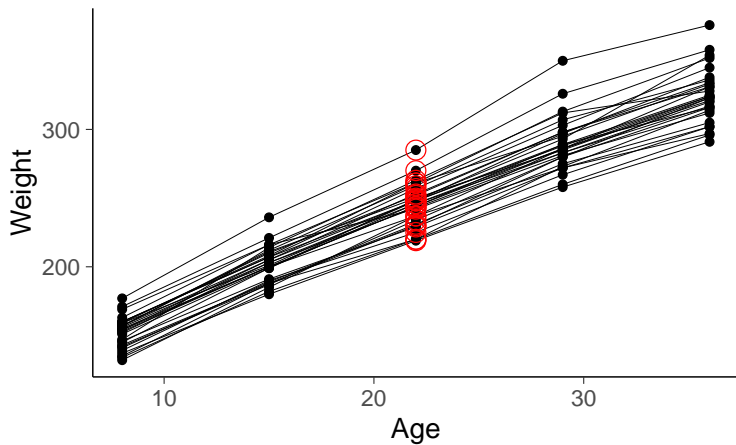
1-step-ahead?



Yes!

# Cross-validation for hierarchical data

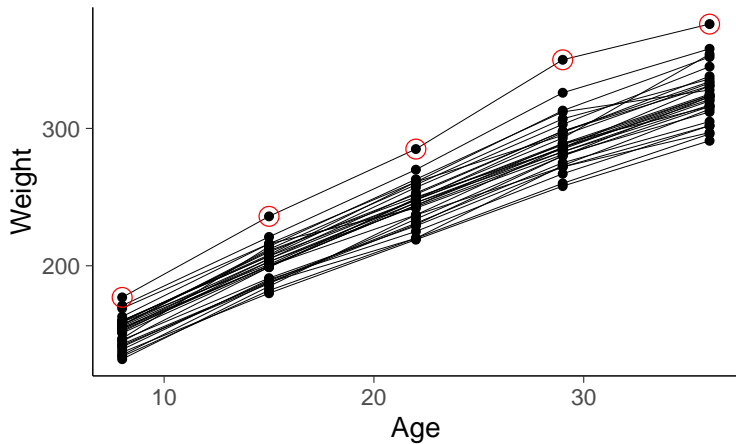
Leave-one-time-point-out?



Yes!

# Cross-validation for hierarchical data

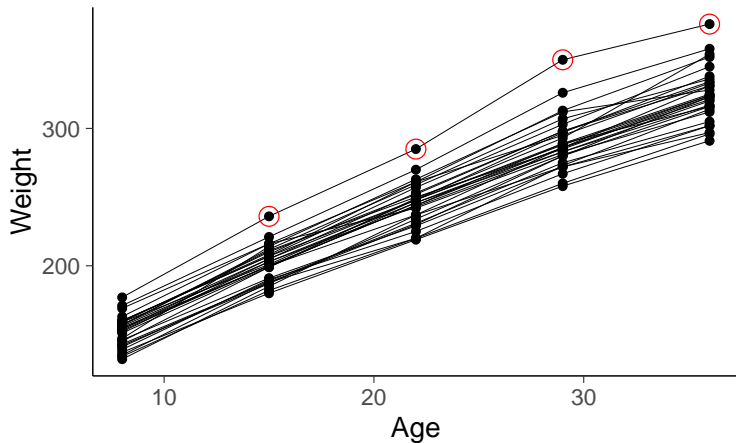
Leave-one-rat-out?



Yes!

# Cross-validation for hierarchical data

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 [CV-FAQ](#)

# Fast cross-validation

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

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

# Importance sampling leave-one-out cross-validation

- We want to compute

$$p(y_i | x_i, x_{-i}, y_{-i}) = \int p(y_i | x_i, \theta) p(\theta | x_{-i}, y_{-i}) d\theta$$

# Importance sampling leave-one-out cross-validation

- We want to compute

$$p(y_i | x_i, x_{-i}, y_{-i}) = \int p(y_i | x_i, \theta) p(\theta | x_{-i}, y_{-i}) d\theta$$

- Proposal distribution is full posterior  $\theta^{(s)} \sim p(\theta | x, y)$
- Target distribution is LOO-posterior  $p(\theta | x_{-i}, y_{-i})$



# Importance sampling leave-one-out cross-validation

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- Target distribution is LOO-posterior  $p(\theta | x_{-i}, y_{-i})$
- Importance ratio

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

# Importance sampling leave-one-out cross-validation

- We want to compute

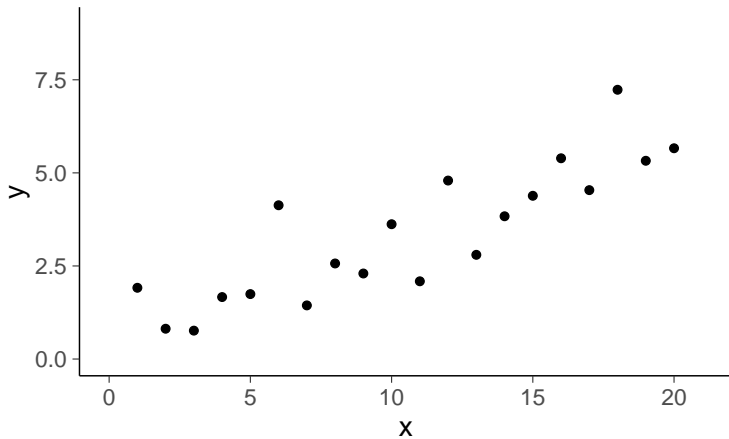
$$p(y_i | x_i, x_{-i}, y_{-i}) = \int p(y_i | x_i, \theta) p(\theta | x_{-i}, y_{-i}) d\theta$$

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- Target distribution is LOO-posterior  $p(\theta | x_{-i}, y_{-i})$
- Importance ratio

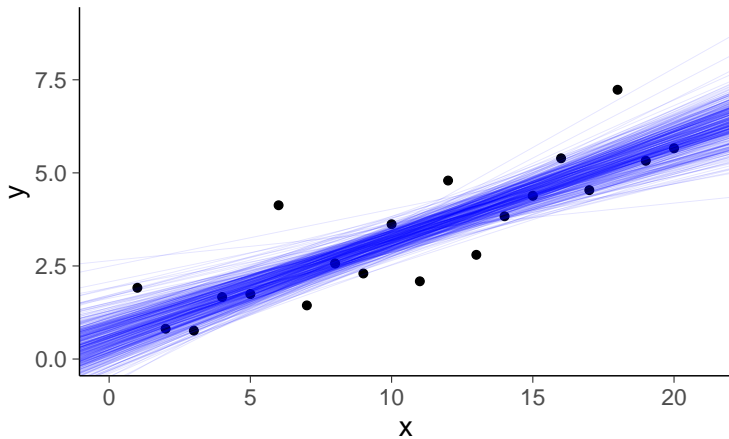
$$w_i^{(s)} = \frac{p(\theta^{(s)} | x_{-i}, y_{-i})}{p(\theta^{(s)} | x, y)} \propto \frac{1}{p(y_i | x_i, \theta^{(s)})}$$

$$\tilde{w}_i^{(s)} = \frac{w_i^{(s)}}{\sum_{s'=1}^S w_i^{(s')}}$$

Data

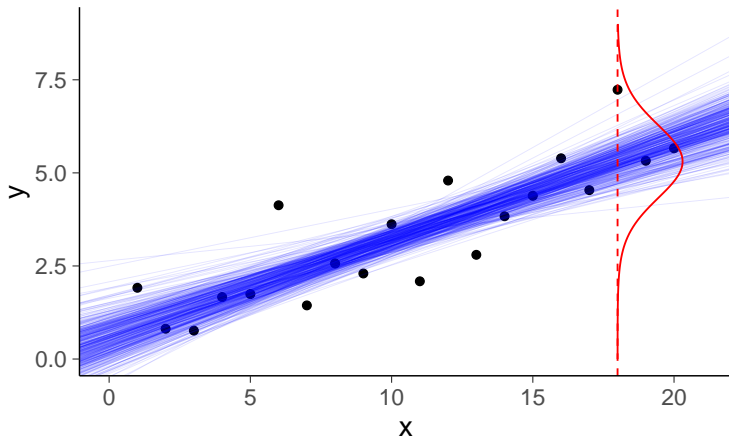


## Posterior draws



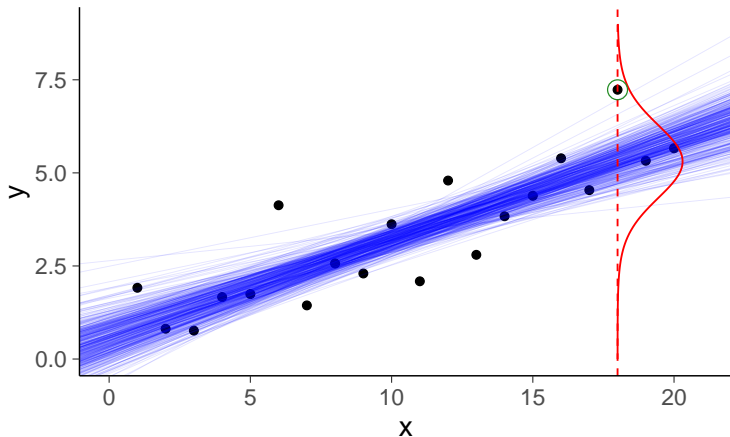
$$\theta^{(s)} \sim p(\theta \mid x, y)$$

## Posterior predictive distribution



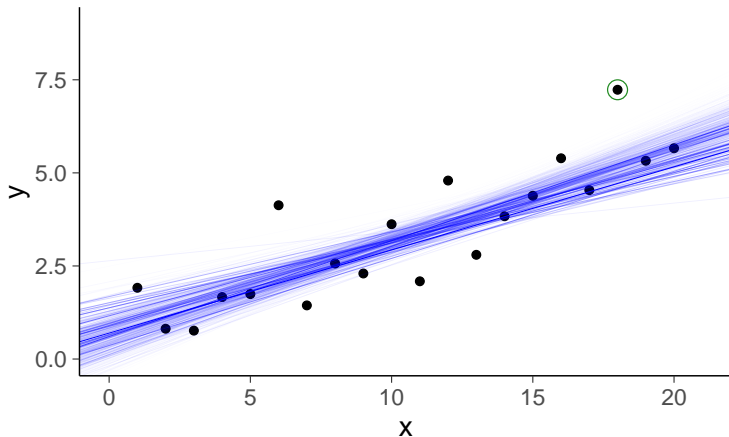
$$\theta^{(s)} \sim p(\theta \mid x, y), \quad p(\tilde{y} \mid \tilde{x}, x, y) \approx \frac{1}{S} \sum_{s=1}^S p(\tilde{y} \mid \tilde{x}, \theta^{(s)})$$

## Posterior predictive distribution



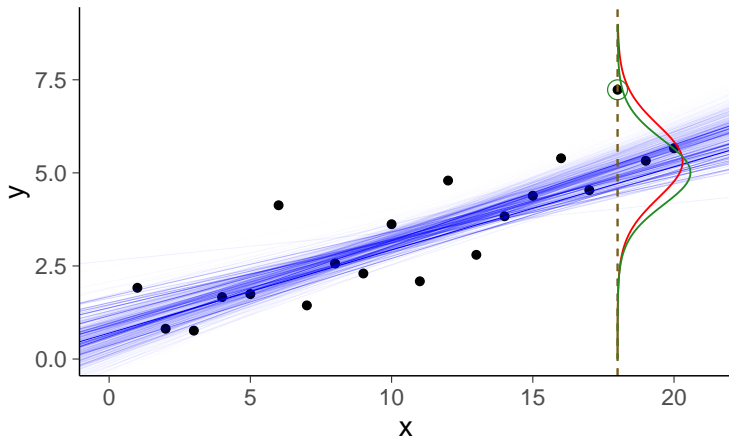
$$\theta^{(s)} \sim p(\theta \mid x, y), \quad p(\tilde{y} \mid \tilde{x}, x, y) \approx \frac{1}{S} \sum_{s=1}^S p(\tilde{y} \mid \tilde{x}, \theta^{(s)})$$

## PSIS-LOO weighted draws



$$\theta^{(s)} \sim p(\theta \mid x, y), \quad w_i^{(s)} = p(\theta^{(s)} \mid x_{-i}, y_{-i}) / p(\theta^{(s)} \mid x, y)$$

## PSIS-LOO weighted predictive distribution



$$\theta^{(s)} \sim p(\theta \mid x, y), \quad \tilde{w}_i^{(s)} = p(\theta^{(s)} \mid x_{-i}, y_{-i}) / p(\theta^{(s)} \mid x, y)$$

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



# Pareto smoothed importance sampling LOO

- $p(y_i | x_i, x_{-i}, y_{-i}) = \int p(y_i | x_i, \theta) p(\theta | x_{-i}, y_{-i}) d\theta$
- Proposal  $p(\theta | x, y)$  and target  $p(\theta | x_{-i}, y_{-i})$
- Importance ratio

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

$$\tilde{w}_i^{(s)} = \frac{w_i^{(s)}}{\sum_{s'=1}^S w_i^{(s')}}}$$

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

# Pareto smoothed importance sampling LOO

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$$\tilde{w}_i^{(s)} = \frac{w_i^{(s)}}{\sum_{s'=1}^S w_i^{(s')}}}$$

$$\begin{aligned} p(y_i | x_i, x_{-i}, y_{-i}) &\approx \sum_{s=1}^S \left[ \tilde{w}_i^{(s)} p(y_i | x_i, \theta^{(s)}) \right] \\ &\approx \frac{\sum_{s=1}^S \left[ w_i^{(s)} p(y_i | x_i, \theta^{(s)}) \right]}{\sum_{s'=1}^S w_i^{(s')}} \end{aligned}$$

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

$$\approx \frac{\sum_{s=1}^S \left[ w_i^{(s)} p(y_i | x_i, \theta^{(s)}) \right]}{\sum_{s'=1}^S w_i^{(s')}}}$$

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

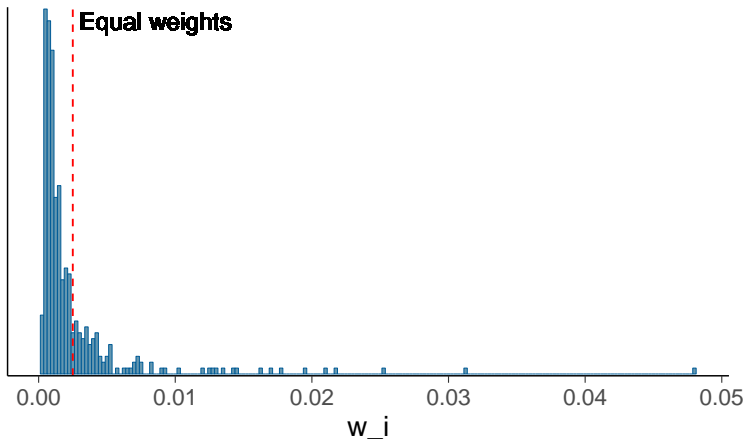
# Pareto smoothed importance sampling LOO

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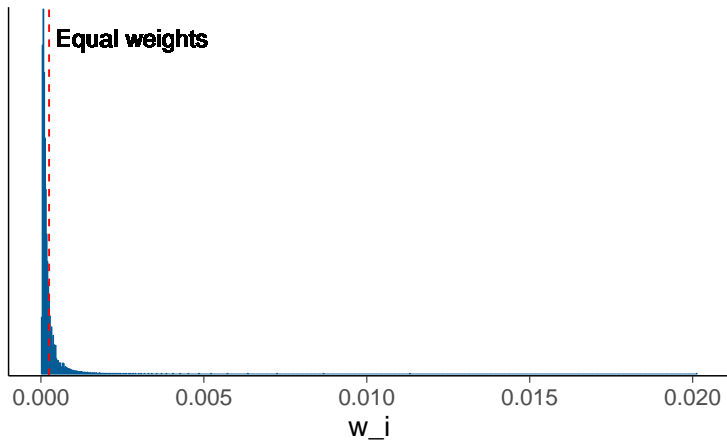
$$\begin{aligned} p(y_i | x_i, x_{-i}, y_{-i}) &\approx \sum_{s=1}^S \left[ \tilde{w}_i^{(s)} p(y_i | x_i, \theta^{(s)}) \right] \\ &\approx \frac{1}{\frac{1}{S} \sum_{s'=1}^S w_i^{(s')}} \end{aligned}$$

- The variability of importance weights matter
  - Pareto- $k$  diagnostic
  - Pareto smoothed importance sampling LOO (PSIS-LOO)

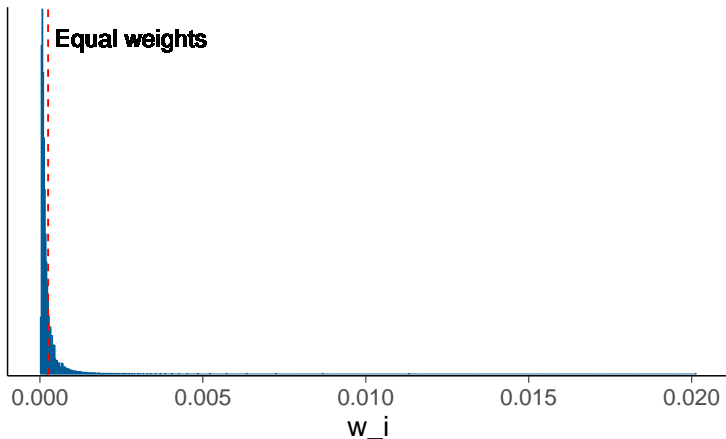
## 400 importance weights for leave-18th-out



## 4000 importance weights for leave-18th-out



## 4000 importance weights for leave-18th-out

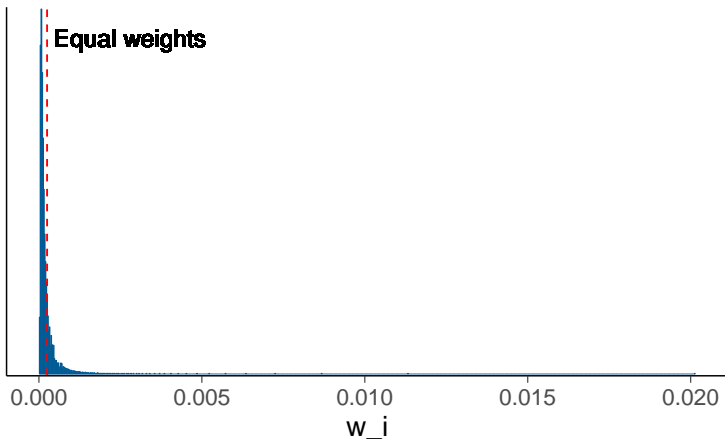


$$\text{ESS} \approx 1 / \sum_{s=1}^S (\tilde{w}^{(s)})^2 \approx 459$$

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



## 4000 importance weights for leave-18th-out



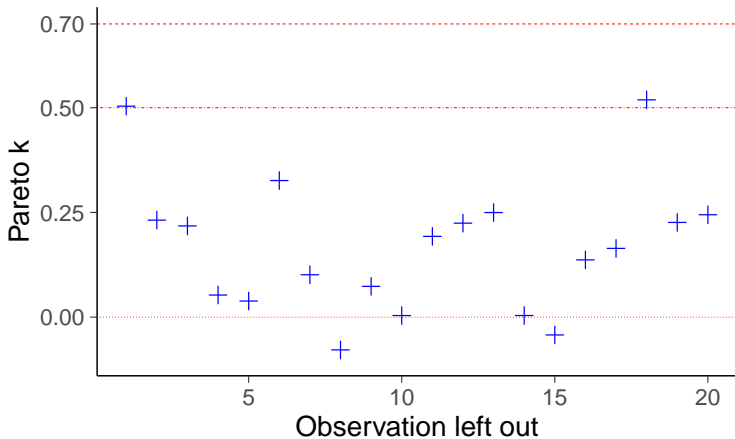
$$\text{ESS} \approx 1 / \sum_{s=1}^S (\tilde{w}^{(s)})^2 \approx 459$$

$$\text{Pareto } \hat{k} \approx 0.52$$

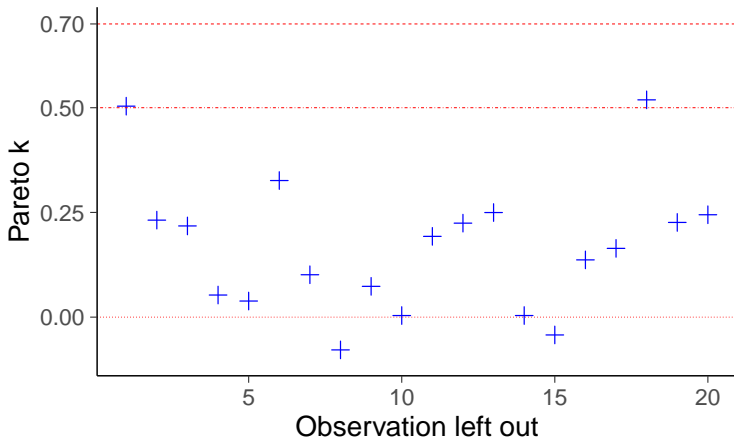
- Pareto  $\hat{k}$  estimates the tail shape which determines the convergence rate of PSIS. Less than 0.7 is ok.

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

## PSIS-LOO diagnostics



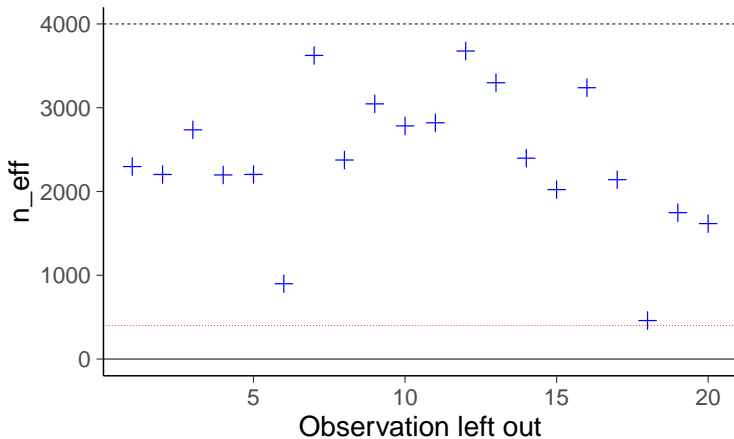
## PSIS-LOO diagnostics



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 \(2017b\)](#)

# Pareto smoothed importance sampling (PSIS)

- Replace the largest weights with ordered statistics of the fitted Pareto distribution
  - equivalent to using model to filter the noise out of the weights

See more in [Vehtari, Simpson, Gelman, Yao & Gabry \(2021\)](#)

## Pareto smoothed importance sampling (PSIS)

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- Reduced variability compared to the plain IS
- Reduced bias compared to the truncated IS

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# Pareto smoothed importance sampling (PSIS)

- Replace the largest weights with ordered statistics of the fitted Pareto distribution
  - equivalent to using model to filter the noise out of the weights
- Reduced variability compared to the plain IS
- Reduced bias compared to the truncated IS
- Asymptotically consistent under some mild conditions

See more in [Vehtari, Simpson, Gelman, Yao & Gabry \(2021\)](#)



## Stan code

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

## Stan code

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

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

## Stan code

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}
```

- RStanARM and brms compute `log_lik` by default

## loo()

- RStan (`log_lik` in gen. quantities), RStanARM, brms  
`loo(fit)`

## loo()

- RStan (`log_lik` in gen. quantities), RStanARM, brms  
`loo(fit)`

- CmdStanR (eventually will work as others)

```
loocmd <- function(fit, ...) {  
  loo(fit$draws("log_lik"),  
    r_eff=relative_eff(fit$draws("log_lik"))),  
  ...  
}  
loocmd(fit)
```

## What if many high Pareto- $\hat{k}$ 's

- `rstan::loo(..., moment_match = TRUE)`  
`brms::loo(..., moment_match = TRUE)`  
support implicitly adaptive importance sampling with  
moment matching algorithm by Paananen et al. (2021). See  
<http://mc-stan.org/loo/articles/loo2-moment-matching.html>

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- `rstanarm::loo(..., k_threshold = 0.7)`  
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- Use K-fold-CV (more about this soon)



# Pareto smoothed importance sampling CV variants

- 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
  - Stan demo of the challenges and integrated LOO at <https://avehtari.github.io/modelselection/roaches.html>

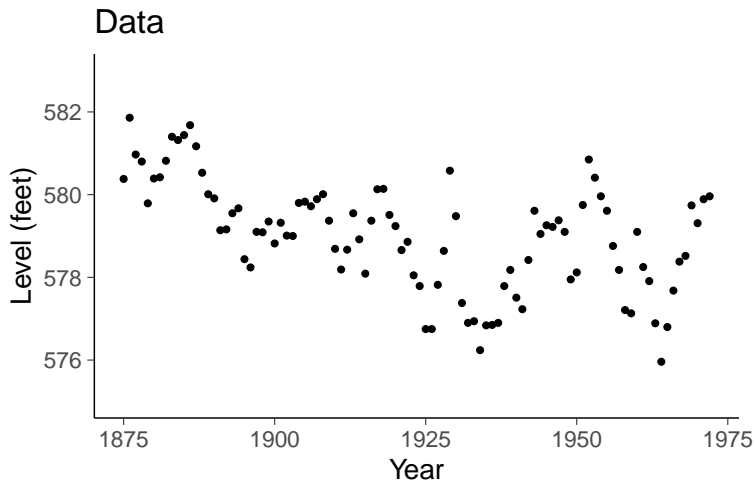
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- PSIS-LOO for non-factorized models
  - [mc-stan.org/loo/articles/loo2-non-factorizable.html](https://mc-stan.org/loo/articles/loo2-non-factorizable.html)

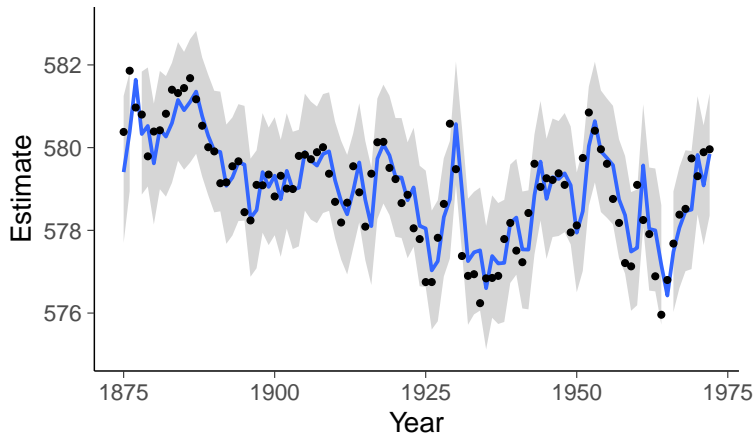
# Pareto smoothed importance sampling CV variants

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- PSIS-LOO for non-factorized models
  - [mc-stan.org/loo/articles/loo2-non-factorizable.html](https://mc-stan.org/loo/articles/loo2-non-factorizable.html)
- PSIS-LOO for time series
  - Approximate leave-future-out cross-validation (LFO-CV)  
[mc-stan.org/loo/articles/loo2-lfo.html](https://mc-stan.org/loo/articles/loo2-lfo.html)

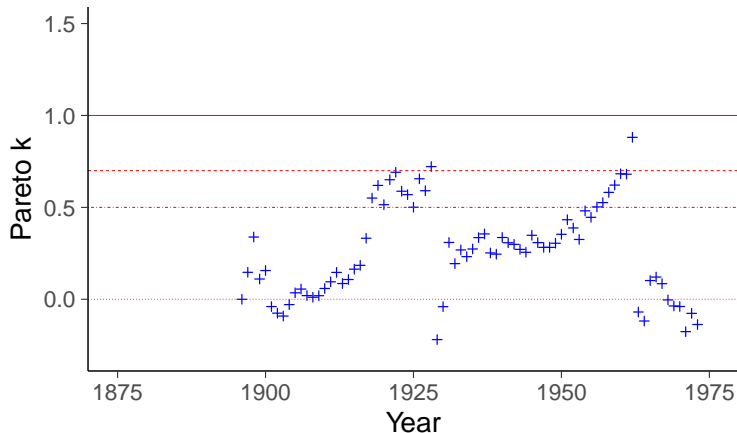
# LFO-CV



AR-4 prediction with 95% interval



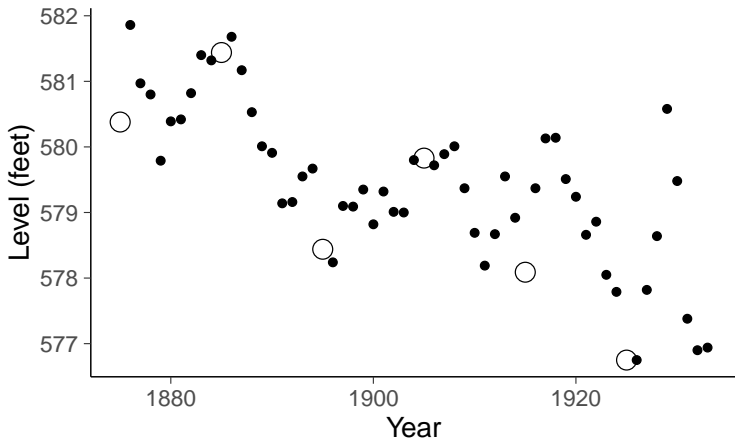
## PSIS-1-step-ahead with refits



# K-fold cross-validation

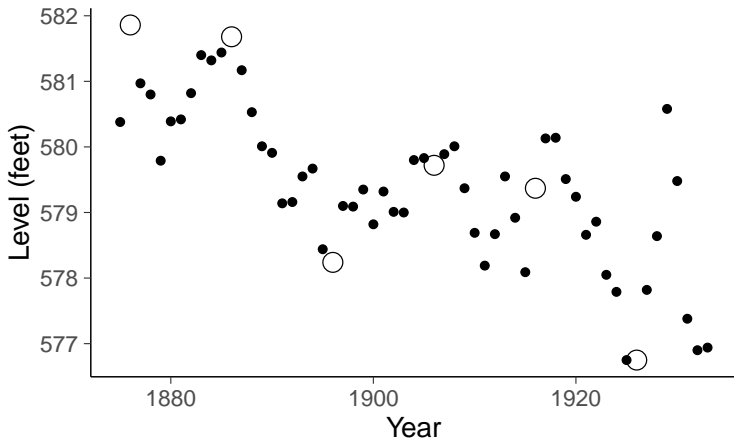
- K-fold cross-validation can approximate LOO
  - the same use cases as with LOO
- K-fold cross-validation can be used for hierarchical models
  - good for leave-one-group-out
- K-fold cross-validation can be used for time series
  - with leave-block-out

## Balance k-fold approximation of LOO

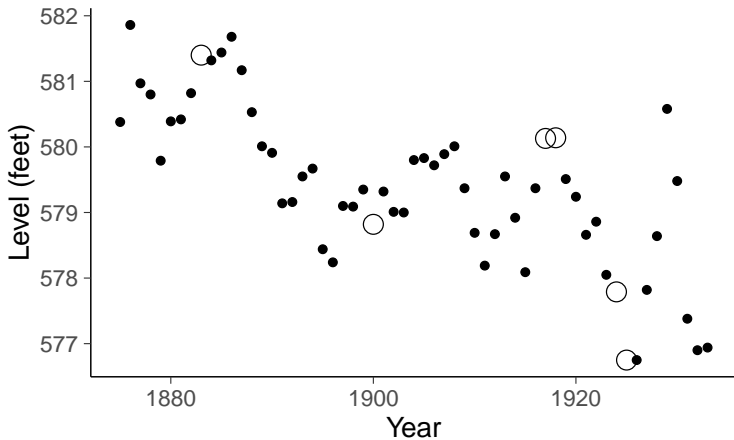




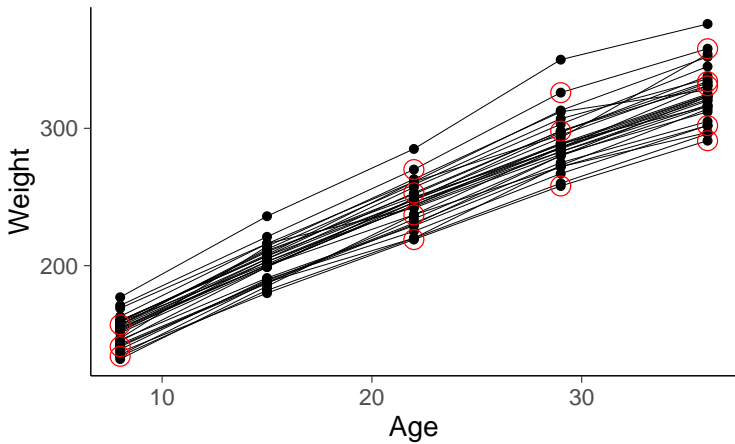
## Balance k-fold approximation of LOO



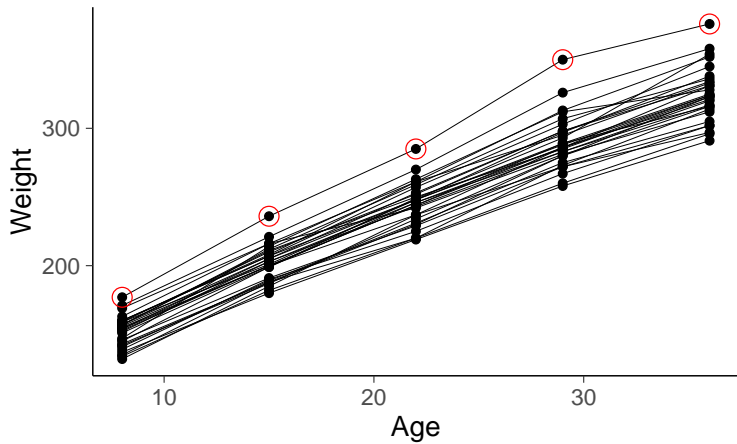
## Random k-fold approximation of LOO



## Random kfold approximation of LOO



## Leave-one-rat-out



## K-fold-CV code

- RStan, CmdStanR  
See vignette <http://mc-stan.org/loo/articles/loo2-elpd.html>
- RStanARM, brms  
`kfold(fit)`
- Alternative data divisions  
`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 \(2017a\)](#)



## WAIC vs PSIS-LOO

- WAIC has same assumptions as LOO
- PSIS-LOO is more accurate
- PSIS-LOO has much better diagnostics

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

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- WAIC has same assumptions as LOO
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- PSIS-LOO has much better diagnostics
- 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

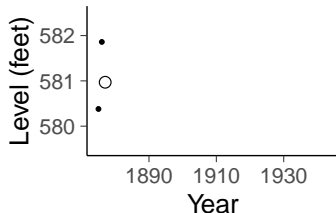
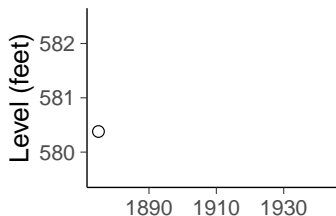
- AIC uses maximum likelihood estimate for prediction
- DIC uses posterior mean for prediction
- BIC is an approximation for marginal likelihood
- TIC, NIC, RIC, PIC, BPIC, QIC, AIC<sub>c</sub>, ...

## Marginal likelihood / Bayes factor

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

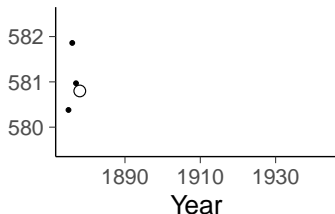
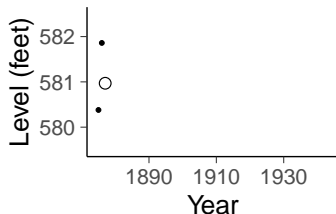
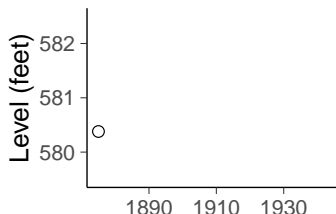
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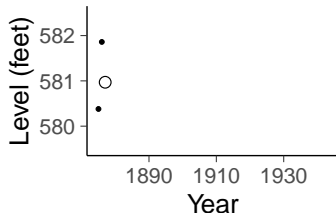
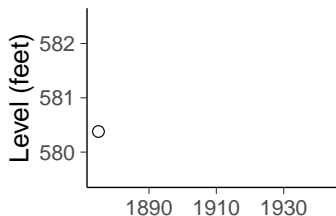
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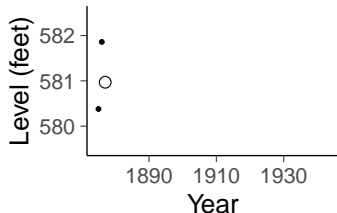
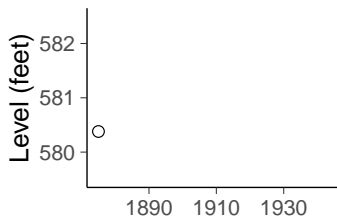
- Like leave-future-out 1-step-ahead cross-validation but starting with 0 observations
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## Marginal likelihood / Bayes factor

- 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

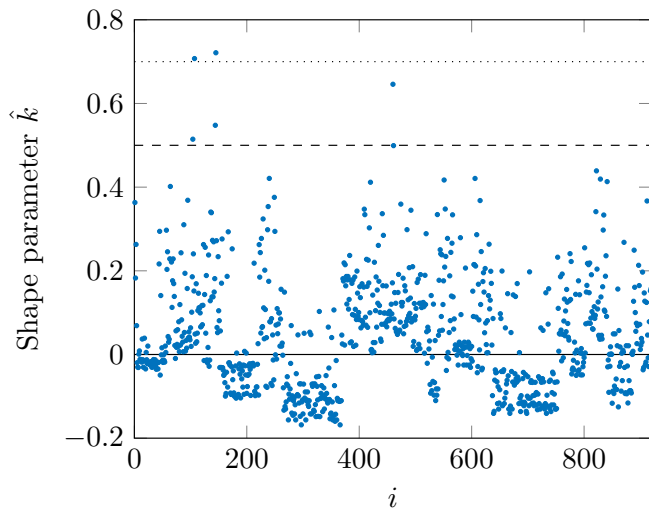
# Cross-validation for model assessment

- 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  $p_{\text{loo}}$ )
  - checking calibration of leave-one-out predictive posteriors (`ppc_loo_pit` in `bayesplot`)

see demos [avehtari.github.io/modelselection/](https://avehtari.github.io/modelselection/)

# Radon example

## PSIS-LOO diagnostics

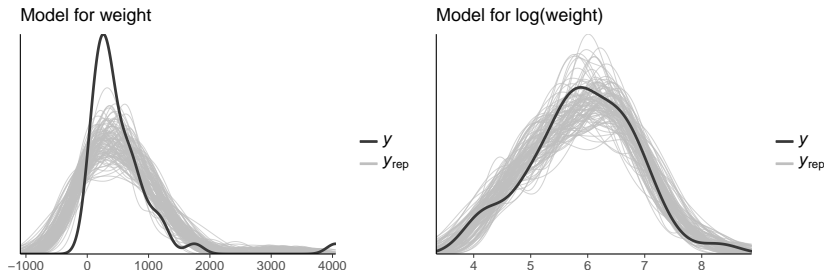


see [Vehtari, Gelman & Gabry \(2017a\)](#)

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- Posterior predictive checking is often sufficient

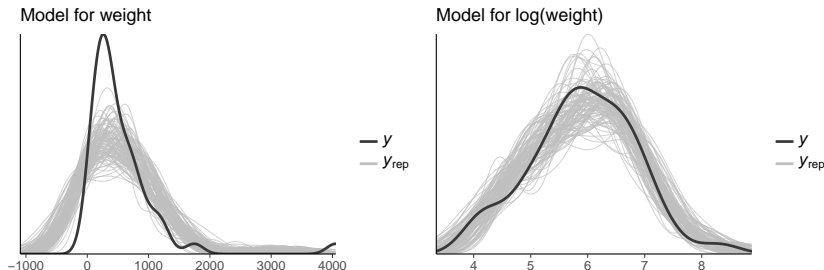


Predicting the yields of mesquite bushes.

Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 11.

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- BDA3, Chapter 6
- Gabry, Simpson, Vehtari, Betancourt, Gelman (2019). Visualization in Bayesian workflow. JRSS A, <https://doi.org/10.1111/rssa.12378>
- [mc-stan.org/bayesplot/articles/graphical-ppcs.html](https://mc-stan.org/bayesplot/articles/graphical-ppcs.html)

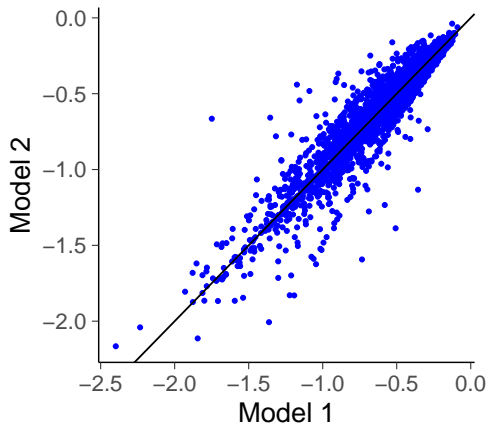
## Arsenic well example – Model comparison

- Logistic regression for predicting probability of switching well with high arsenic level in rural Bangladesh
  - Model 1:  
 $\log(\text{arsenic}) + \text{distance}$
  - Model 2:  
 $\log(\text{arsenic}) + \text{distance} + \text{education level}$



# Arsenic well example – Model comparison

Model 1 vs Model 2

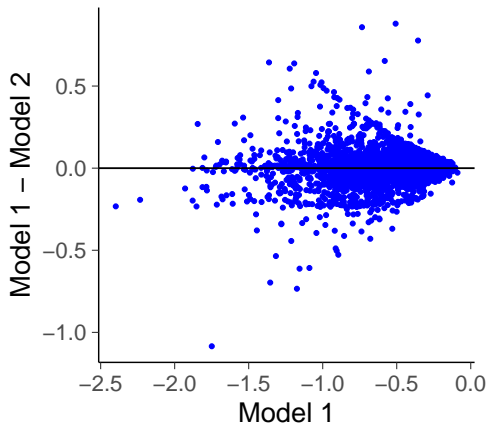


Model 1:  $\widehat{\text{elpd}}_{\text{LOO}}(\mathbf{M}_a | y^{\text{obs}}) \approx -1952, \text{SE}=16$

Model 2:  $\widehat{\text{elpd}}_{\text{LOO}}(\mathbf{M}_b | y^{\text{obs}}) \approx -1938, \text{SE}=17$

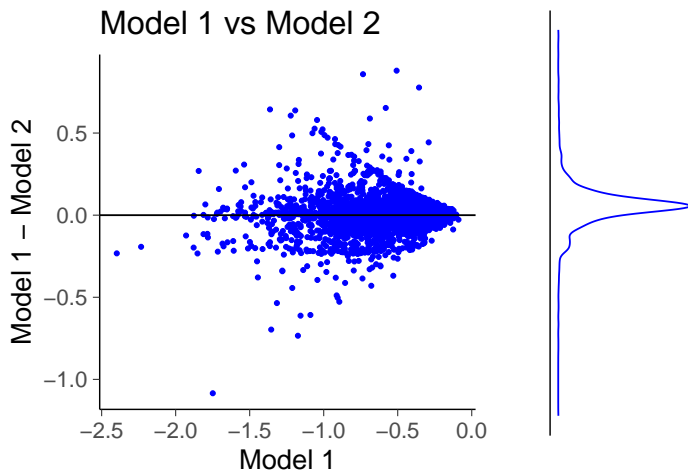
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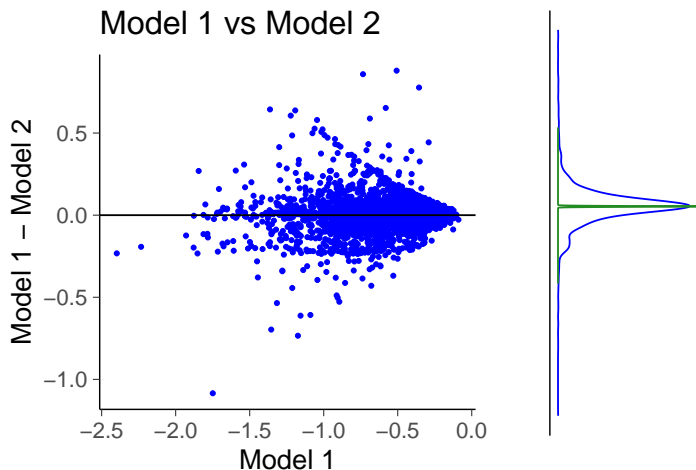
Difference:  $\widehat{\text{elpd}}_{\text{LOO}}(M_a, M_b \mid y^{\text{obs}}) \approx -14.4, \text{SE} = 6.1$

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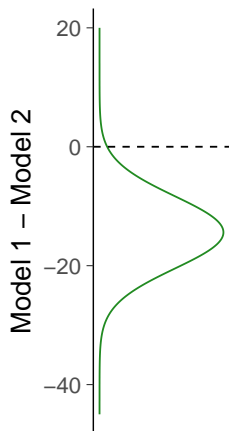
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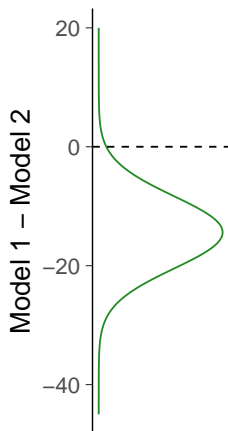
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# Arsenic well example – Model comparison



```
> loo_compare(model1, model2)
```

	elpd_diff	se_diff
model2	0.0	0.0
model1	-14.4	6.1

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

## 8 schools – Model comparison

```
> loo_compare(pooled, hierarchical)
              elpd_diff se_diff
pooled          0.0       0.0
hierarchical -0.3       0.7
```

No difference between pooled and hierarchical for predicting the future observations for a new school (exchangeable with the schools in the data).

## Poisson vs Hurdle-Poisson example

	elpd_diff	se_diff
Hurdle-Poisson	0.0	0.0
Poisson	-215.9	22.1

Clear difference (which was also obvious in posterior predictive checks)



## LOO difference uncertainty estimate reliability

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2. The models are misspecified with outliers in the data
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3. The number of observations is small
  - in nested case the skewness favors the simpler model
  - any inference with small  $n$  is difficult
  - if  $|\widehat{\text{elpd}}_{\text{LOO}}(\mathbf{M}_a, \mathbf{M}_b \mid \mathbf{y}^{\text{obs}})| > 4$ , model is well specified, and  $n > 100$  then the normal approximation is good

# Sometimes cross-validation is not needed

- In nested case, often easier and more accurate to analyse posterior distribution of more complex model directly  
[avehtari.github.io/modelselection/betablockers.html](https://avehtari.github.io/modelselection/betablockers.html)

- instead of comparing

- Model 1:  $y \sim \text{normal}(\alpha, \sigma)$

- vs

- Model 2:  $y \sim \text{normal}(\alpha + \beta x, \sigma)$

- look at the posterior of  $\beta$  directly

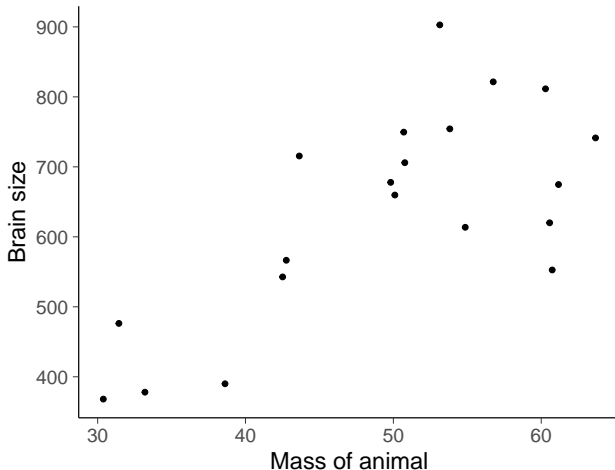
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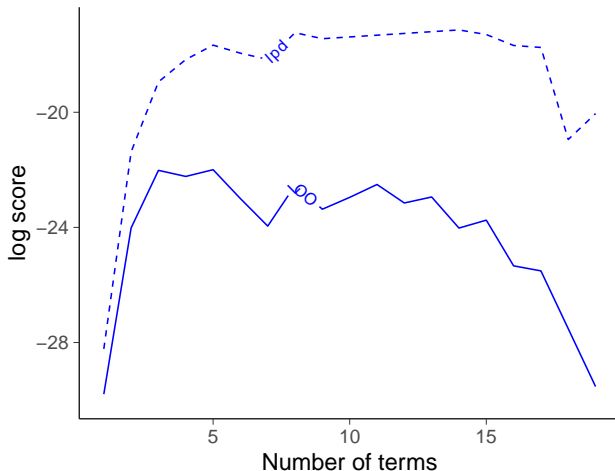
Simulated data by Richard McElreath



# Model selection needed to avoid overfitting?

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Polynomial basis functions





## Model selection needed to avoid overfitting?

- Gaussian process can be used as a prior on function space
  - GP can be approximated with basis functions

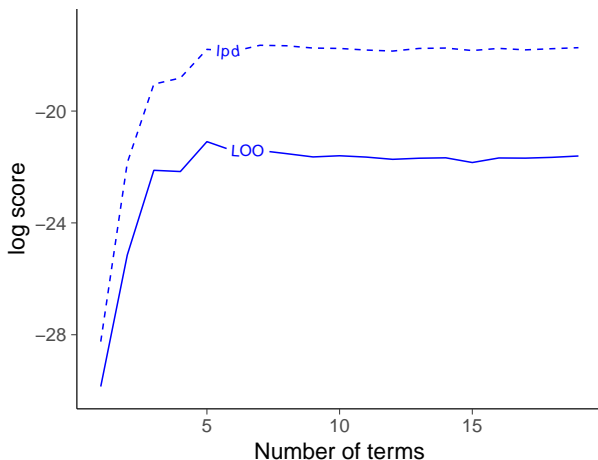
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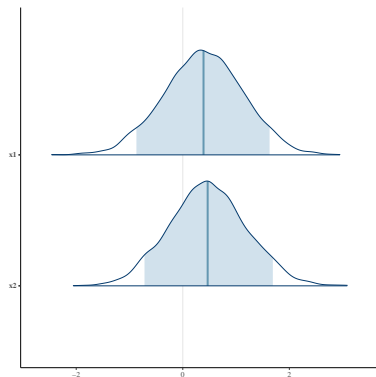
Gaussian process basis functions



## Model is not needed to avoid overfitting

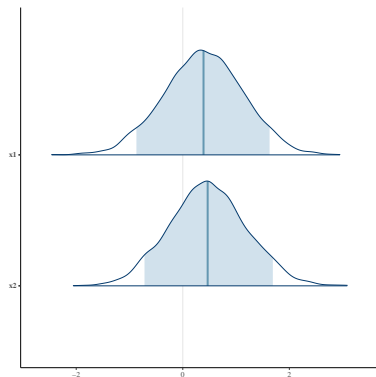
- No overfitting when using good priors that keep the prior on the predictive space approximately constant when more components are added, e.g.
  - Gaussian processes
  - (regularized) Horseshoe for sparsity
  - R2-D2 and R2-D2-M2 for prior on  $R^2$

# Sometimes predictive model comparison can be useful

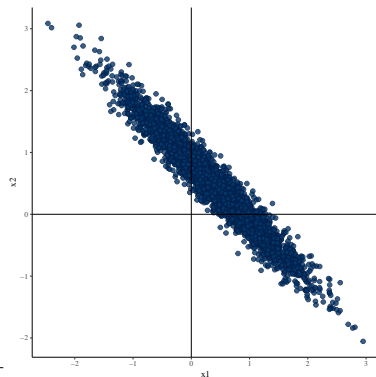


Marginal posterior intervals

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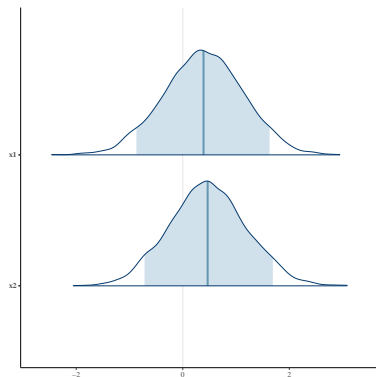
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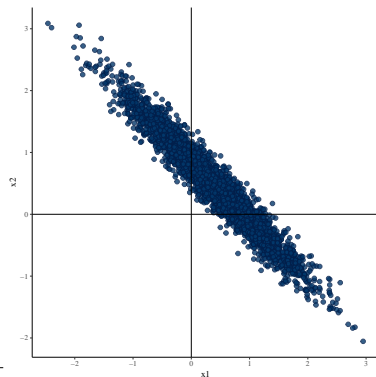
Joint posterior density

`rstanarm + bayesplot`

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Marginal posterior intervals



Joint posterior density

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see also [Collinear demo](#)

What if one is not clearly better than others?



# What if one is not clearly better than others?

- Continuous expansion including all models?
  - and then analyse the posterior distribution directly  
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- In a nested case choose more complex if you want to take into account all the uncertainties.  
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- If needed integrate over the model space = model averaging
- Bayesian stacking may work better than BMA in case of misspecified models or small data
  - Yao, Vehtari, Simpson, & Gelman (2018)

# Cross-validation and model selection

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- Overfitting in selection process is not unique for cross-validation

# Selection induced bias and overfitting

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

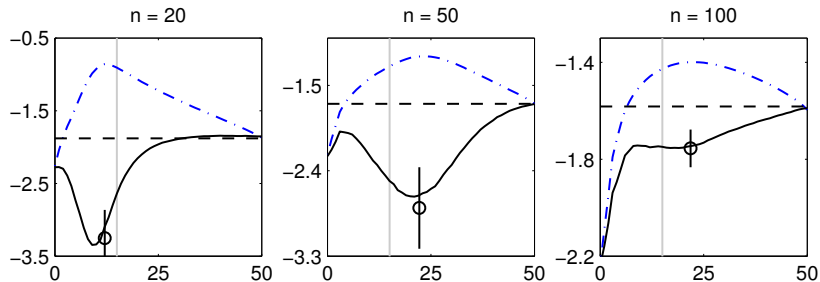
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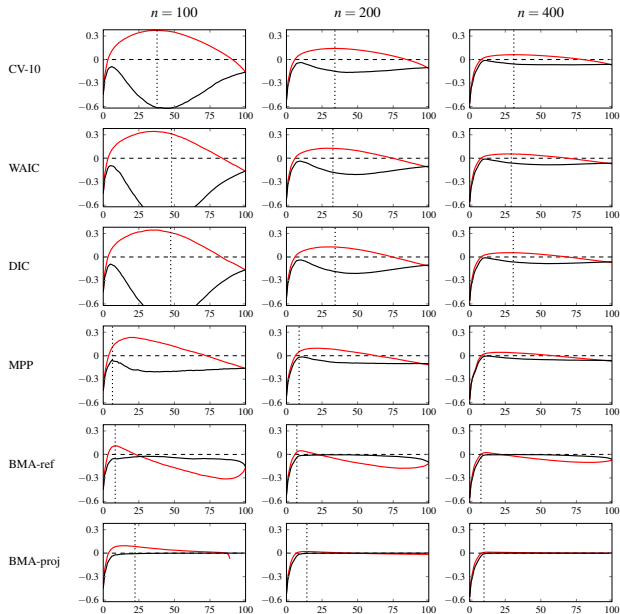
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- Performance of the selection process itself can be assessed using two level cross-validation, but it does not help choosing better models
- Bigger problem if there is a large number of models as in covariate selection

# Selection induced bias in variable selection



# Selection induced bias in variable selection



## Take-home messages

- It's good to think predictions of observables, because observables are the only ones we can observe
- 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
- Cross-validation has high variance, and **if** you trust your model you can beat cross-validation in accuracy



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