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Bayesian Statistics and Data Analysis
Lecture 8b

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Thanks to Aki Vehtari, Aalto University

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

Goal of model evaluation

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

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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

Model choice utility

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

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

Subsection 1

Measures of predictive accuracy

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

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- But how do we evaluate the posterior predictive distribution?

Probabilistic predictions: Scoring rules

- Scoring rules: *How well does the predictive distribution align with observation?*

$$S(F, y),$$

where $S(F, y) \in \mathbb{R}$, F is a density, and y is an observation.

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- Proper scoring rules: $S(F, y)$ is minimized when the forecasted distribution matches the (true) distribution of the observation

$$\mathbb{E}_{y \sim p_{true}}[S(p_{true}, y)] \leq \mathbb{E}_{y \sim p_{true}}[S(F, y)],$$

  where p_{true} is the true data generating process.

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$$\mathbb{E}_{y \sim p_{true}}[S(p_{true}, y)] \leq \mathbb{E}_{y \sim p_{true}}[S(F, y)],$$

  where p_{true} is the true data generating process.
- Local scoring rules: $S(p_{true}, y_i)$ only depend on the actual observation y_i

Probabilistic predictions

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

$$S(p(\tilde{y}|y), y_i) = \log p(y_i|y)$$

Probabilistic predictions

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

$$S(p(\tilde{y}|y), y_i) = \log p(y_i|y)$$

- 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

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

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

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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*):

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

  where $\tilde{y}$ is an unseen observation generated from the true data generating process $p_{\mathrm{true}}(\tilde{y})$, 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)

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

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

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- Analogy: Monte Carlo approximation using our data: $y \sim p_{\text{true}}(\tilde{y})$

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- Analogy: Monte Carlo approximation using our data: $y \sim p_{\text{true}}(\tilde{y})$
- The elpd, lpd and efficient number of parameters (p_{loo})

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

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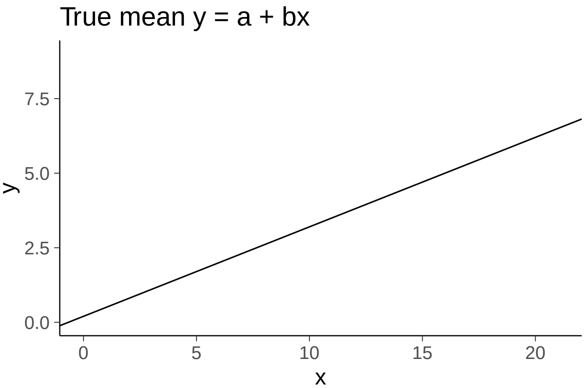
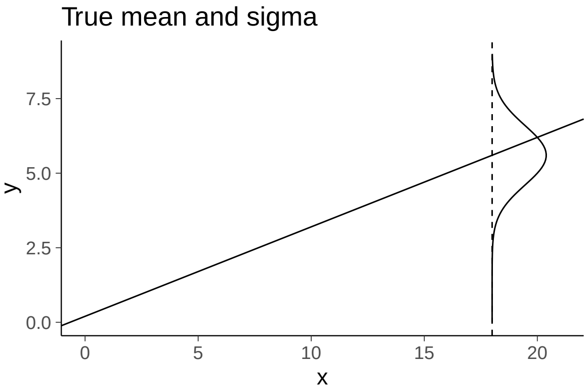
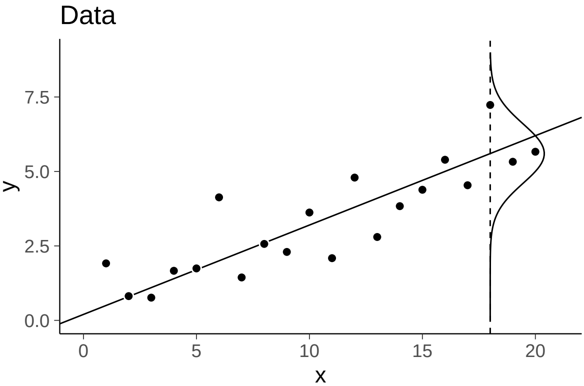
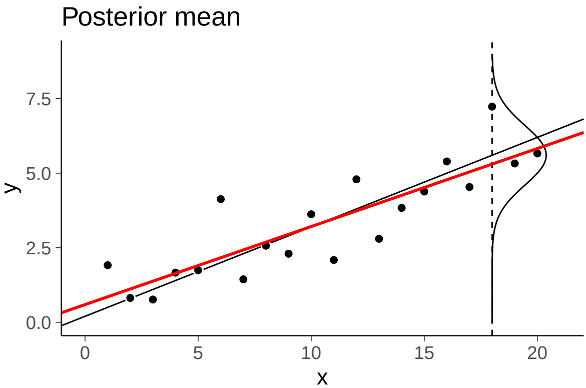
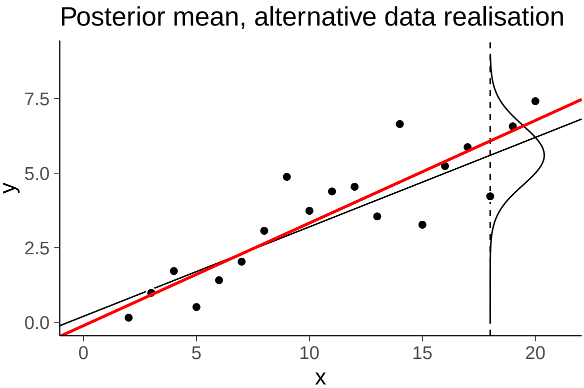



True mean and sigma
y
7.5
5.0
2.5
0.0
0
5
10
15
20
x


Data
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x


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


Posterior mean, alternative data realisation
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

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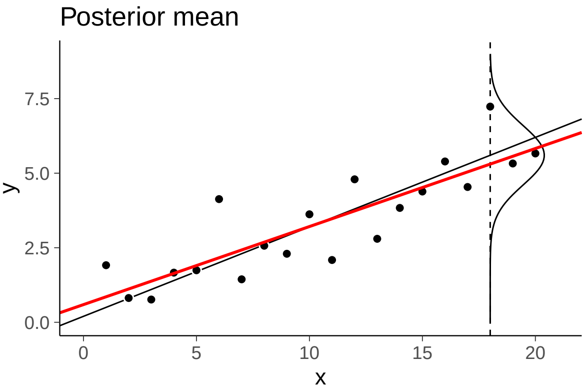
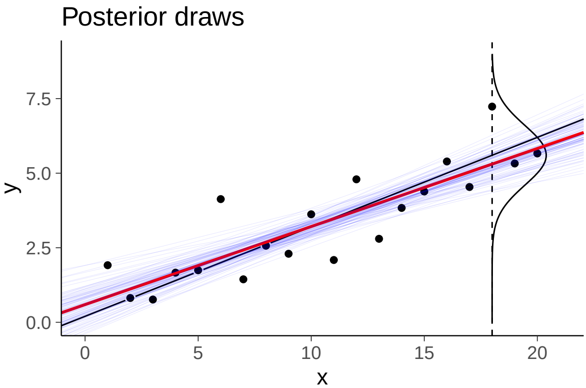
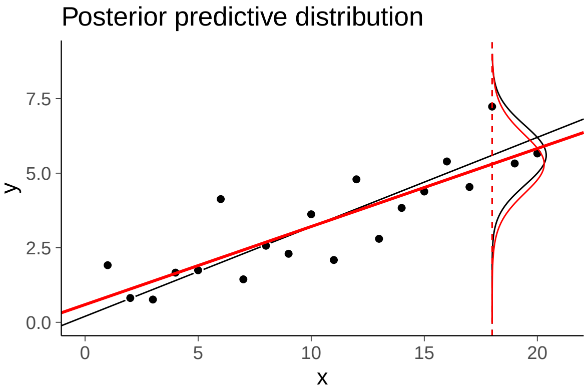



Posterior draws
y
7.5
5.0
2.5
0.0
x
0
5
10
15
20


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

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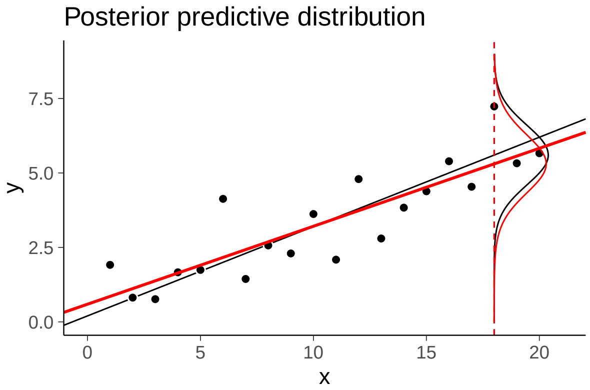

$$p(\tilde{y}|\tilde{x} = 18, x, y) = \int p(\tilde{y}|\tilde{x} = 18, \theta)p(\theta|x, y)d\theta$$

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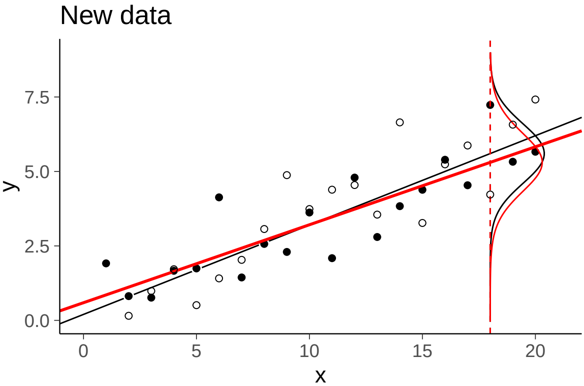
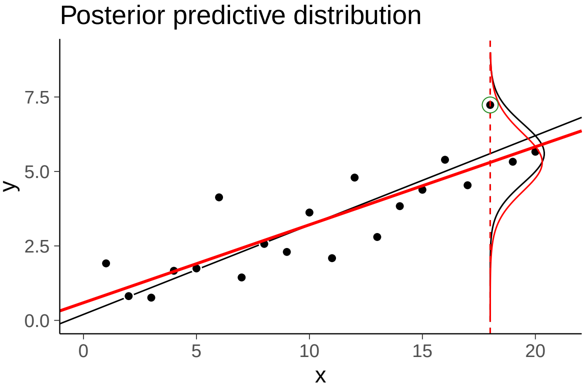
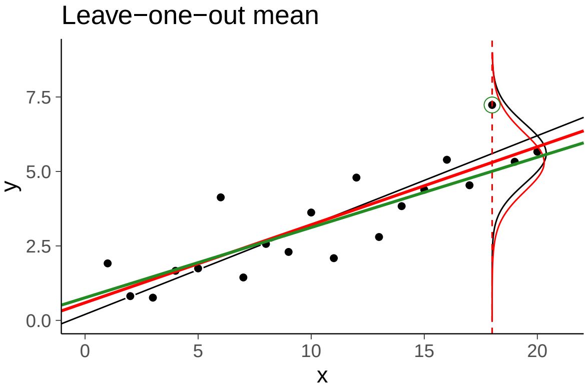
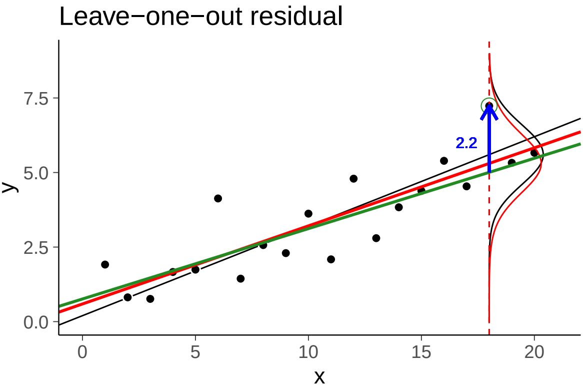
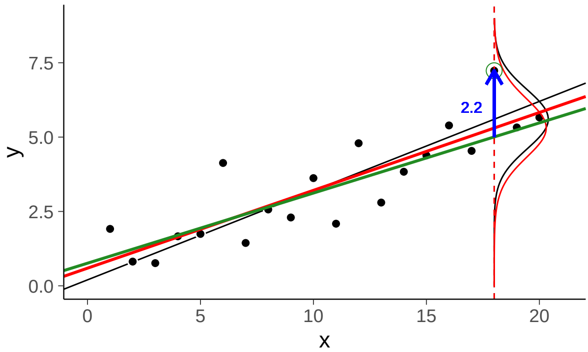



Posterior predictive distribution
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

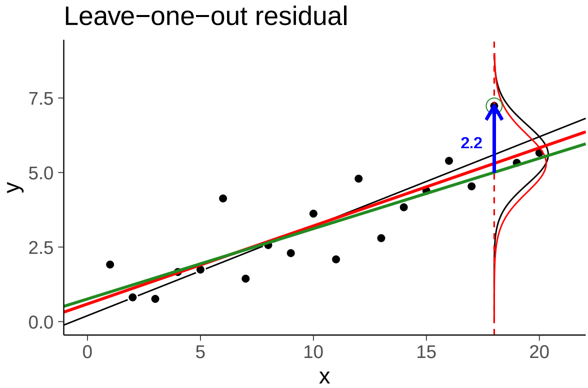

Leave−one−out mean
y
x
0.0
2.5
5.0
7.5
0
5
10
15
20


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

Leave−one−out residual

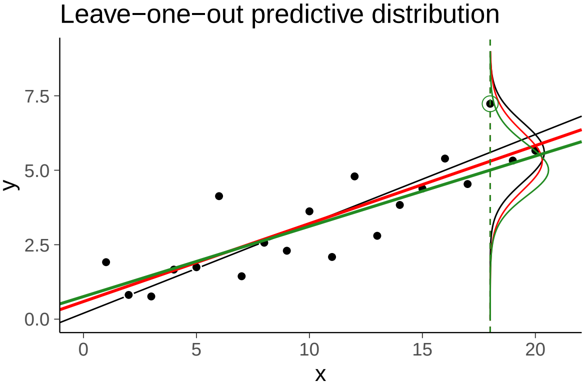


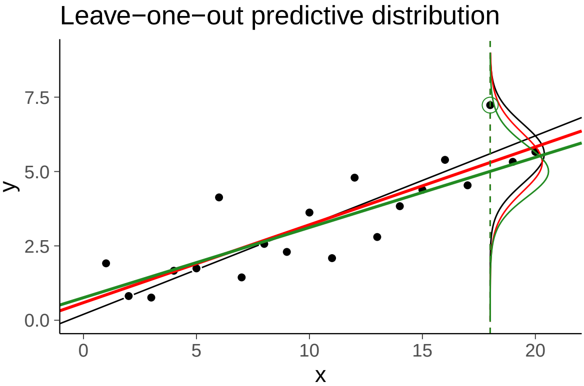
$$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$$



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

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


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



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

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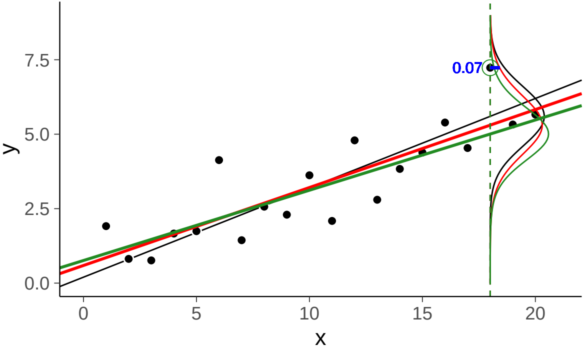
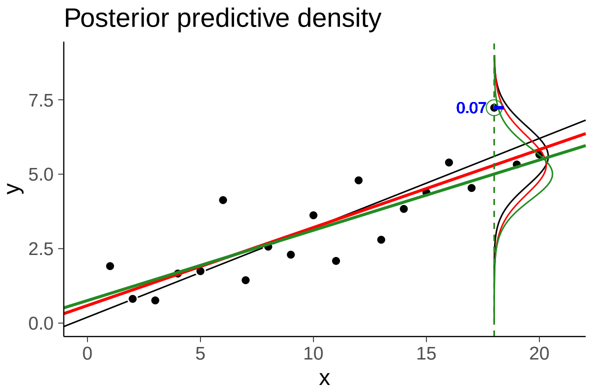
Posterior predictive density





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

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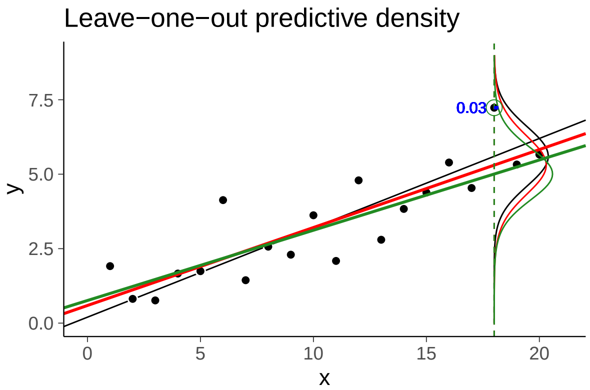
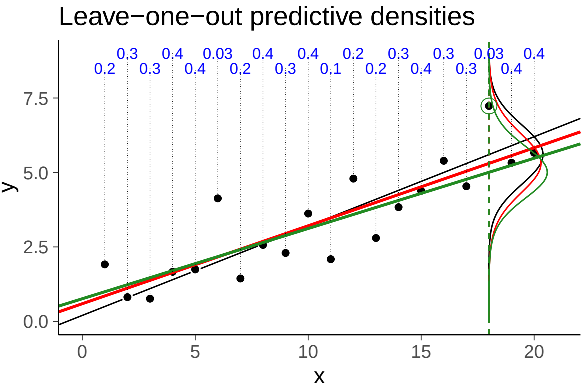


$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$

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



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

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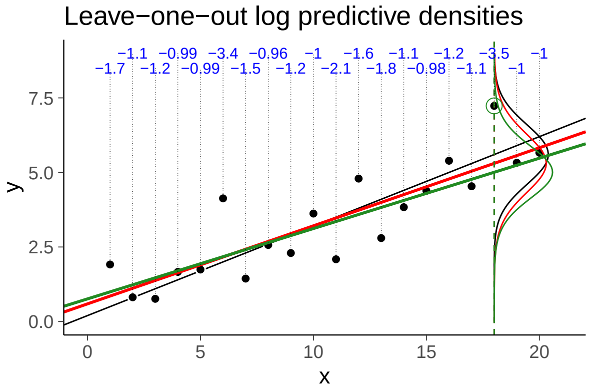
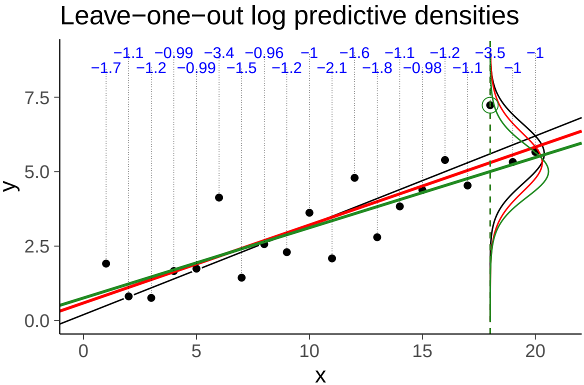


$$\log p(y_i | x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$$



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

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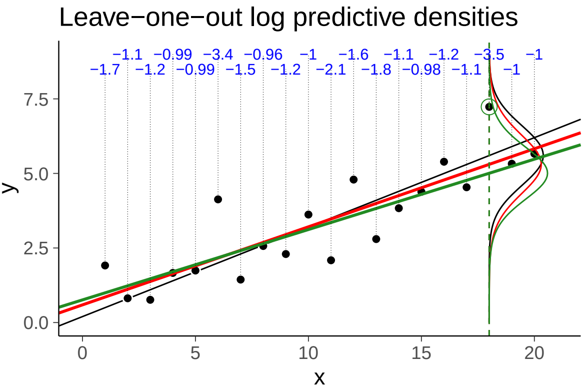

$$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$$

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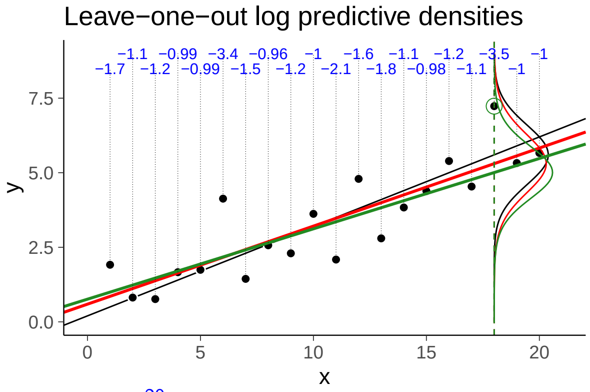

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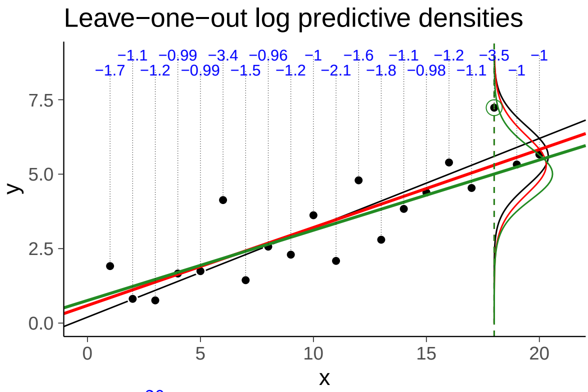
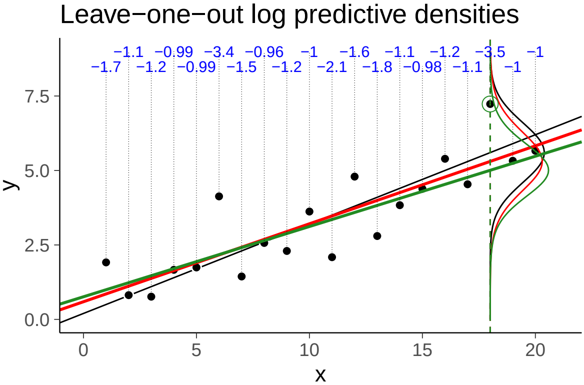
unbiased estimate of log posterior pred. density for new data



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

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



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

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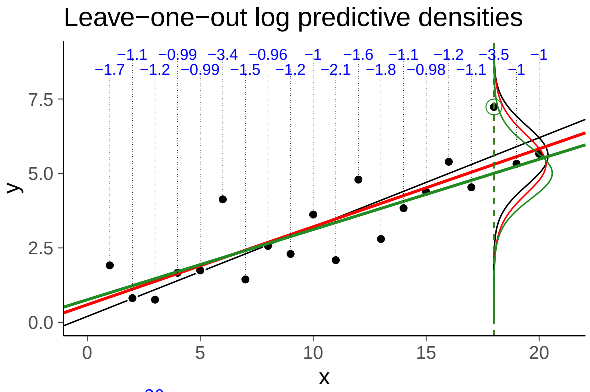

$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

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

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.
```

Subsection 1

When is LOO applicable

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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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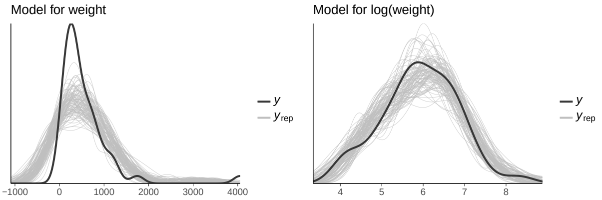
Sometimes cross-validation is not needed

- Posterior predictive checking can be sufficient



Predicting the yields of mesquite bushes.

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

Sometimes cross-validation is not needed

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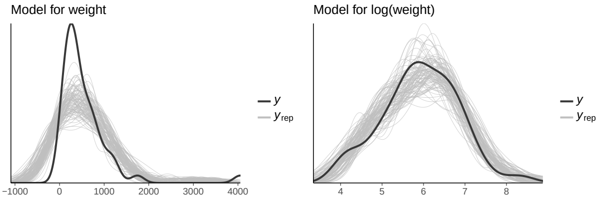


Predicting the yields of mesquite bushes.
Gelman, Hill & Vehtari (2020, Ch. 11)

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

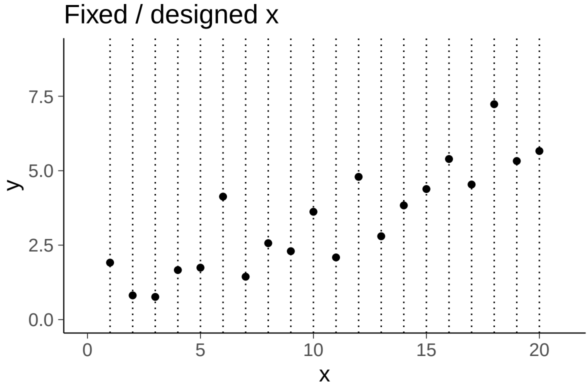
Data generating mechanisms and prediction tasks

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

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

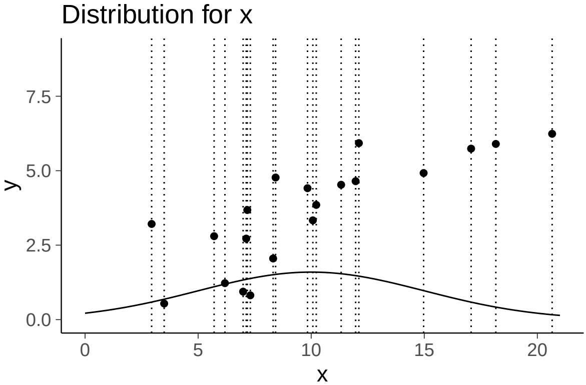
2. Use the knowledge of the prediction task if available
3. Cross-validation can be used to analyse different parts, even if there is no clear prediction task

x in p_{true}



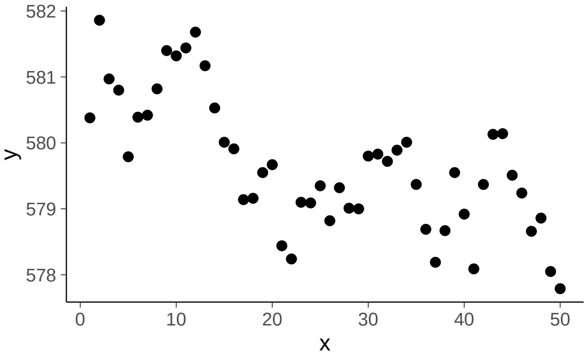
LOO is ok for fixed / designed x: $p_{\text{true}}(y|x)$

x in p_{true}

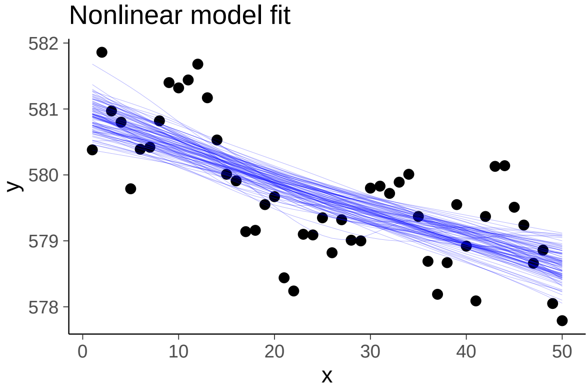


LOO is ok for random x. $p_{\text{true}}(y, x)$

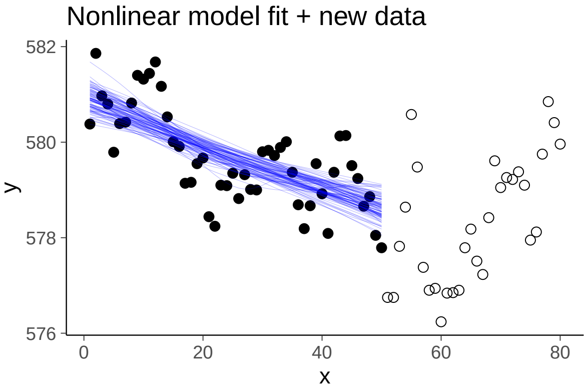
p_{true} extrapolation



p_{true} extrapolation

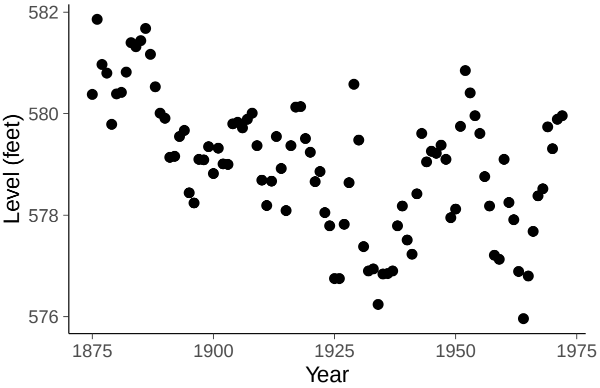


p_{true} extrapolation



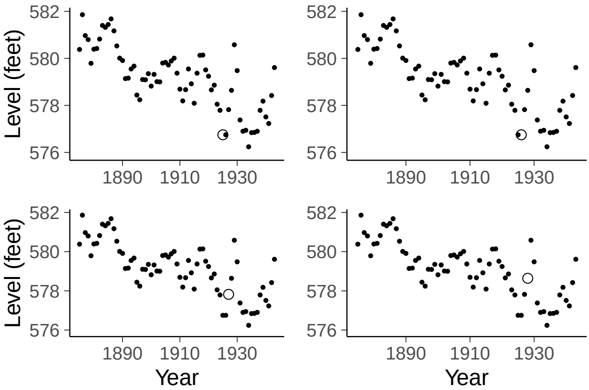
Extrapolation is more difficult

LOO for time series data



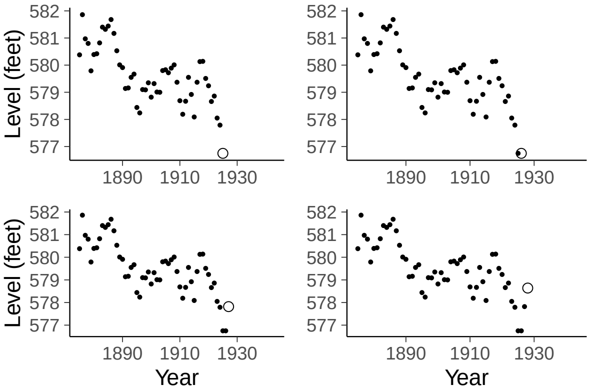
p_{true} for time series?

LOO for time series



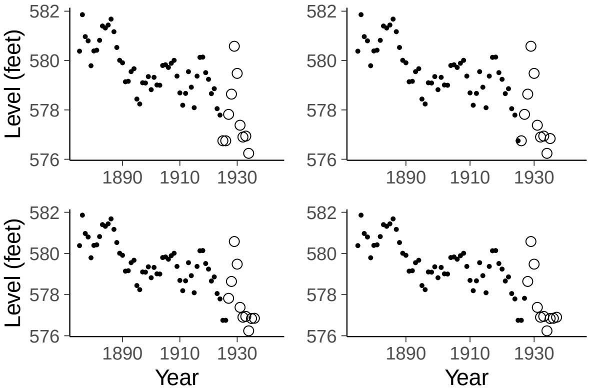
Leave-one-out cross-validation is ok for assessing conditional model

LOO for time series



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

LOO for time series



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

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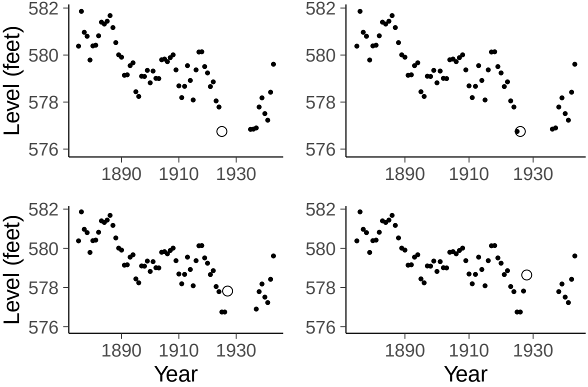
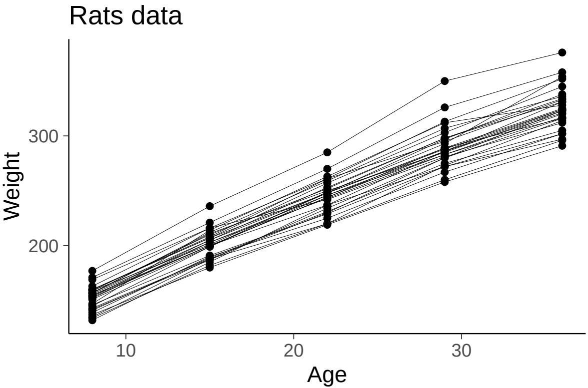
LOO for time series



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

LOO for hiearchical data



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

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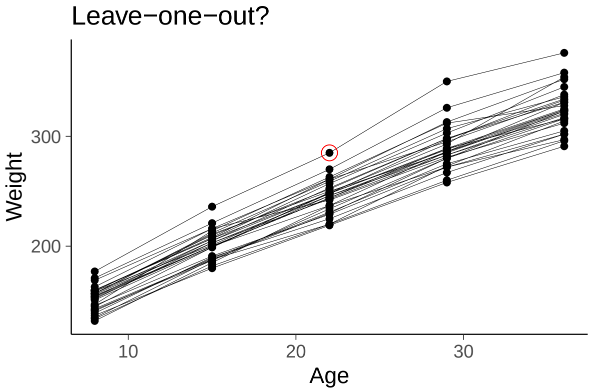
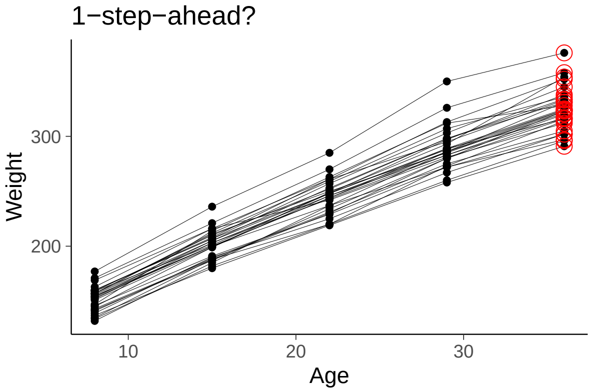
LOO for hiearchical data



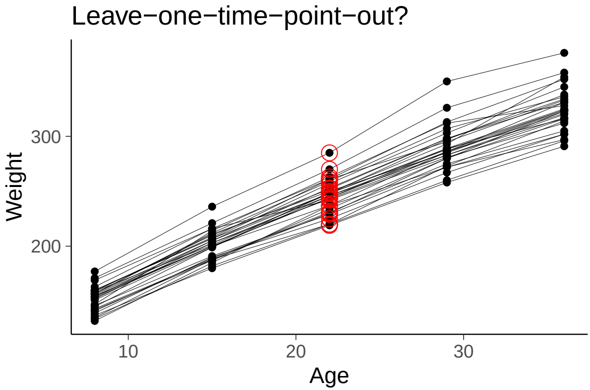
Yes!

LOO for hiearchical data



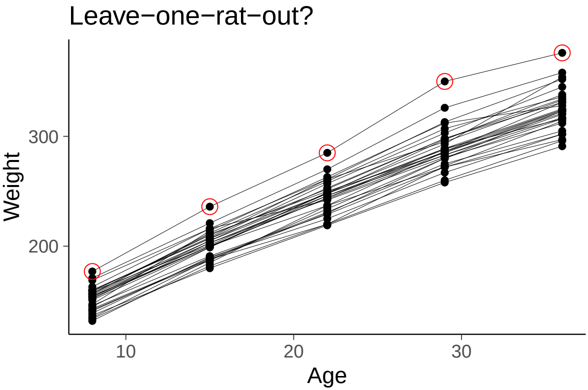
Yes!

LOO for hiearchical data



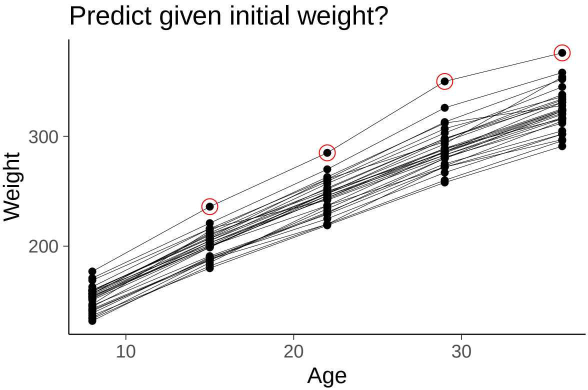
Yes!

LOO for hiearchical data



Yes!

LOO for hiearchical data



Yes!

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Fast cross-validation

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

Fast cross-validation

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

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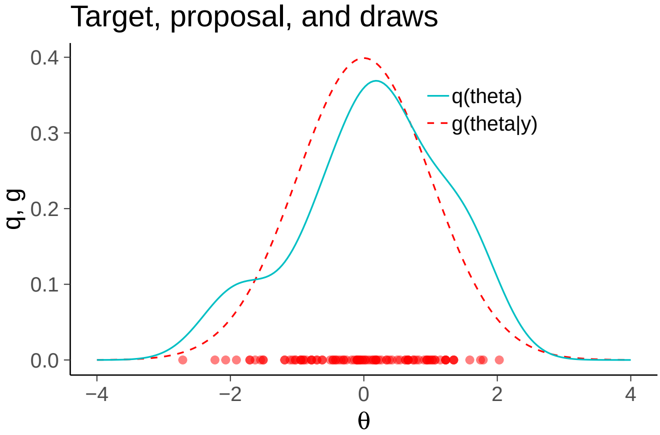
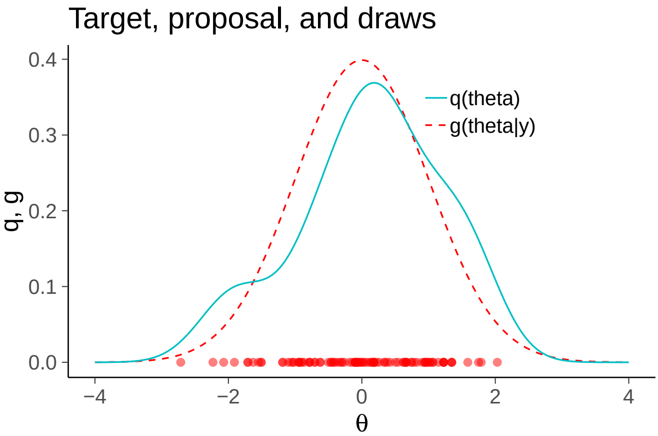
Subsection 2

PSIS LOO-CV

Recap: Importance sampling

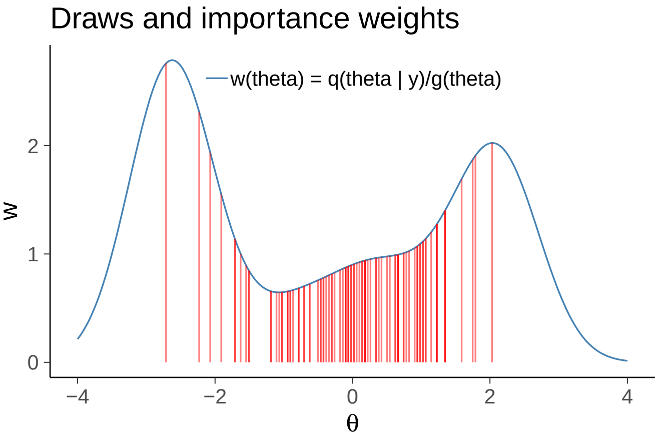


Recap: Importance sampling



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

Recap: Importance sampling



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

Importance sampling for LOO-CV

- Let $f = p(\tilde{y}_i|y_{-i})$, $g = p(\theta|y)$, and $q = p(\theta|y_{-i})$

Importance sampling for LOO-CV

- Let $f = p(\tilde{y}_i|y_{-i})$, $g = p(\theta|y)$, and $q = p(\theta|y_{-i})$
- Having samples θ^s from $p(\theta^s|y)$

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

where w_i^s are importance weights and

$$w_i^s = \frac{p(\theta^s|y_{-i})}{p(\theta^s|y)}.$$

Importance sampling for LOO-CV

- We get a nice solution

$$w_i^s = \frac{p(\theta^s|y_{-i})}{p(\theta^s|y)} = \frac{\frac{p(\theta^s)\prod_{j\neq i} p(y_j|\theta^s)}{p(y_{-i})}}{\frac{p(\theta^s)\prod_j p(y_j|\theta^s)}{p(y)}} \propto \frac{1}{p(y_i|\theta^s)}.$$

Importance sampling for LOO-CV

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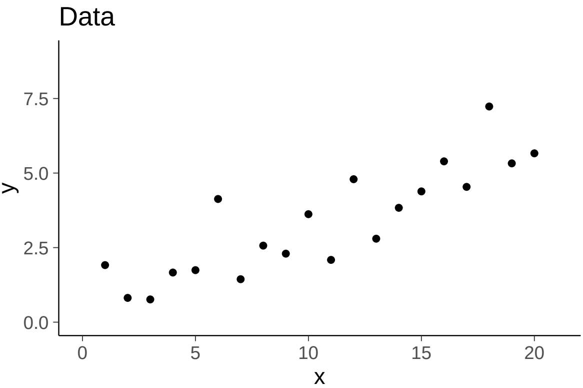
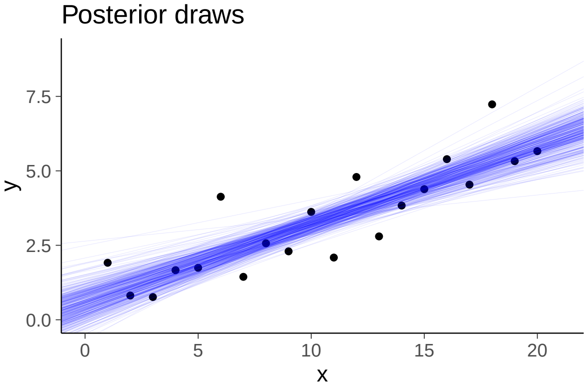
- If evaluated with $\tilde{y}_i = y_i$

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

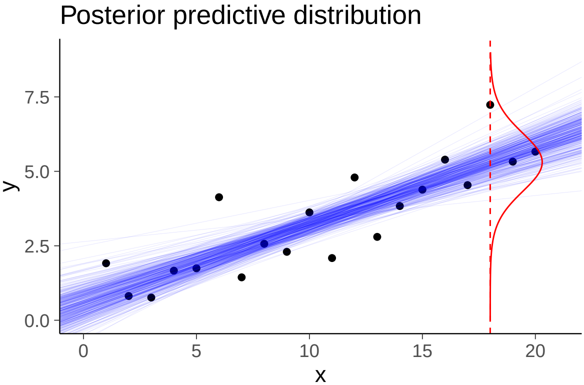
and

$$\log w_i^{(s)} = -\log p(y_i|\theta^{(s)})$$


Data
y
7.5
5.0
2.5
0.0
0
5
10
15
20
x



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



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

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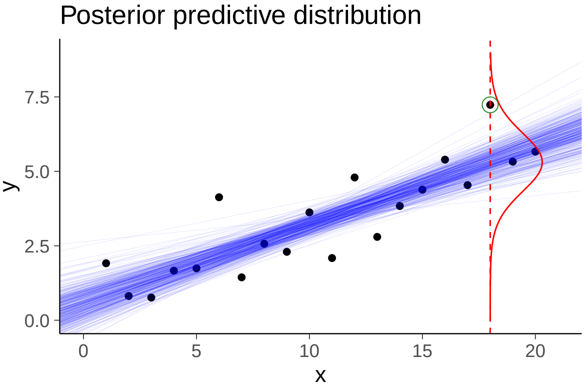

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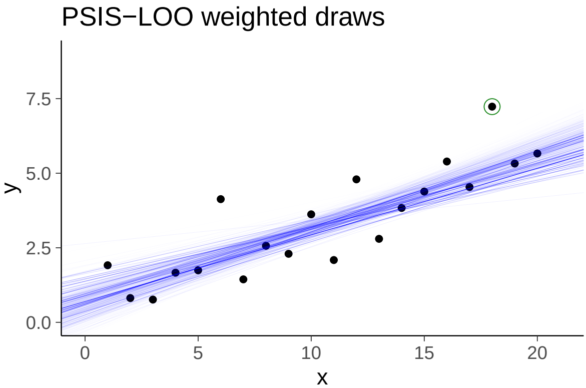
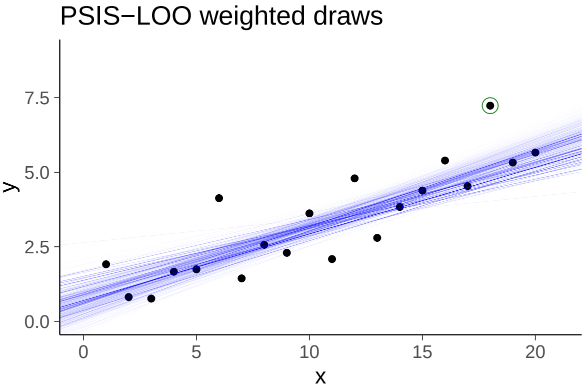


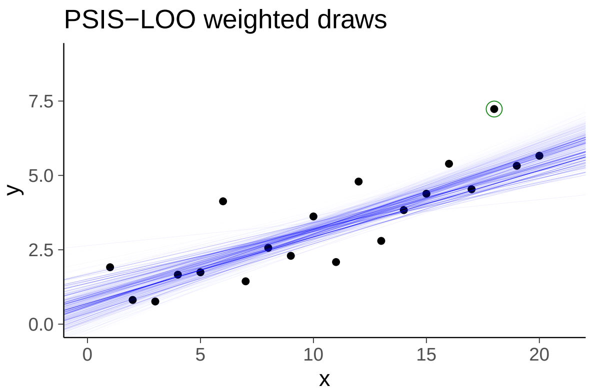
$$\theta^{(s)} \sim p(\theta|x, y)$$

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

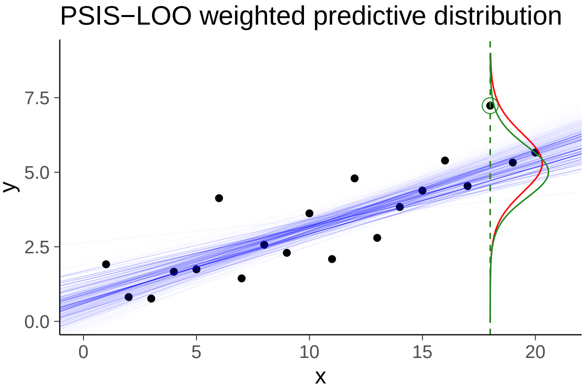


$$\theta^{(s)} \sim p(\theta|x, y)$$

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



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



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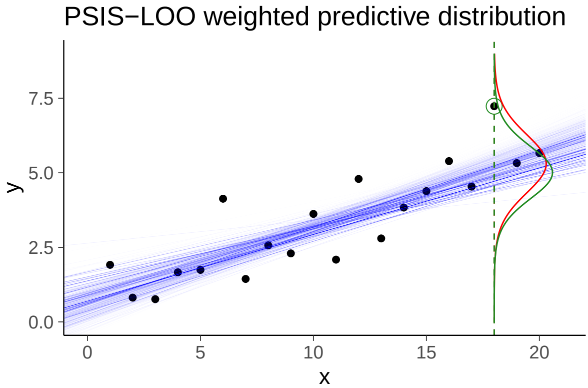
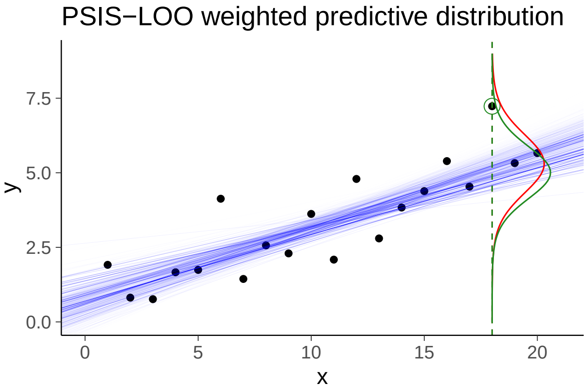


$$\theta^{(s)} \sim p(\theta|x, y)$$

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

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



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Recap: Pareto smoothed importance sampling

- Pareto-Smoothed Importance sampling smooth the weights according to a Generalized Pareto(k) distribution
- Pareto-k diagnostic estimate the number of existing moments ($\lfloor 1/k \rfloor$)

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Recap: Pareto smoothed importance sampling

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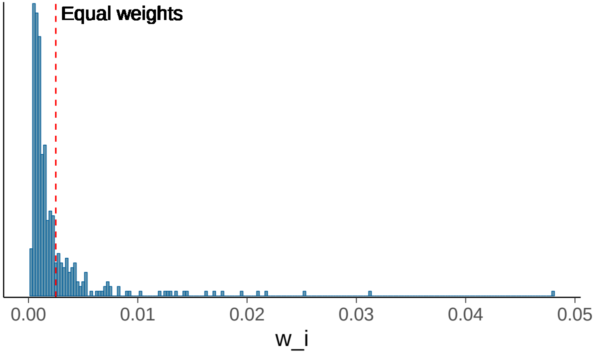
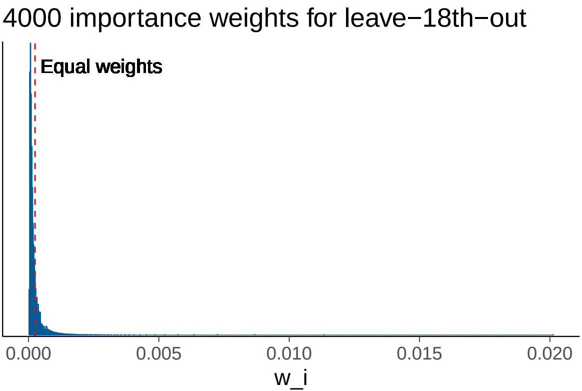
- Pareto-k diagnostic estimate the number of existing moments ($\lfloor 1/k \rfloor$)
- Finite variance and central limit theorem for $k < 1/2$
- Finite mean and generalized central limit theorem for $k < 1$, but pre-asymptotic constant grows impractically large for $k > 0.7$
- Hence $k > 0.7$ can be used to indicate what observation that can be "held-out" using IS

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

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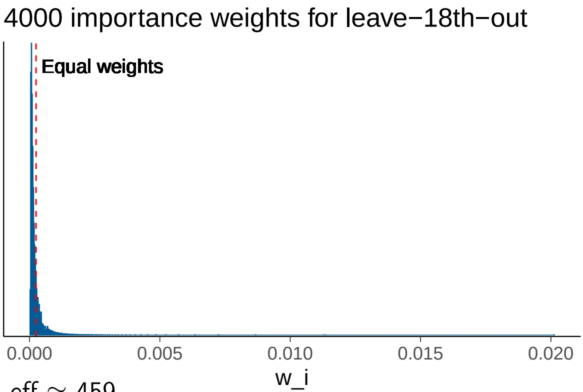
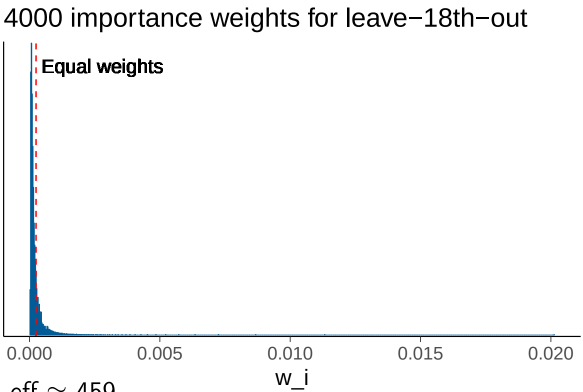
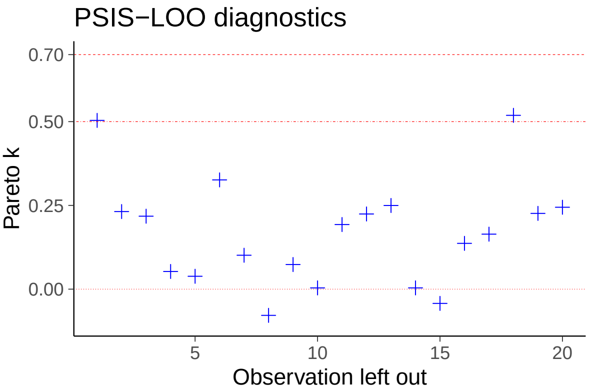


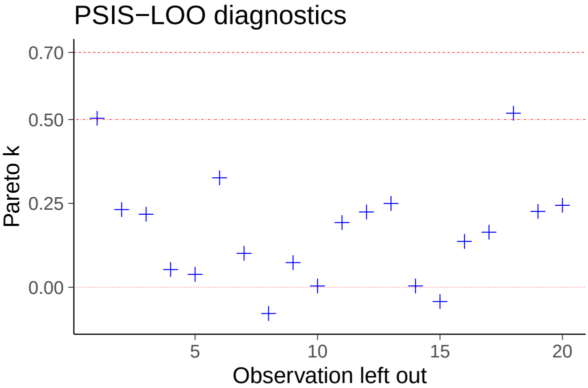
n_eff ≈ 459



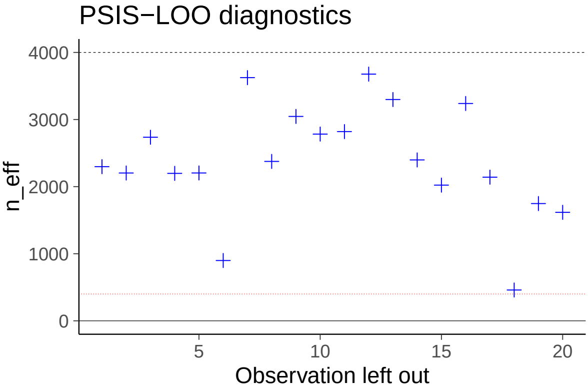
n_eff $\approx$ 459

Pareto $\hat{k} \approx 0.52$ Pareto $\hat{k}$ estimates the tail shape which determines the convergence rate of PSIS. Less than 0.7 is ok.


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




```
  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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                          Count  Pct.    Min. n_eff
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 (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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Stan code

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

Stan code

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

```
...
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 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
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 (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.
```

PSIS-LOO

1. PSIS-LOO for hierarchical models
   1.1 leave-one-group out is challenging for PSIS-LOO

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PSIS-LOO

1. PSIS-LOO for hierarchical models
   1.1 leave-one-group out is challenging for PSIS-LOO
2. PSIS-LOO for non-factorizable models

PSIS-LOO

1. PSIS-LOO for hierarchical models
   1.1 leave-one-group out is challenging for PSIS-LOO
2. PSIS-LOO for non-factorizable models
3. PSIS-LOO for time series
   3.1 Approximate leave-future-out cross-validation

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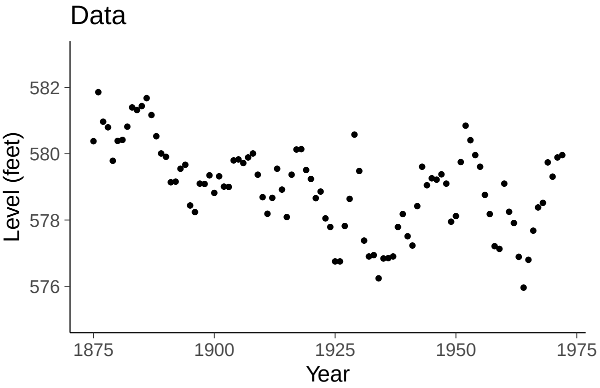
PSIS-LOO for time series



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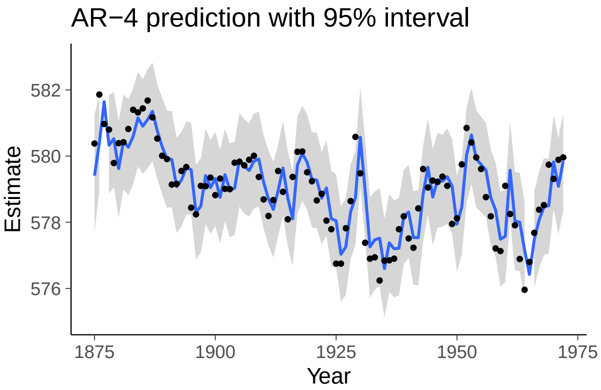
PSIS-LOO for time series



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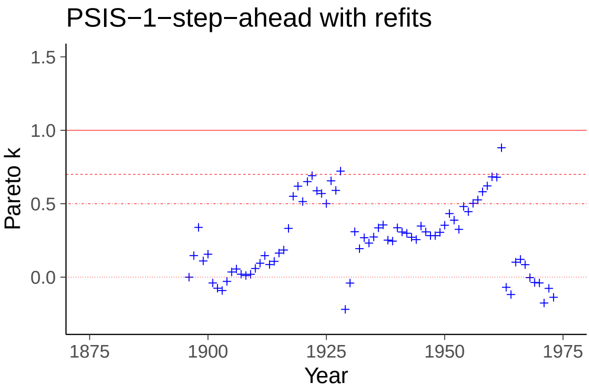

mc-stan.org/loo/articles/loo2-lfo.html

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Subsection 3

K-fold CV

K-fold cross-validation

- We can approximate $elpd_{\text{loo}}$ using K-fold CV

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K-fold cross-validation

- We can approximate $elpd_{\text{loo}}$ using K-fold CV
  1. `for k in K`
     1.1 hold $1/K$ observations out (i.e. $y_{-y(k)}$)
     1.2 compute $p(\theta|y_{-y(k)})$
     1.3 compute lpd for $y_{-y(k)}$
  2. sum the lpd over K folds

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     1.3 compute lpd for $y_{-y(k)}$
  2. sum the lpd over K folds
- We only need to estimate K models

K-fold cross-validation

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

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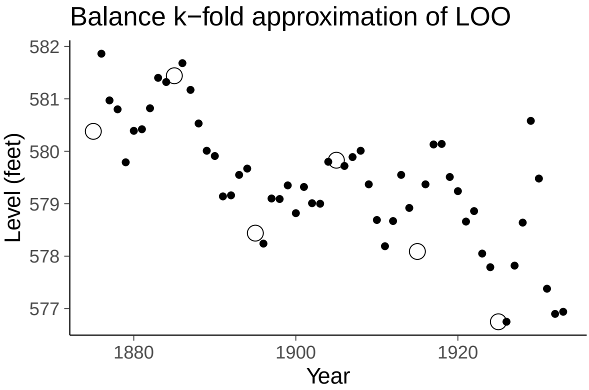
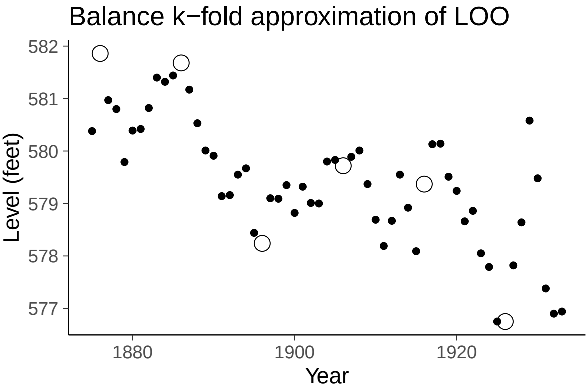
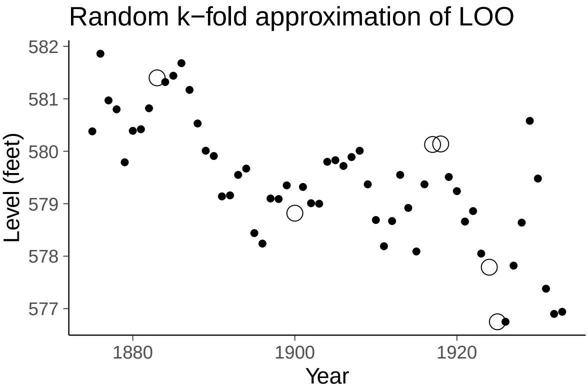
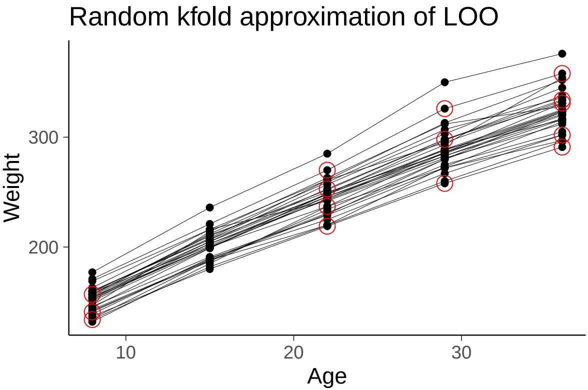
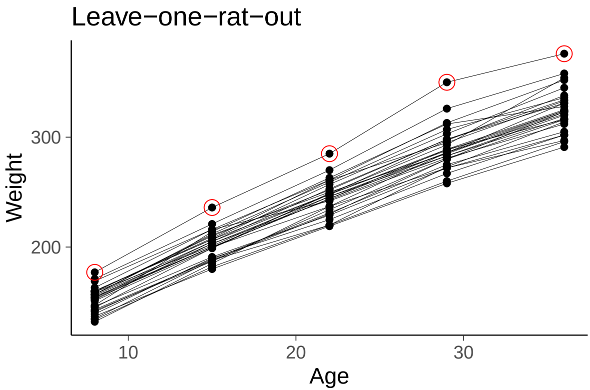



Balance k−fold approximation of LOO
Level (feet)
582
581
580
579
578
577
1880
1900
1920
Year


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


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


Leave−one−rat−out
Weight
300
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30
Age

Cross-validation for model assessment

1. CV is good for model assessment when application specific utility/cost functions are used

Cross-validation for model assessment

1. CV is good for model assessment when application specific utility/cost functions are used
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)

Subsection 4

Model Comparison

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 (blue): formula = kcal.per.g $\sim$ neocortex
   1.2 Model 2 (red): formula = kcal.per.g $\sim$ neocortex + log(mass)

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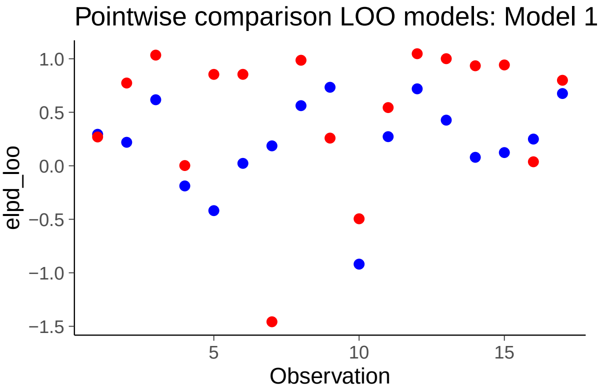
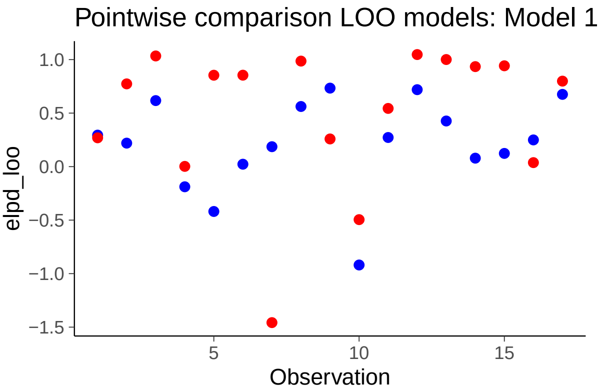
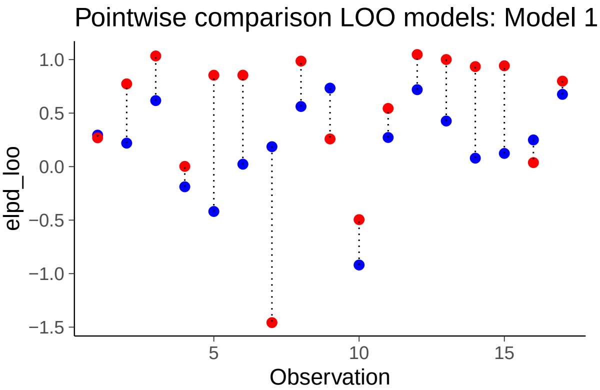




Model 1 elpd_loo $\approx$ 3.7, SE=1.8
Model 2 elpd_loo $\approx$ 8.4, SE=2.8



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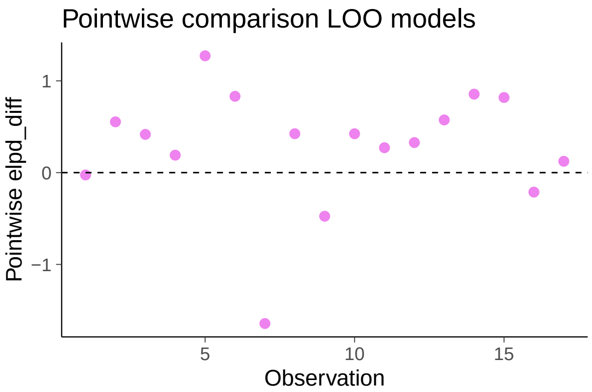


```
Model comparison:
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff        se
      4.7       2.7
```

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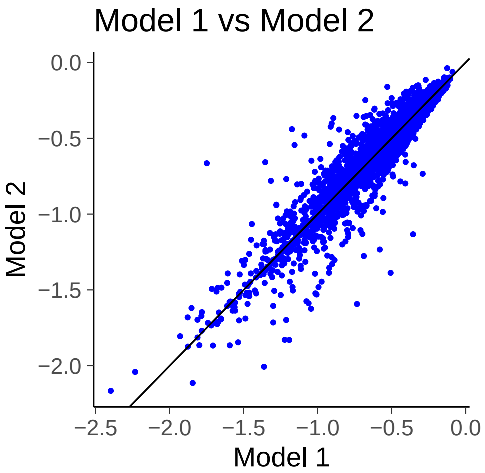
Arsenic well example – Model comparison

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

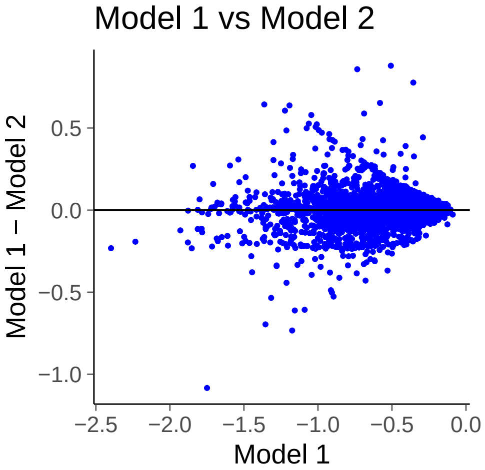
Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 13.

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
```

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Arsenic well example – Model comparison

```
> loo_compare(model1, model2)
       elpd_diff se_diff
model2    0.0       0.0
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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.

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What if one is not clearly better than others?

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   1.1 and then analyse the posterior distribution directly
   1.2 sparse priors like regularized horseshoe prior instead of variable selection

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4. In a nested case choose more complex if you want to take into account all the uncertainties.

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Cross-validation and model selection

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2. Do not use cross-validation to choose from a large set of models
   2.1 selection process leads to overfitting
3. Overfitting in selection process is not unique for cross-validation

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

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Section 3

Information criteria

Akaike Information Criteria

1. Remember the relationship between the elpd and the lpd

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2. Akaike information criteria

$$\mathrm{elpd}_{\mathrm{AIC}} = \sum_i \log p(y_i|\hat{\theta}_{\mathrm{MLE}}) - k$$

3. AIC

$$\mathrm{AIC} = -2\mathrm{elpd}_{\mathrm{AIC}}$$

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Deviance Information Criteria

1. Deviance information criteria

$$\mathrm{elpd}_{\mathrm{DIC}} = \sum_i \log p(y_i|\hat{\theta}_{\mathrm{Bayes}}) - p_{\mathrm{DIC}}$$

2. We estimate the number of effeicient parameters with

$$p_{\mathrm{DIC1}} = 2(\log p(y|\hat{\theta}_{\mathrm{Bayes}}) - \mathrm{E}_{p(\theta|y)}(\log p(y|\theta)))$$

or

$$p_{\mathrm{DIC2}} = 2V_{p(\theta|y)}(\log p(y|\theta))$$

3. DIC

$$\mathrm{DIC} = -2\mathrm{elpd}_{\mathrm{DIC}}$$

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Watanabe Information Criteria

1. Watanabe information criteria

$$\text{elpd}_{\text{WAIC}} = \sum_i \log p(y_i|y) - p_{\text{WAIC}}$$

2. We estimate the number of efficient parameters with

$$p_{\text{WAIC1}} = 2\sum_i^n (\log \mathrm{E}_{p(\theta|y)}(p(y_i|\theta)) - \mathrm{E}_{p(\theta|y)}(\log p(y_i|\theta)))$$

or

$$p_{\text{WAIC2}} = 2\sum_i^n (V_{p(\theta|y)}(\log p(y_i|\theta)))$$

3. WAIC

$$\text{WAIC} = -2\text{elpd}_{\text{WAIC}}$$

4. WAIC can be seen as an approximation of the $elpd_{\text{loo}}$

WAIC vs PSIS-LOO

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2. PSIS-LOO is more accurate
3. PSIS-LOO has much better diagnostics
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)

Section 4

Model averaging and Stacking

Special lecture!

1. Special lecture on model averaging and stacking next week!

Section 5

Summary

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

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