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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

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Predictive performance

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

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- True predictive performance is found out by using it to make predictions and comparing predictions to true observations
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  All models are wrong... but some are useful.
- 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

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  - eg. money, life years, quality adjusted life years, etc.

Predictive performance

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- Choose the model function to maximize our utility
- Application specific utility/cost functions are important
  - eg. money, life years, quality adjusted life years, etc.
- General utility: overall in the goodness of the predictive distribution
  - we don't know (yet) the application specific utility

then good information theoretically justified choice is log-score

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

Background and Motivation

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

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

where $\tilde{y}_i$ is an unseen observation generated from the true data generating process $p_t(\tilde{y}_i)$, and y are observed data.

Section 2

Cross-validation

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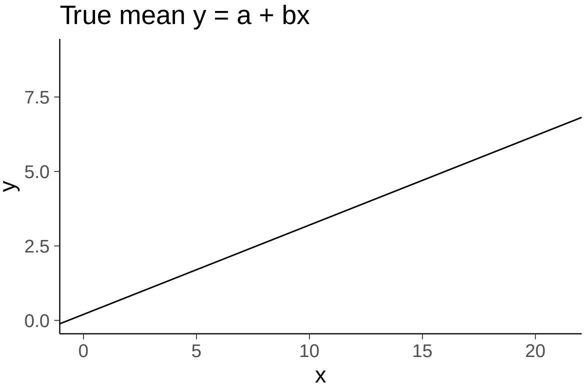
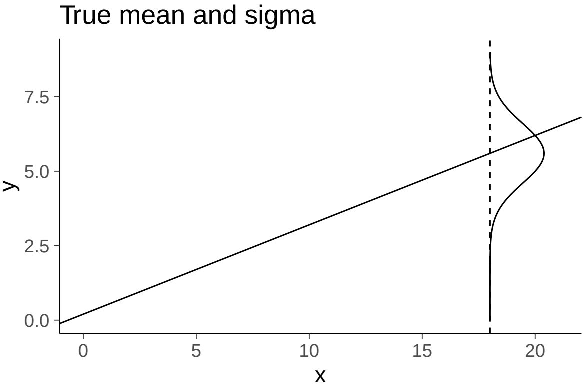
Leave-one-out cross-validation (LOO-CV)

- 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

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

- Pareto-Smoothed Importance Sampling (PSIS) can be used to efficiently compute each π_i (see Gelfand, 1996 and Vehtari et. al., 2019)


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
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y
0
5
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20
x

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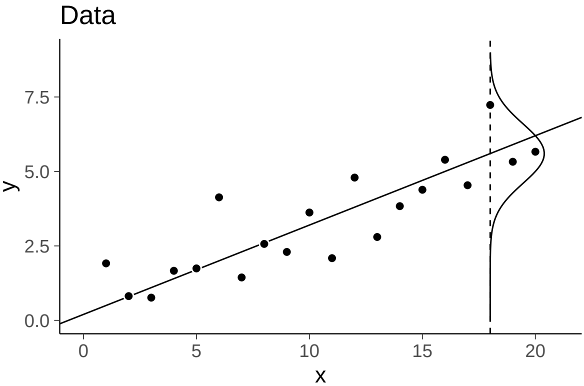

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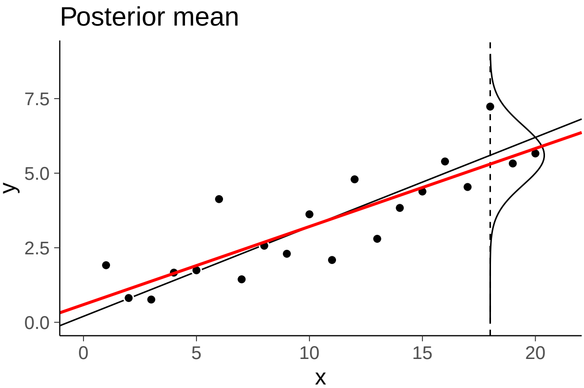
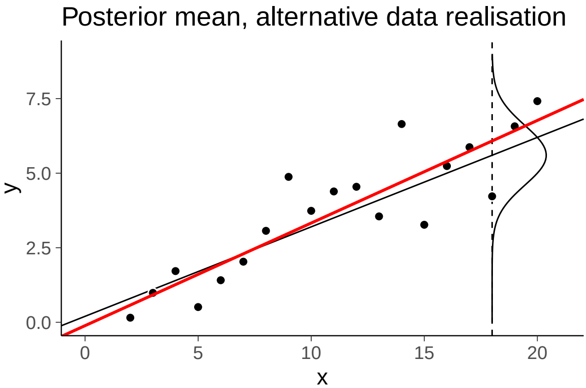
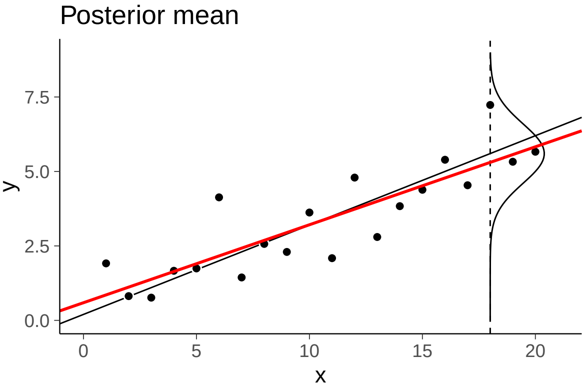



Posterior mean, alternative data realisation
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x


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

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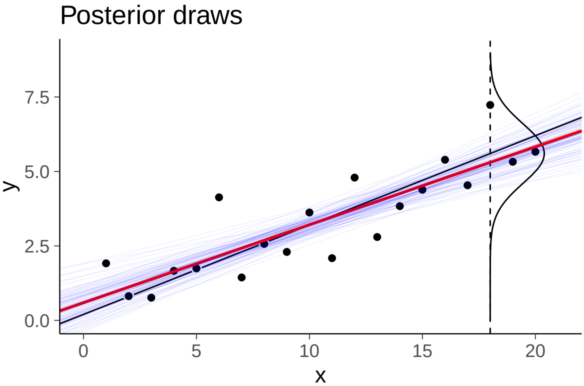
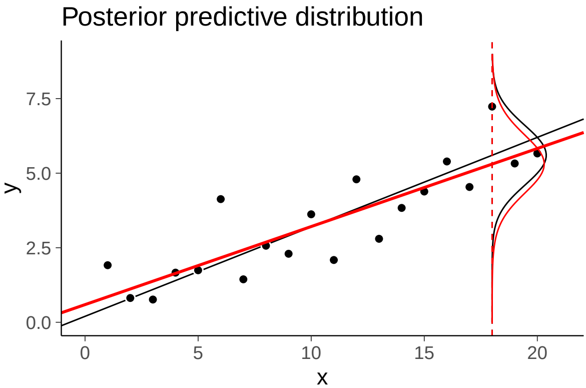
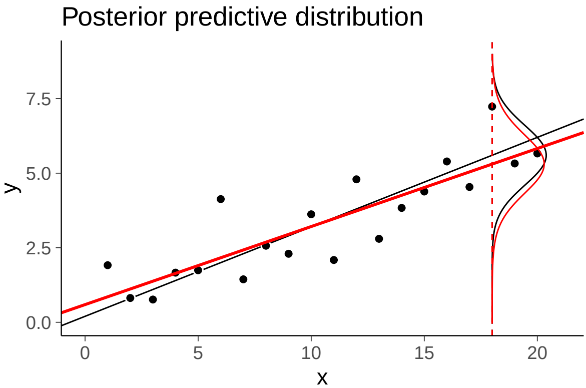
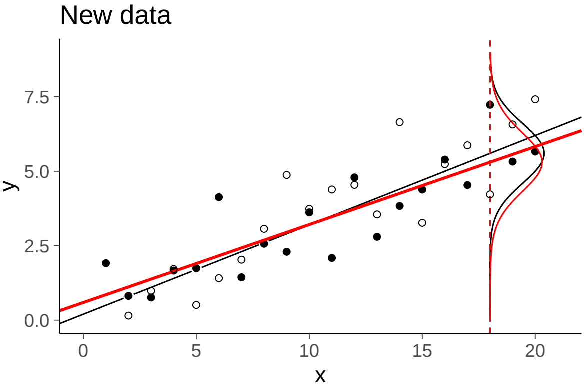
  - Measures of predictive accuracy
- Cross-validation
  - When is LOO applicable
  - PSIS-LOO and `loo`
  - Comparison and selection
  - Additional reading
- Information criteria
- To move up

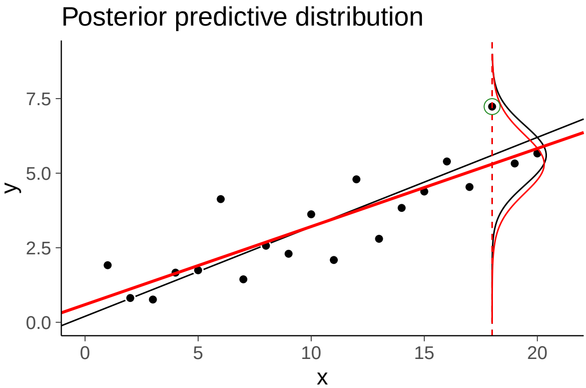



Posterior predictive distribution
y
x
0.0
2.5
5.0
7.5
0
5
10
15
20



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


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


Posterior predictive distribution
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5.0
2.5
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y
0
5
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20
x

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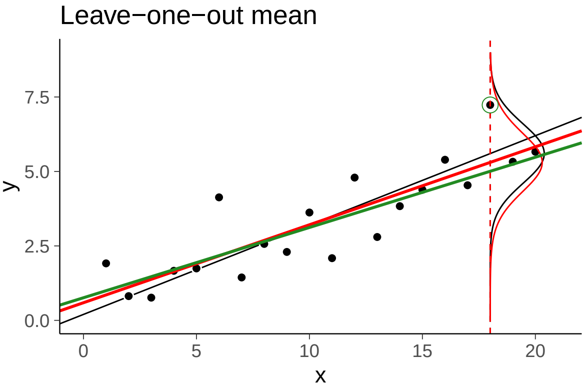

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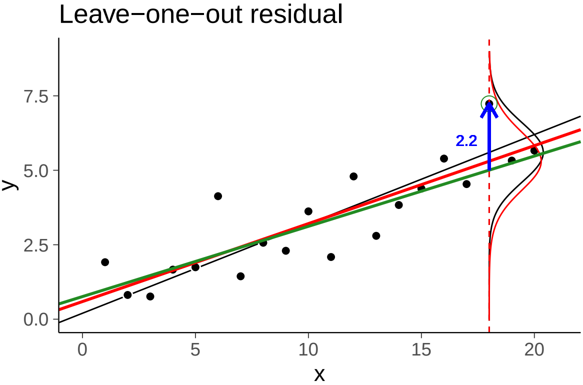
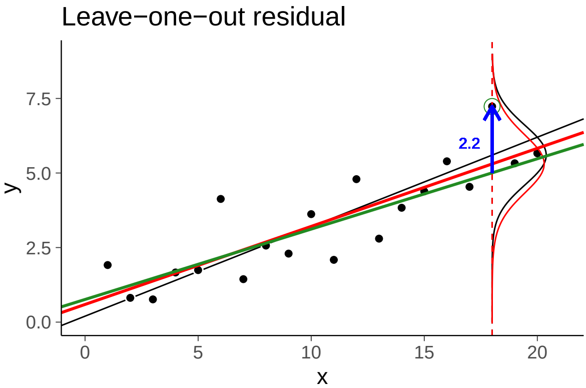
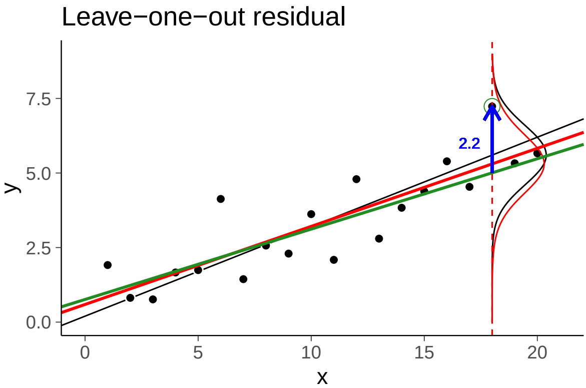




$$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$$



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

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

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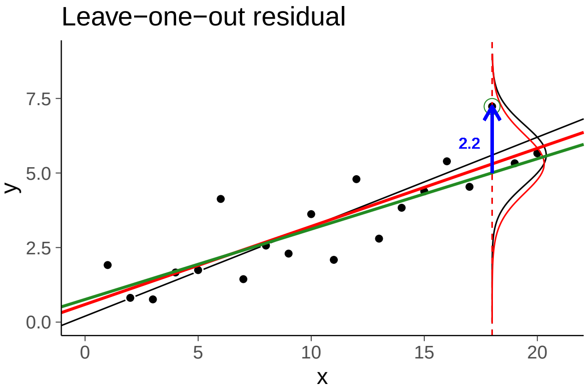
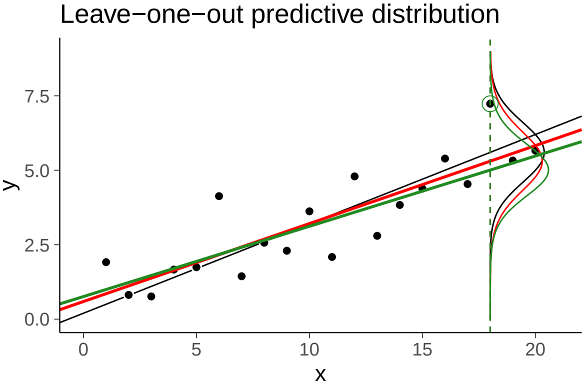
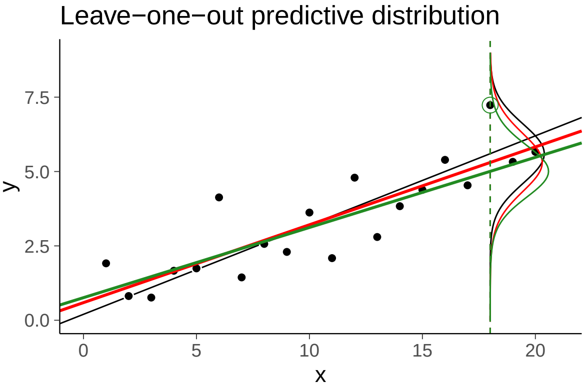


$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$

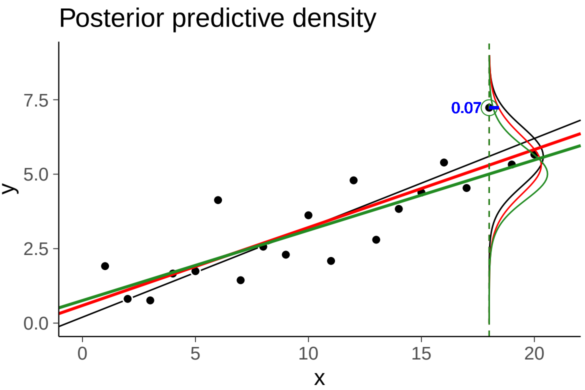
Can be use to compute, e.g., RMSE, R^2, 90% error

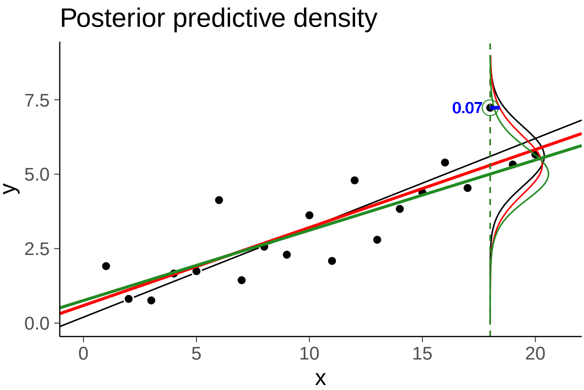
See LOO-R^2 at avehtari.github.io/bayes_R2/bayes_R2.html


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

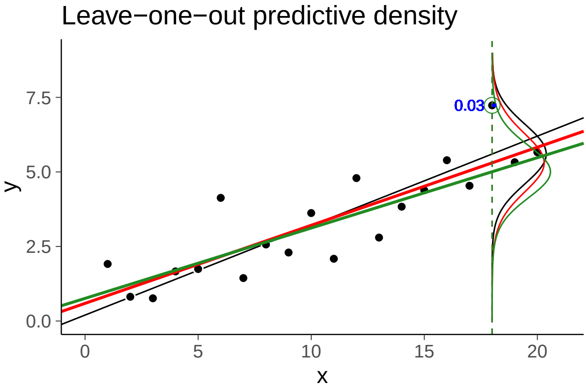


$$p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18}) = \int p(\tilde{y}|\tilde{x} = 18, \theta)p(\theta|x_{-18}, y_{-18})d\theta$$


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



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



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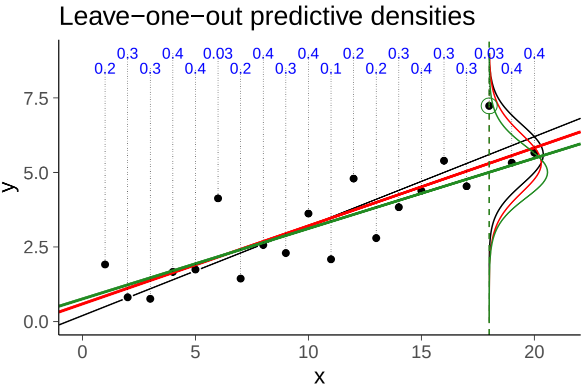
$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$



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

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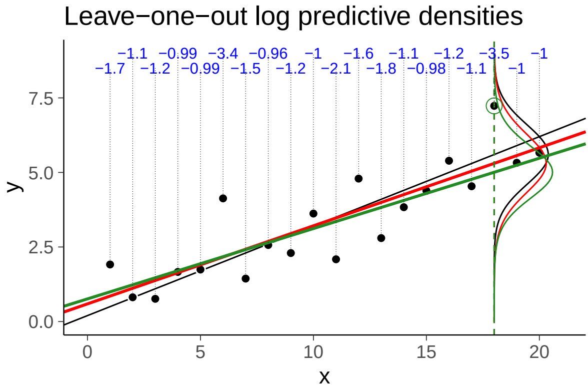
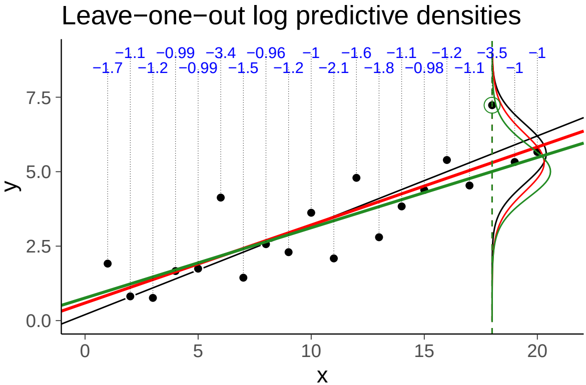
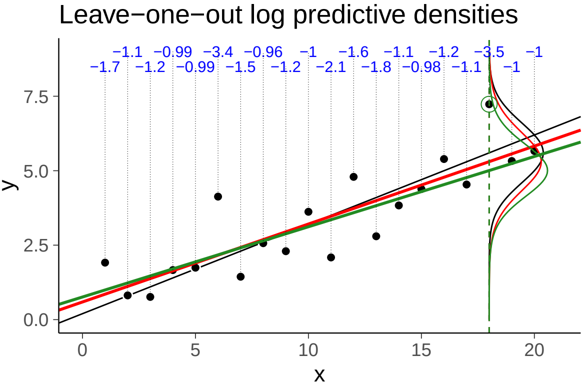


$$\log p(y_i | x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$$



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



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

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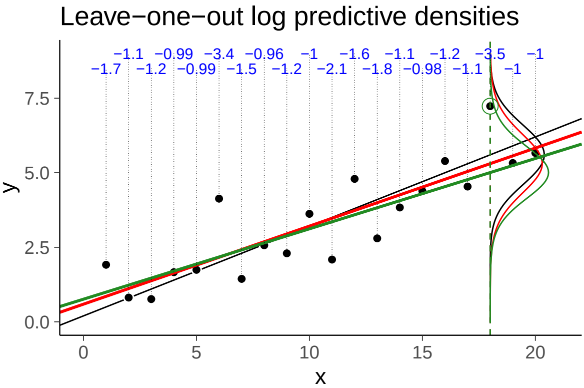
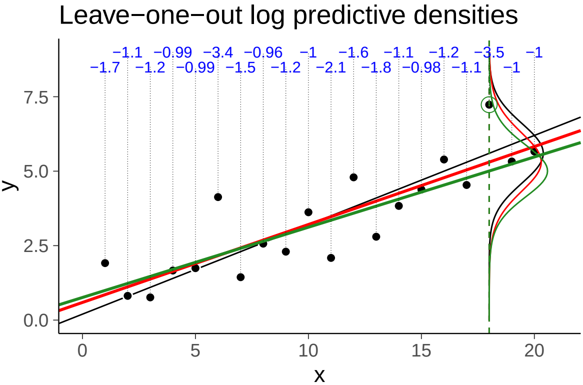


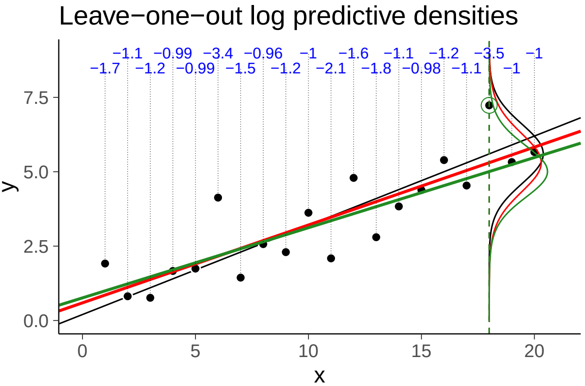
$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$

unbiased estimate of log posterior pred. density for new data



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

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



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

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

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

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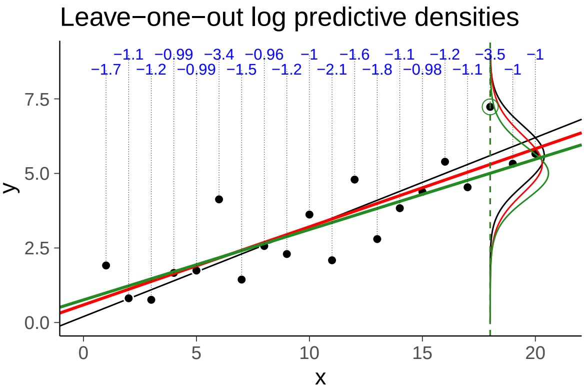
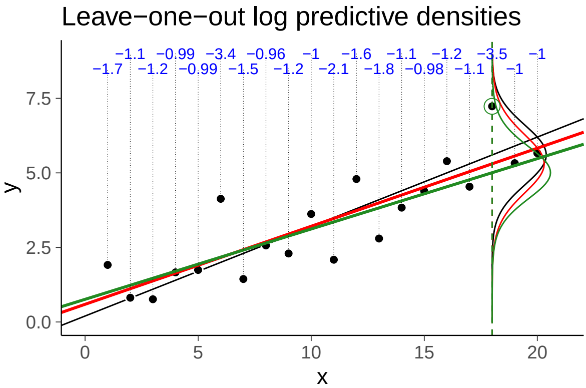


$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

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



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

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Stan and loo package

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

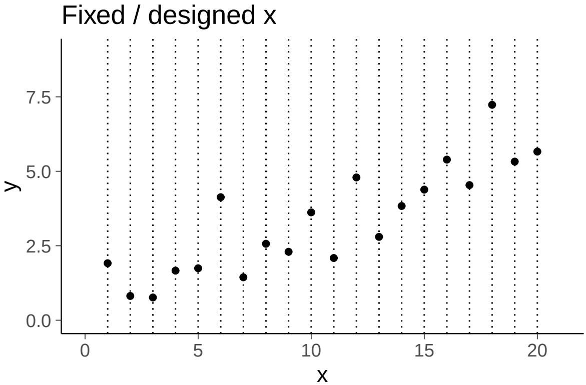
         Estimate  SE
elpd_loo    -29.5 3.3
p_loo         2.7 1.0
------
Monte Carlo SE of elpd_loo is 0.1.

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.

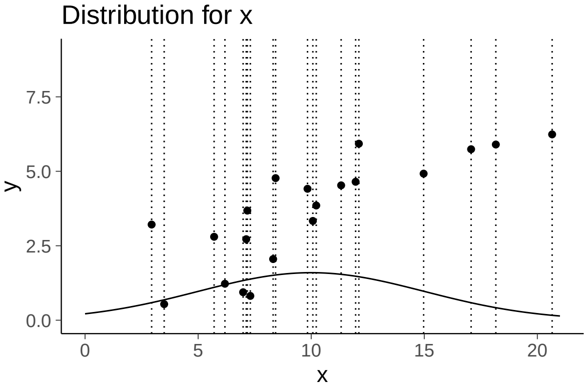
Model comparison:
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff        se
     -0.2       0.1
```



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.

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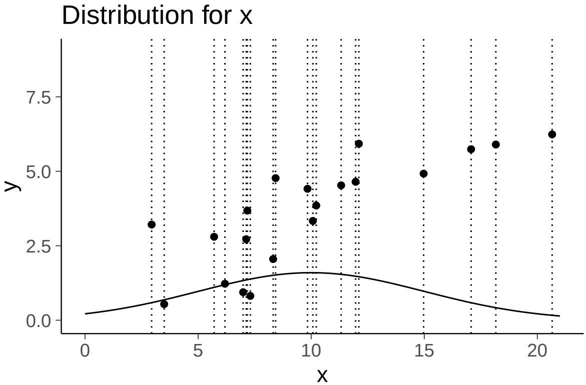

LOO is ok for random x. SE is uncertainty about $y|x$ and x.

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/`

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Section 3

Information criteria

Section 4

To move up

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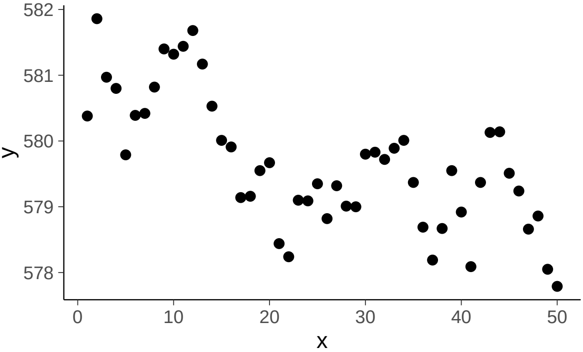

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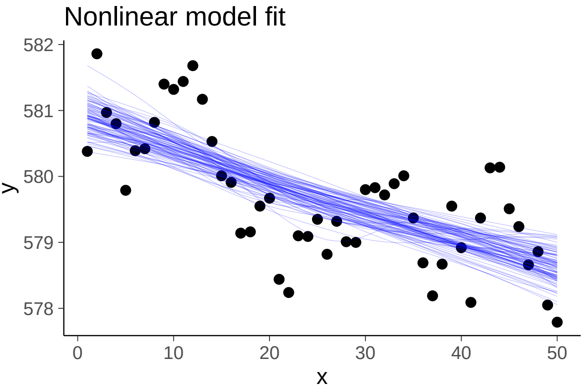

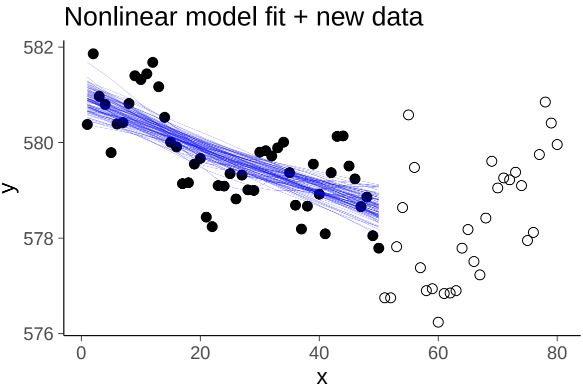
Nonlinear model fit + new data
582
580
578
576
y
0
20
40
60
80
x

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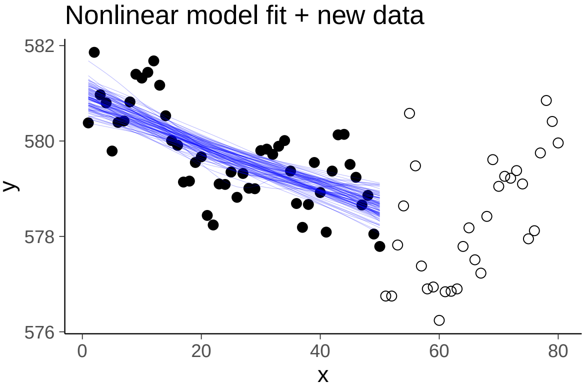
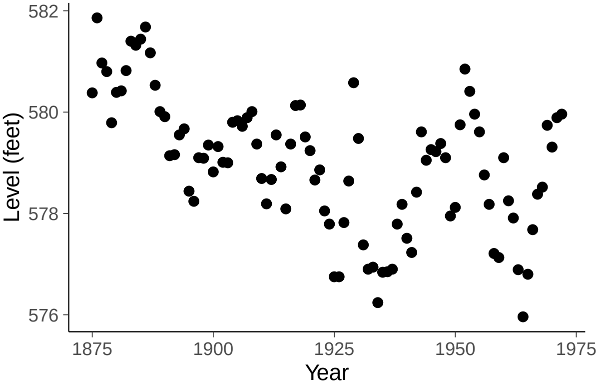
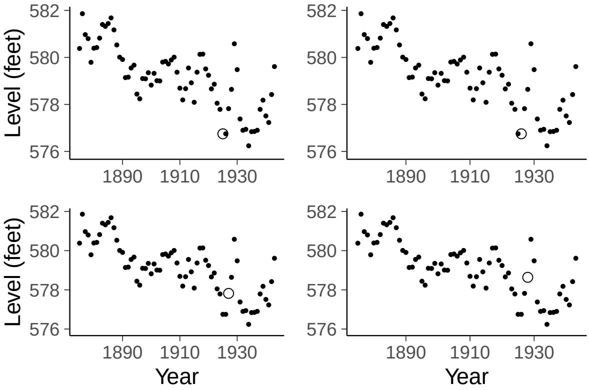


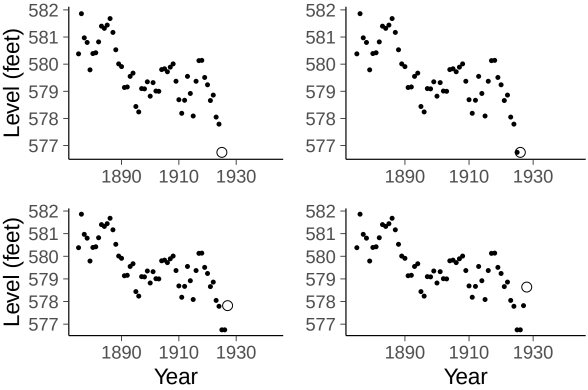
Extrapolation is more difficult



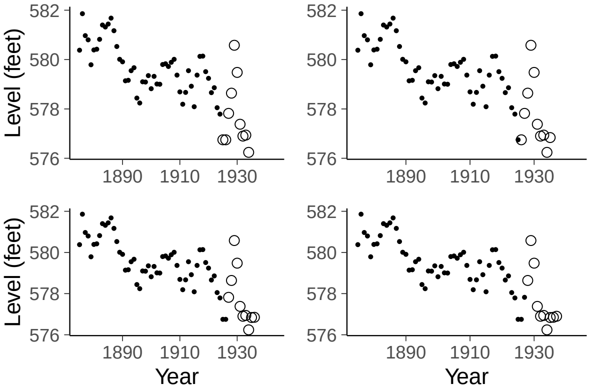
Can LOO or other cross-validation be used with time series?



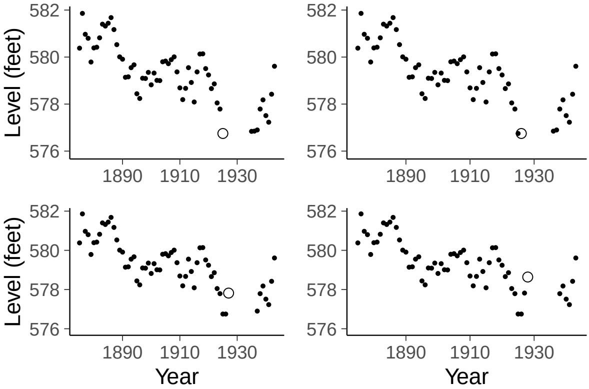
Leave-one-out cross-validation is ok for assessing conditional model



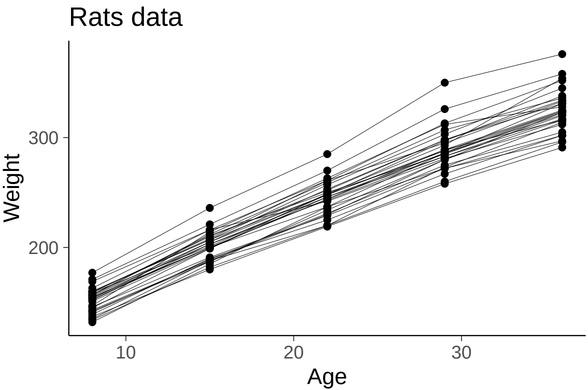
Leave-future-out cross-validation is better for predicting future



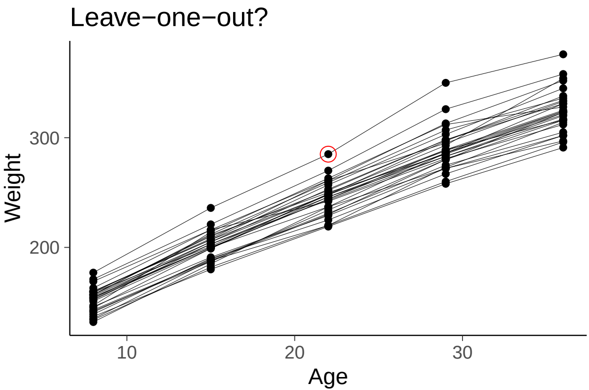
m-step-ahead cross-validation is better for predicting further future



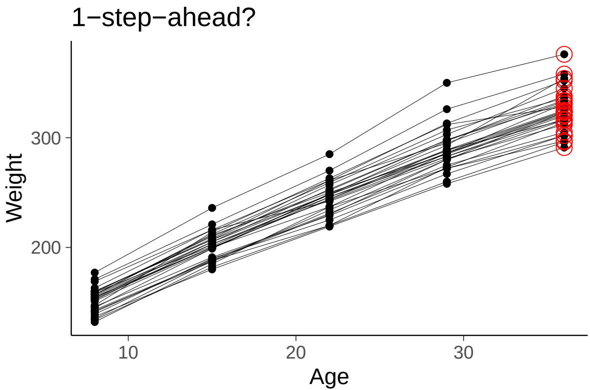
m-step-ahead leave-a-block-out cross-validation



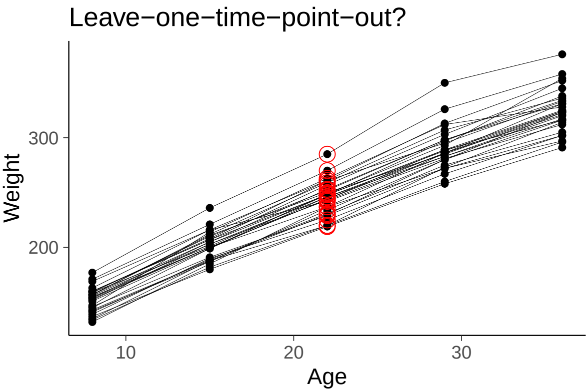
Can LOO or other cross-validation be used with hierarchical data?



Yes!



Yes!



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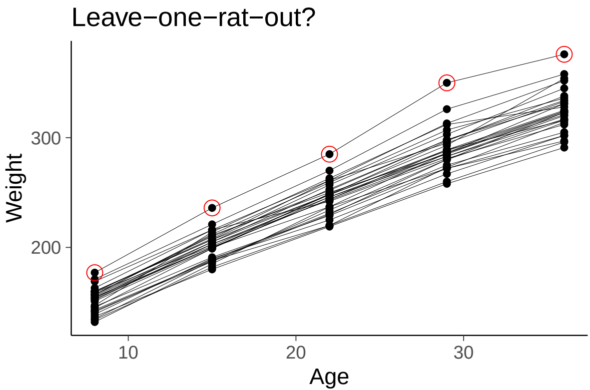

Yes!

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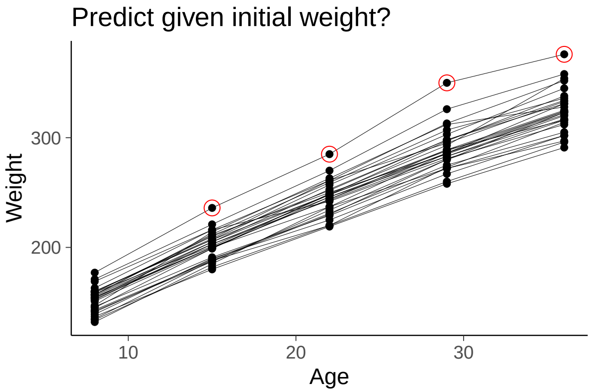

Yes!

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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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/`

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 code

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

Stan code

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

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

Stan code

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```

1. RStanARM and BRMS compute log_lik by default

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

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Pareto smoothed importance sampling LOO

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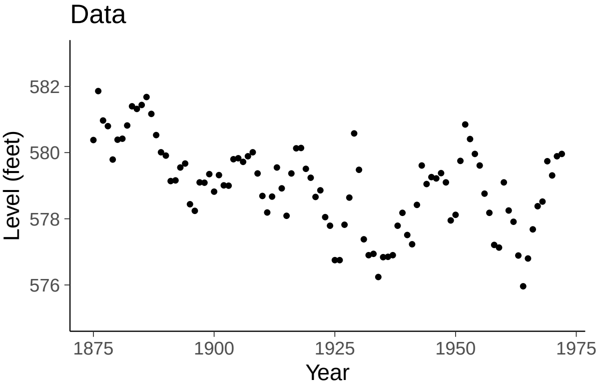
2. PSIS-LOO for non-factorizable models
   2.1 `mc-stan.org/loo/articles/loo2-non-factorizable.html`
3. PSIS-LOO for time series
   3.1 Approximate leave-future-out cross-validation
   `mc-stan.org/loo/articles/loo2-lfo.html`


Data
582
580
578
576
Level (feet)
1875
1900
1925
1950
1975
Year

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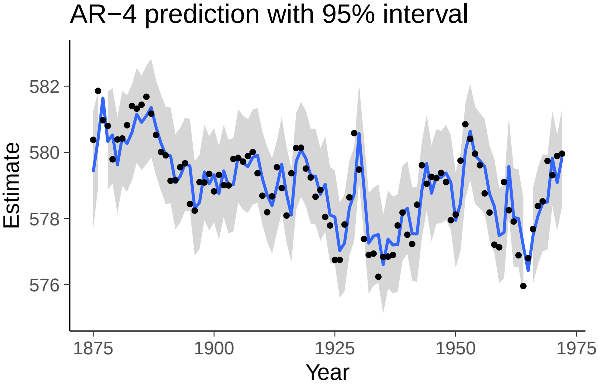
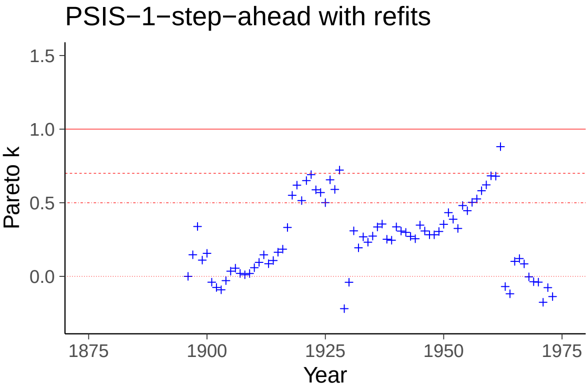
- Model assessment and selection
  - Measures of predictive accuracy
- Cross-validation
  - When is LOO applicable
  - PSIS-LOO and `loo`
  - Comparison and selection
  - Additional reading
- Information criteria
- To move up





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

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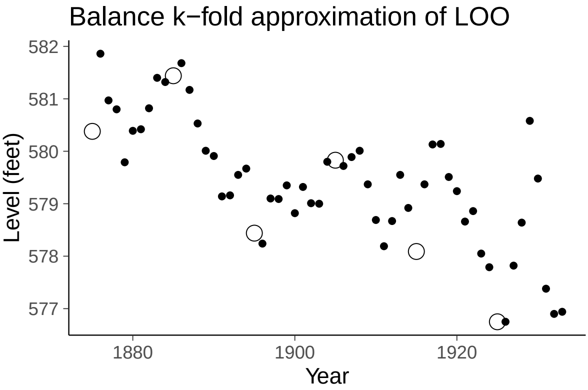

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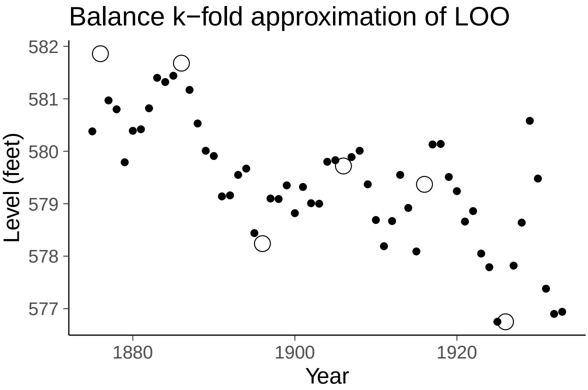

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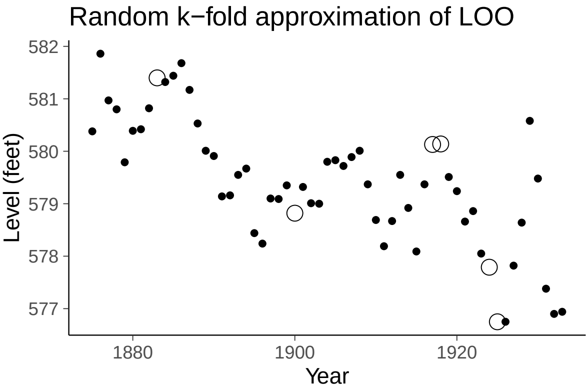

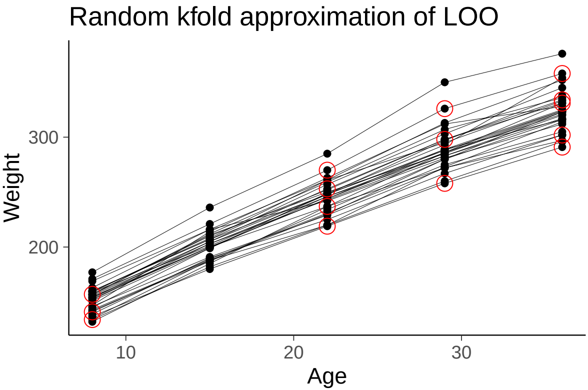
Random kfold approximation of LOO
Weight
300
200
10
20
30
Age

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- Model assessment and selection
  - Measures of predictive accuracy
- Cross-validation
  - When is LOO applicable
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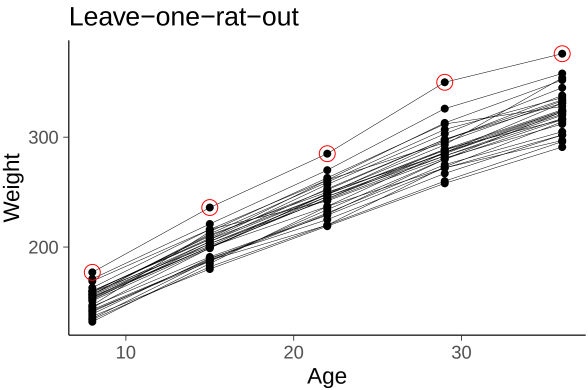

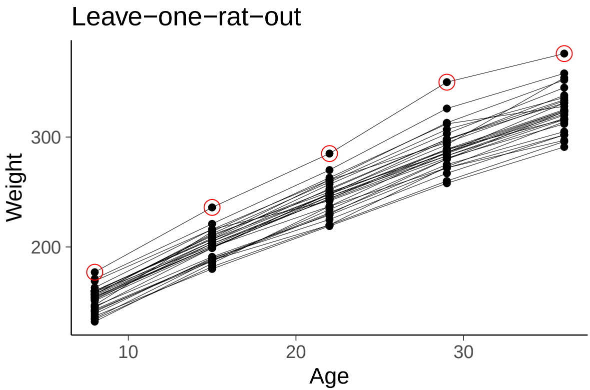

kfold_split_random()

kfold_split_balanced()

kfold_split_stratified()

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)

WAIC vs PSIS-LOO

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

see Vehtari, Gelman & Gabry (2017a)

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WAIC vs PSIS-LOO

1. WAIC has same assumptions as LOO
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)

see Vehtari, Gelman & Gabry (2017a)

*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, ...

Marginal likelihood / Bayes factor

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

Marginal likelihood / Bayes factor

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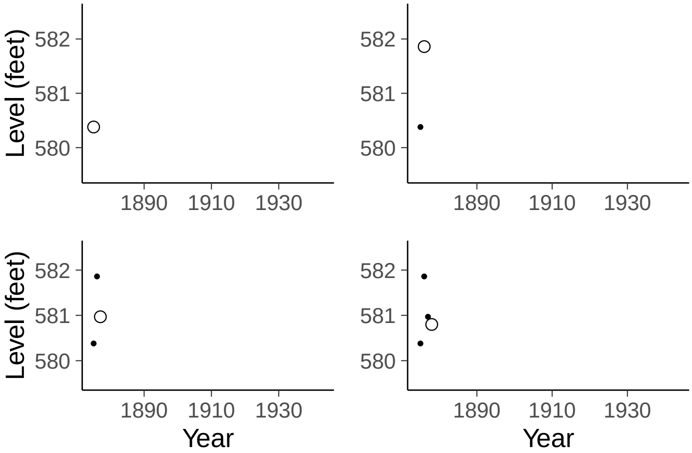

Marginal likelihood / Bayes factor

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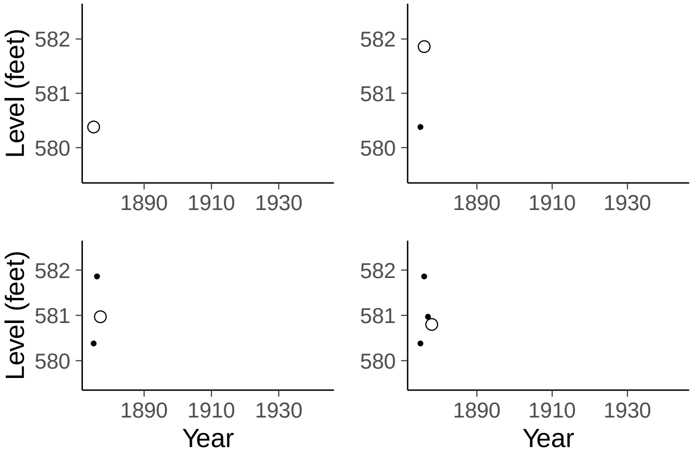
   - which makes it very sensitive to prior



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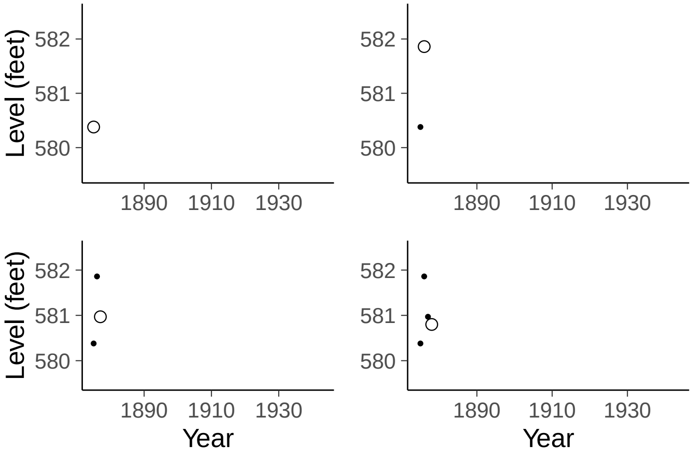
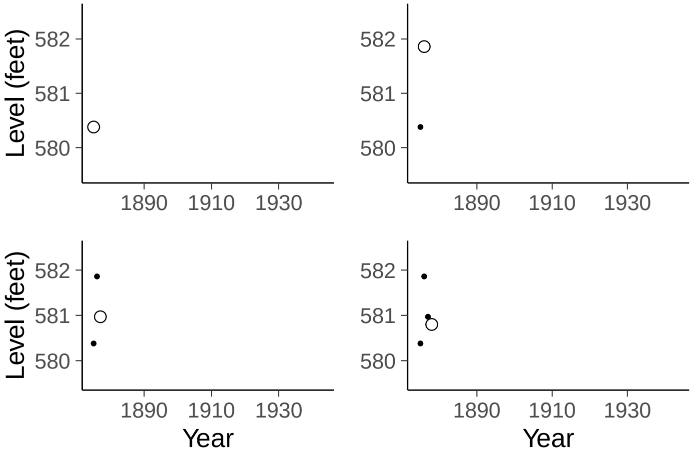


Marginal likelihood / Bayes factor

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



Cross-validation for model assessment

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

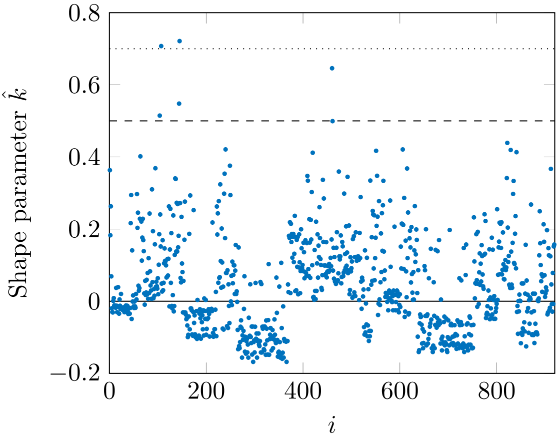
Cross-validation for model assessment

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/`

Radon example

PSIS-LOO diagnostics



see Vehtari, Gelman & Gabry (2017a)

Sometimes cross-validation is not needed

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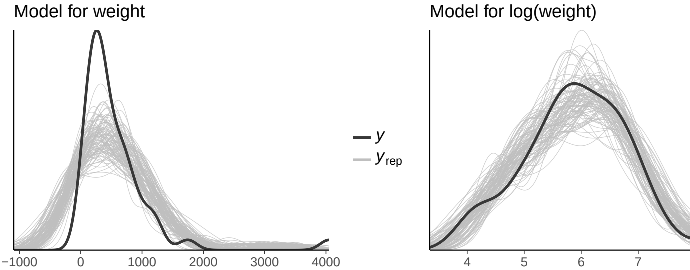
1. Posterior predictive checking is often sufficient



Predicting the yields of mesquite bushes.

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

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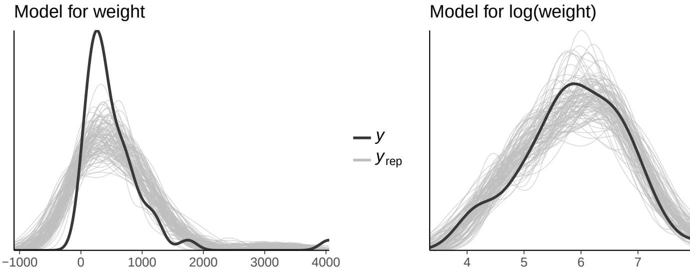

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1. BDA3, Chapter 6
2. Gabry, Simpson, Vehtari, Betancourt, Gelman (2019). Visualization in Bayesian workflow. JRSS A, https://doi.org/10.1111/rssa.12378
3. mc-stan.org/bayesplot/articles/graphical-ppcs.html
4. betanalpha.github.io/assets/case_studies/principled_bayesian_workflow.html

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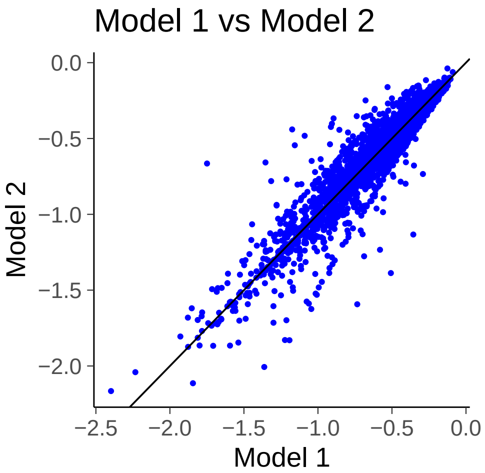
Arsenic well example – Model comparison

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

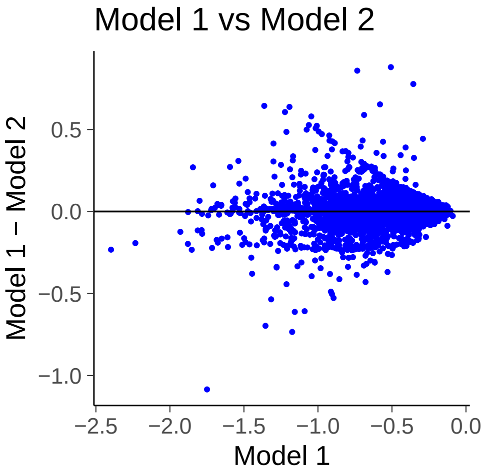
Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 13.

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
```

see Vehtari, Gelman & Gabry (2017a)

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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 (more details in a forthcoming article).

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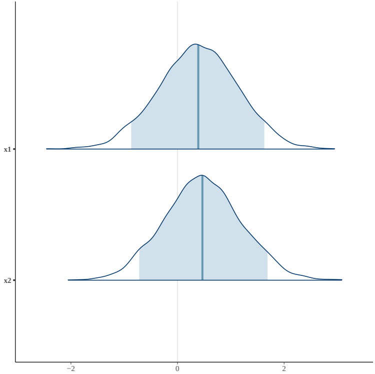
   1.1 see predictive model selection in M-closed case by San Martini and Spezzaferri (1984)
   1.2 but you should not force your design of experiment or analysis to stay in the simplified world
2. In nested case, often easier and more accurate to analyse posterior distribution of more complex model directly
   `avehtari.github.io/modelselection/betablockers.html`

Sometimes predictive model comparison can be useful



Marginal posterior intervals

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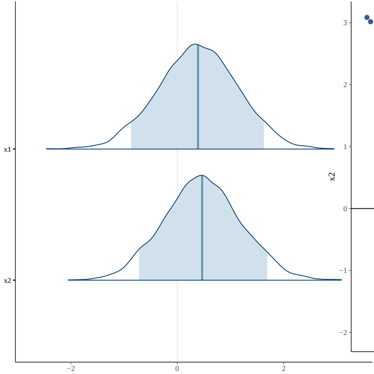

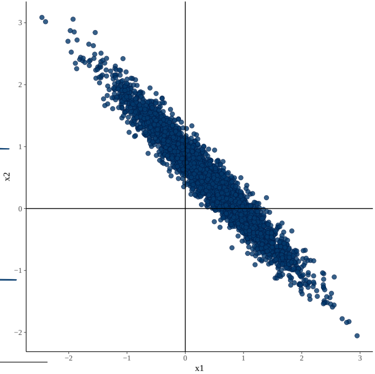

Marginal posterior intervals   Joint posterior density

rstanarm + bayesplot

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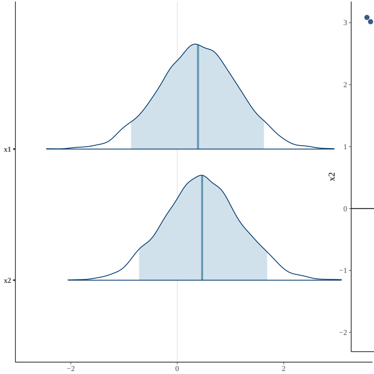

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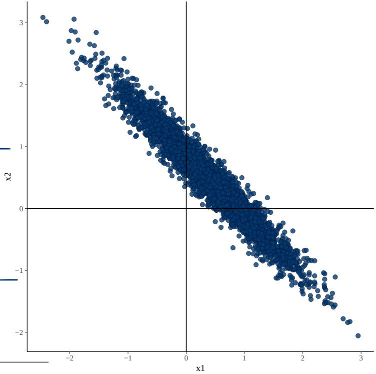

Joint posterior density

rstanarm + bayesplot

see also Collinear demo

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
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Model averaging

1. Prefer continuous model expansion

Model averaging

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2. If needed integrate over the model space = model averaging

Model averaging

1. Prefer continuous model expansion
2. If needed integrate over the model space = model averaging
3. Bayesian stacking may work better than BMA
   3.1 Yao, Vehtari, Simpson, & Gelman (2018)

Cross-validation and model selection

1. Cross-validation can be used for model selection if
   1.1 small number of models
   1.2 the difference between models is clear

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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

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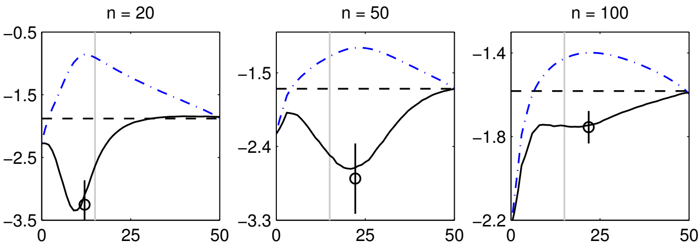
Selection induced bias in variable selection



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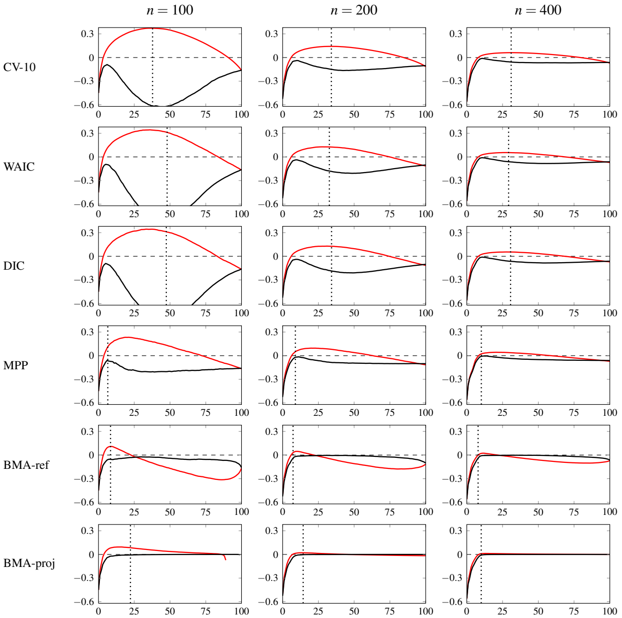

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Take-home messages

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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