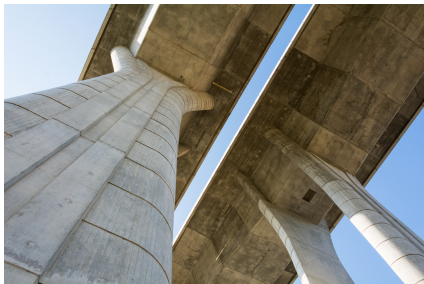


Predicting concrete quality



- How accurate the model is?
- Is it better than predicting with random guess?
- Is it possible that the model has overfitted?
- Is model B better than model A? (next week)

Outline

- What is cross-validation
 - Leave-one-out cross-validation (elpd_loo, p_loo)
 - Uncertainty in LOO (SE)
- Fast cross-validation
 - PSIS and diagnostics in loo package (Pareto k, n_eff, Monte Carlo SE)
 - K-fold cross-validation
- When is cross-validation applicable?
 - data generating mechanisms and prediction tasks
 - leave-many-out cross-validation

Next week

- Model comparison and selection (elpd_diff, se)
- Related methods (WAIC, *IC, BF)
- Model averaging
- Potential overfitting in model selection

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. preprint at arxiv.org/abs/1507.04544.
 - See also
<https://users.aalto.fi/~ave/modelselection/CV-FAQ.html>

Next week

- 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)

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
 - more about these in lecture 10
- 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
 - more about these in lecture 10
- 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

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

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 ($k < 0.7$).

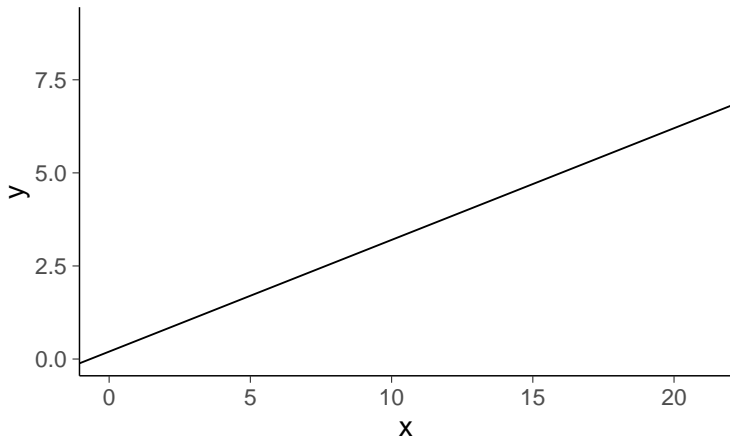
See `help('pareto-k-diagnostic')` for details.

Model comparison:

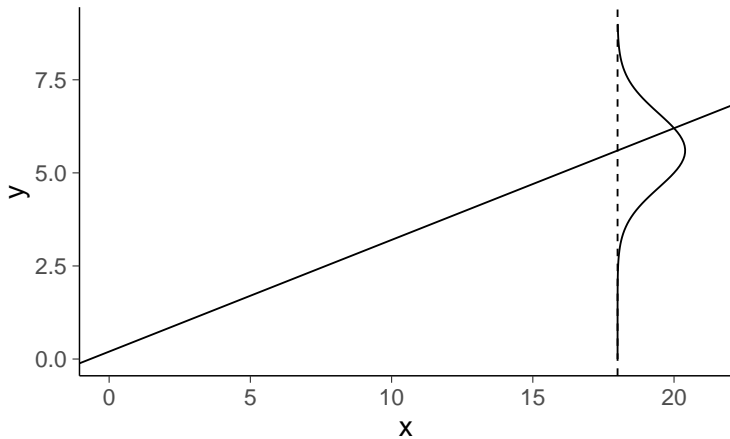
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff	se
-0.2	0.1

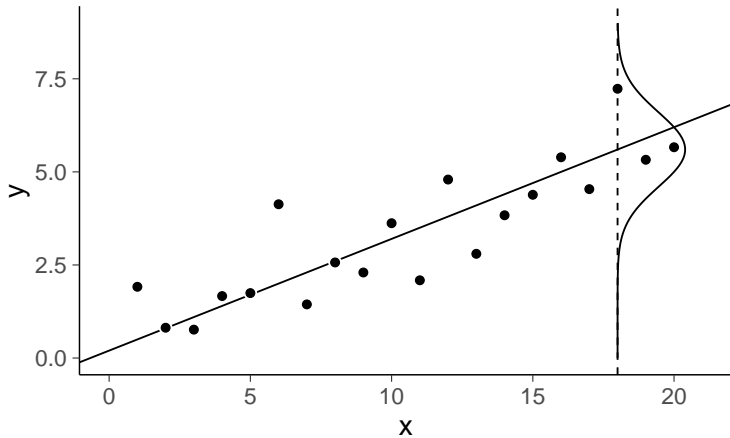
True mean $y = a + bx$



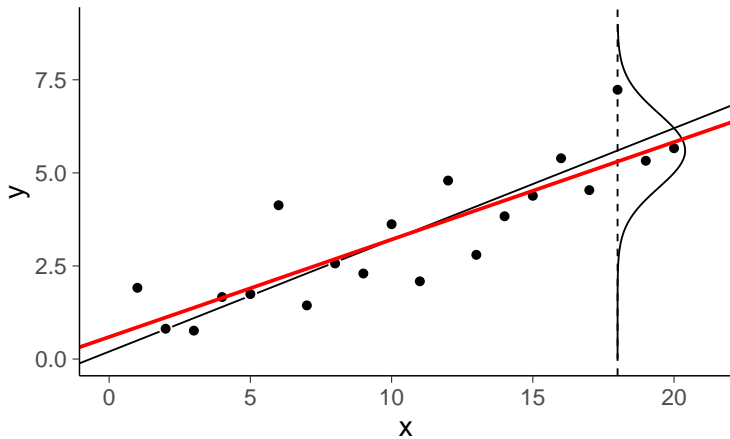
True mean and sigma



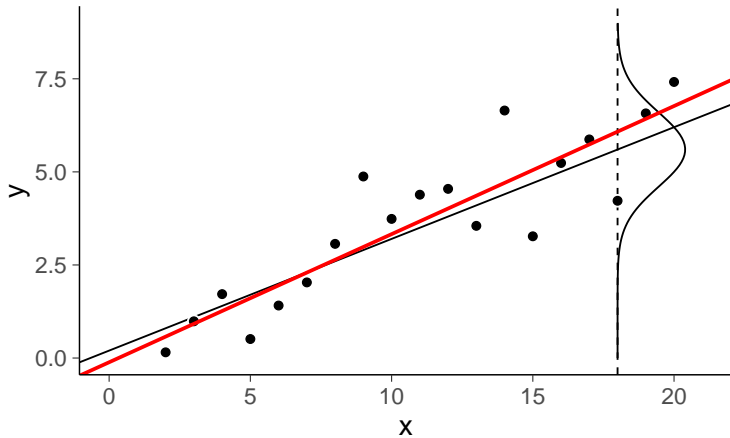
Data



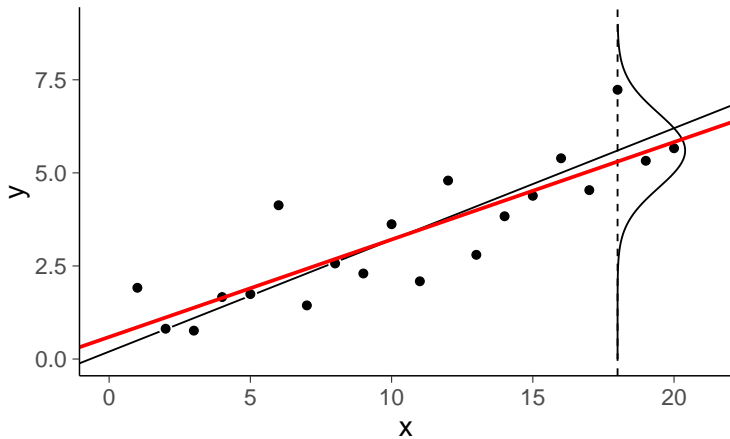
Posterior mean



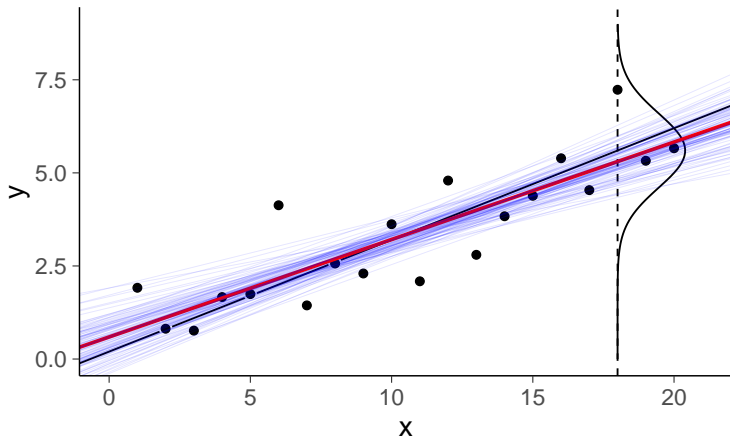
Posterior mean, alternative data realisation



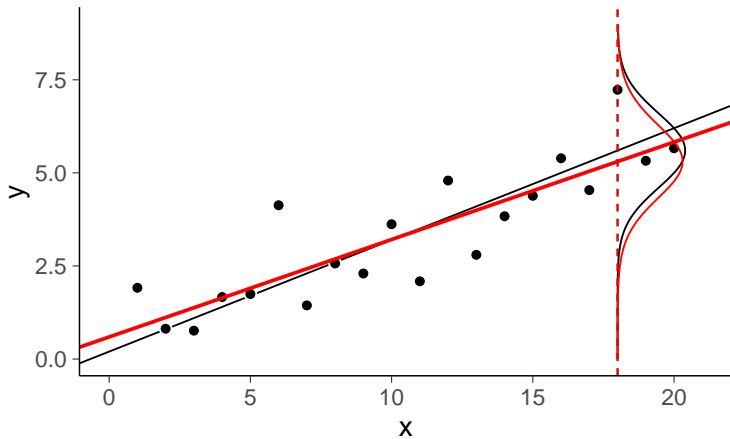
Posterior mean



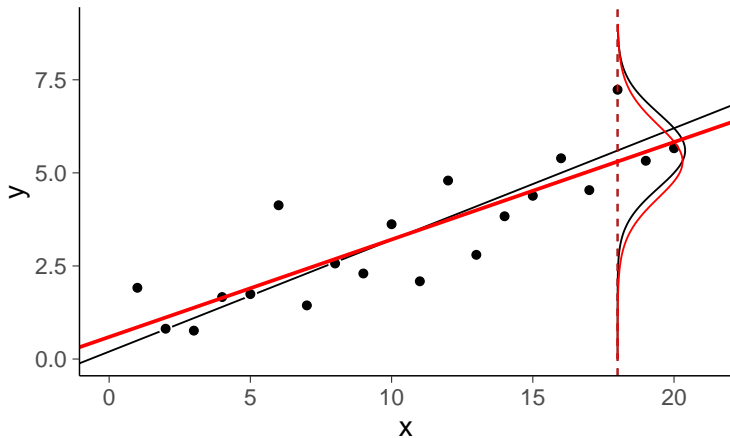
Posterior draws



Posterior predictive distribution

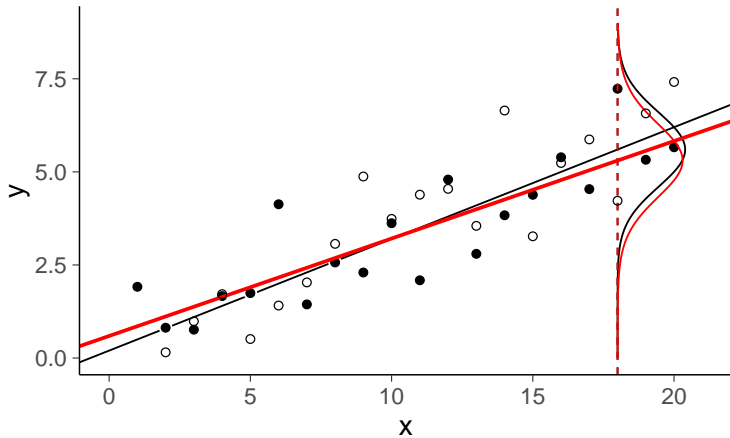


Posterior predictive distribution

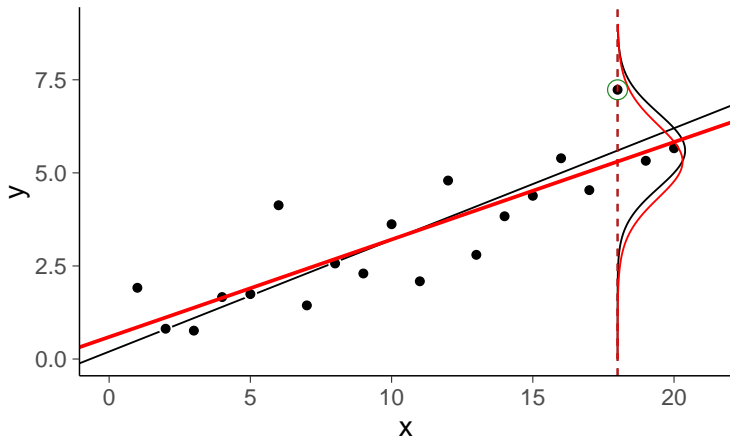


$$p(\tilde{y} \mid \tilde{x} = 18, x, y) = \int p(\tilde{y} \mid \tilde{x} = 18, \theta) p(\theta \mid x, y) d\theta$$

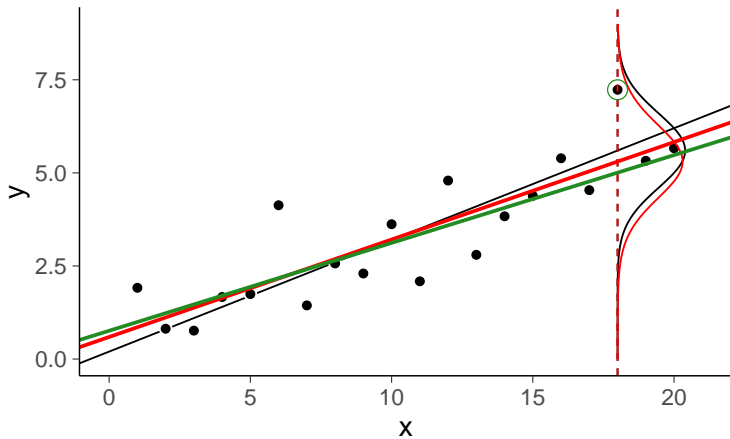
New data



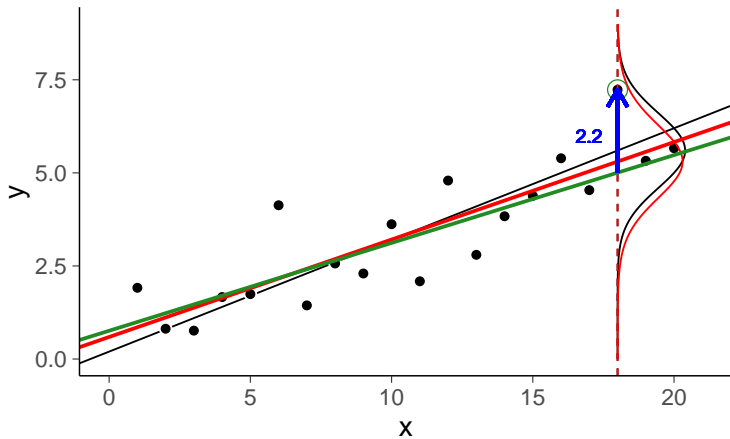
Posterior predictive distribution



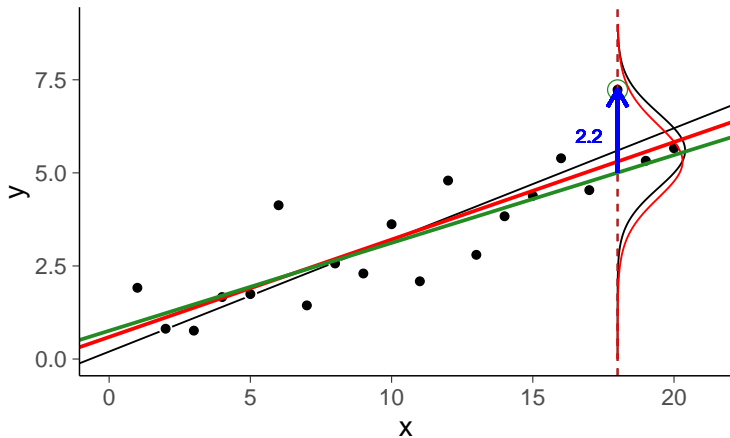
Leave-one-out mean



Leave-one-out residual

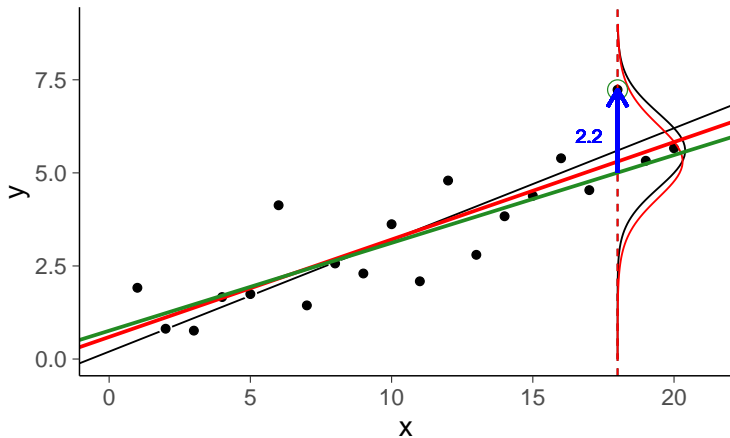


Leave-one-out residual



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

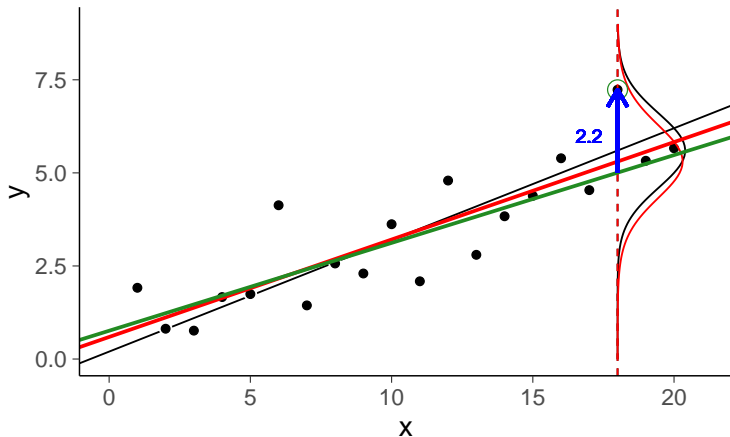
Leave-one-out residual



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

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

Leave-one-out residual

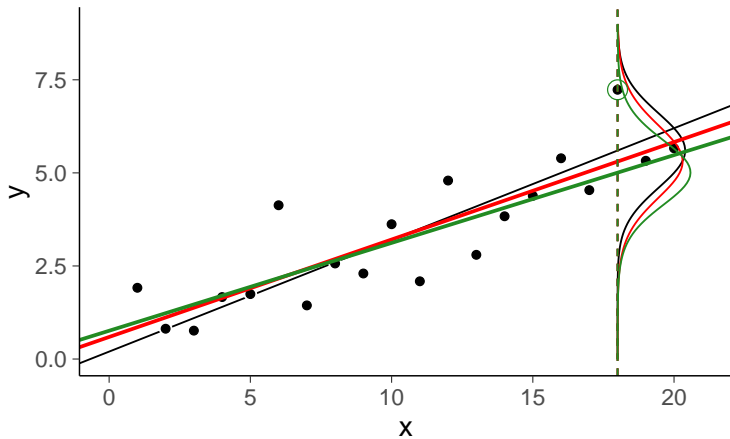


$$y_{18} - E[p(\tilde{y} \mid \tilde{x} = 18, x_{-18}, y_{-18})]$$

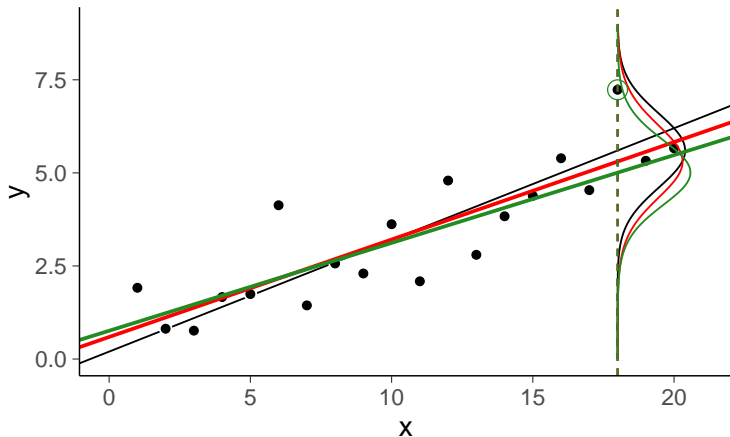
Can be used to compute, e.g., RMSE, R^2 , 90% error

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

Leave-one-out predictive distribution

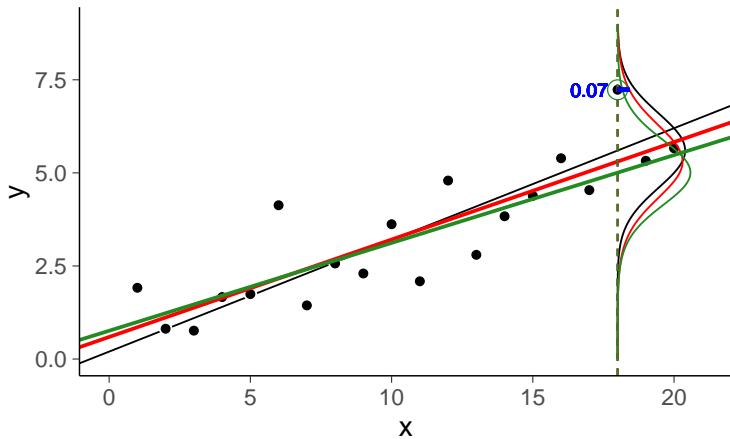


Leave-one-out predictive distribution

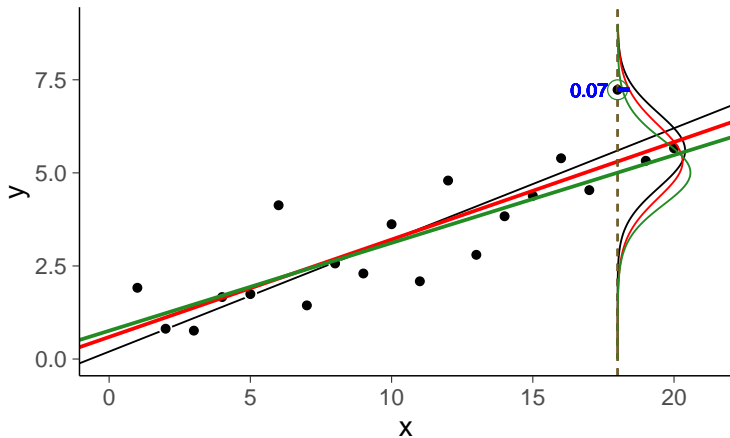


$$p(\tilde{y} \mid \tilde{x} = 18, x_{-18}, y_{-18}) = \int p(\tilde{y} \mid \tilde{x} = 18, \theta) p(\theta \mid x_{-18}, y_{-18}) d\theta$$

Posterior predictive density

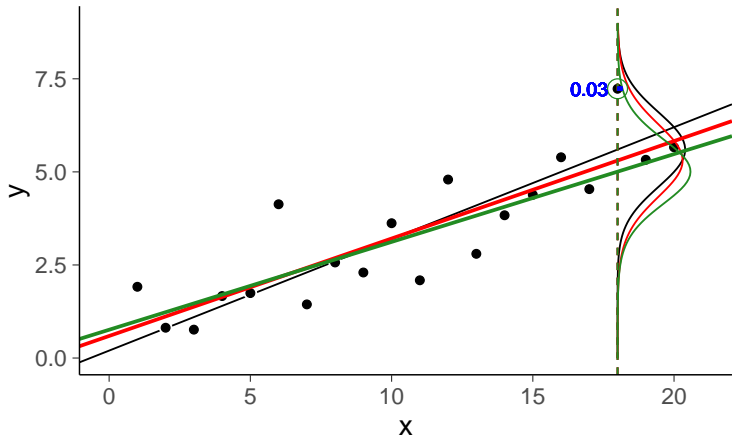


Posterior predictive density



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

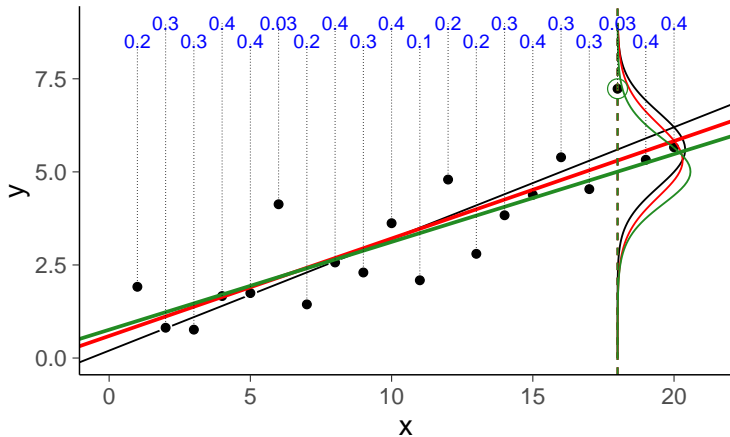
Leave-one-out predictive density



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

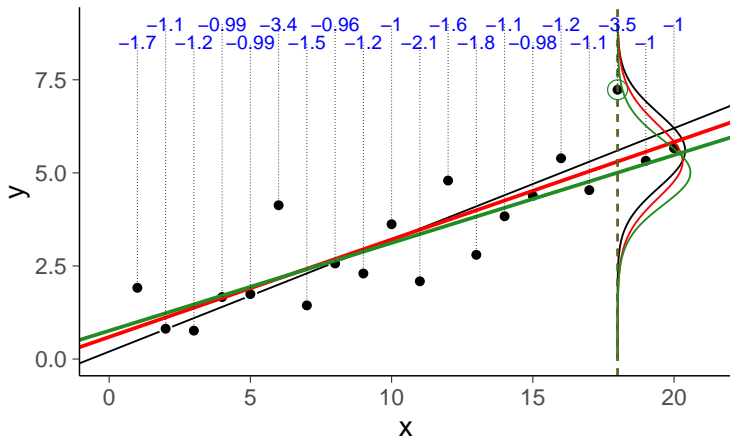
$$p(\tilde{y} = y_{18} \mid \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$$

Leave-one-out predictive densities



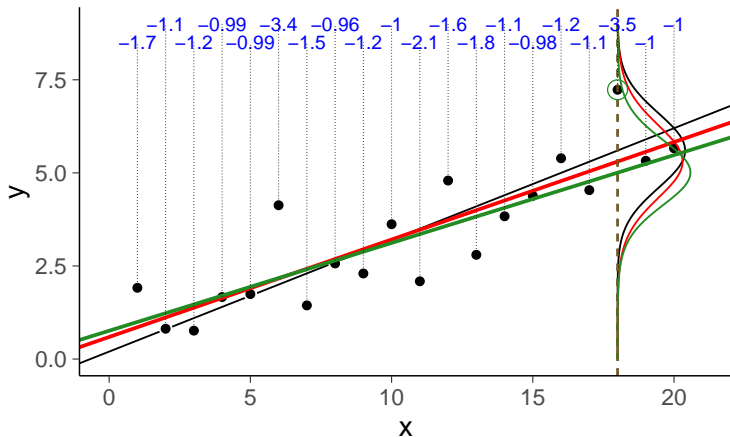
$$p(y_i | x_i, x_{-i}, y_{-i}), \quad i = 1, \dots, 20$$

Leave-one-out log predictive densities



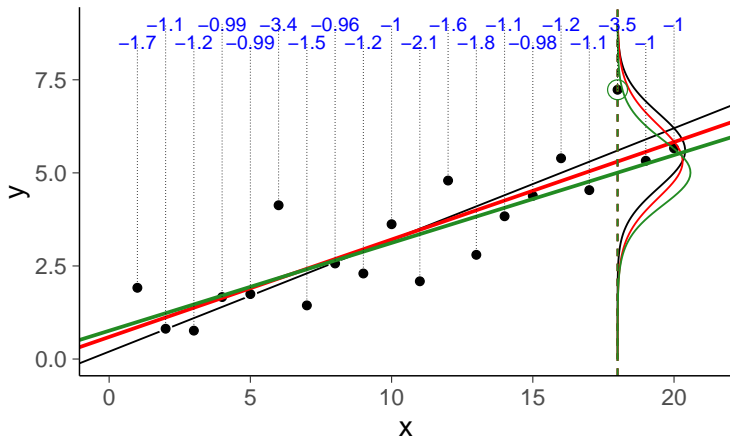
$$\log p(y_i | x_i, x_{-i}, y_{-i}), \quad i = 1, \dots, 20$$

Leave-one-out log predictive densities



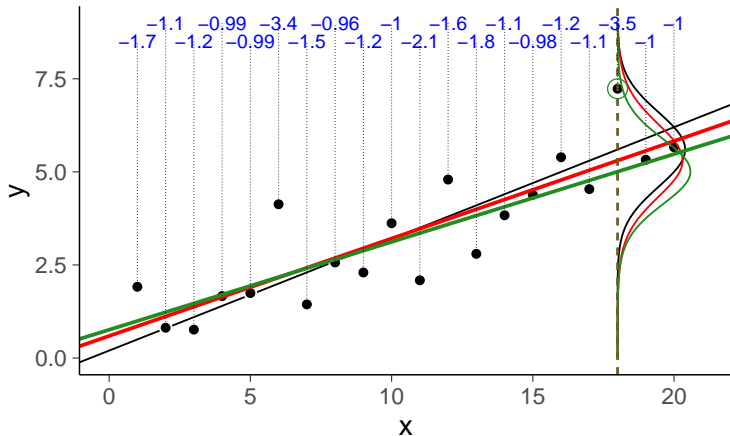
$$\sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

Leave-one-out log predictive densities



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

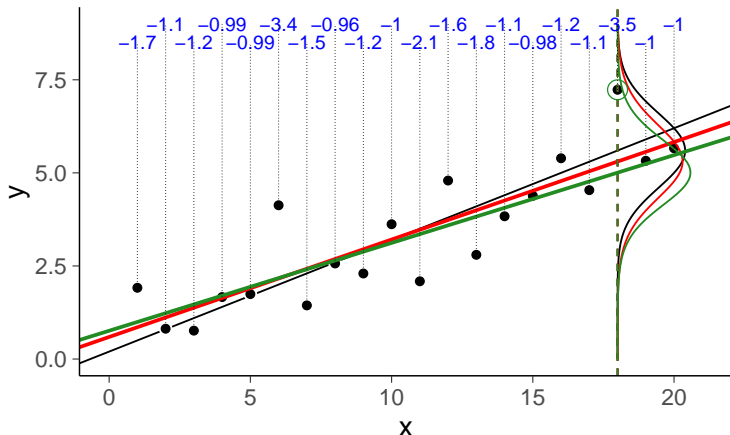
Leave-one-out log predictive densities



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

an estimate of log posterior pred. density for new data

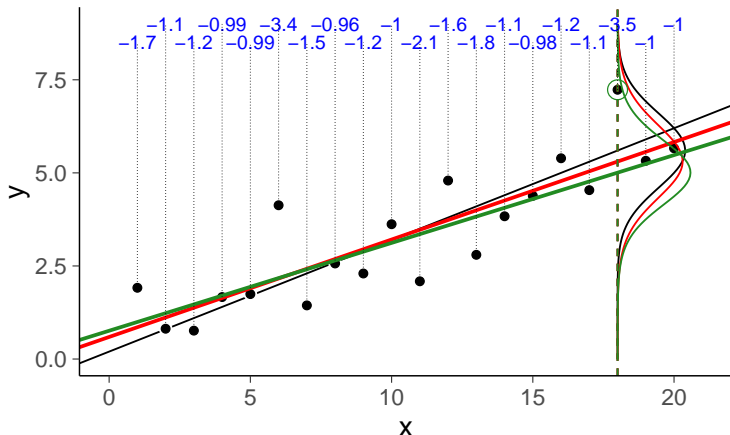
Leave-one-out log predictive densities



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

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

Leave-one-out log predictive densities

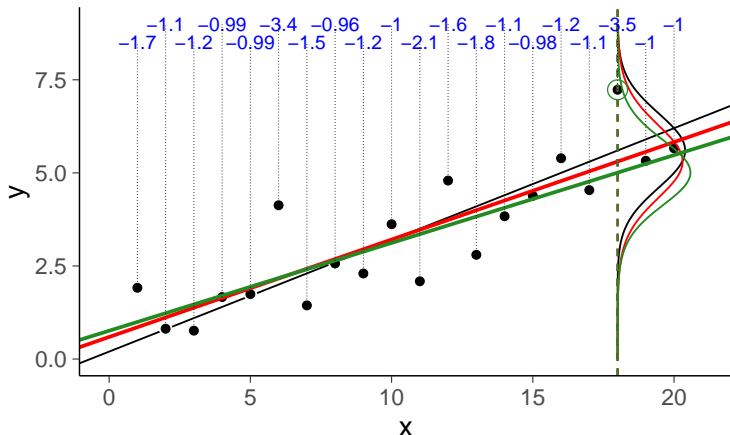


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$$\text{lpd} = \sum_{i=1}^{20} \log p(y_i | x_i, x, y) \approx -26.8$$

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

Leave-one-out log predictive densities

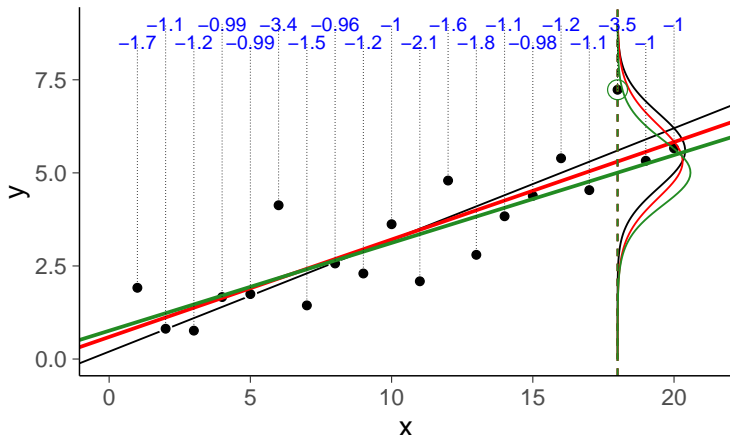


$$\text{elpd_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

asymptotically approaches p in case of regular faithful model

Leave-one-out log predictive densities

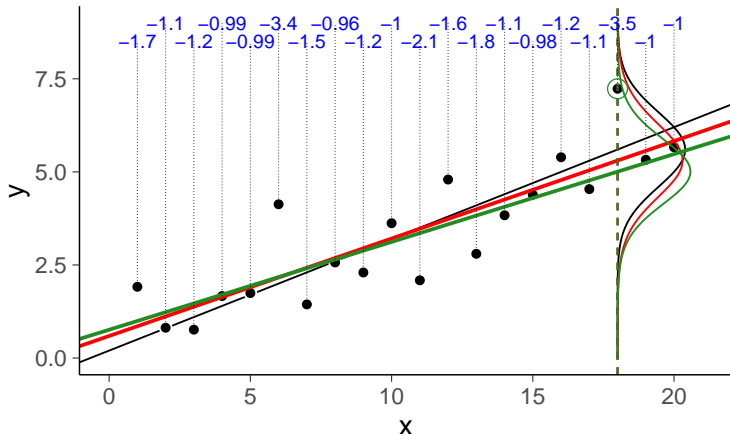


$$\text{elpd_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

asymptotically approaches p in case of regular faithful model

Leave-one-out log predictive densities



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

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

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

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.

Helicopter flight time – elpd

Computed from 4000 by 145 log-likelihood matrix

	Estimate	SE
elpd_loo	-52.9	10.1
p_loo	9.0	1.3
looic	105.8	20.1

Monte Carlo SE of elpd_loo is 0.1.

All Pareto k estimates are good ($k < 0.5$).
See `help('pareto-k-diagnostic')` for details.

Helicopter flight time – R^2

```
> bayes_R2(fit) |> round(digits=2)
```

```
  Estimate Est. Error Q2.5 Q97.5
```

```
R2      0.41      0.05 0.31  0.5
```

```
> loo_R2(fit) |> round(digits=2)
```

```
  Estimate Est. Error Q2.5 Q97.5
```

```
R2      0.36      0.07 0.22  0.48
```

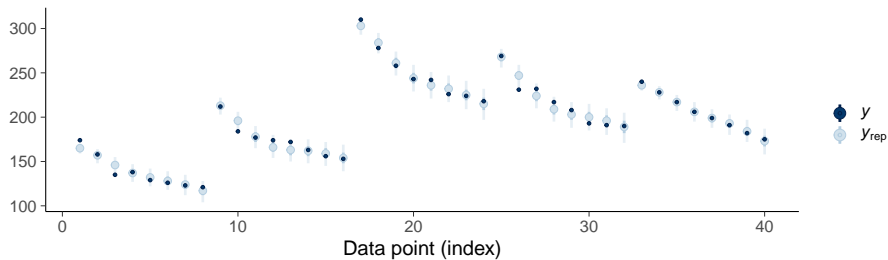
Student retention – R^2

```
> bayes_R2( fit6 )|> round( digits =2)
  Estimate Est. Error Q2.5 Q97.5
R2      0.98          0 0.97  0.98
```

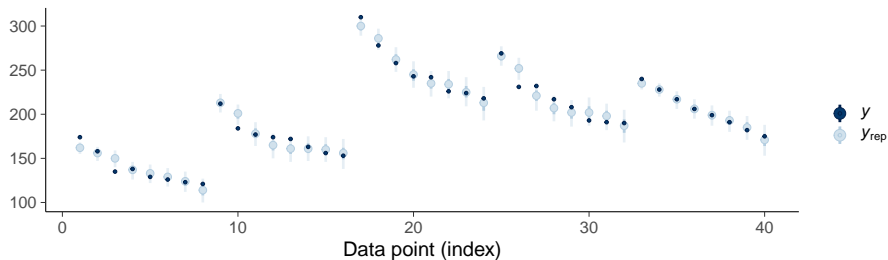
```
> loo_R2( fit6 ) |> round( digits =2)
  Estimate Est. Error Q2.5 Q97.5
R2      0.97          0.01 0.95  0.98
```

Student retention

Posterior predictive intervals



LOO predictive intervals



Student retention – R^2

Latent hierarchical linear vs. latent hierarchical linear + spline

```
> loo_R2(fit4) |> round(digits=2)
```

	Estimate	Est. Error	Q2.5	Q97.5
R2	0.92	0.02	0.88	0.95

```
> loo_R2(fit6) |> round(digits=2)
```

	Estimate	Est. Error	Q2.5	Q97.5
R2	0.97	0.01	0.95	0.98

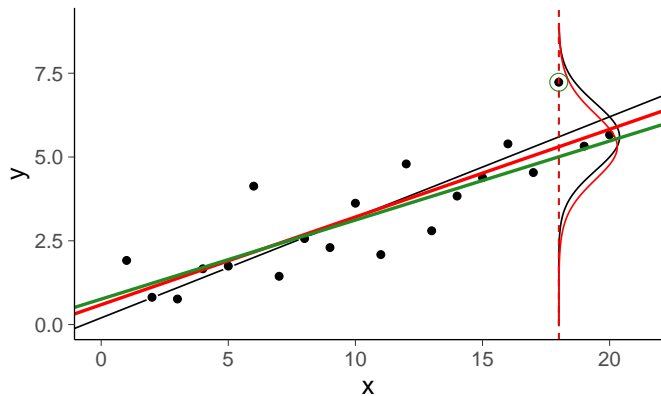
Student retention – elpd (log score)

Latent hierarchical linear vs. latent hierarchical linear + spline

```
> loo_compare(fit4 , fit6 )
      elpd_diff se_diff
fit6    0.0     0.0
fit4 -43.2    14.4
```

Next week more about this

LOO-PIT predictive checking



- LOO probability integral transform (LOO-PIT)

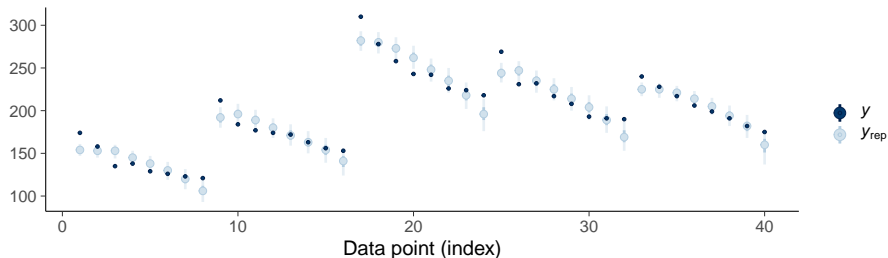
$$p_i = p(y_i^{\text{rep}} \leq y_i | y_{-i})$$

- If $p(\tilde{y}_i | y_{-i})$ is well calibrated, distribution of p_i 's would be uniform between 0 and 1

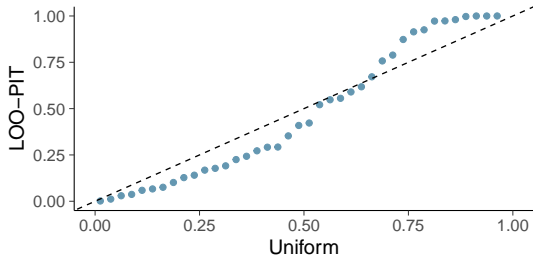
Student retention – LOO-PIT checking

```
pp_check(fit, type = "loo_pit_qq", ndraws=4000)
```

Latent hierarchical linear – LOO predictive intervals



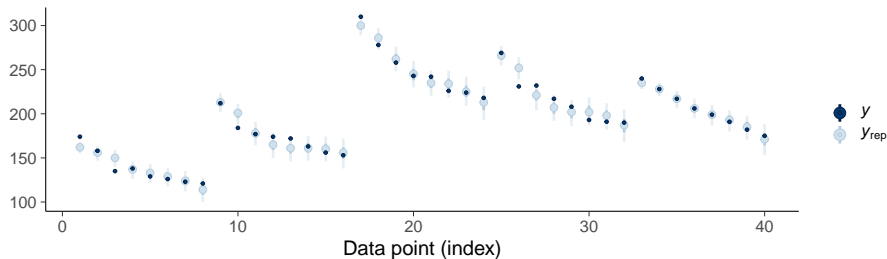
LOO-PIT check



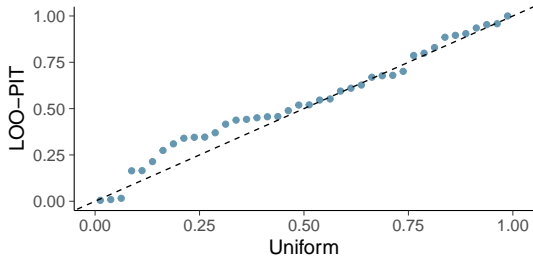
Student retention – LOO-PIT checking

```
pp_check(fit, type = "loo_pit_qq", ndraws=4000)
```

Latent hierarchical linear + spline – LOO predictive intervals/



LOO-PIT check



Brute-force LOO

- Re-run MCMC n times to sample from $p(\theta | x_{-i}, y_{-i})$
 - can take a lot of time

Brute-force LOO

- Re-run MCMC n times to sample from $p(\theta \mid x_{-i}, y_{-i})$
 - can take a lot of time
 - or high parallelization

Cooper, Vehtari, Forbes, Kennedy, and Simpson (2023).
Bayesian cross-validation by parallel Markov chain Monte
Carlo. arXiv:2310.07002.

Fast cross-validation

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

see Vehtari, Gelman & Gabry (2017a) and 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

- 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 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

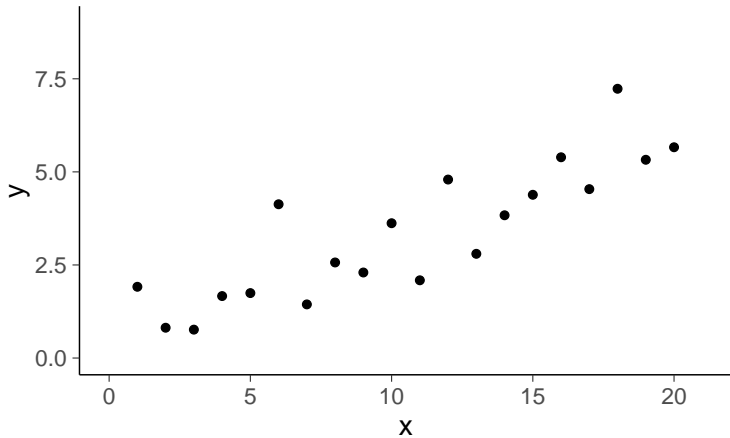
$$p(y_i | x_i, x_{-i}, y_{-i}) = \int p(y_i | x_i, \theta) p(\theta | x_{-i}, y_{-i}) d\theta$$

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

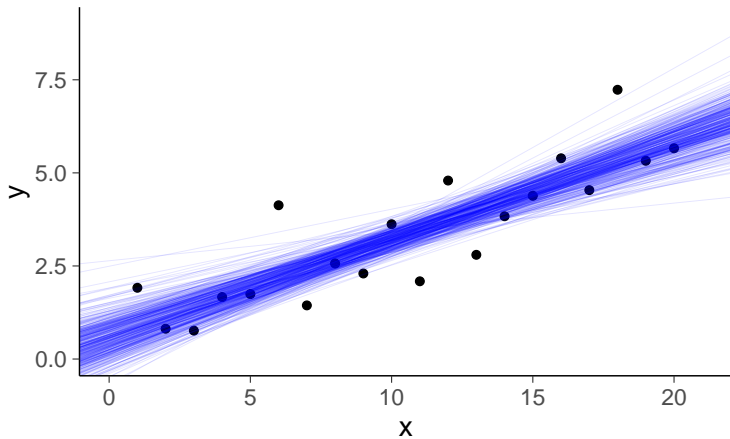
$$w_i^{(s)} = \frac{p(\theta^{(s)} | x_{-i}, y_{-i})}{p(\theta^{(s)} | x, y)} \propto \frac{1}{p(y_i | x_i, \theta^{(s)})}$$

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

Data

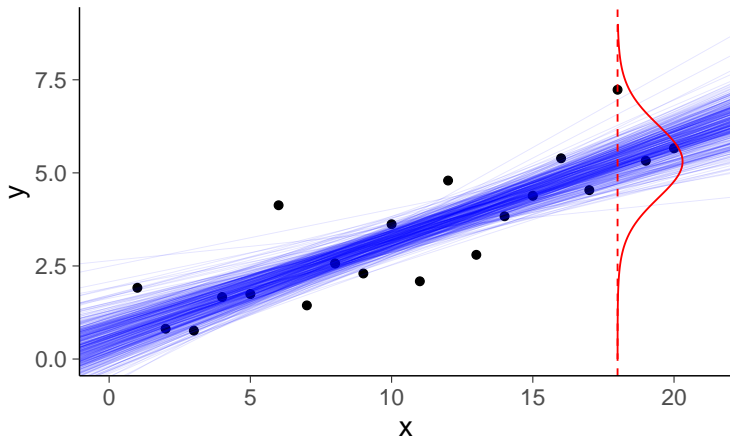


Posterior draws



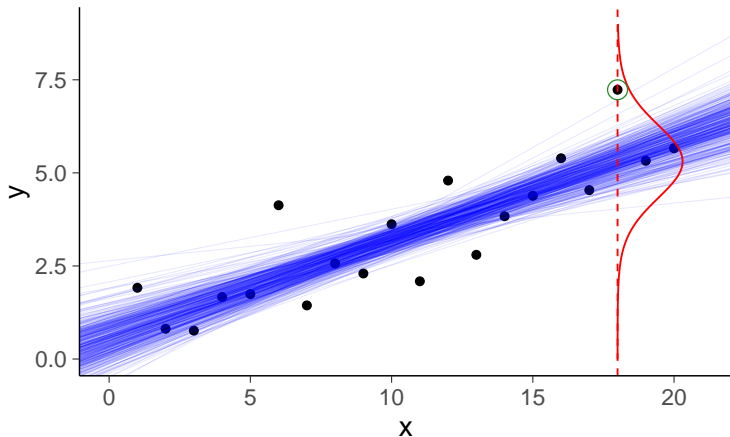
$$\theta^{(s)} \sim p(\theta | x, y)$$

Posterior predictive distribution



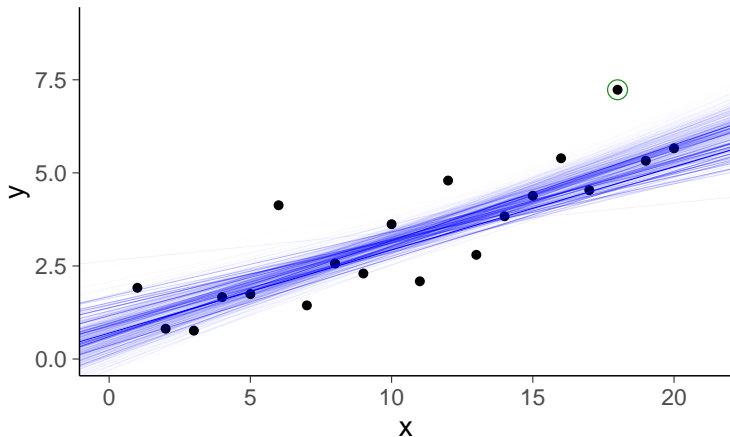
$$\theta^{(s)} \sim p(\theta | x, y), \quad p(\tilde{y} | \tilde{x}, x, y) \approx \frac{1}{S} \sum_{s=1}^S p(\tilde{y} | \tilde{x}, \theta^{(s)})$$

Posterior predictive distribution



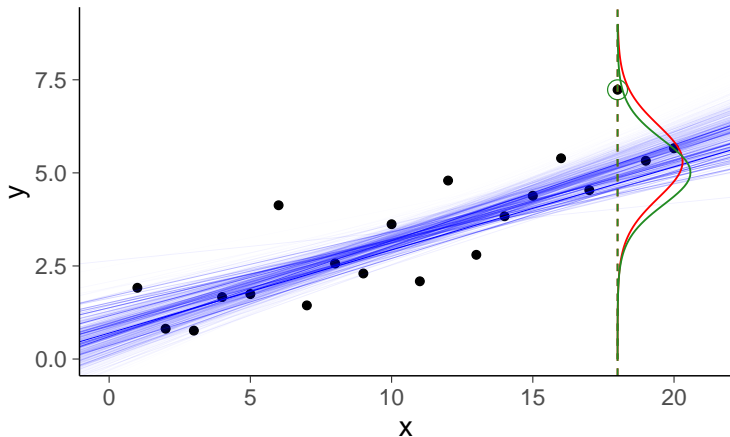
$$\theta^{(s)} \sim p(\theta | x, y), \quad p(\tilde{y} | \tilde{x}, x, y) \approx \frac{1}{S} \sum_{s=1}^S p(\tilde{y} | \tilde{x}, \theta^{(s)})$$

PSIS-LOO weighted draws



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

PSIS-LOO weighted predictive distribution



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

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

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

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

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

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

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

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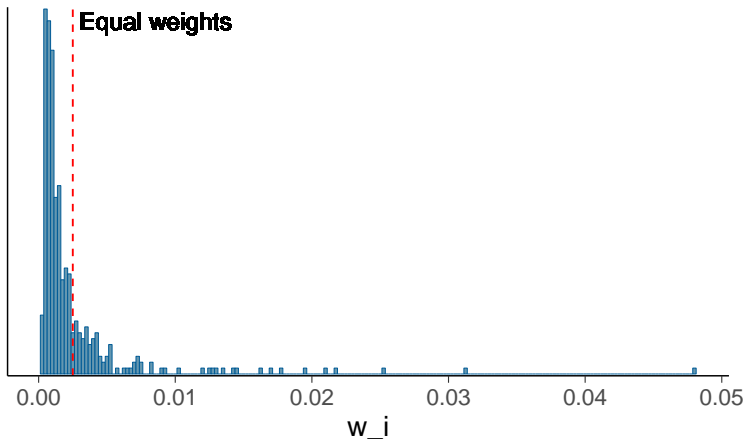
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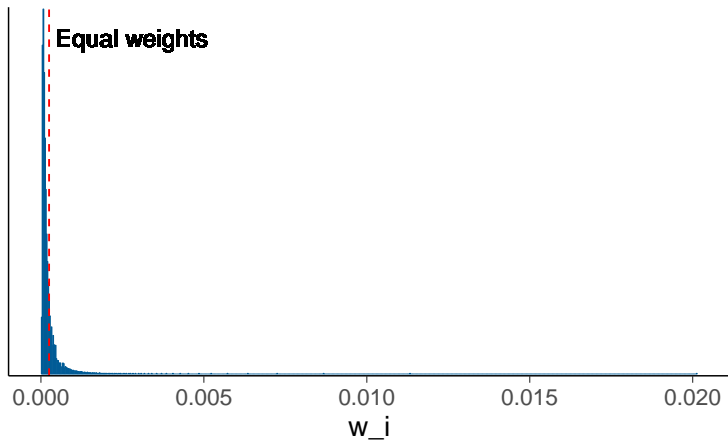
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- The variability of importance weights matter
 - Pareto- k diagnostic
 - Pareto smoothed importance sampling LOO (PSIS-LOO)

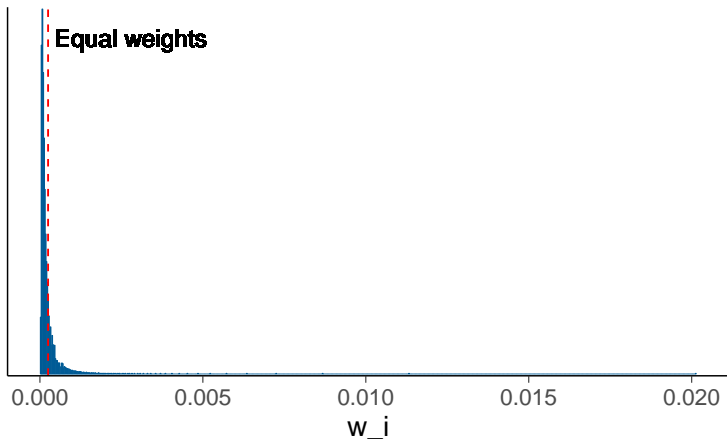
400 importance weights for leave-18th-out



4000 importance weights for leave-18th-out



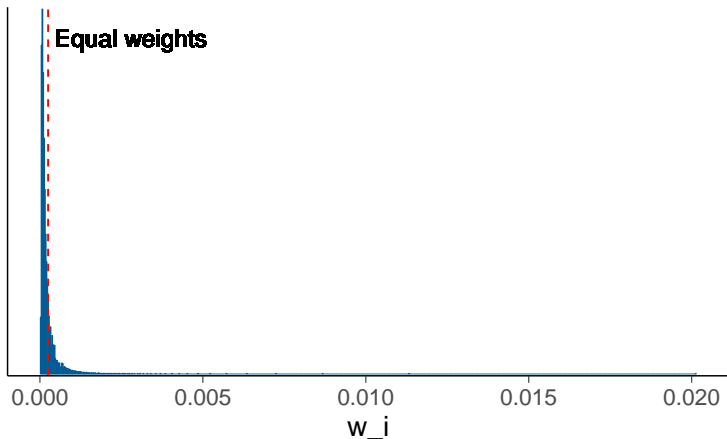
4000 importance weights for leave-18th-out



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

see Vehtari, Gelman & Gabry (2017b)

4000 importance weights for leave-18th-out



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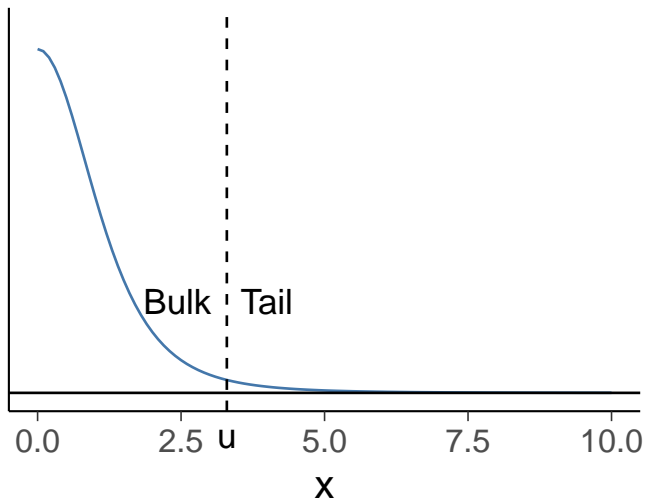
$$\text{Pareto } \hat{k} \approx 0.52$$

- 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)

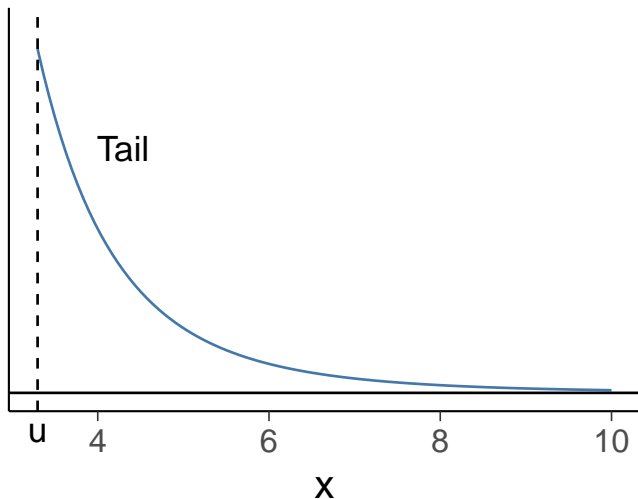
Pareto- \hat{k} diagnostic

Pickands (1975): many distributions have tail ($x > u$) that is well approximated with Generalized Pareto distribution (GPD)



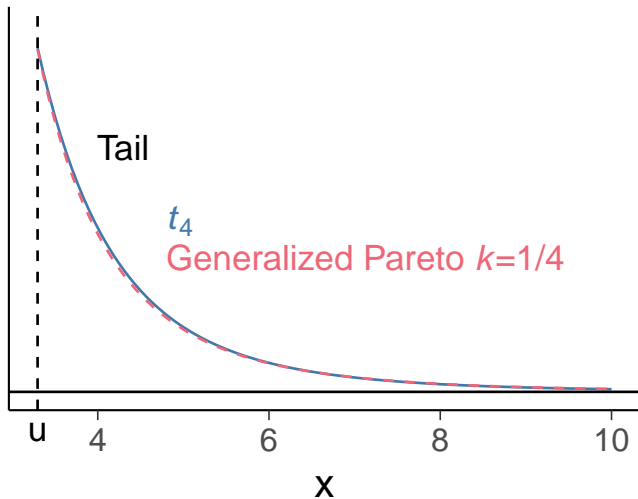
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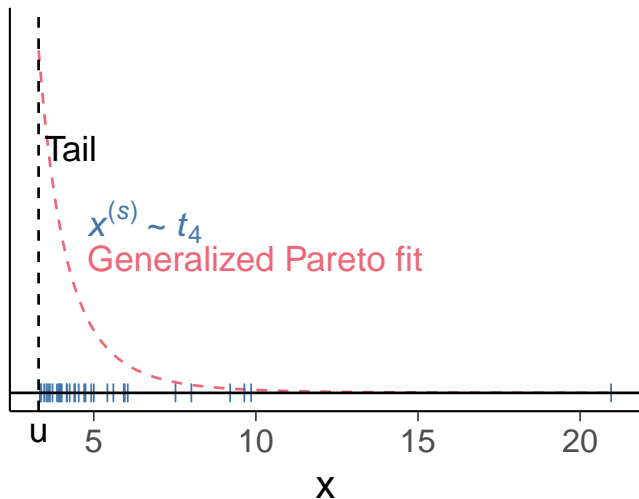
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Pareto- \hat{k} and convergence rate of PSIS

- CLT says that to half the MCSE, need 4 times bigger S

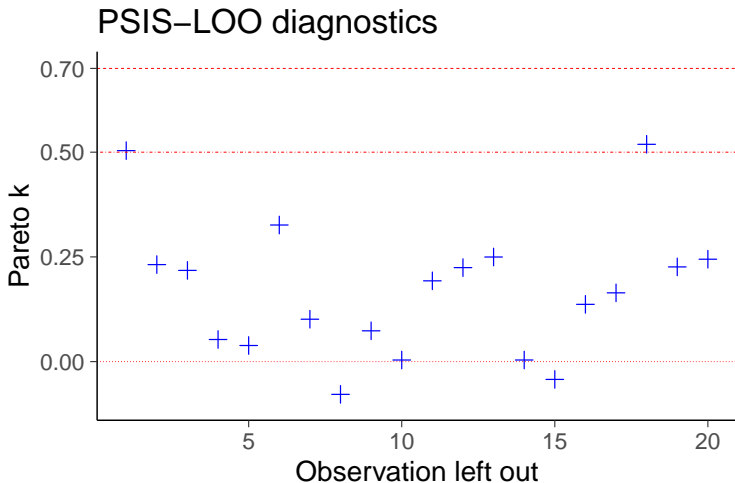
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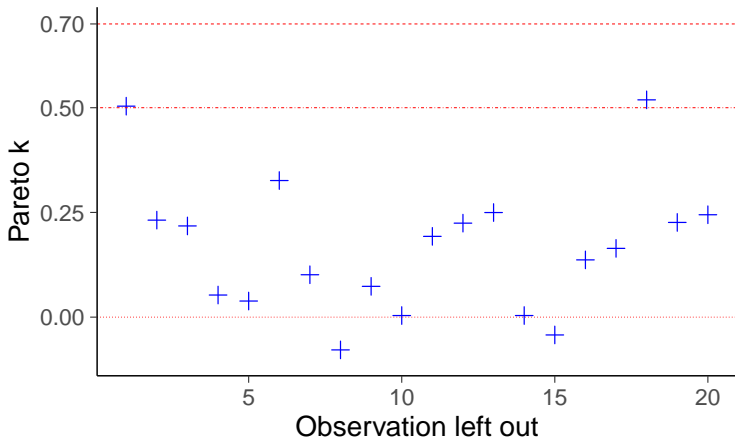
Pareto- \hat{k} and convergence rate of PSIS

- CLT says that to half the MCSE, need 4 times bigger S
- If Pareto- $\hat{k} \approx 0.7$, to half the MCSE, need 10 times bigger S
- If Pareto- $\hat{k} > 1$, to half the MCSE, nothing helps

- Pareto- \hat{k} for each leave-one-out fold indicates reliability of the PSIS-LOO approximation



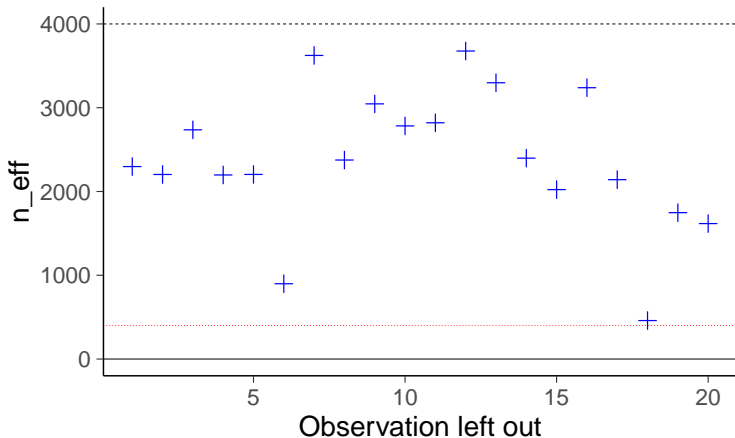
PSIS-LOO diagnostics



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
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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:

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

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

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

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)

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- 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

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

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```
...
model {
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  beta ~ normal(pmubeta, psbeta);
  y ~ normal(mu, sigma);
}
generated quantities {
  vector[N] log_lik;
  for (i in 1:N)
    log_lik[i] = normal_lpdf(y[i] | mu[i], sigma);
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- RStanARM and brms compute `log_lik` by default

loo()

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

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fit\$loo()
- RStanARM, brms
loo(fit)
- brms alternative
fit <- add_criterion(fit, 'loo')

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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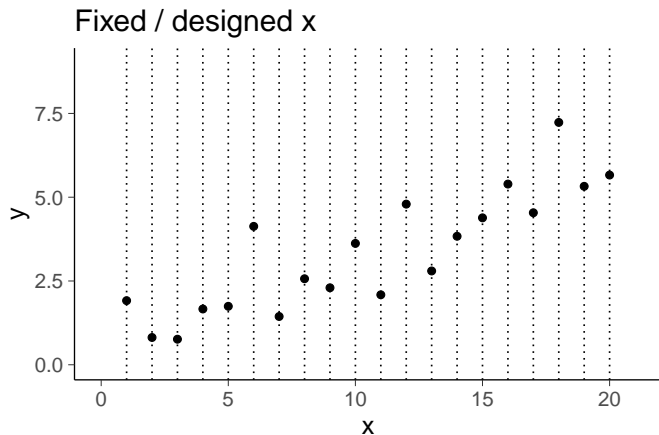
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See <https://users.aalto.fi/~ave/modelselection/roaches.html>
- Use K-fold-CV (more about this later)
`rstanarm::kfold(..., K=10)`
`brms::kfold(..., K=10)`
RStan/CmdStanR vignette
<http://mc-stan.org/loo/articles/loo2-elpd.html>

Assumptions about the future observations



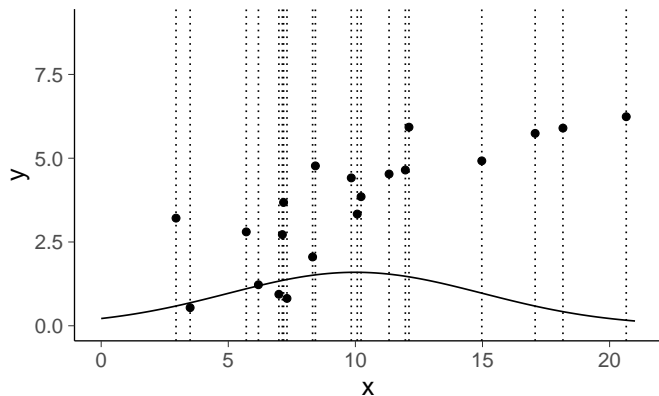
$$\text{elpd_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

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

Assumptions about the future observations

Distribution for x



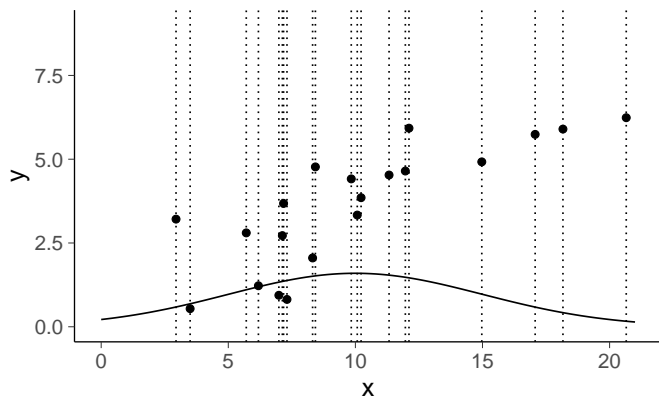
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Distribution for x



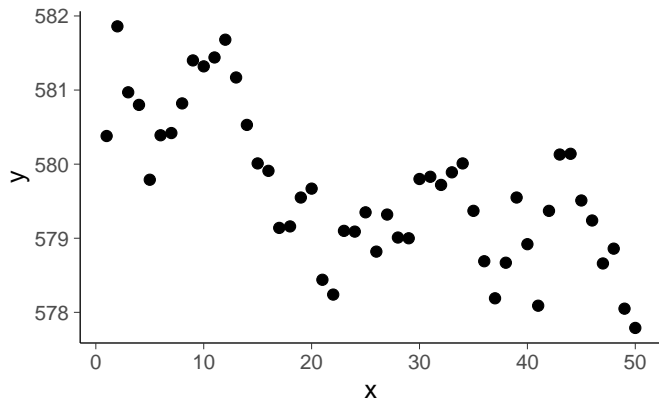
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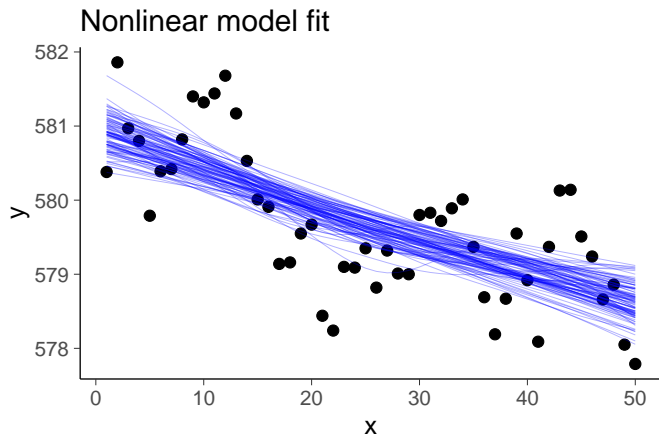
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Covariate shift can be handled with importance weighting or modelling

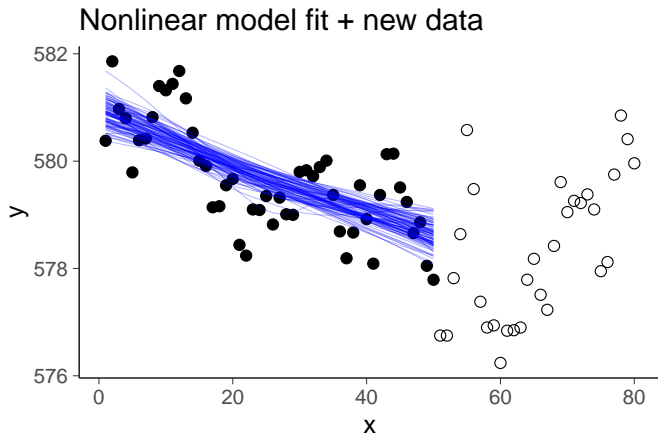
Interpolation vs extrapolation



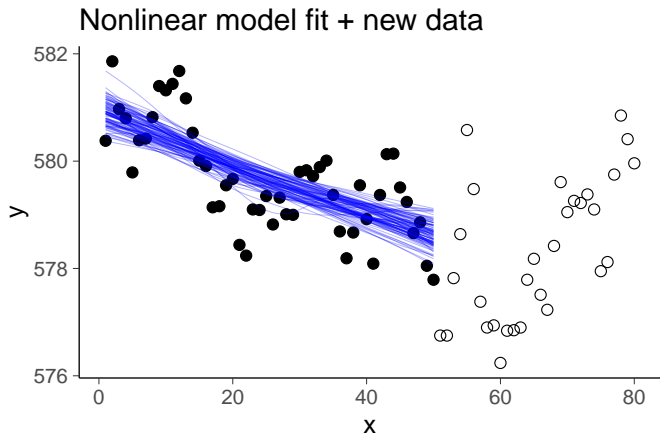
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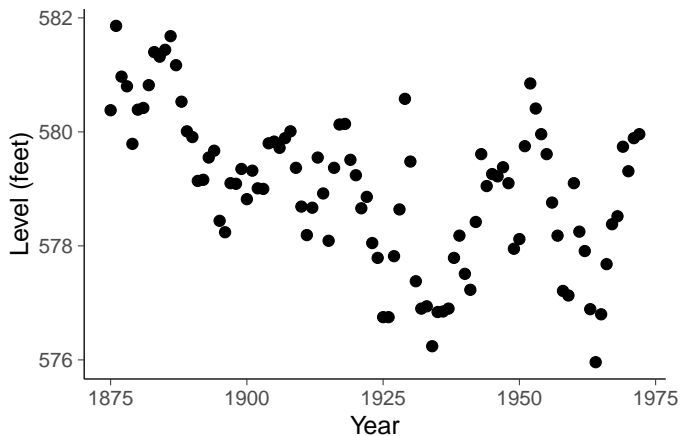


Interpolation vs extrapolation



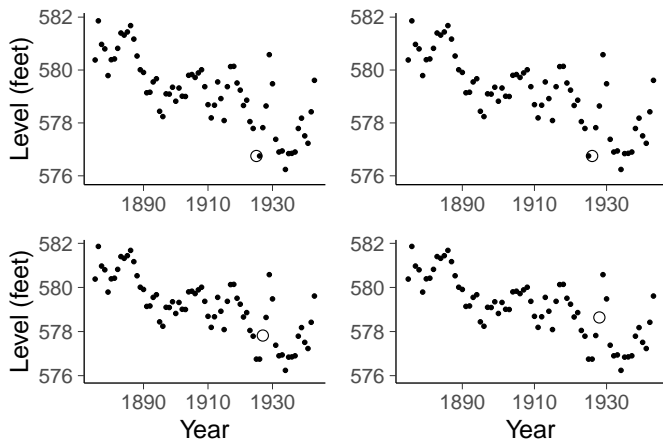
Extrapolation is more difficult

Cross-validation for time series?



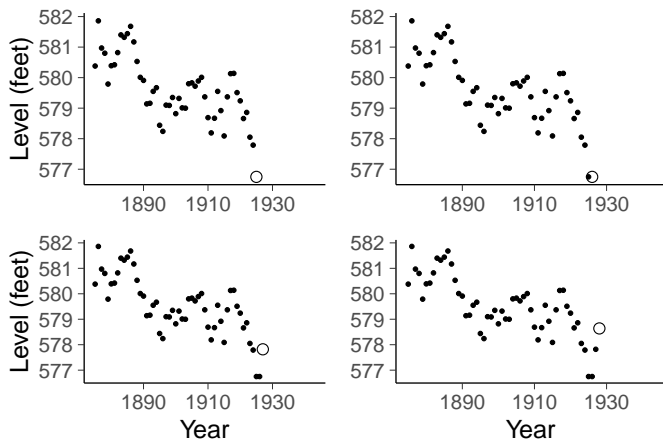
Can LOO or other cross-validation be used with time series?

Cross-validation for time series



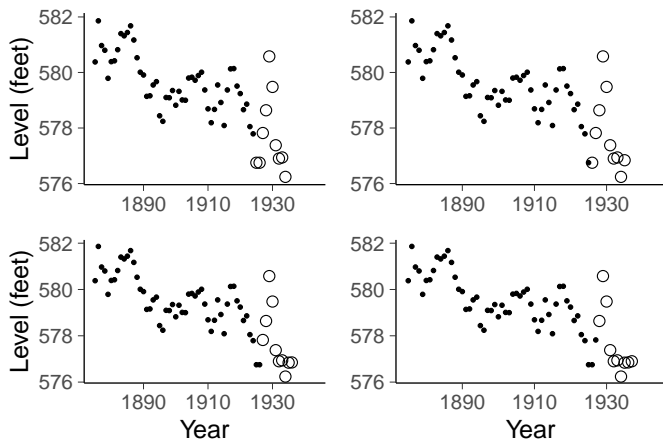
Leave-one-out cross-validation is ok for assessing conditional model

Cross-validation for time series



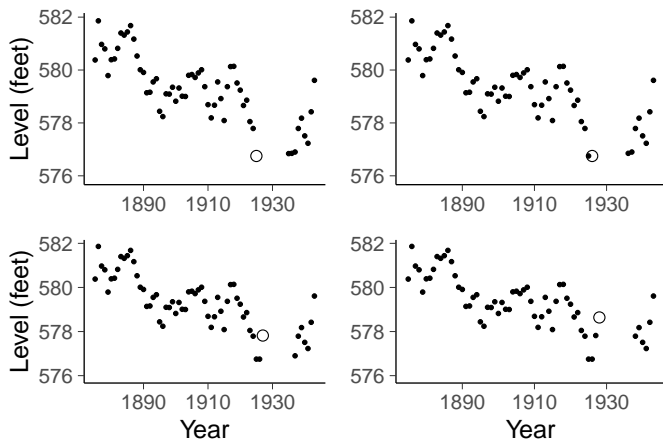
Leave-future-out (LFO) cross-validation is better for predicting future

Cross-validation for time series



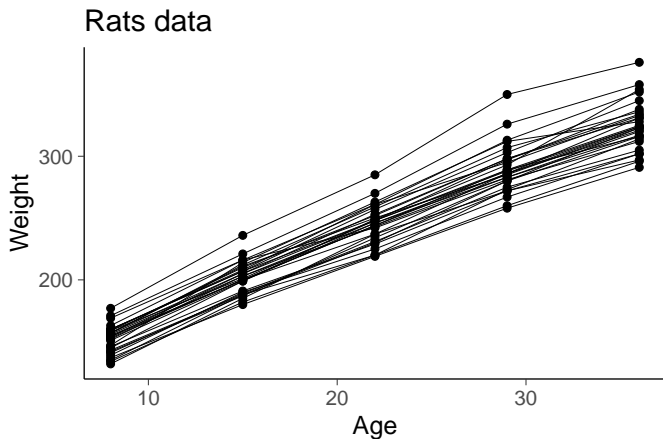
m-step-ahead cross-validation is better for predicting further future

Cross-validation for time series



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

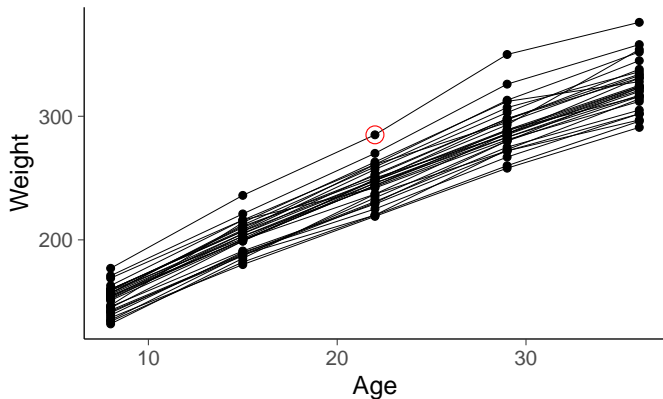
Cross-validation for hierarchical data



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

Cross-validation for hierarchical data

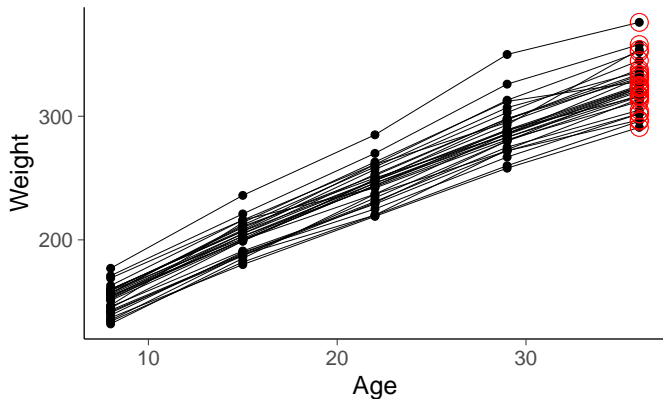
Leave-one-out?



Yes!

Cross-validation for hierarchical data

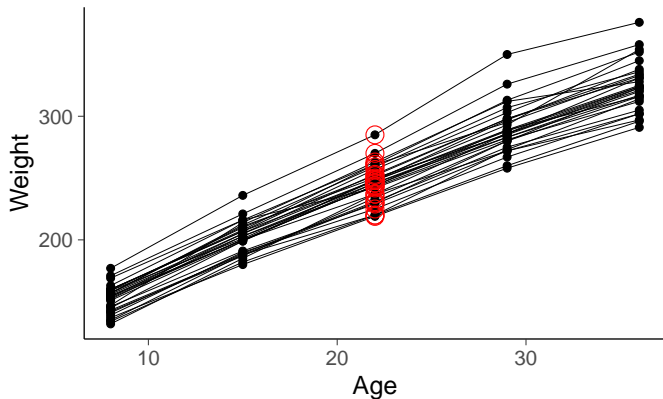
1-step-ahead?



Yes!

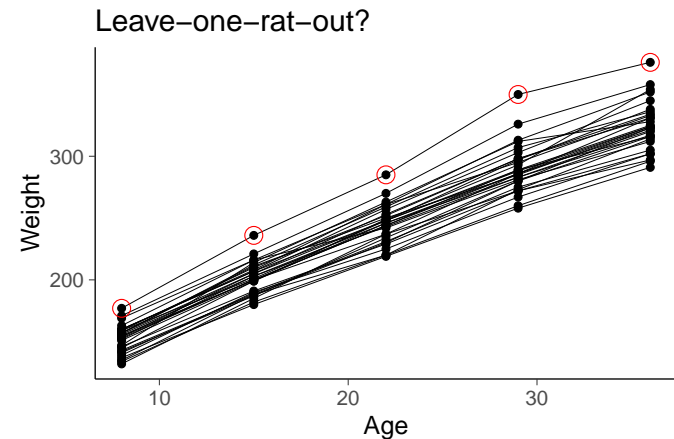
Cross-validation for hierarchical data

Leave-one-time-point-out?



Yes!

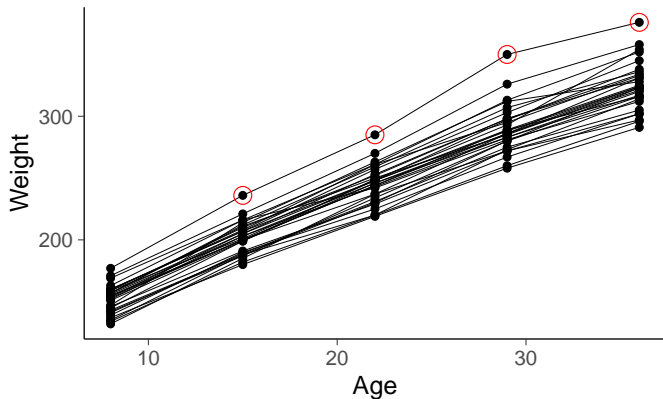
Cross-validation for hierarchical data



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

Pareto smoothed importance sampling CV variants

- PSIS-LOO for hierarchical models
 - leave-one-group out is challenging for PSIS-LOO
 - Stan demo of the challenges and integrated LOO at <https://users.aalto.fi/~ave/modelselection/roaches.html>
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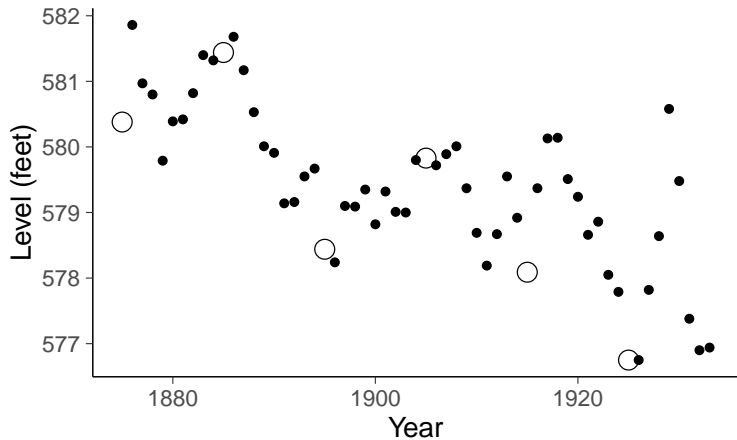
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- PSIS-LOO for time series
 - Approximate leave-future-out cross-validation (LFO-CV)
mc-stan.org/loo/articles/loo2-lfo.html

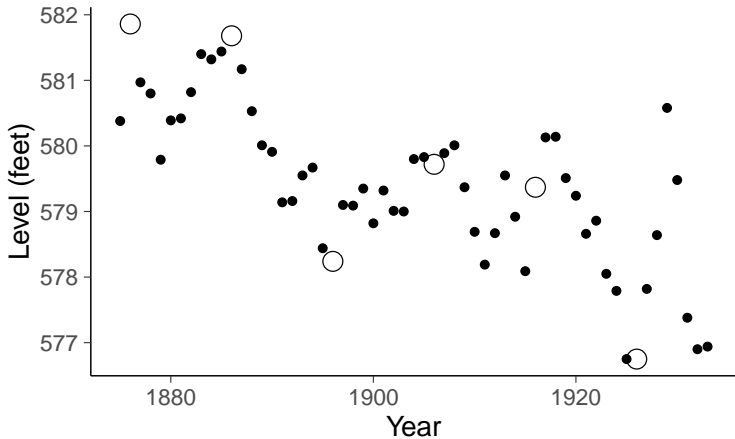
K-fold cross-validation

- 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

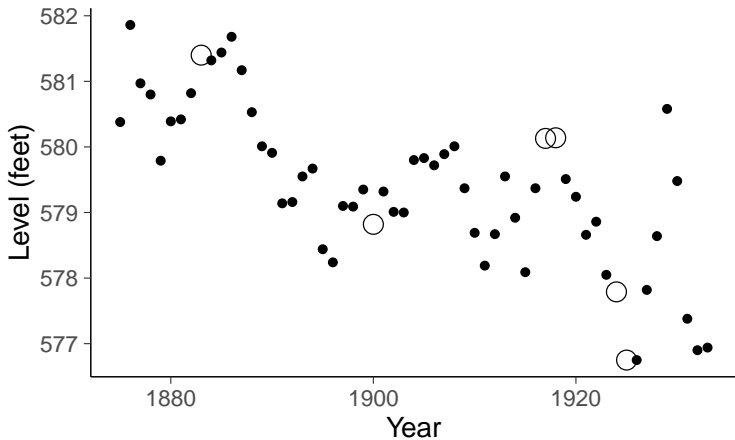
Balance k-fold approximation of LOO



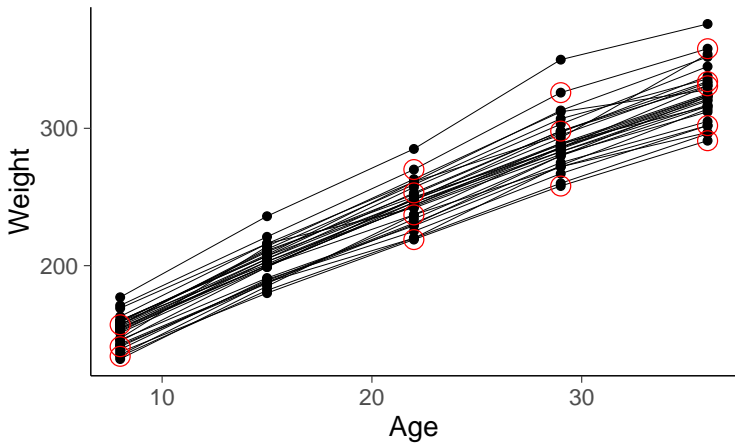
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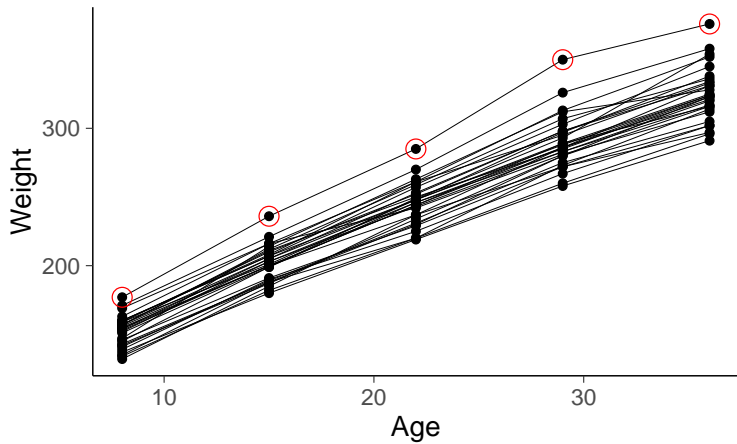
Random k-fold approximation of LOO



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()`

Cross-validation for model assessment

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 - e.g. in concrete quality prediction reported that the absolute error is smaller than X with 90% probability
- Also useful in model checking in similar way as posterior predictive checking (PPC)
 - checking calibration of leave-one-out predictive posteriors (ppc_loo_pit in bayesplot)
 - model misspecification diagnostics (e.g. Pareto- k and p_loo)

see demos <https://users.aalto.fi/~ave/casestudies.html>

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 - e.g. hierarchical model with one parameter per observation
 - indicated by large p and p_{loo} (e.g. $N/5 < p, p_{\text{loo}} < p$)
 - moment matching or integrated LOO may help

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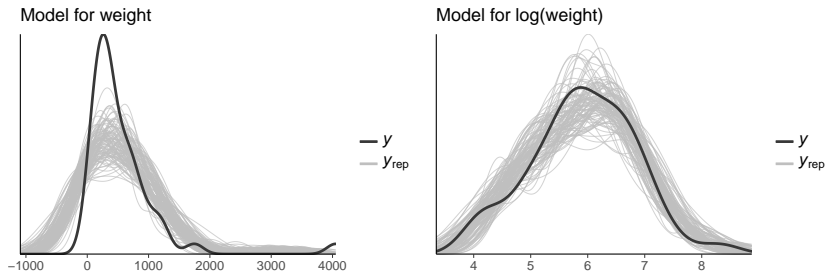
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- See more in CV-FAQ

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- Posterior predictive checking is often sufficient

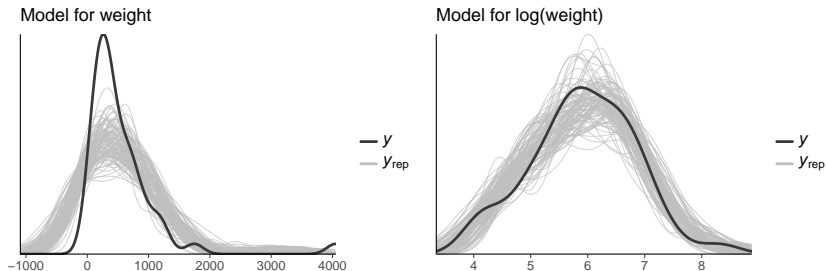


Predicting the yields of mesquite bushes.

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

Model comparison and selection

Next lecture

- Model comparison and selection (elpd_diff, se)
- Related methods (WAIC, *IC, BF)
- Model averaging
- Potential overfitting in model selection