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Bayesian Statistics and Data Analysis
Lecture 8b

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Thanks to Aki Vehtari, Aalto University

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Section 1

Model assessment and selection

Predictive performance

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

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  - external validation

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  All models are wrong... but some are useful.
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  - external validation
- Expected predictive performance
  - approximates the external validation

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

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

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

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

Subsection 1

Measures of predictive accuracy

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(Bayesian) Points Prediction Accuracy

- Point residuals

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

where

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

i.e. the expected predicted value

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i.e. the expected predicted value

- Mean squared (prediction) error (MSE)

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

Probabilistic predictions

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

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

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- The log predictive density (lpd)

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

Probabilistic predictions

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

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

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Probabilistic predictions

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

- Estimation using MCMC

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

Subsection 2

Model selection

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Model selection

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

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

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

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

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Section 2

Cross-validation

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

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

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

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

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

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

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- Hold out observation i and try to predict y_i based on $\mathbf{y}_{-i}$
- Estimation of elpd_M using leave-one-out cross-validation

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

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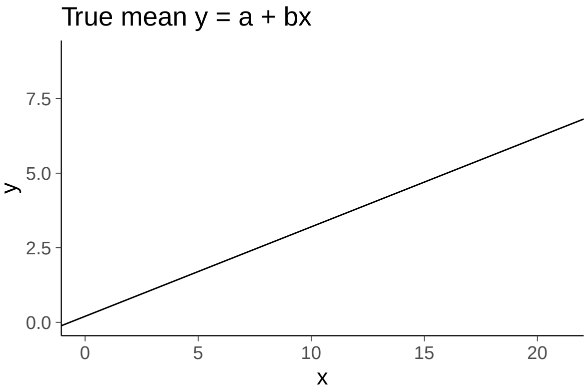
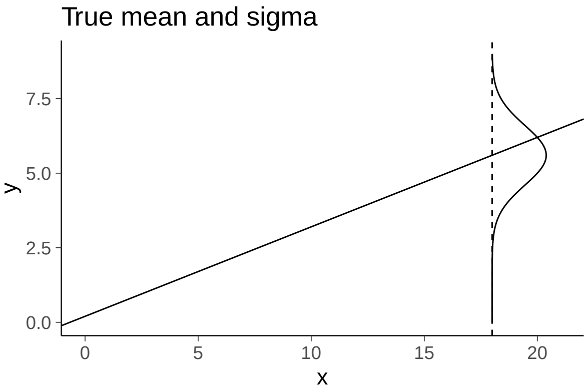
- Analogy: Monte Carlo approximation using our data
- Similar to jack-knife resampling
- The elpd, lpd and efficient number of parameters (p_{loo})

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


True mean y = a + bx
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x


True mean and sigma
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

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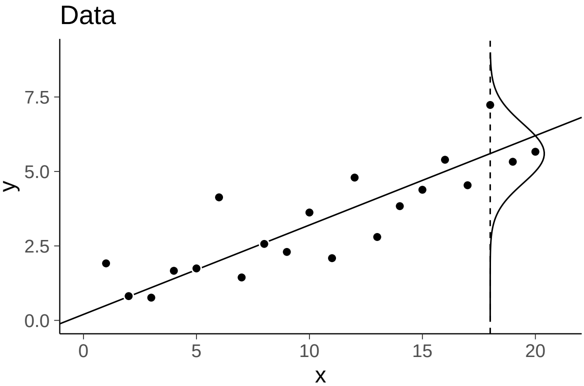

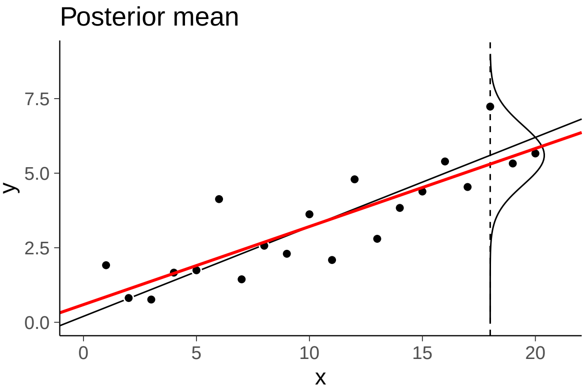
Posterior mean
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

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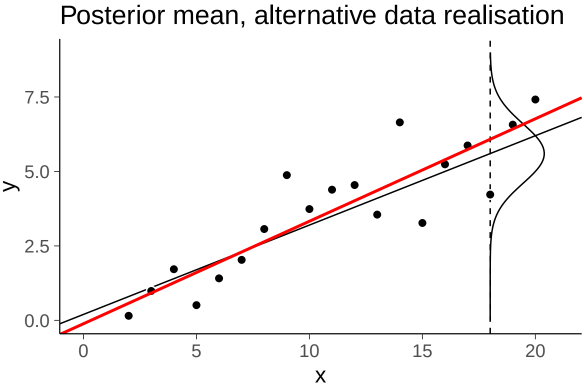

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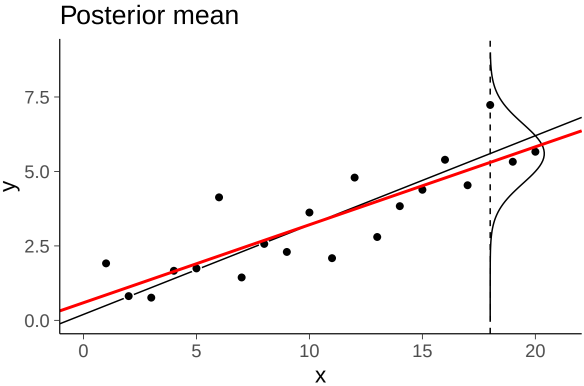

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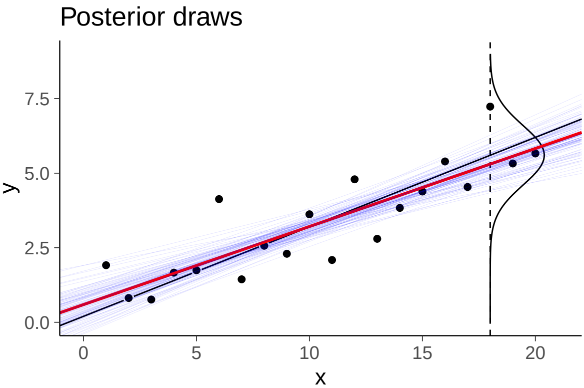
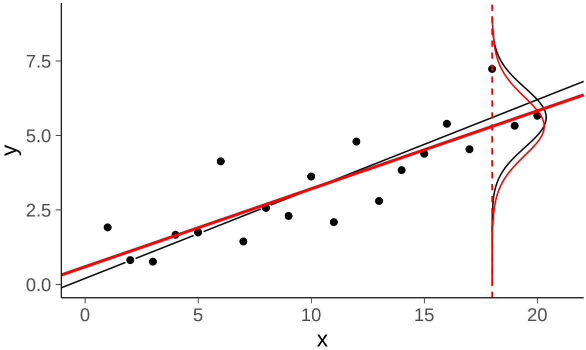


Posterior predictive distribution



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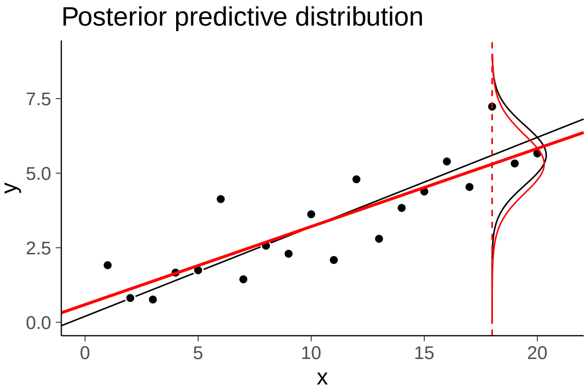
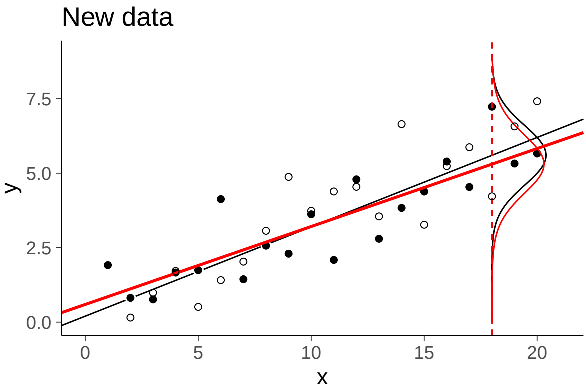
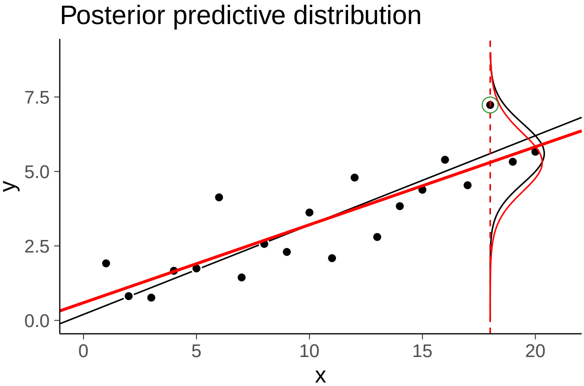


$$p(\tilde{y}|\tilde{x} = 18, x, y) = \int p(\tilde{y}|\tilde{x} = 18, \theta)p(\theta|x, y)d\theta$$


New data
y
7.5
5.0
2.5
0.0
0
5
10
15
20
x


Posterior predictive distribution
7.5
5.0
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20
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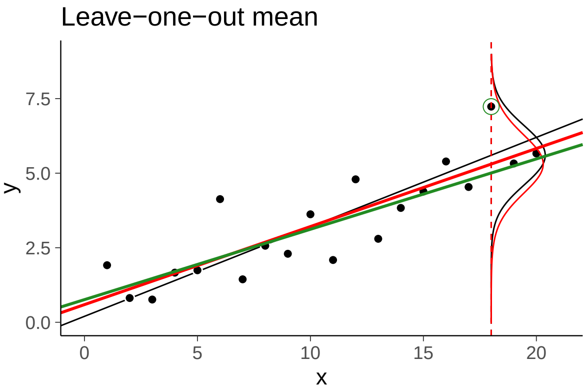

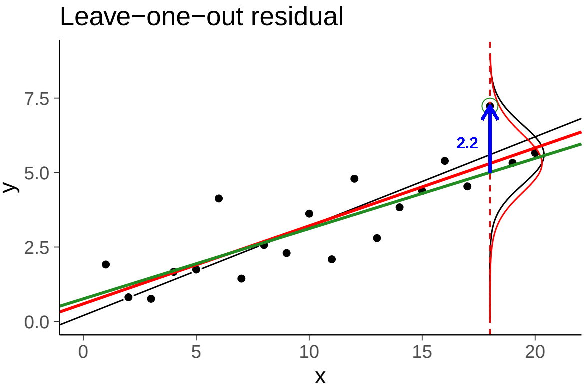
Leave−one−out residual
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x
2.2

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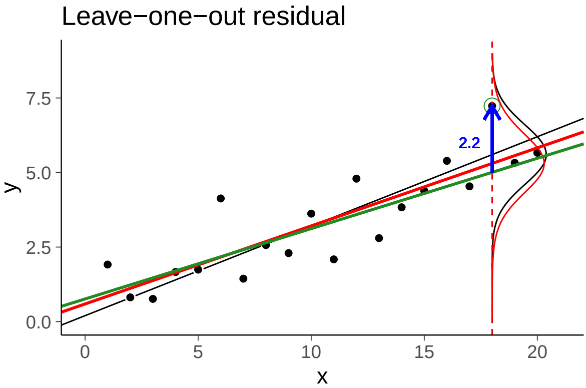
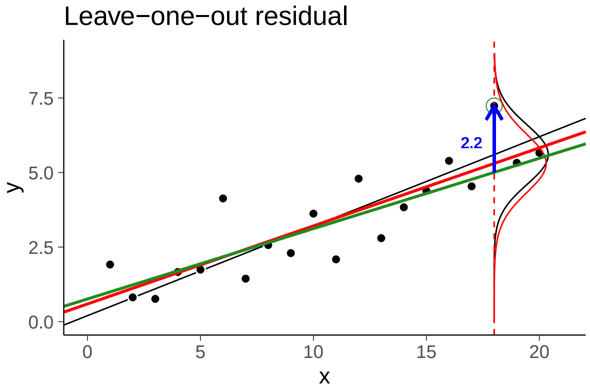
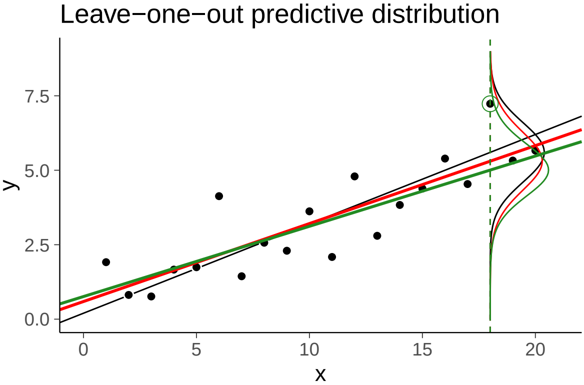


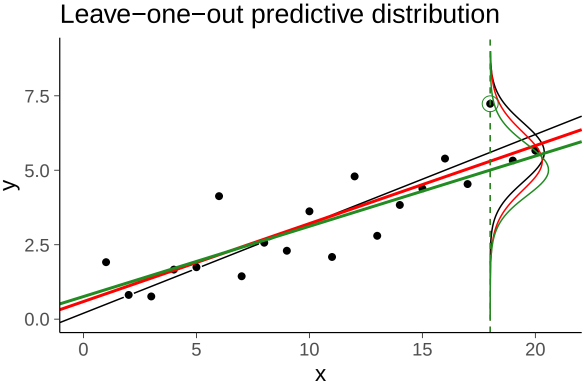
$$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$$



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

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


Leave−one−out predictive distribution
y
x
0.0
2.5
5.0
7.5
0
5
10
15
20



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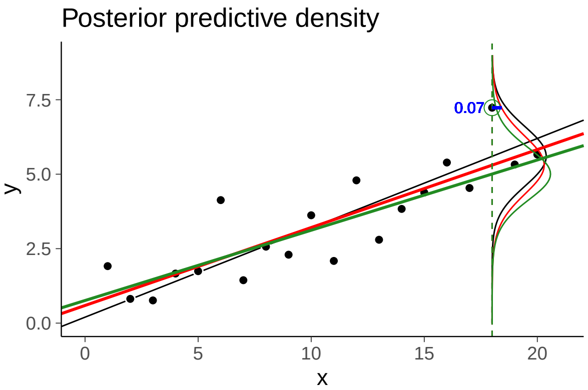
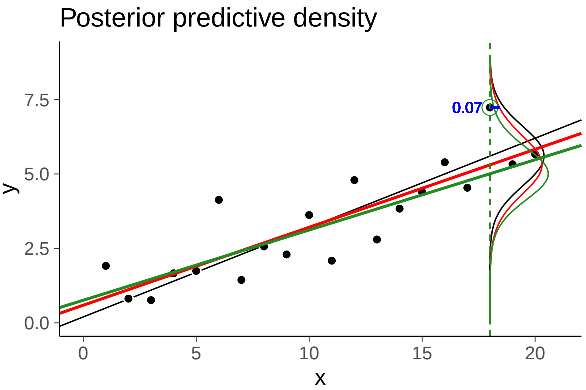

Posterior predictive density
0.07
y
x
7.5
5.0
2.5
0.0
0
5
10
15
20



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

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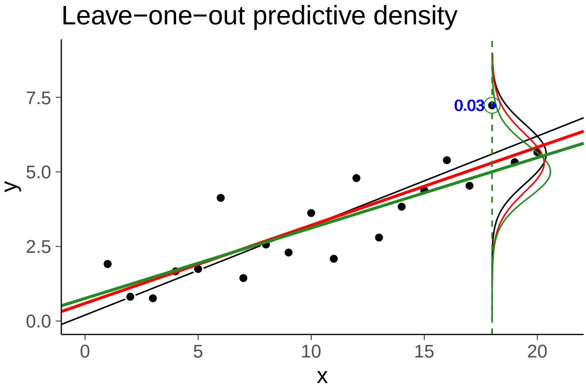
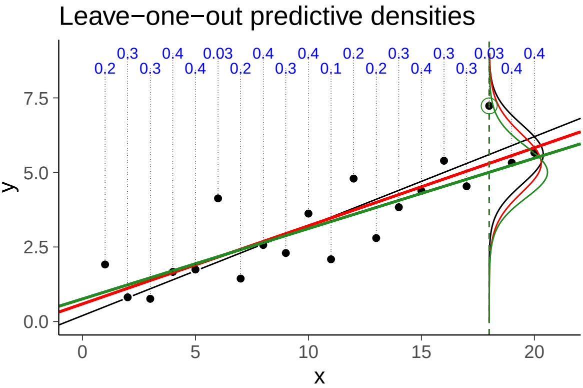
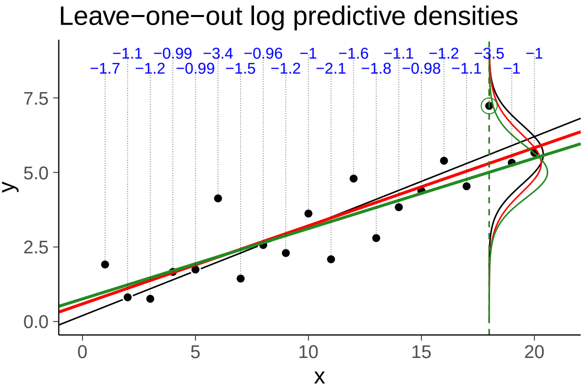


$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$$

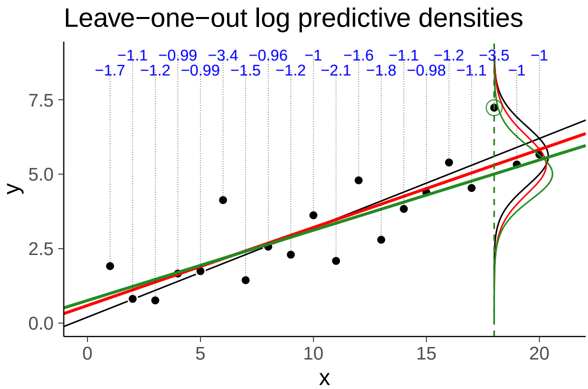
$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$$



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



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



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

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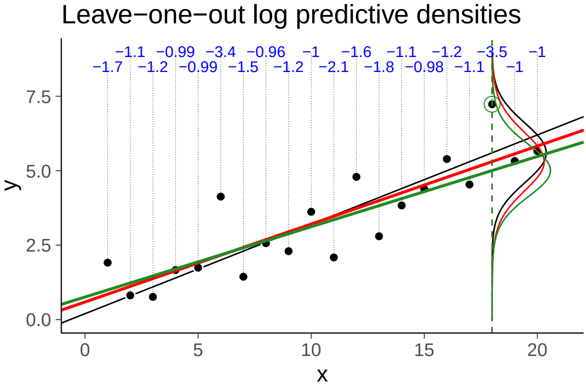
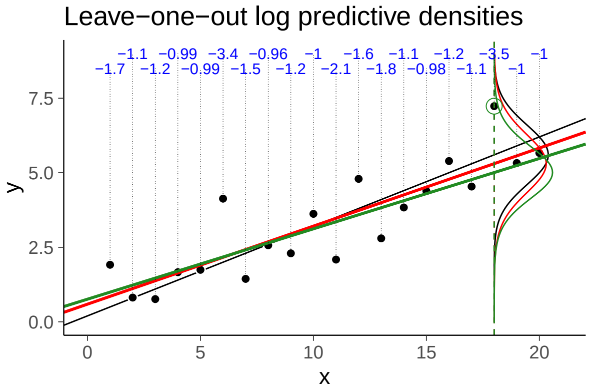


$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$



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

unbiased estimate of log posterior pred. density for new data

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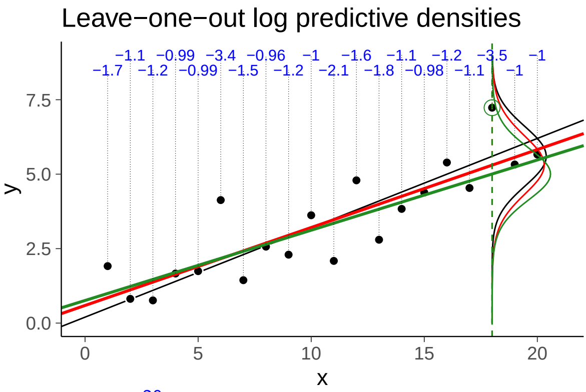
- Model assessment and selection
  - Measures of predictive accuracy
  - Model selection
- Cross-validation
  - When is LOO applicable
  - PSIS-LOO and `loo`
  - K-fold cross-validation
  - Comparison and selection
  - Additional reading
- Information criteria
- Model averaging
- Summary



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

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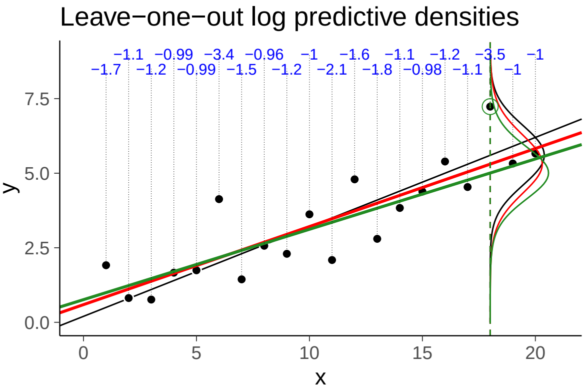
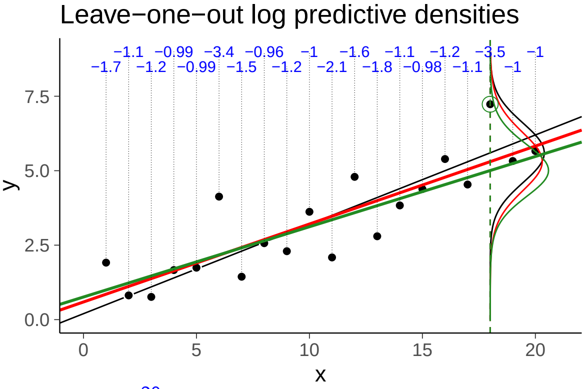


$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$$

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

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



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

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

Stan and `loo` package

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

         Estimate  SE
elpd_loo    -29.5 3.3
p_loo         2.7 1.0
------
Monte Carlo SE of elpd_loo is 0.1.

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

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

Pro and cons with LOO-CV

+ Intuitive
+ Robust
+ Good theoretical properties

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Pro and cons with LOO-CV

\+ Intuitive

\+ Robust

\+ Good theoretical properties

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

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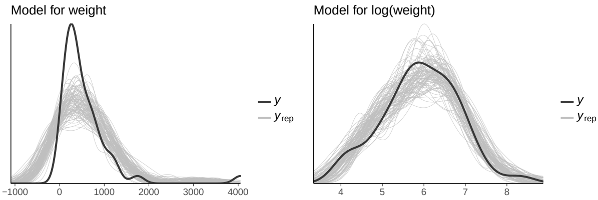
Sometimes cross-validation is not needed

- Posterior predictive checking can be sufficient



Predicting the yields of mesquite bushes.

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

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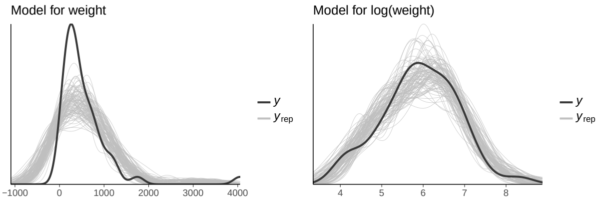

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Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 11.

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

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Subsection 1

When is LOO applicable

Summary of data generating mechanisms and prediction tasks

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

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

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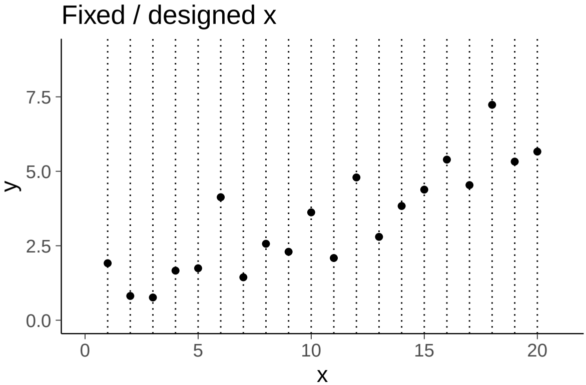
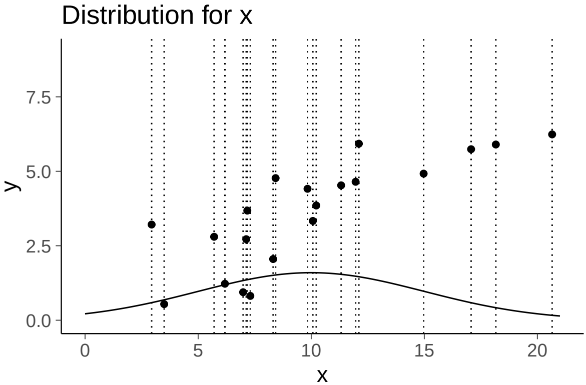


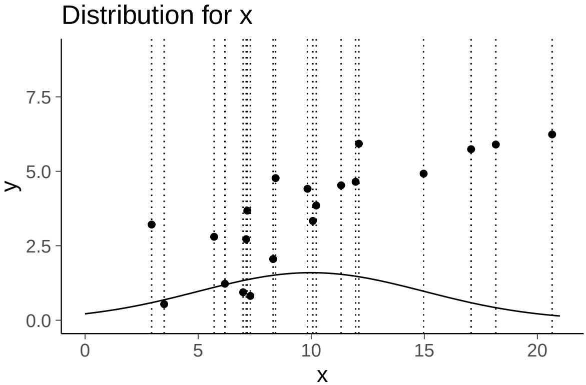
LOO is ok for fixed / designed x. SE is uncertainty about $y|x$.

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



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

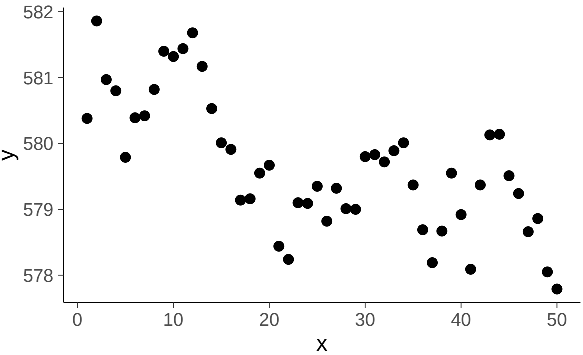
see Vehtari & Ojanen (2012) and andrewgelman.com/2018/08/03/loo-cross-validation-approaches-valid/

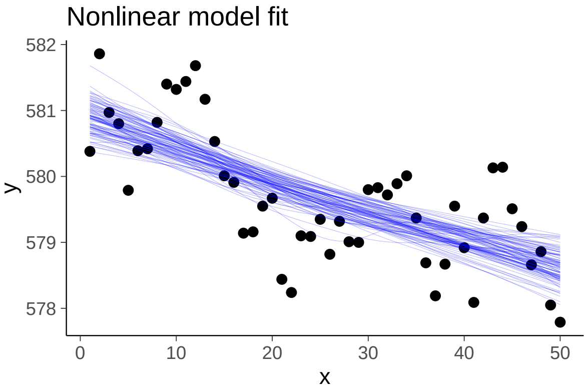


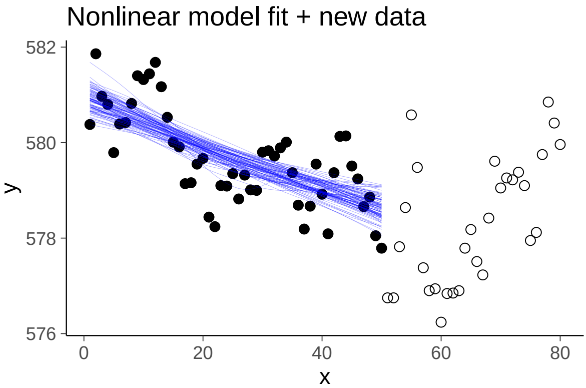
LOO is ok for random x. SE is uncertainty about $y|x$ and x.

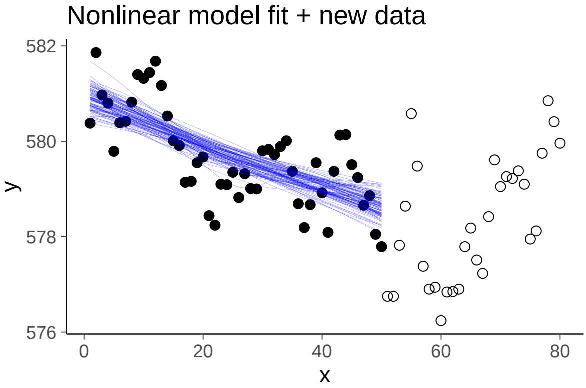
Covariate shift can be handled with importance weighting or modelling

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

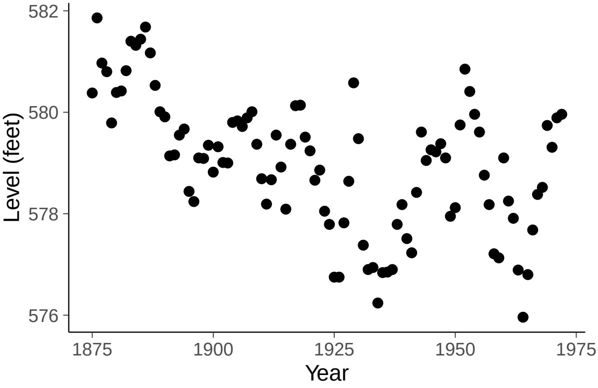

582
581
580
579
578
y
0
10
20
30
40
50
x


Nonlinear model fit
582
581
580
579
578
y
0
10
20
30
40
50
x

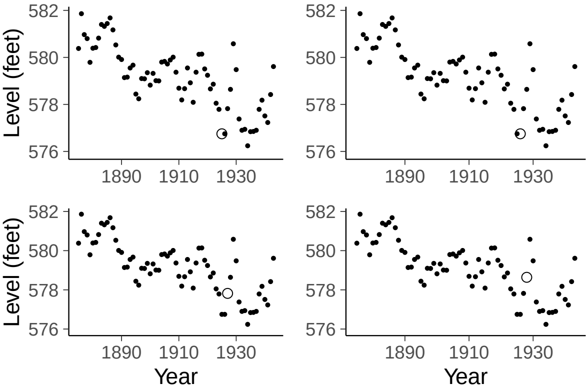

Nonlinear model fit + new data
582
580
578
576
y
0
20
40
60
80
x



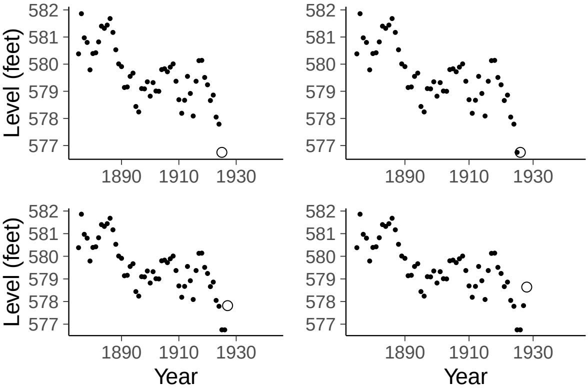
Extrapolation is more difficult



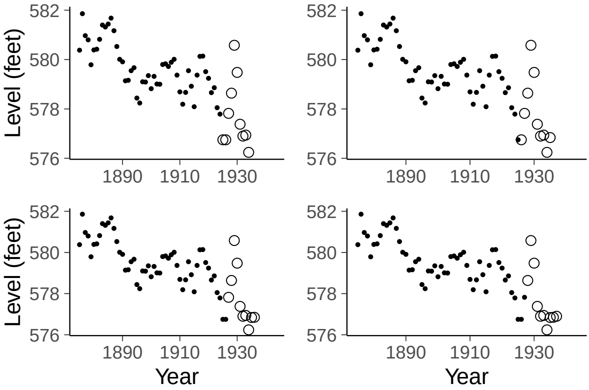
Can LOO or other cross-validation be used with time series?



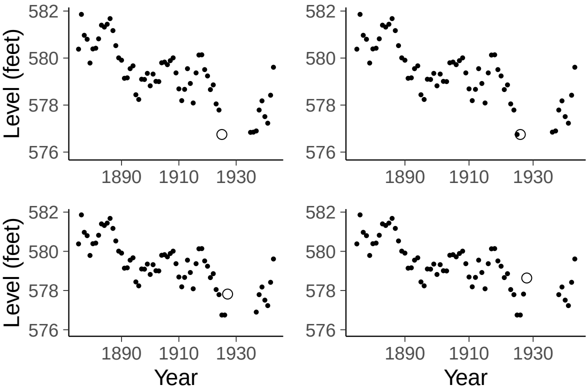
Leave-one-out cross-validation is ok for assessing conditional model



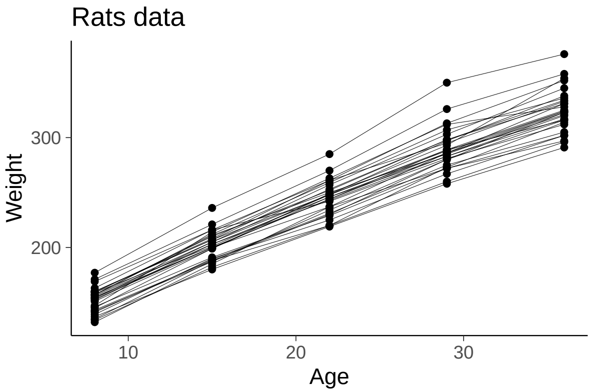
Leave-future-out cross-validation is better for predicting future



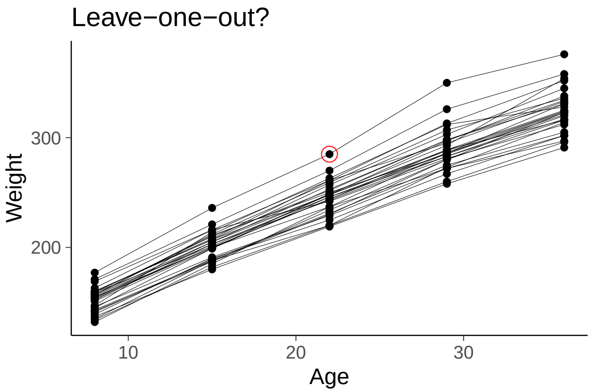
m-step-ahead cross-validation is better for predicting further future



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



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



Yes!

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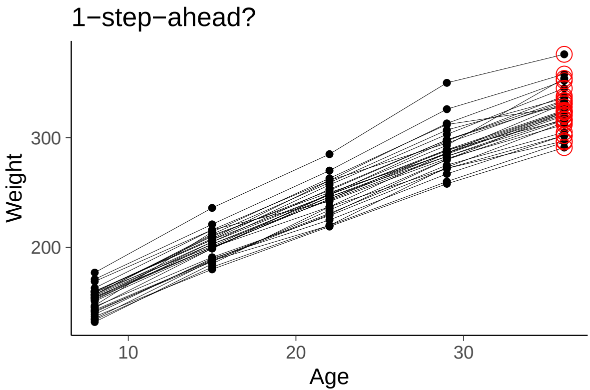
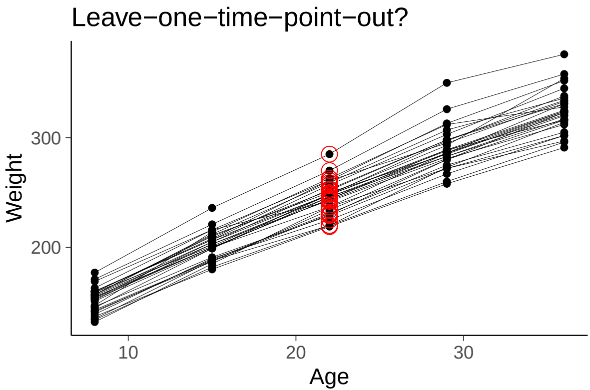
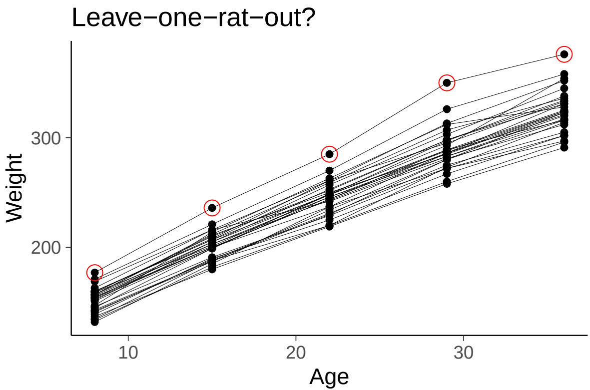


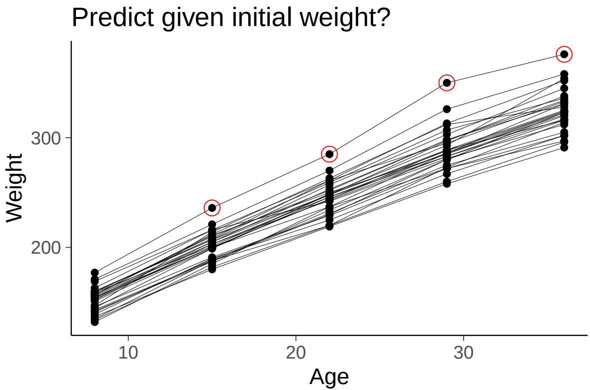
Yes!



Yes!



Yes!



Yes!

Fast cross-validation

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

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

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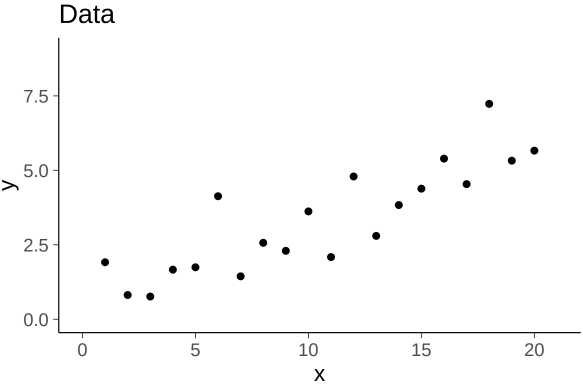
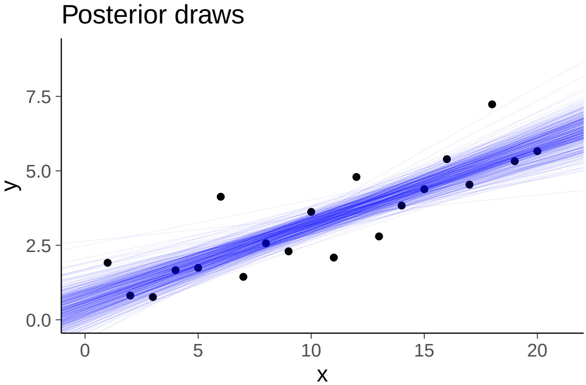
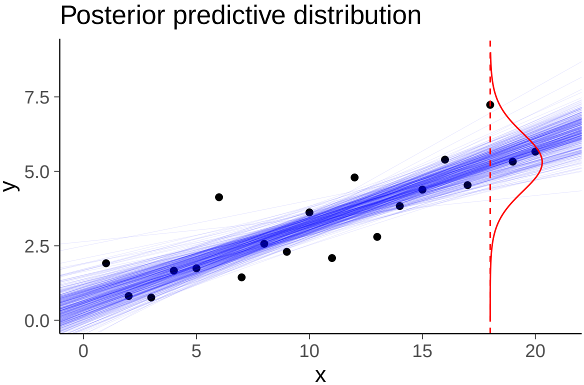
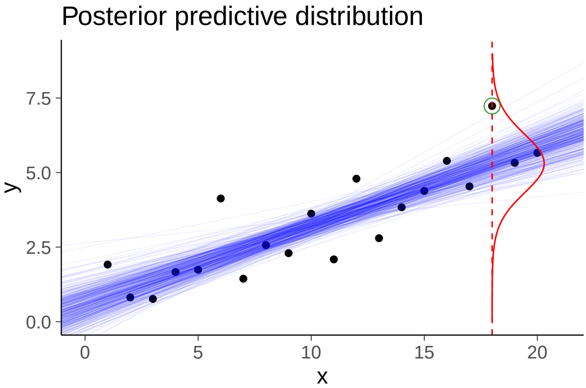




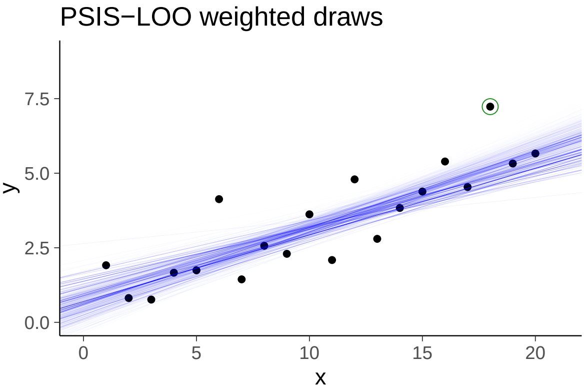
$$\theta^{(s)} \sim p(\theta|x, y)$$



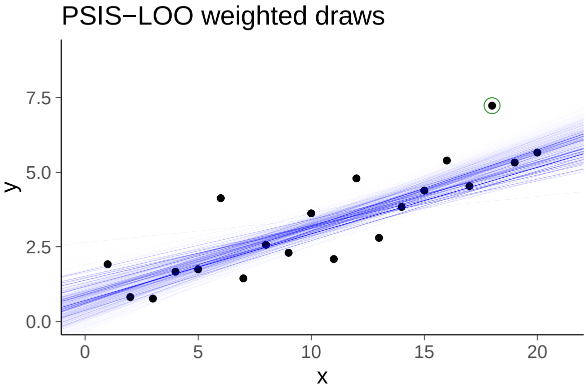
$$\theta^{(s)} \sim p(\theta|x,y), \quad p(\tilde{y}|\tilde{x},x,y) \approx \frac{1}{S}\sum_{s=1}^{S} p(\tilde{y}|\tilde{x},\theta^{(s)})$$



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

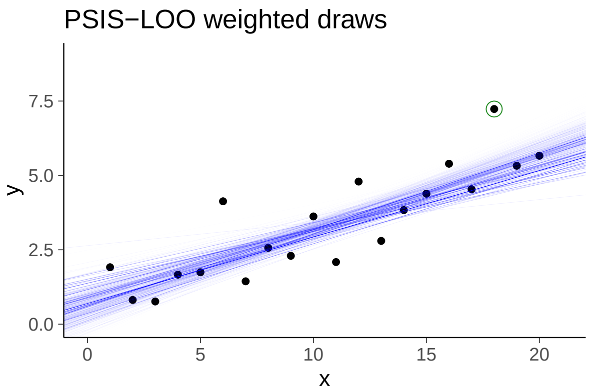


$$\theta^{(s)} \sim p(\theta|x,y)$$
$$r_i^{(s)} = p(\theta^{(s)}|x_{-i},y_{-i})/p(\theta^{(s)}|x,y)$$

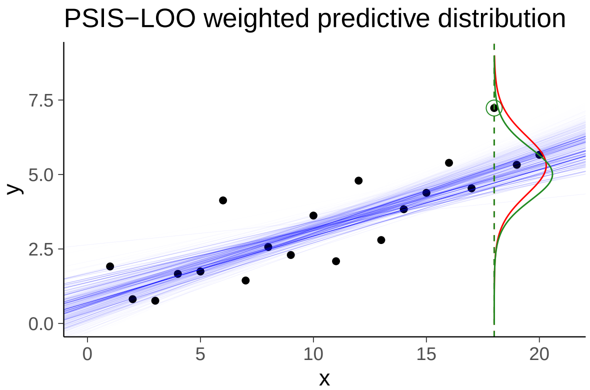


$$\theta^{(s)} \sim p(\theta|x, y)$$

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



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



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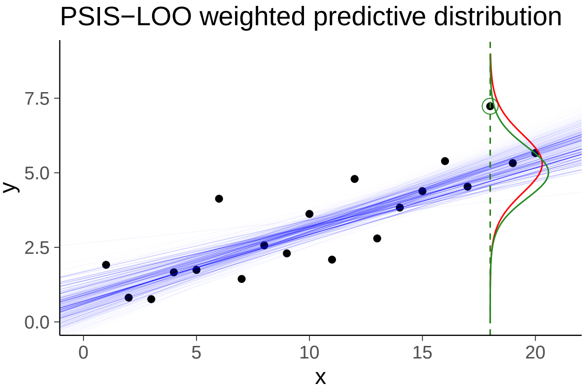
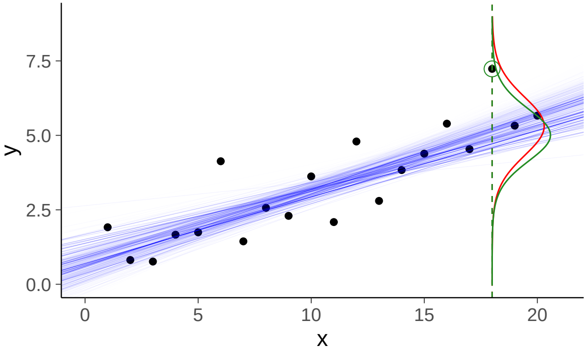


$$\theta^{(s)} \sim p(\theta|x, y)$$
$$r_i^{(s)} = p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y) \propto 1/p(y_i|x_i, \theta^{(s)})$$
$$p(y_i|x_i, x_{-i}, y_{-i}) \approx \sum_{s=1}^{S}[w_i^{(s)} p(y_i|x_i, \theta^{(s)})]$$

PSIS−LOO weighted predictive distribution

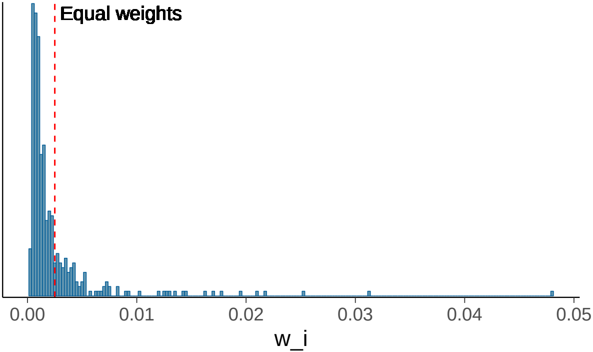


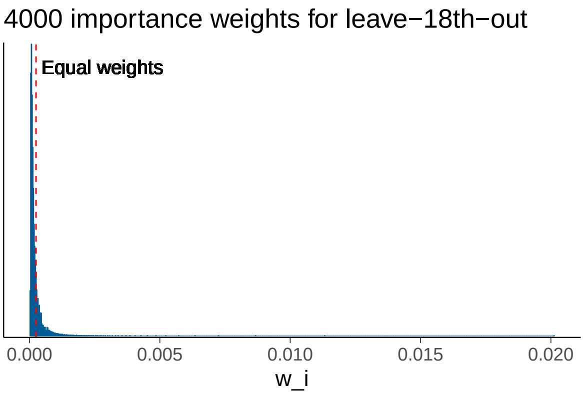
$$\theta^{(s)} \sim p(\theta|x, y)$$

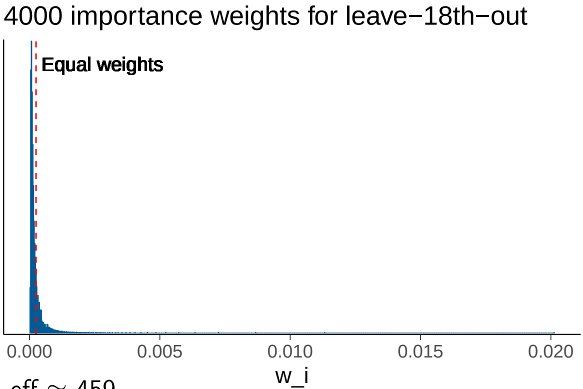
$$r_i^{(s)} = p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y) \propto 1/p(y_i|x_i, \theta^{(s)})$$

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

400 importance weights for leave−18th−out

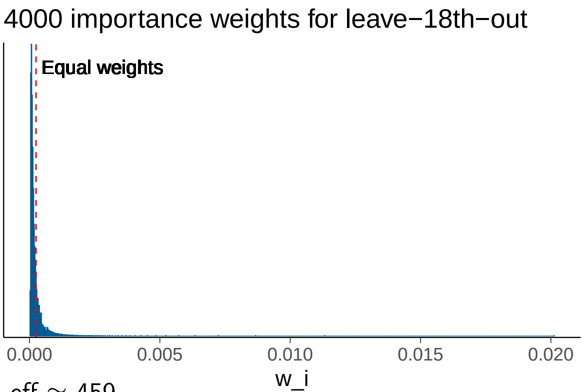



4000 importance weights for leave−18th−out
Equal weights
0.000
0.005
0.010
0.015
0.020
w_i



n_eff $\approx$ 459

see Vehtari, Gelman & Gabry (2017b)

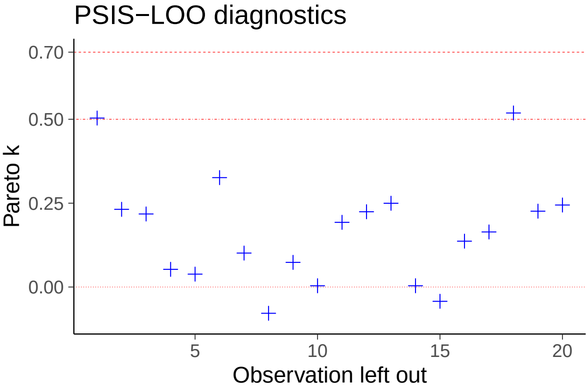


n_eff $\approx$ 459

Pareto $\hat{k} \approx 0.52$

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

see Vehtari, Gelman & Gabry (2017b)


PSIS−LOO diagnostics
0.70
0.50
0.25
0.00
Pareto k
5
10
15
20
Observation left out

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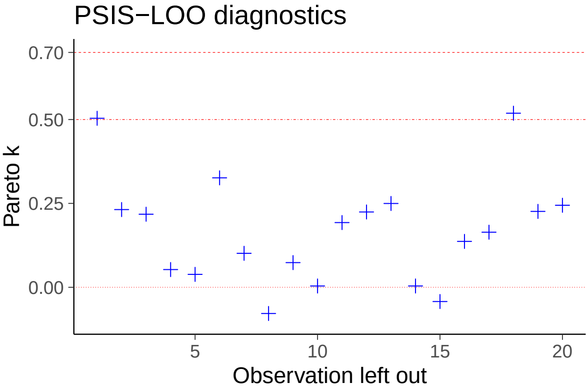
- Model assessment and selection
  - Measures of predictive accuracy
  - Model selection
- Cross-validation
  - When is LOO applicable
  - PSIS-LOO and `loo`
  - K-fold cross-validation
  - Comparison and selection
  - Additional reading
- Information criteria
- Model averaging
- Summary




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

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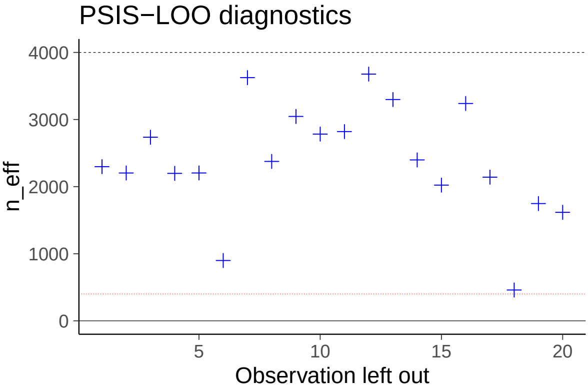


```
Pareto k diagnostic values:
                         Count  Pct.    Min. n_eff
(-Inf, 0.5]   (good)     18     90.0%   899
 (0.5, 0.7]   (ok)        2     10.0%   459
   (0.7, 1]   (bad)       0      0.0%   <NA>
   (1, Inf)   (very bad)  0      0.0%   <NA>
```

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.
```

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

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.

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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.

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

elpd_diff        se
     -0.2       0.1
```

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

Importance sampling

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

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

where w_i^s are importance weights and

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

Importance sampling

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

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

where w_i^s are importance weights and

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

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

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

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Stan code

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

Stan code

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

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

Pareto smoothed importance sampling LOO

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

Pareto smoothed importance sampling LOO

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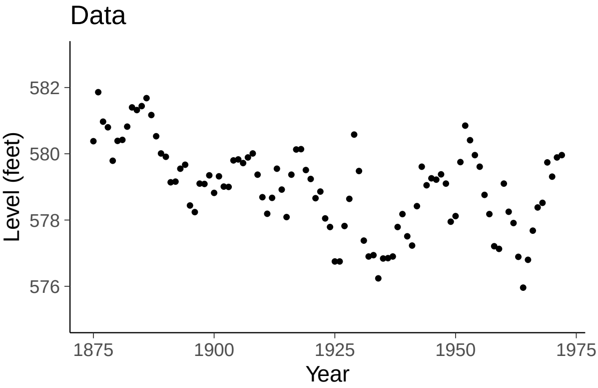
   1.1 leave-one-group out is challenging for PSIS-LOO
       see Merkel, Furr and Rabe-Hesketh (2018) for an approach using quadrature integration
2. PSIS-LOO for non-factorizable models
   2.1 `mc-stan.org/loo/articles/loo2-non-factorizable.html`

Pareto smoothed importance sampling LOO

1. PSIS-LOO for hierarchical models
   1.1 leave-one-group out is challenging for PSIS-LOO
   see Merkel, Furr and Rabe-Hesketh (2018) for an approach using quadrature integration
2. PSIS-LOO for non-factorizable models
   2.1 mc-stan.org/loo/articles/loo2-non-factorizable.html
3. PSIS-LOO for time series
   3.1 Approximate leave-future-out cross-validation
   mc-stan.org/loo/articles/loo2-lfo.html

PSIS-LOO for time series



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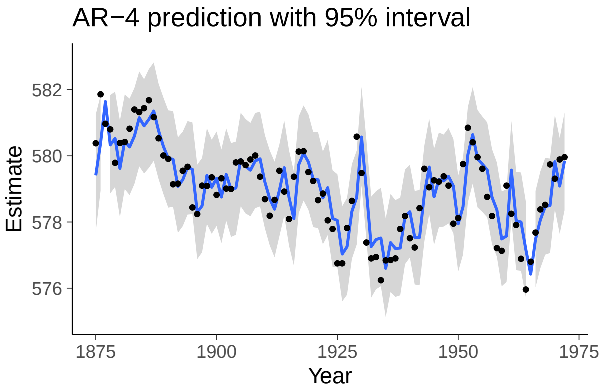
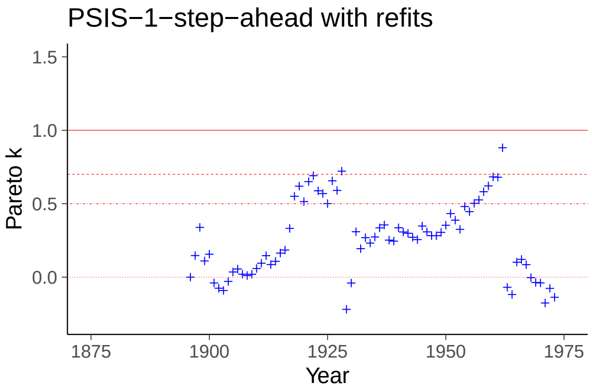
PSIS-LOO for time series



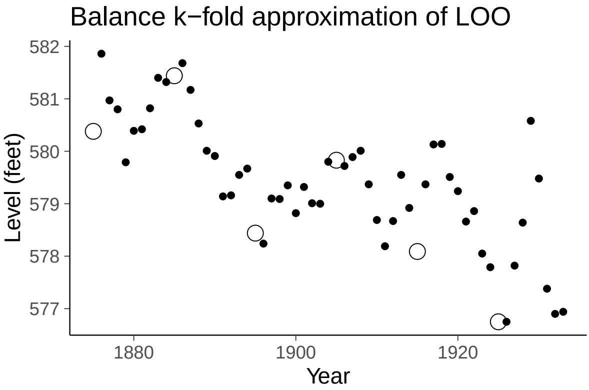
PSIS-LOO for time series

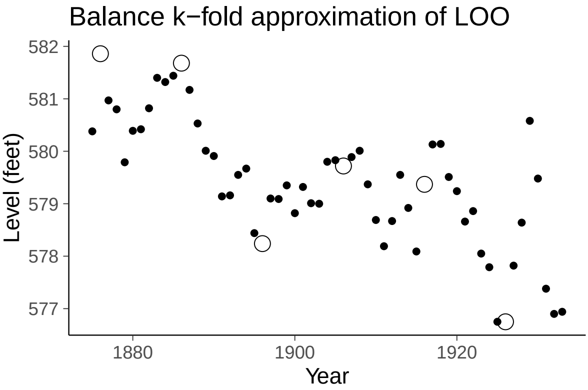


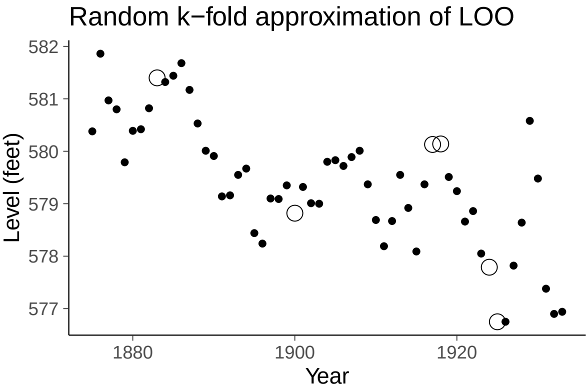
mc-stan.org/loo/articles/loo2-lfo.html

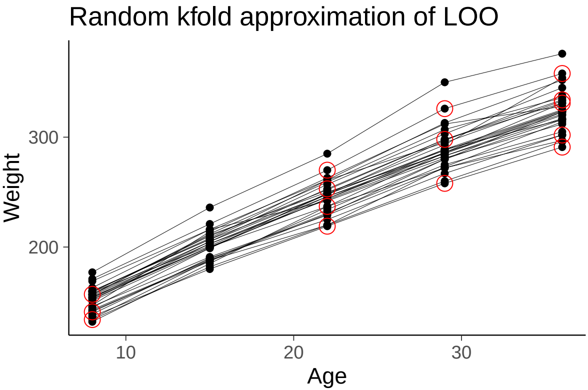
K-fold cross-validation

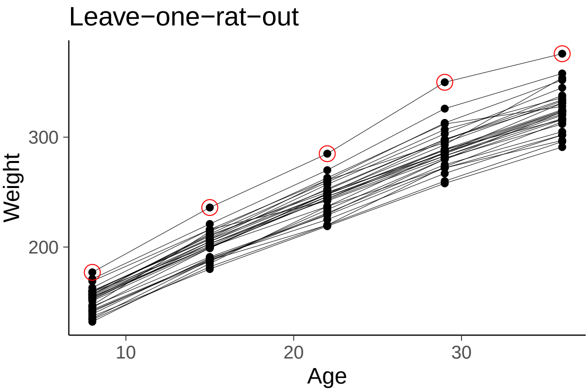
1. K-fold cross-validation can approximate LOO
   1.1 all uses for LOO
2. K-fold cross-validation can be used for hierarchical models
   2.1 good for leave-one-group-out
3. K-fold cross-validation can be used for time series
   3.1 with leave-block-out

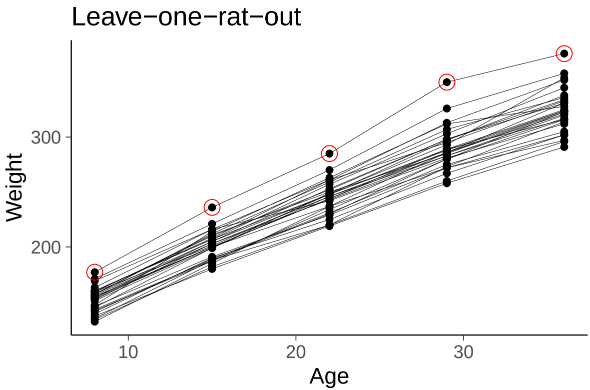

Balance k−fold approximation of LOO
Level (feet)
582
581
580
579
578
577
1880
1900
1920
Year


Balance k−fold approximation of LOO
Level (feet)
582
581
580
579
578
577
1880
1900
1920
Year


Random k−fold approximation of LOO
582
581
580
579
578
577
Level (feet)
1880
1900
1920
Year


Random kfold approximation of LOO
Weight
300
200
10
20
30
Age


Leave−one−rat−out
Weight
300
200
10
20
30
Age



kfold_split_random()

kfold_split_balanced()

kfold_split_stratified()

Cross-validation for model assessment

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

Cross-validation for model assessment

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

see demos `avehtari.github.io/modelselection/`

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Model comparison

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

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

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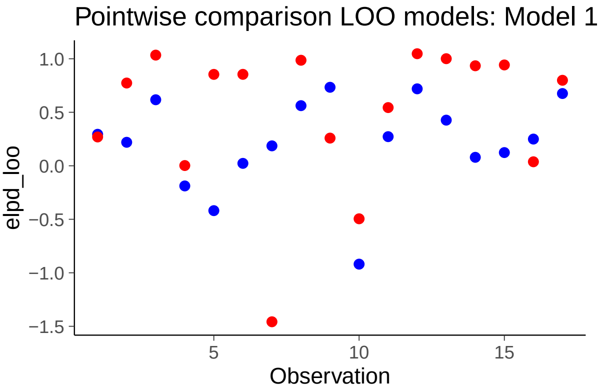
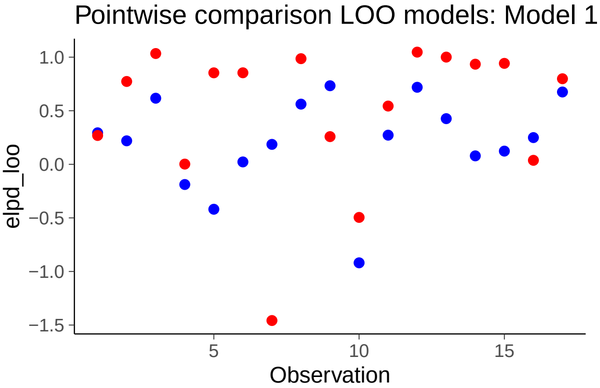
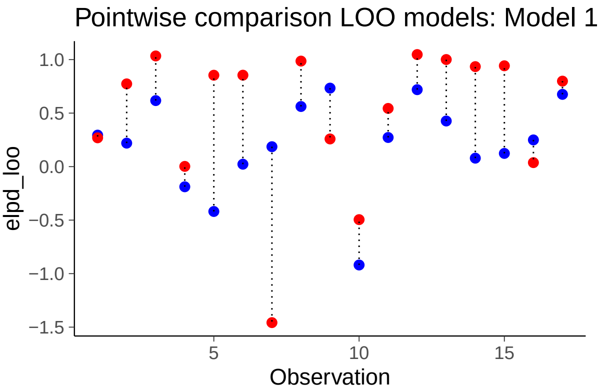




Model 1 elpd_loo $\approx$ 3.7, SE=1.8
Model 2 elpd_loo $\approx$ 8.4, SE=2.8



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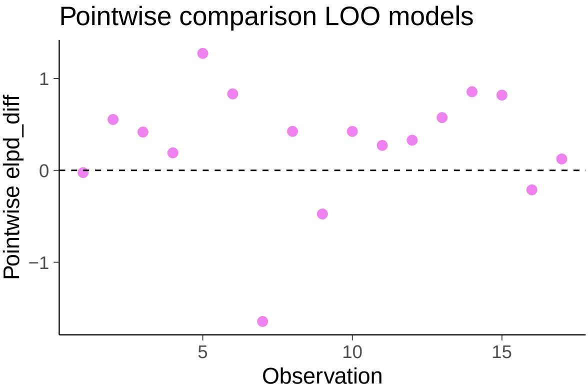


```
Model comparison:
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff        se
      4.7       2.7
```

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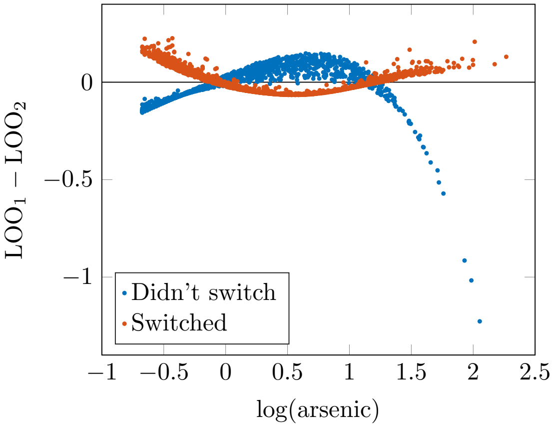
Arsenic well example – Model comparison



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

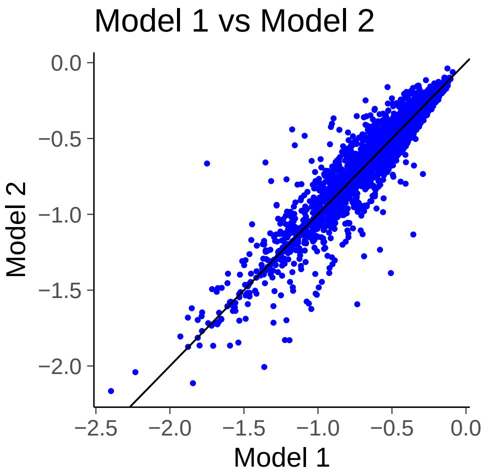
see Vehtari, Gelman & Gabry (2017a)

Arsenic well example – Model comparison

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

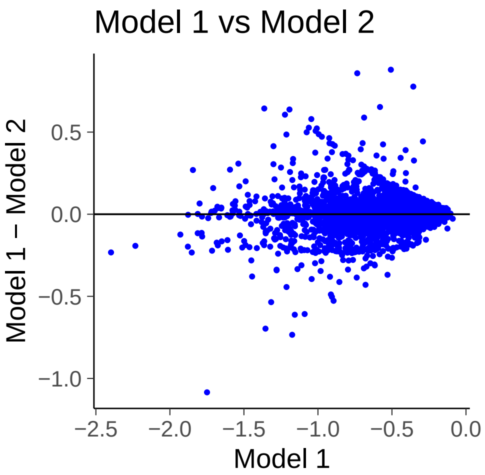
Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 13.

Arsenic well example – Model comparison



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

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)

Arsenic well example – Model comparison

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> loo_compare(model1, model2)
       elpd_diff  se_diff
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`se_diff` and normal approximation for the uncertainty in the difference is good only if models are well specified and the number of observations is relatively big (more details in a forthcoming article).

What if one is not clearly better than others?

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1. Continuous expansion including all models?
   1.1 and then analyse the posterior distribution directly
   avehtari.github.io/modelselection/betablockers.html
   1.2 sparse priors like regularized horseshoe prior instead of variable selection
   video, refs and demos at
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   2.1 selection process leads to overfitting
3. Overfitting in selection process is not unique for cross-validation

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Selection induced bias and overfitting

- Selection induced bias in cross-validation
  - same data is used to assess the performance and make the selection
  - the selected model fits more to the data
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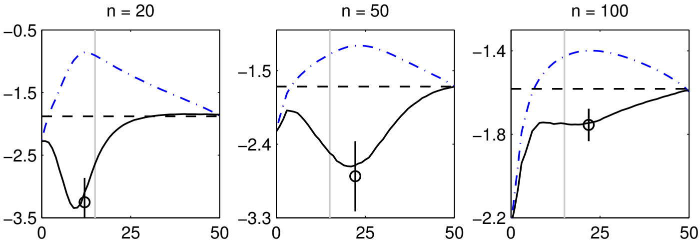
- Performance of the selection process itself can be assessed using two level cross-validation, but it does not help choosing better models
- Bigger problem if there is a large number of models as in covariate selection

Selection induced bias in variable selection



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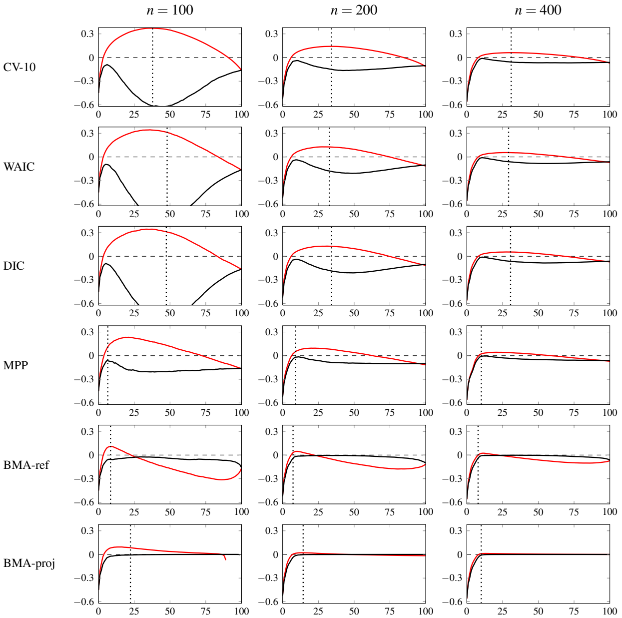

Section 3

Information criteria

WAIC vs PSIS-LOO

see Vehtari, Gelman & Gabry (2017a)

WAIC vs PSIS-LOO

1. WAIC has same assumptions as LOO

see Vehtari, Gelman & Gabry (2017a)

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

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4. LOO makes the prediction assumption more clear, which helps if K-fold-CV is needed instead
5. Multiplying by -2 doesn't give any benefit (Watanabe didn't multiply by -2)

see Vehtari, Gelman & Gabry (2017a)

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*IC

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

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Section 4

Model averaging

Section 5

Summary

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Take-home messages

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

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