Chapter 7

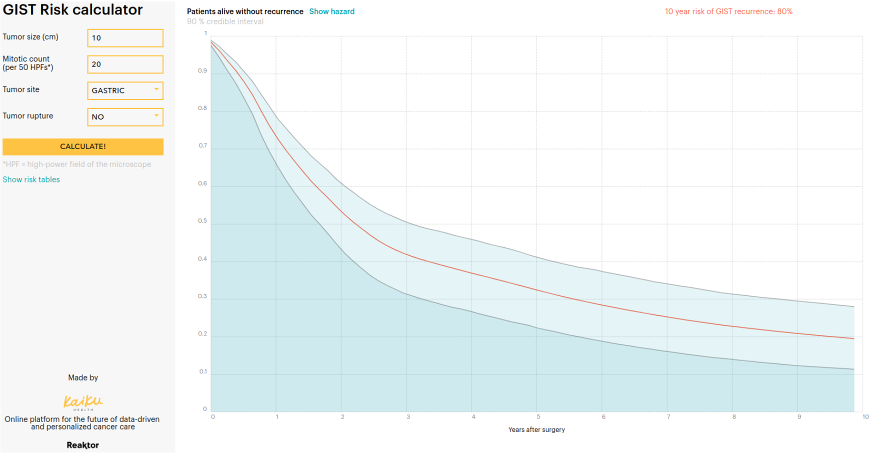
- 7.1 Measures of predictive accuracy
- 7.2 Information criteria and cross-validation
    - Instead of 7.2, read:
      Vehtari, A., Gelman, A., Gabry, J. (2017). Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC. Statistics and Computing. 27(5):1413–1432. arXiv preprint.
- 7.3 Model comparison based on predictive performance
- 7.4 Model comparison using Bayes factors
- 7.5 Continuous model expansion / sensitivity analysis
- 7.5 Example (may be skipped)

Model assessment, selection and inference after selection

- Extra material at https://avehtari.github.io/modelselection/
  - Videos, Slides, Notebooks, References
  - The most relevant for the course is the first part of the talk “Model assessment, comparison and selection at Master class in Bayesian statistics, CIRM, Marseille”

Predicting concrete quality

Predicting cancer recurrence



Predictive performance

- True predictive performance is found out by using it to make predictions and comparing predictions to true observations
  - external validation

Predictive performance

- True predictive performance is found out by using it to make predictions and comparing predictions to true observations
  - external validation
- Expected predictive performance
  - approximates the external validation

Predictive performance

- We need to choose the utility/cost function
- Application specific utility/cost functions are important
  - eg. money, life years, quality adjusted life years, etc.

Predictive performance

- We need to choose the utility/cost function
- Application specific utility/cost functions are important
  - eg. money, life years, quality adjusted life years, etc.
- If are interested overall in the goodness of the predictive distribution, or we don't know (yet) the application specific utility, then good information theoretically justified choice is log-score

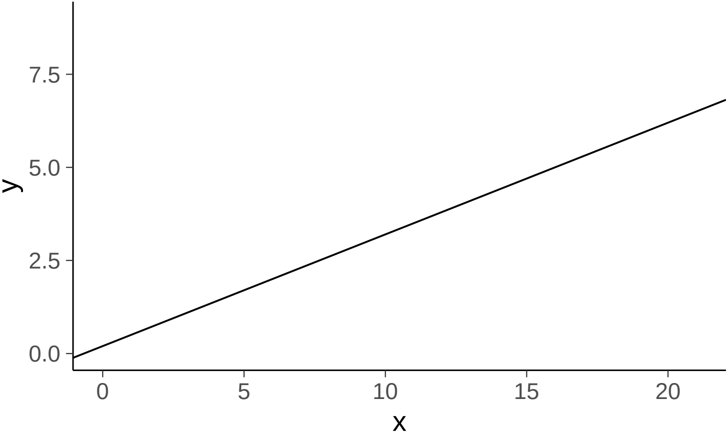
$$\log p(y^{\mathrm{rep}}|y, M),$$

- What is cross-validation
  - Leave-one-out cross-validation (elpd_loo, p_loo)
  - Uncertainty in LOO (SE)
- When is cross-validation applicable?
  - data generating mechanisms and prediction tasks
  - leave-many-out cross-validation
- Fast cross-validation
  - PSIS and diagnostics in loo package (Pareto k, n_eff, Monte Carlo SE)
  - K-fold cross-validation
- Related methods (WAIC, *IC, BF)
- Model comparison and selection (elpd_diff, se)
- Model averaging with Bayesian stacking

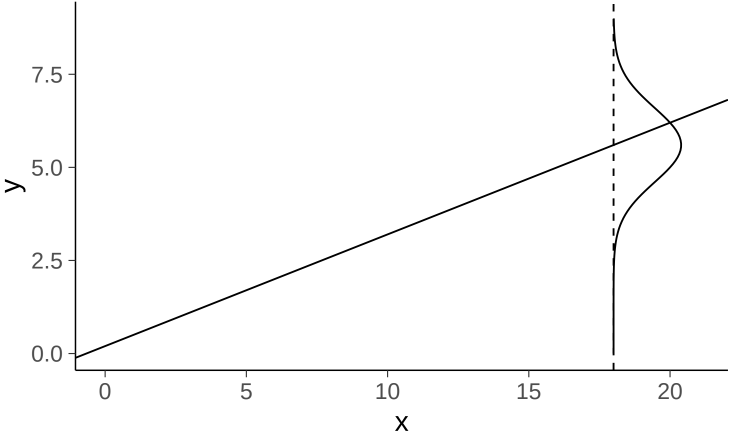
Stan and `loo` package

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

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

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

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

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

elpd_diff        se
     -0.2       0.1
```

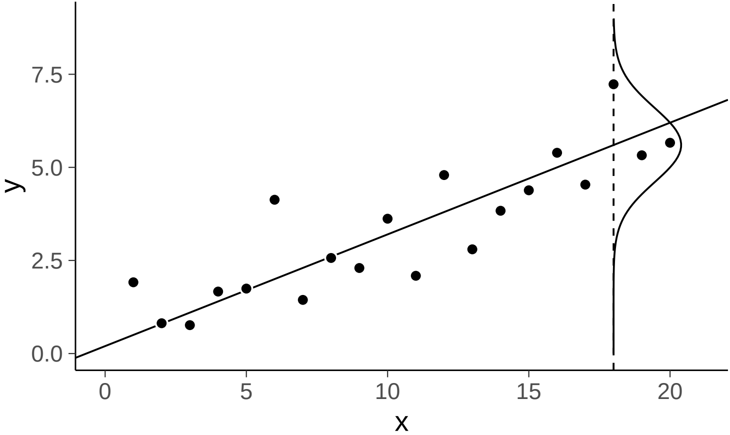
True mean y = a + bx



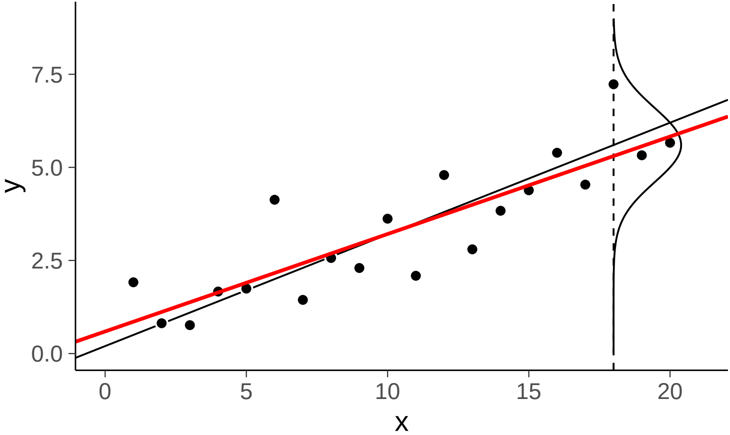
True mean and sigma



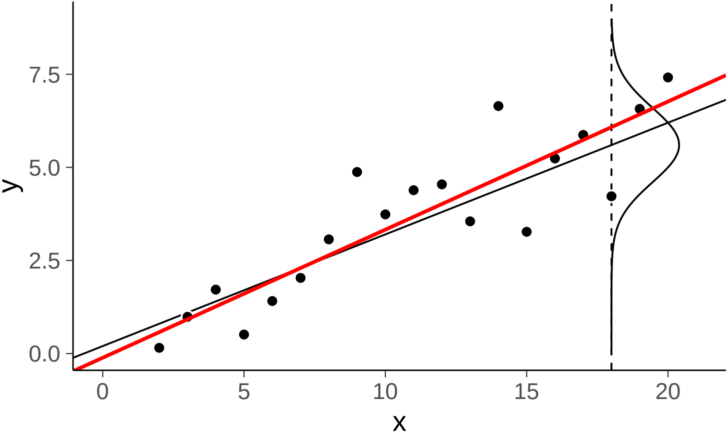
Data



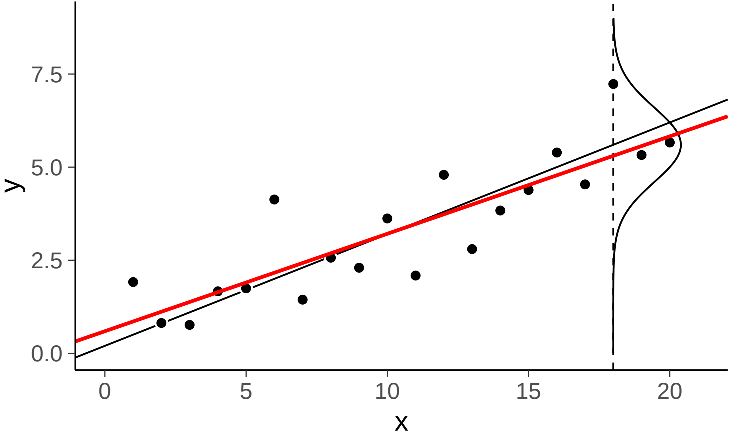
Posterior mean



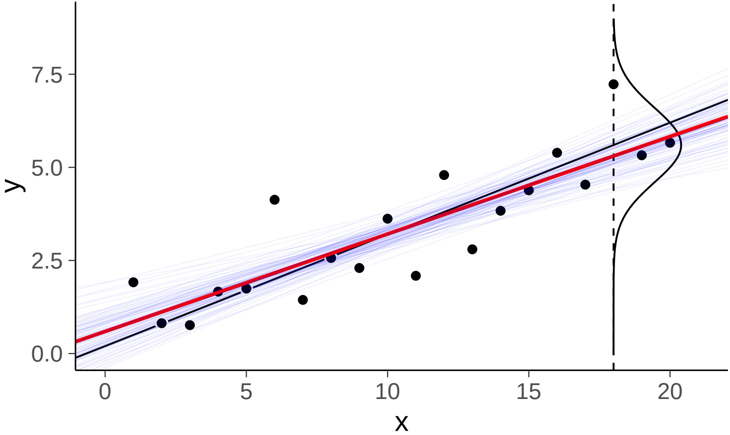
Posterior mean, alternative data realisation



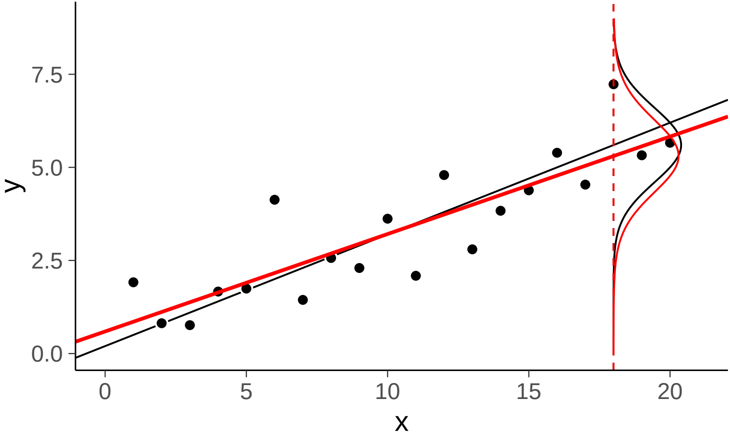
Posterior mean



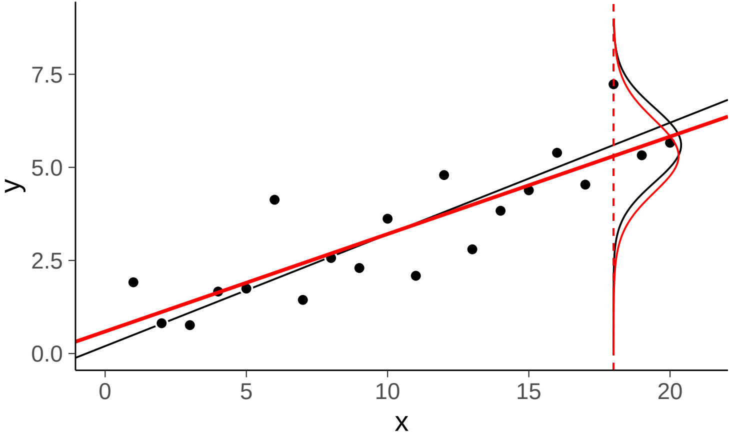
Posterior draws



Posterior predictive distribution

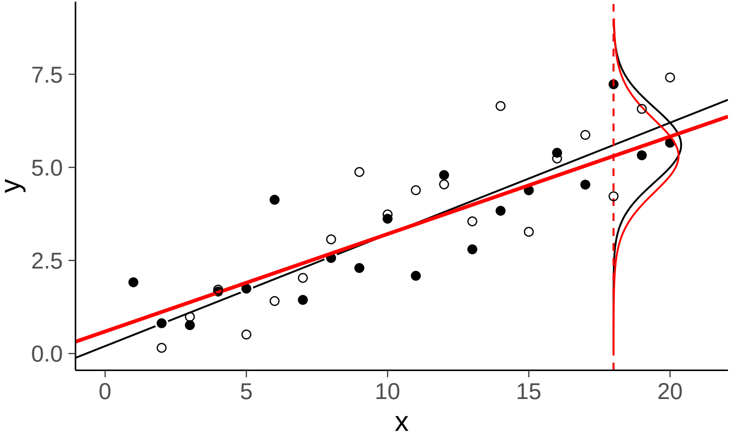


Posterior predictive distribution

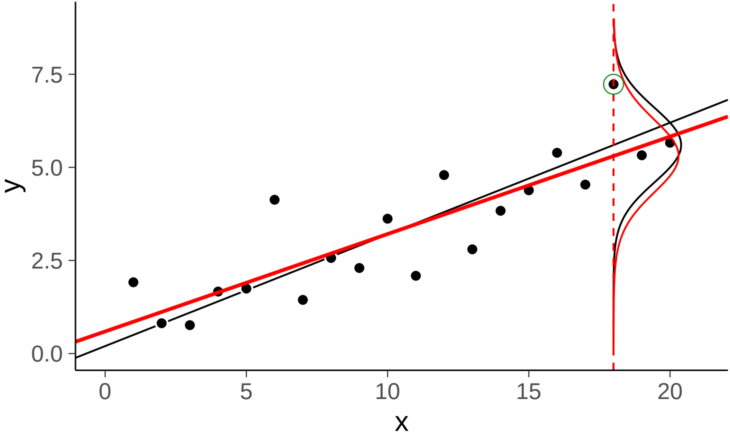


$$p(\tilde{y}|\tilde{x} = 18, x, y) = \int p(\tilde{y}|\tilde{x} = 18, \theta)p(\theta|x, y)d\theta$$

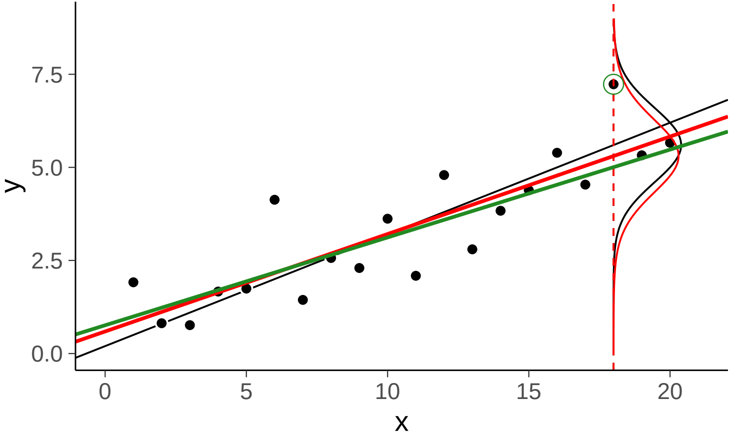
New data



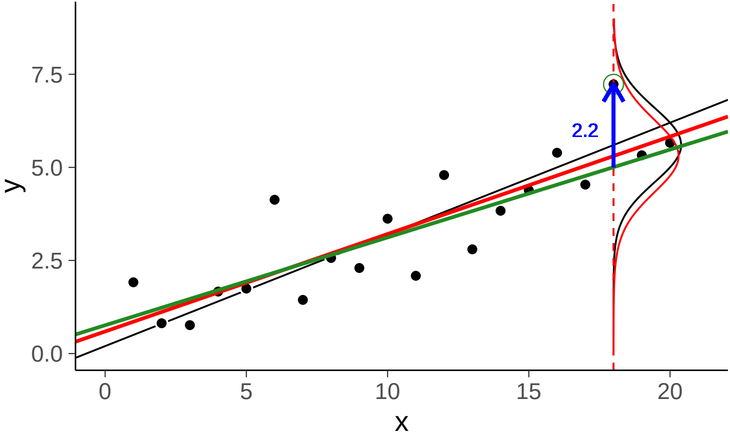
Posterior predictive distribution

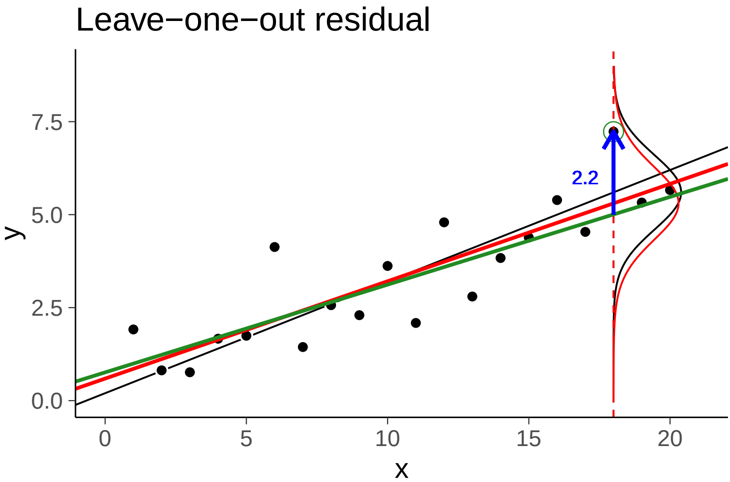


Leave−one−out mean

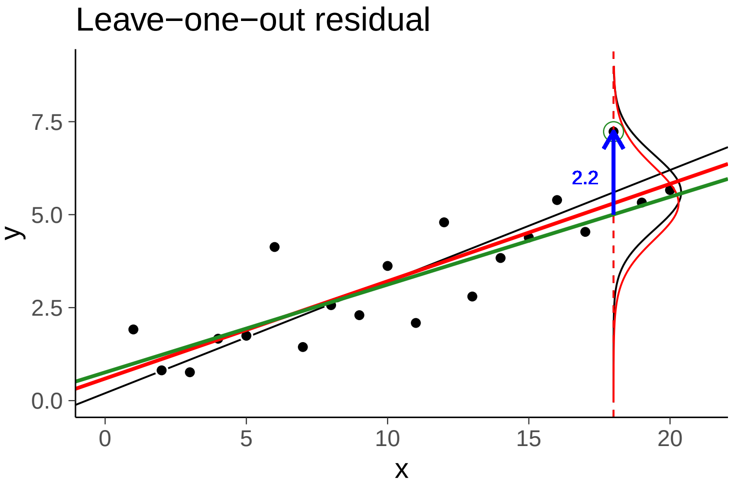


Leave−one−out residual



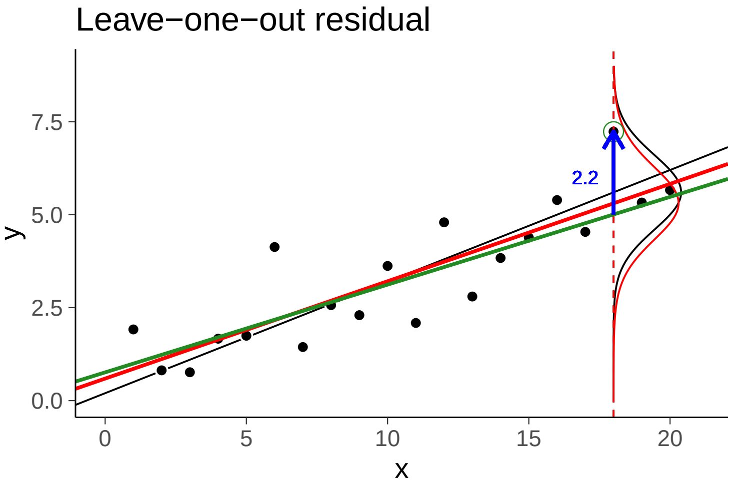


$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$



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

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

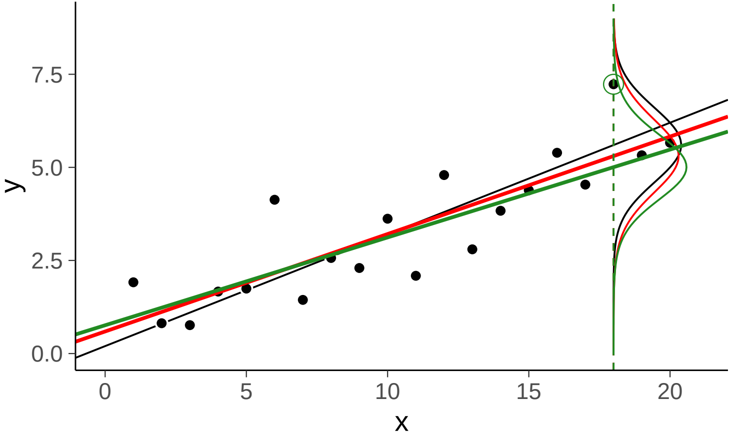


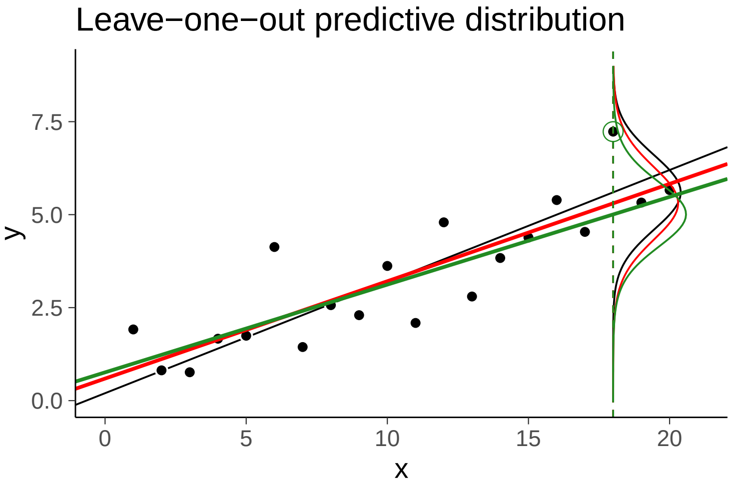
$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$

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

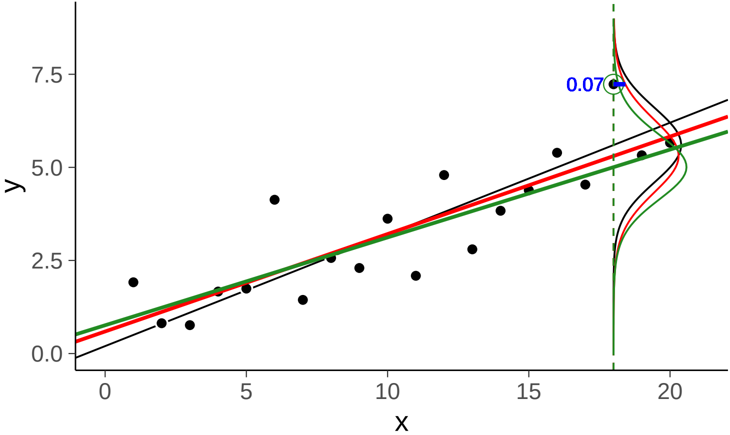
Leave−one−out predictive distribution



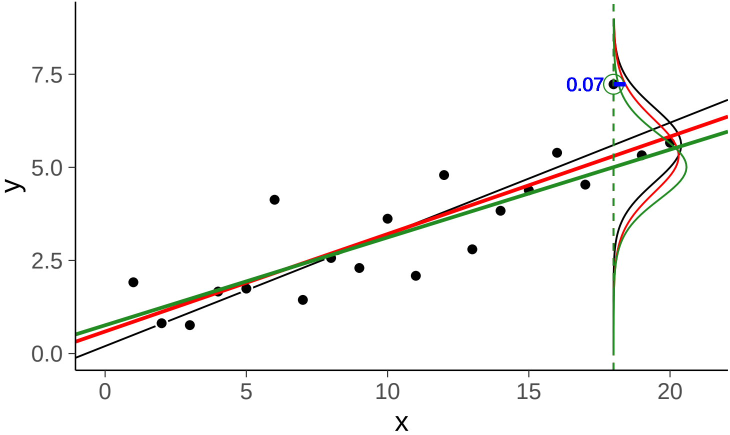


$$p(\tilde{y}|\tilde{x}=18, x_{-18}, y_{-18}) = \int p(\tilde{y}|\tilde{x}=18,\theta)p(\theta|x_{-18},y_{-18})d\theta$$

Posterior predictive density

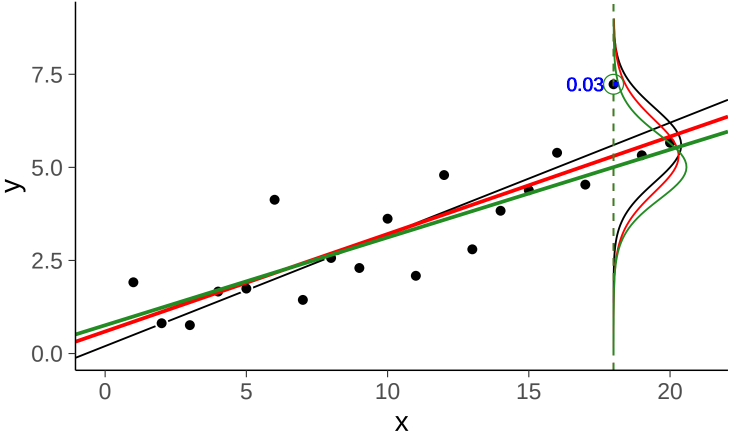


Posterior predictive density



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

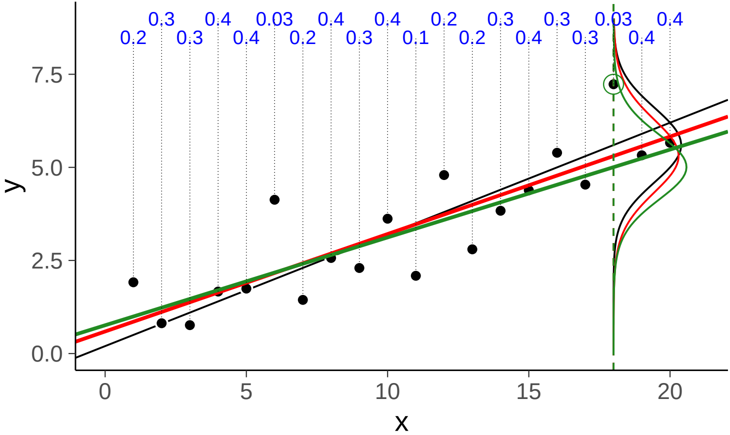
Leave−one−out predictive density



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

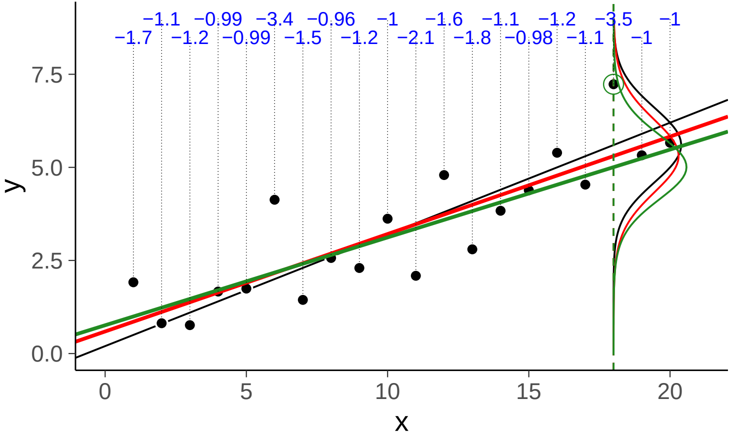
$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$

Leave−one−out predictive densities



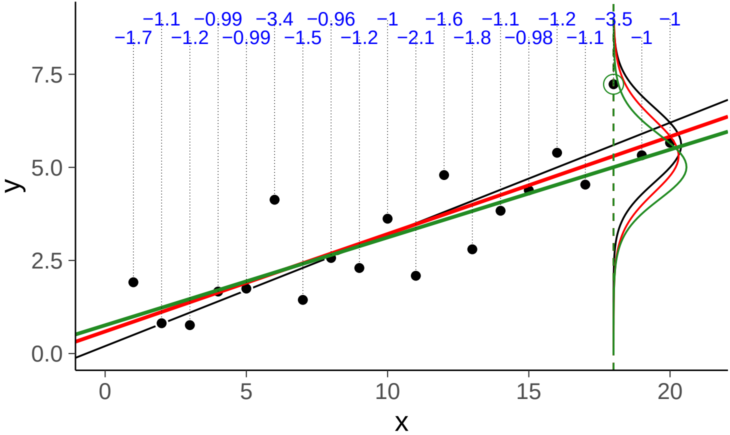
$p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$

Leave−one−out log predictive densities

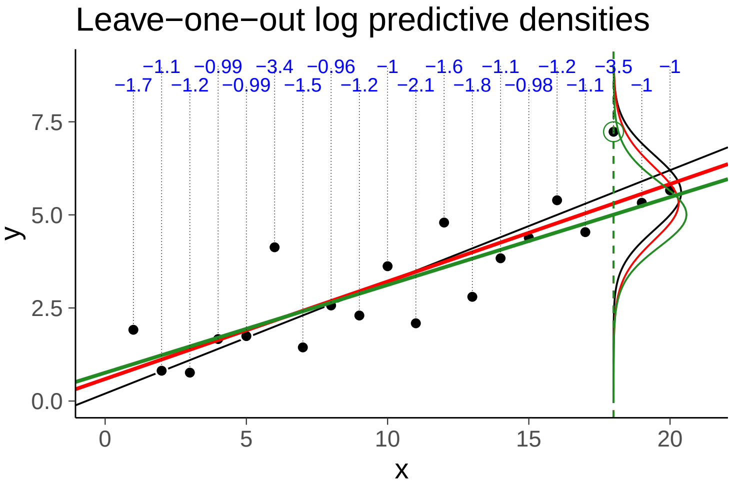


$\log p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$

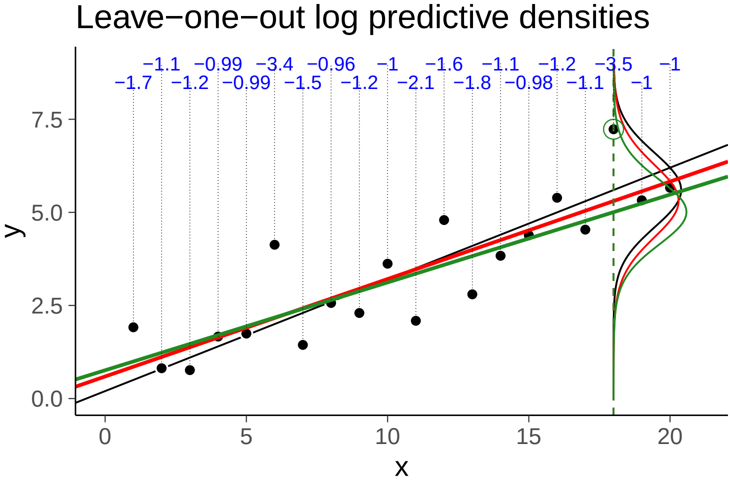
Leave−one−out log predictive densities



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



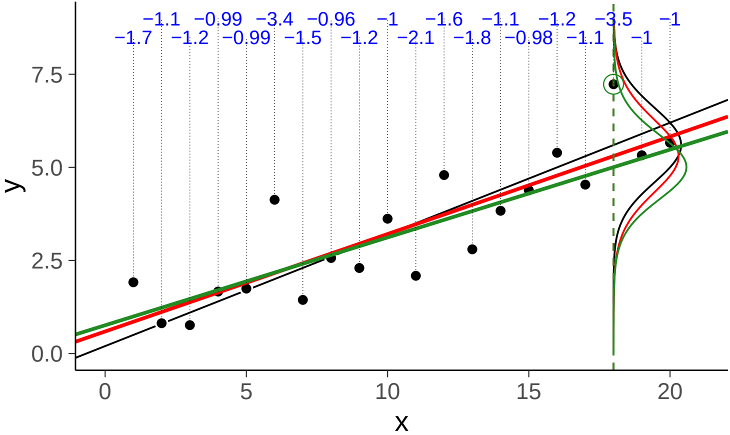
$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$



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

unbiased estimate of log posterior pred. density for new data

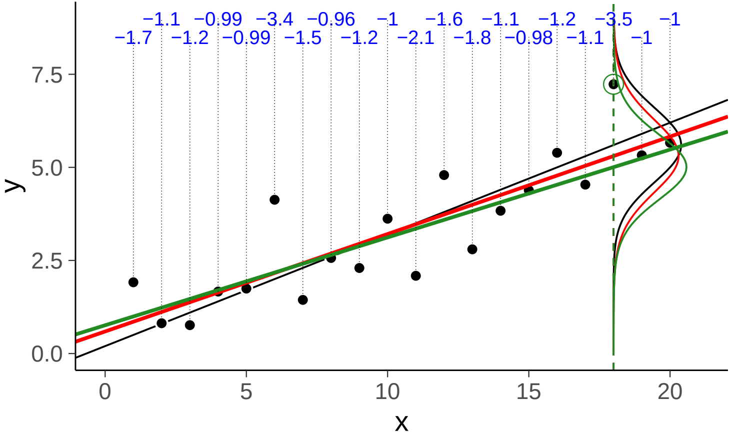
Leave−one−out log predictive densities



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

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

Leave−one−out log predictive densities

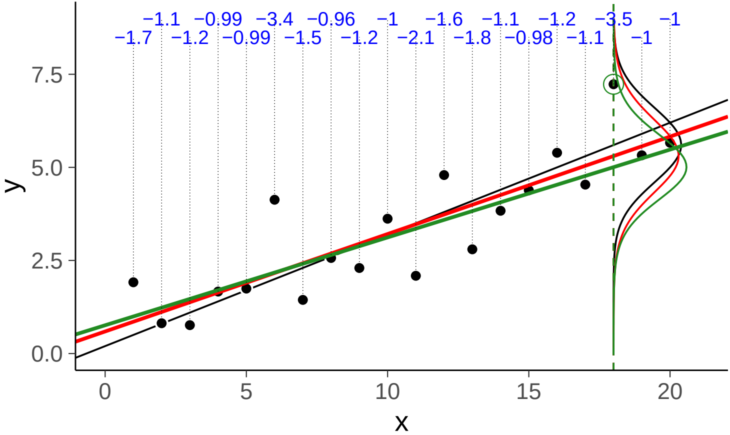


$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$

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

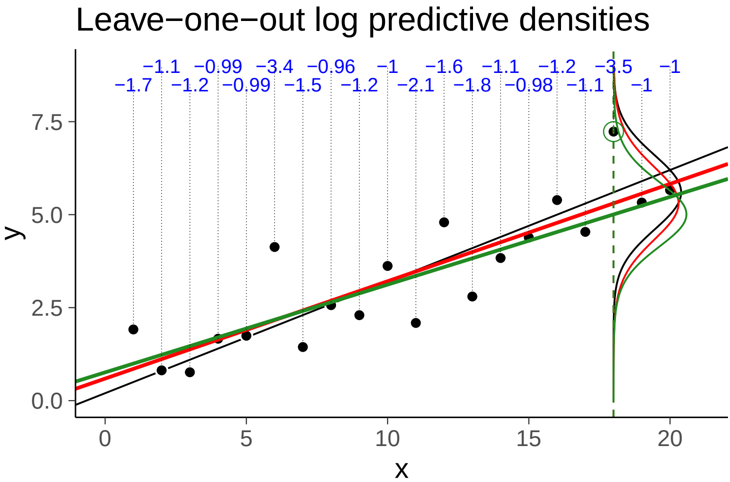
$\text{p\_loo} = \text{lpd} - \text{elpd\_loo} \approx 2.7$

Leave−one−out log predictive densities



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

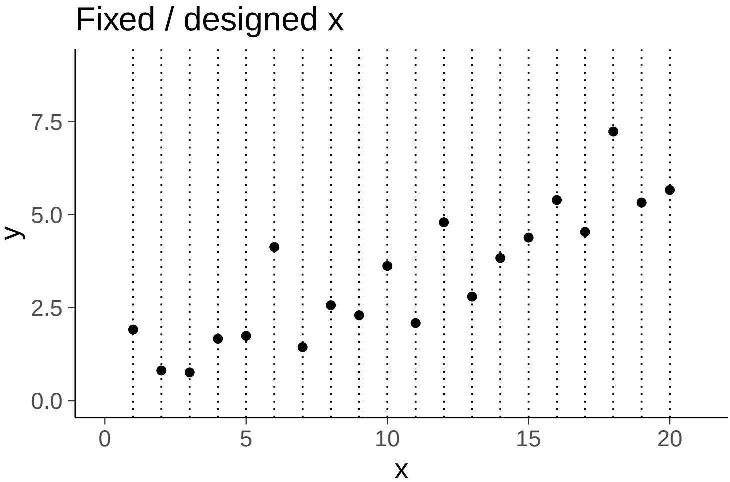
$$\text{SE} = \text{sd}(\log p(y_i|x_i, x_{-i}, y_{-i})) \cdot \sqrt{20} \approx 3.3$$



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

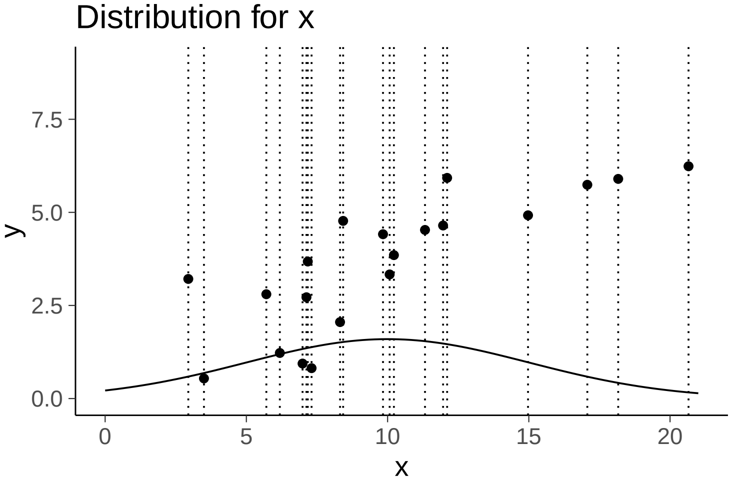
$$\text{SE} = \text{sd}(\log p(y_i|x_i, x_{-i}, y_{-i})) \cdot \sqrt{20} \approx 3.3$$

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



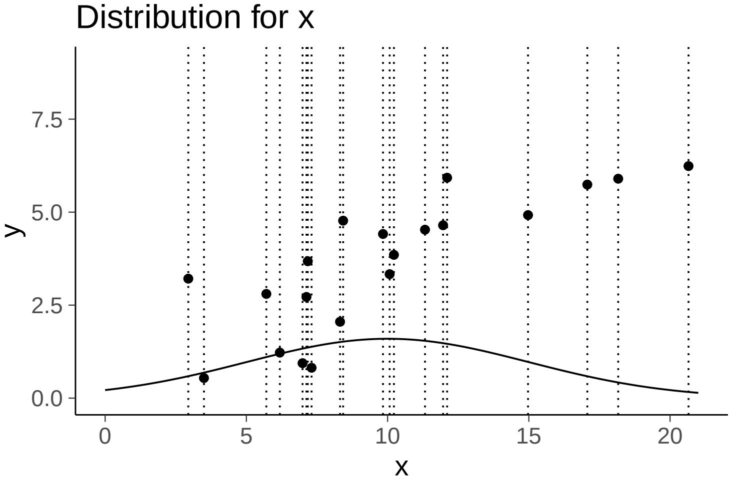
LOO is ok for fixed / designed x. SE is uncertainty about $y|x$.

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/



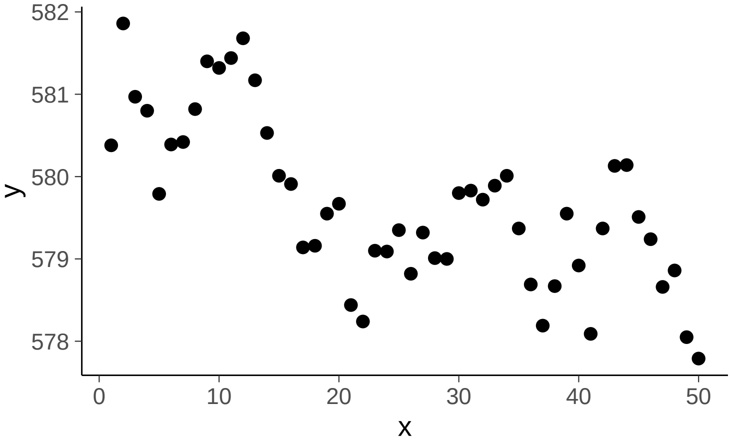
LOO is ok for random x. SE is uncertainty about $y|x$ and x.

Covariate shift can be handled with importance weighting or modelling

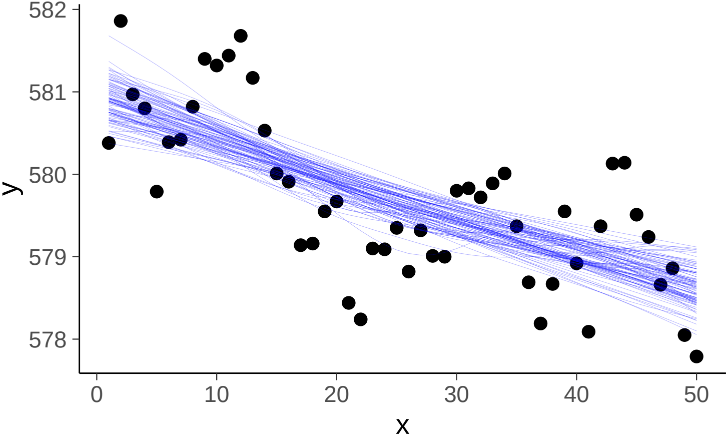
see Vehtari & Ojanen (2012) and andrewgelman.com/2018/08/03/loo-cross-validation-approaches-valid/

`loo` package

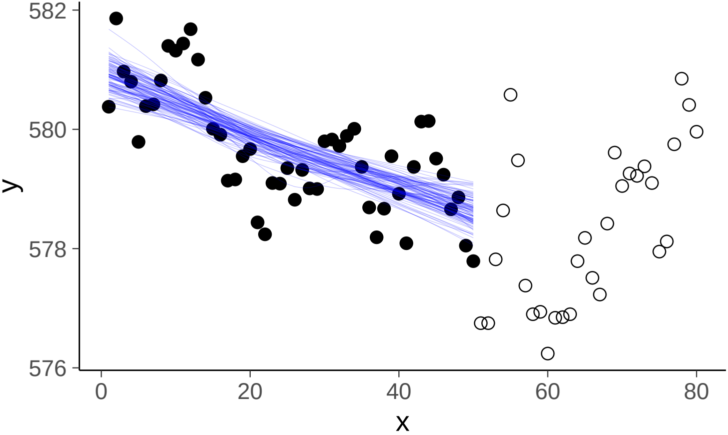
```
Computed from 4000 by 20 log-likelihood matrix

         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.
```

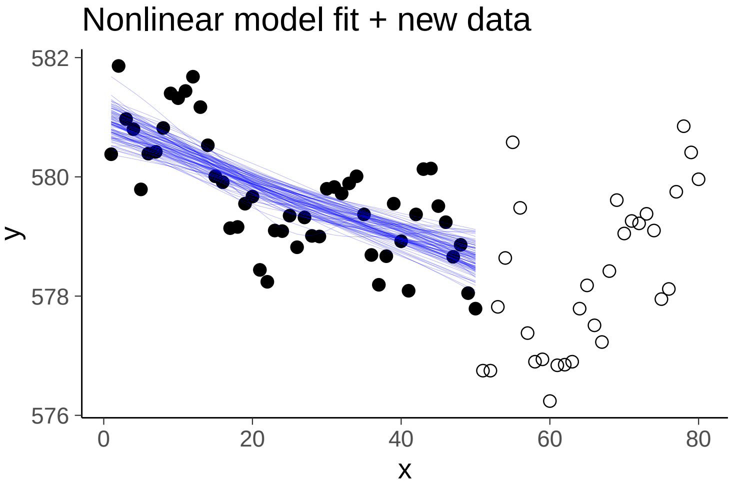

582
581
580
579
578
y
0
10
20
30
40
50
x

Nonlinear model fit

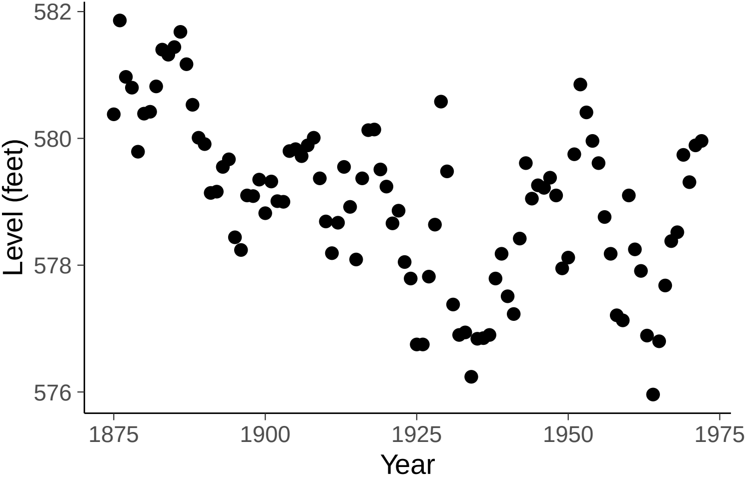


Nonlinear model fit + new data

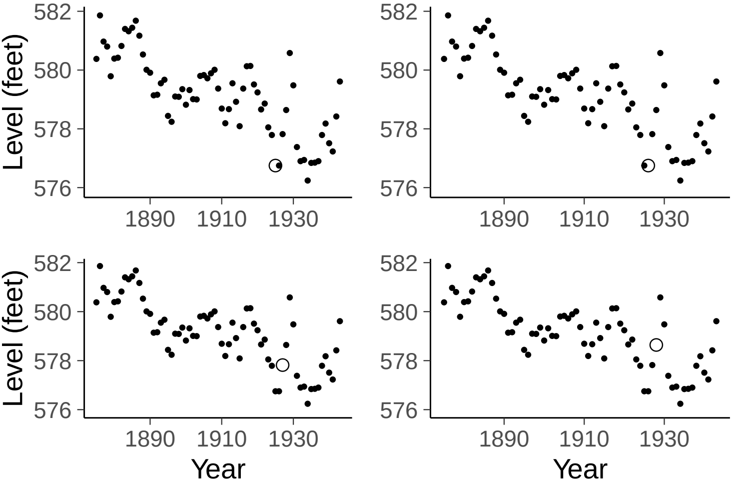




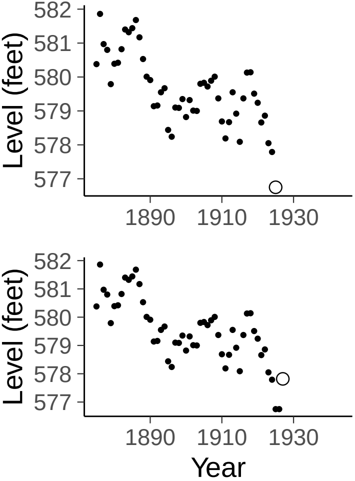
Extrapolation is more difficult



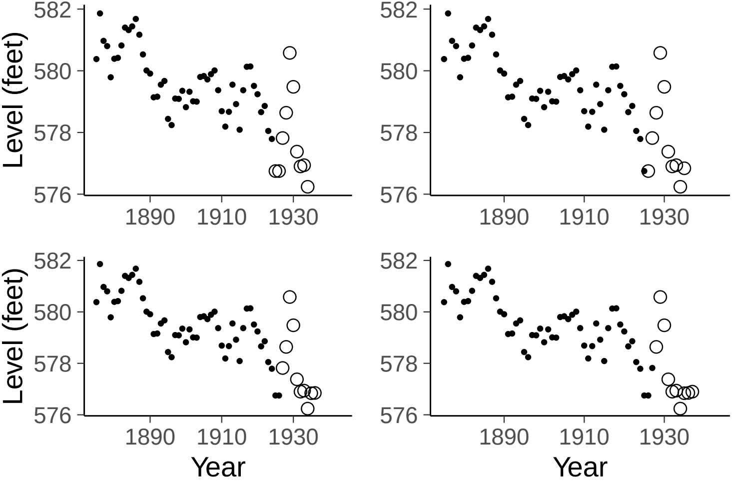
Can LOO or other cross-validation be used with time series?



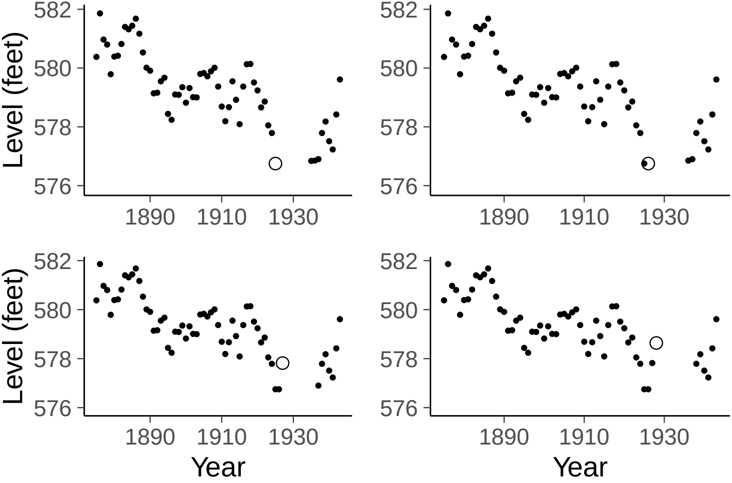
Leave-one-out cross-validation is ok for assessing conditional model



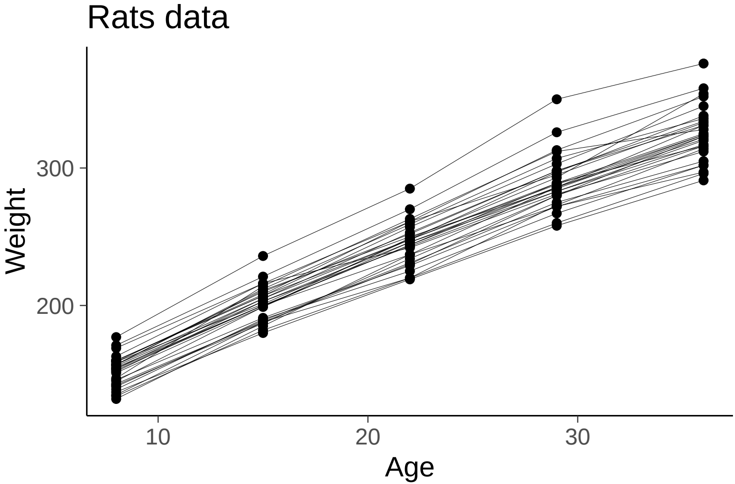
Leave-future-out cross-validation is better for predicting future



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

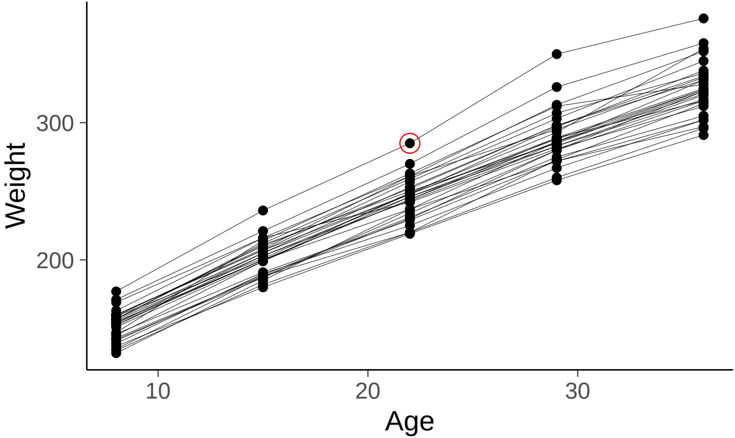


m-step-ahead leave-a-block-out cross-validation



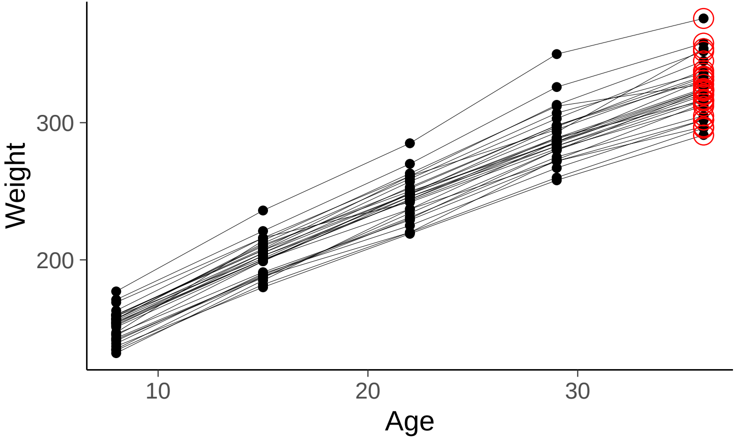
Can LOO or other cross-validation be used with hierarchical data?

Leave−one−out?



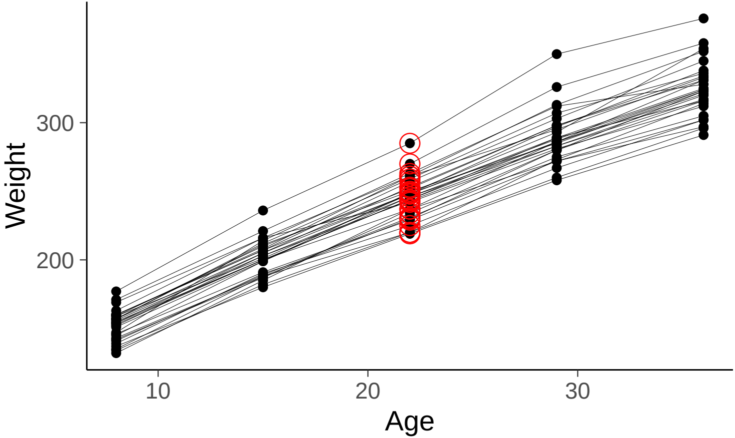
Yes!

1−step−ahead?



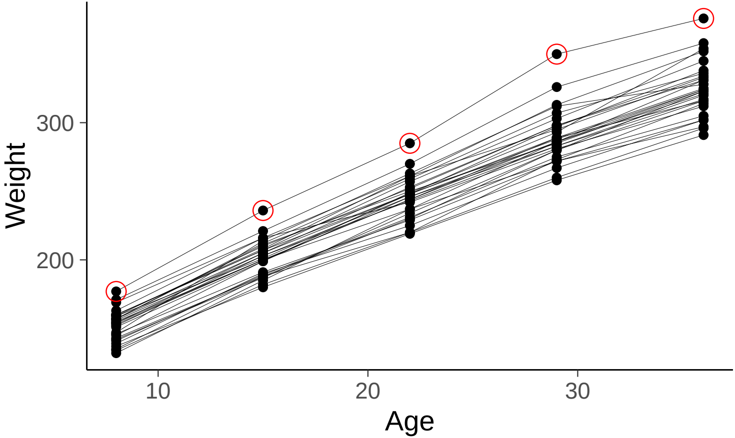
Yes!

Leave−one−time−point−out?



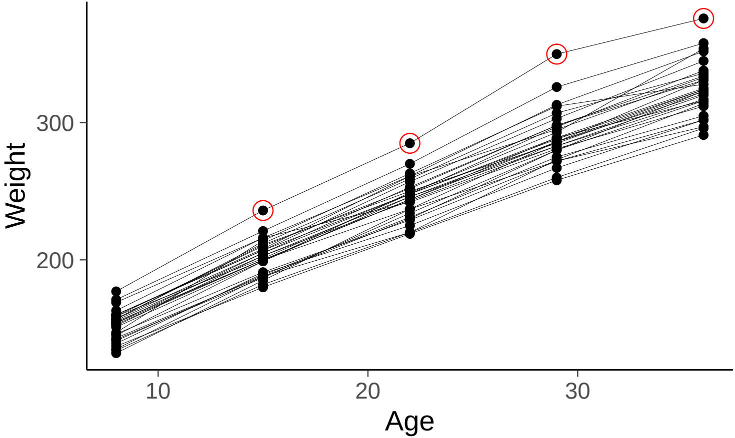
Yes!

Leave−one−rat−out?



Yes!

Predict given initial weight?



Yes!

Summary of data generating mechanisms and prediction tasks

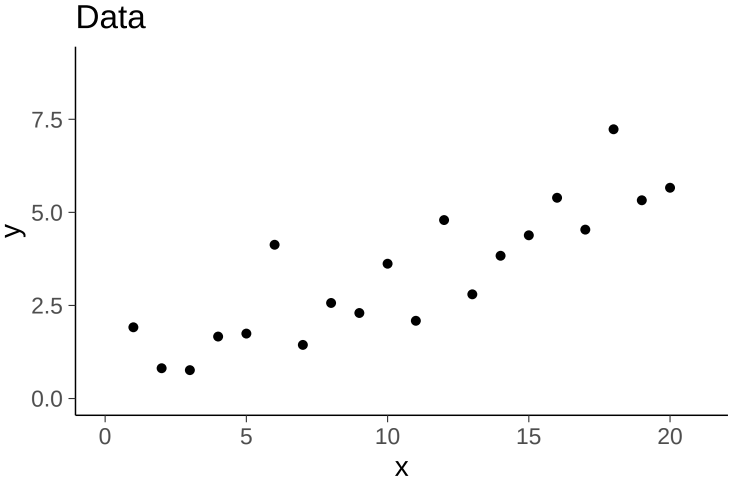
- You have to make some assumptions on data generating mechanism
- Use the knowledge of the prediction task if available
- Cross-validation can be used to analyse different parts, even if there is no clear prediction task

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

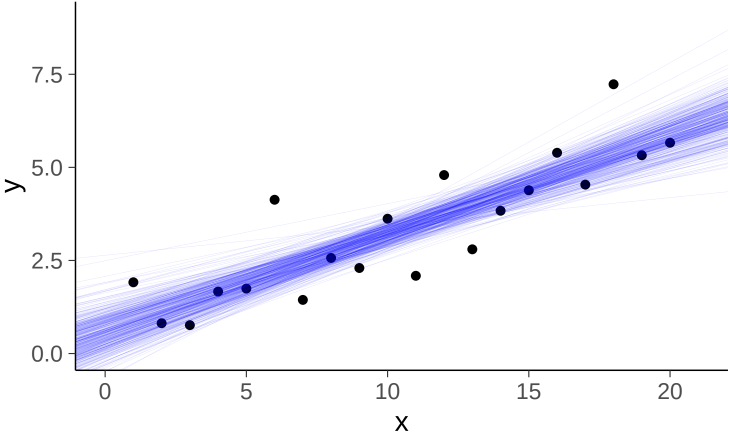
Fast cross-validation

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

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

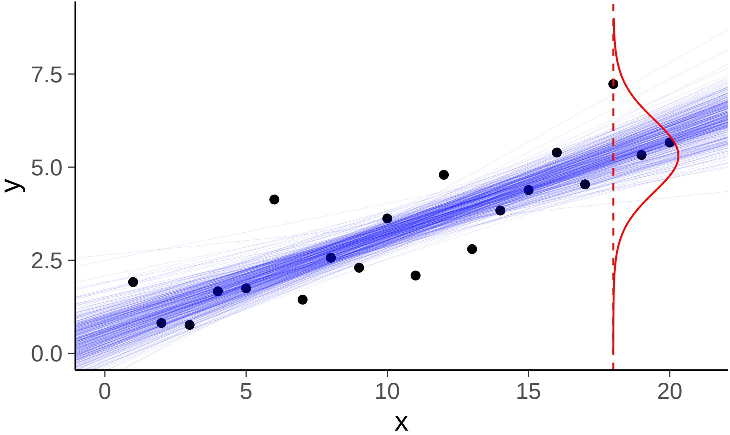

Data
7.5
5.0
2.5
0.0
y
0
5
10
15
20
x

Posterior draws



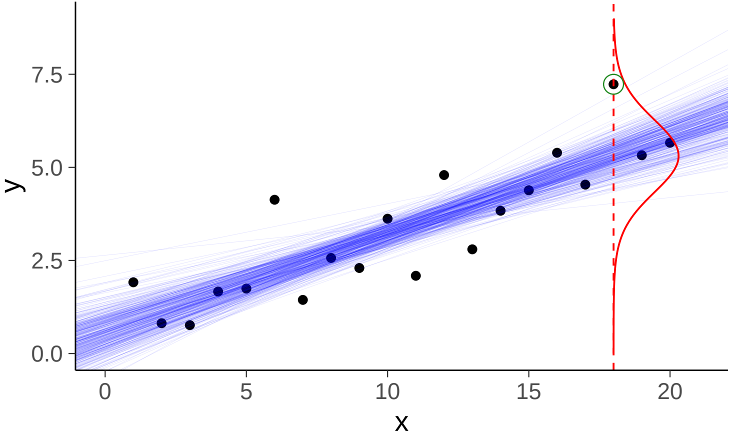
$\theta^{(s)} \sim p(\theta|x, y)$

Posterior predictive distribution



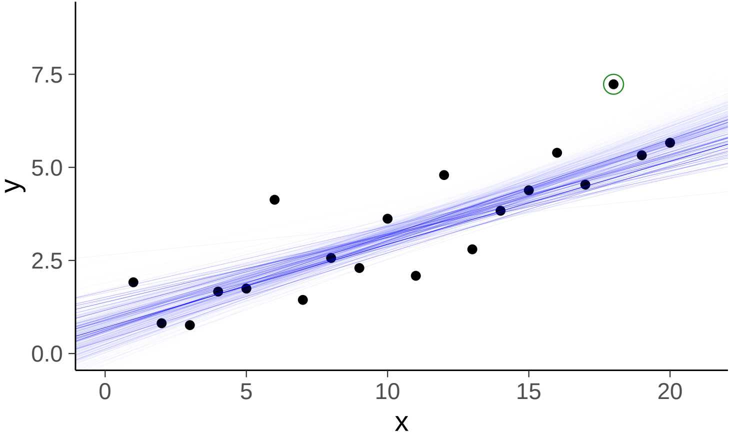
$$\theta^{(s)} \sim p(\theta|x, y), \quad p(\tilde{y}|\tilde{x}, x, y) \approx \frac{1}{S}\sum_{s=1}^{S} p(\tilde{y}|\tilde{x}, \theta^{(s)})$$

Posterior predictive distribution



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

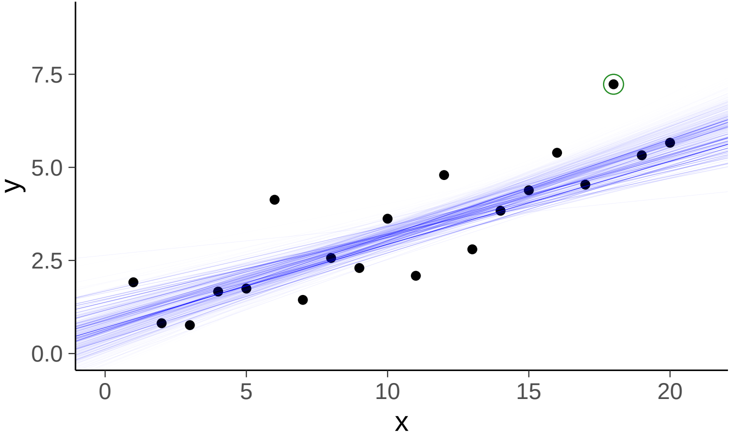
PSIS−LOO weighted draws



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

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

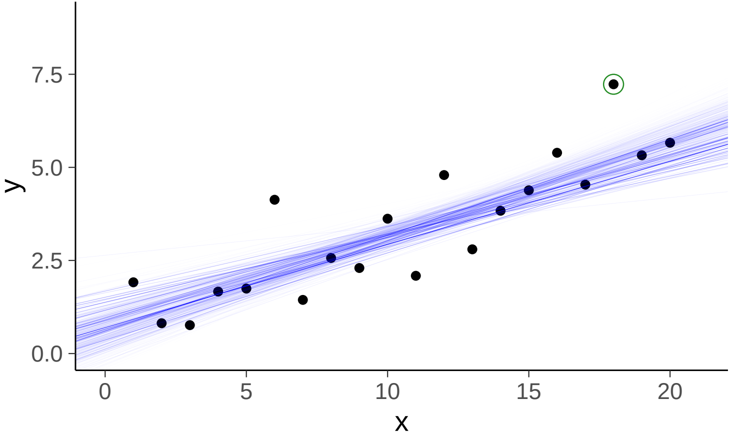
PSIS−LOO weighted draws



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

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

PSIS−LOO weighted draws

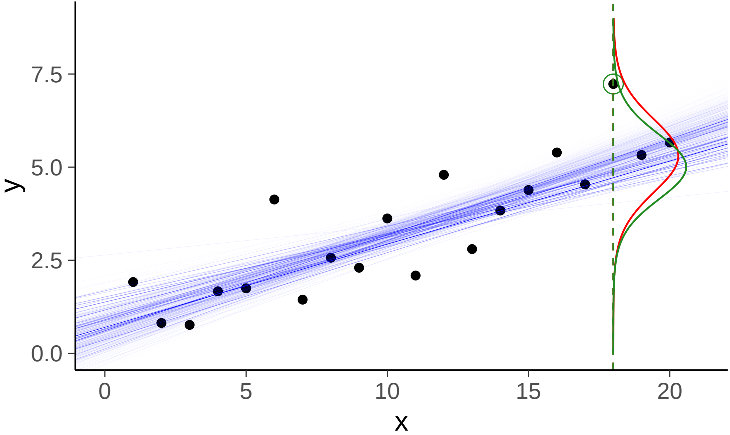


$\theta^{(s)} \sim p(\theta|x, y)$

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

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

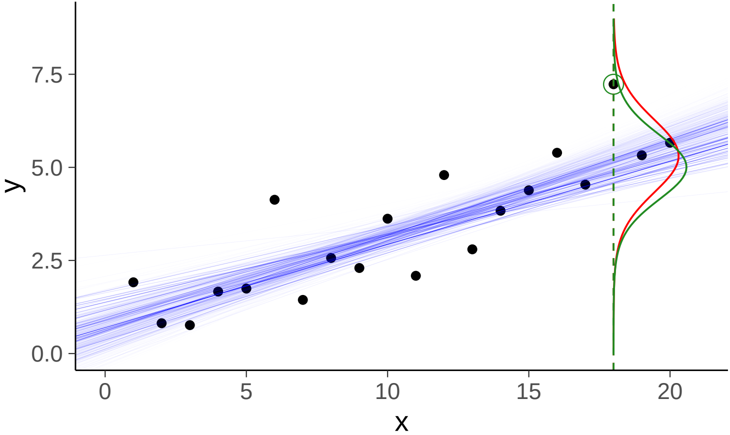
PSIS−LOO weighted predictive distribution



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

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

PSIS−LOO weighted predictive distribution

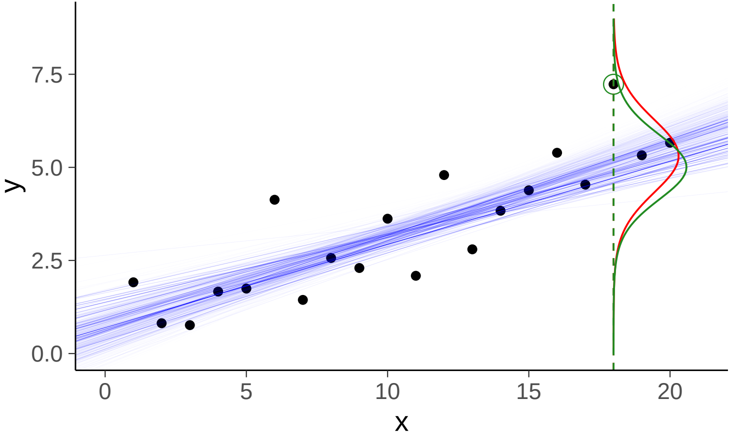


$\theta^{(s)} \sim p(\theta|x, y)$

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

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

PSIS−LOO weighted predictive distribution

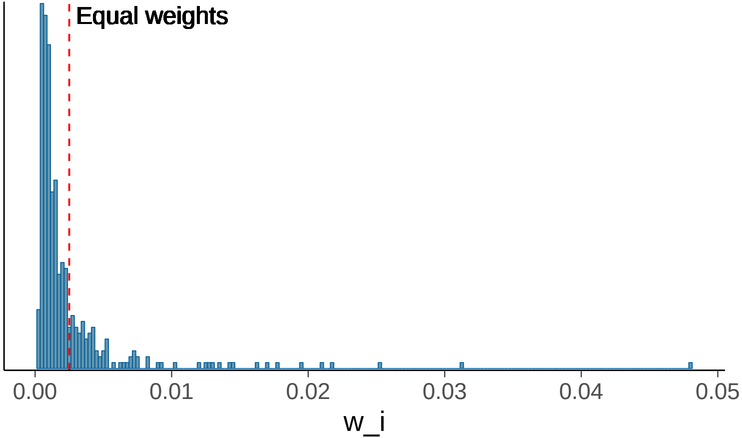


$\theta^{(s)} \sim p(\theta|x, y)$

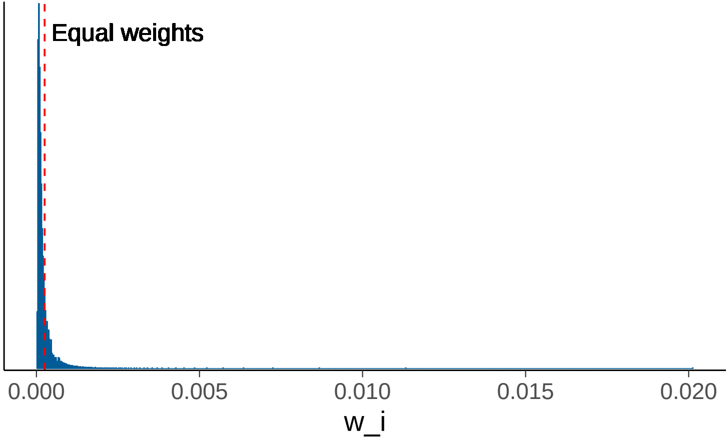
$r_i^{(s)} = p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y) \propto 1/p(y_i|x_i, \theta^{(s)})$

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

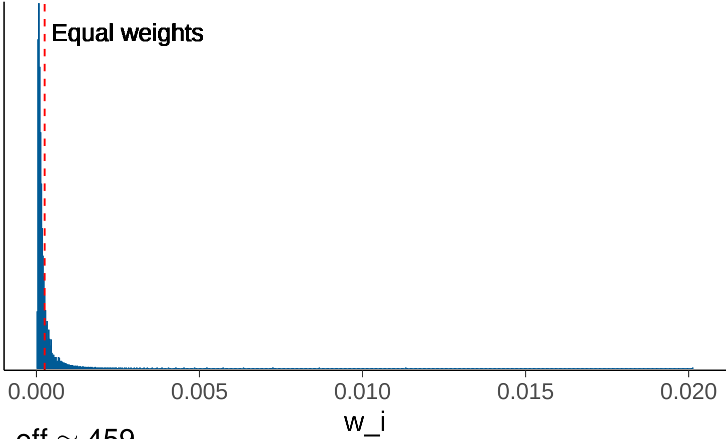
400 importance weights for leave−18th−out



4000 importance weights for leave−18th−out



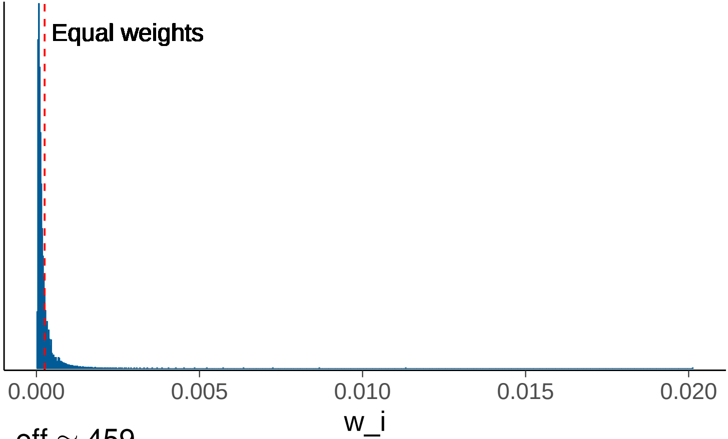
4000 importance weights for leave−18th−out



n_eff ≈ 459

see Vehtari, Gelman & Gabry (2017b)

4000 importance weights for leave−18th−out



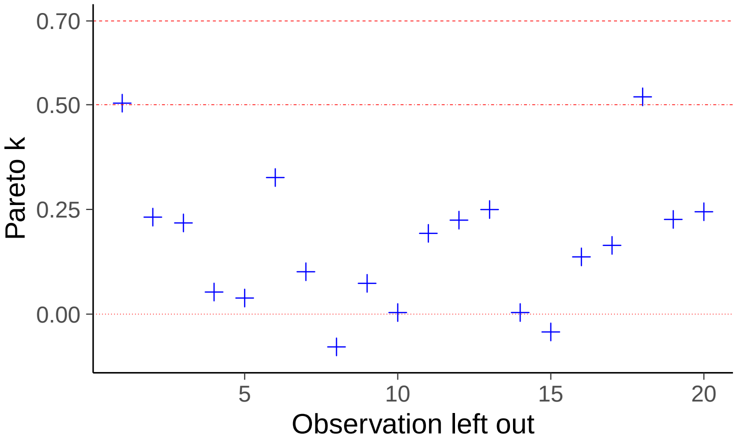
n_eff $\approx$ 459

Pareto $\hat{k} \approx 0.52$

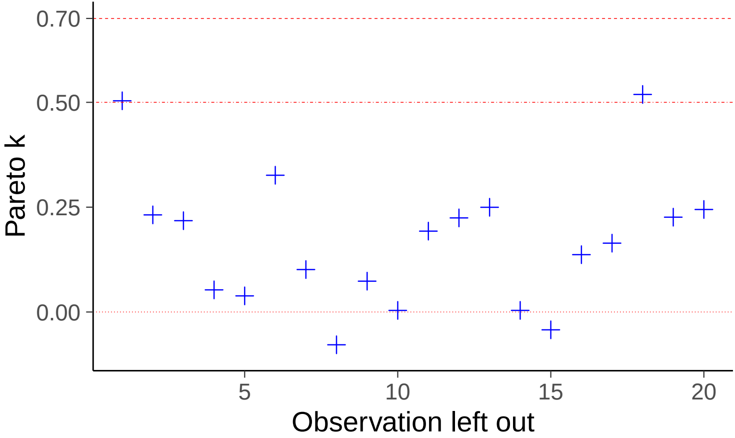
- Pareto $\hat{k}$ estimates the tail shape which determines the convergence rate of PSIS. Less than 0.7 is ok.

see Vehtari, Gelman & Gabry (2017b)

PSIS−LOO diagnostics

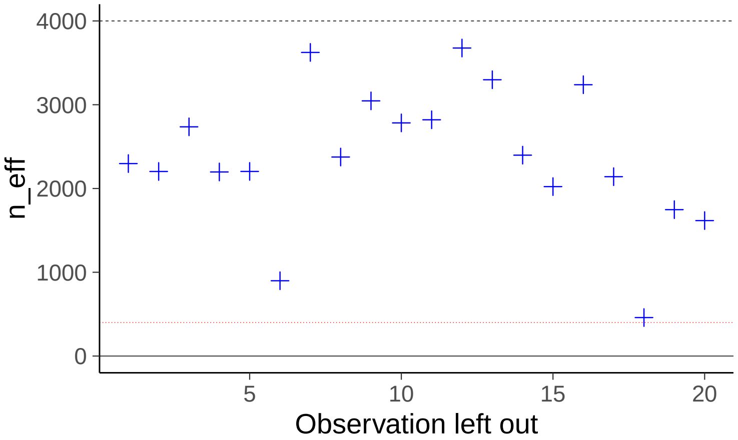


PSIS−LOO diagnostics




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

PSIS−LOO diagnostics




```
    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 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);
}
```

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);
}
```

- RStanARM and BRMS compute log_lik by default

Pareto smoothed importance sampling LOO

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

    see Merkel, Furr and Rabe-Hesketh (2018) for an approach using quadrature integration

Pareto smoothed importance sampling LOO

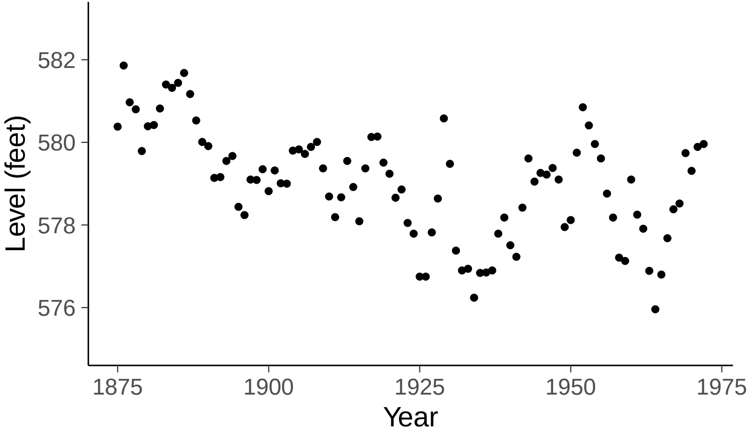
- PSIS-LOO for hierarchical models
  - leave-one-group out is challenging for PSIS-LOO

    see Merkel, Furr and Rabe-Hesketh (2018) for an approach using quadrature integration
- PSIS-LOO for non-factorizable models
  - mc-stan.org/loo/articles/loo2-non-factorizable.html

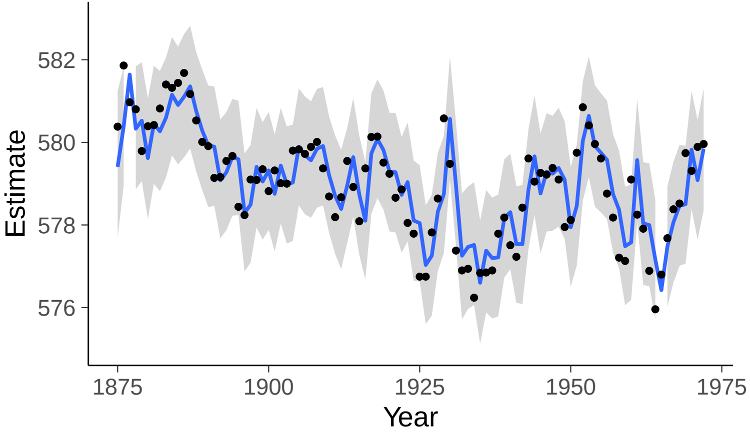
Pareto smoothed importance sampling LOO

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

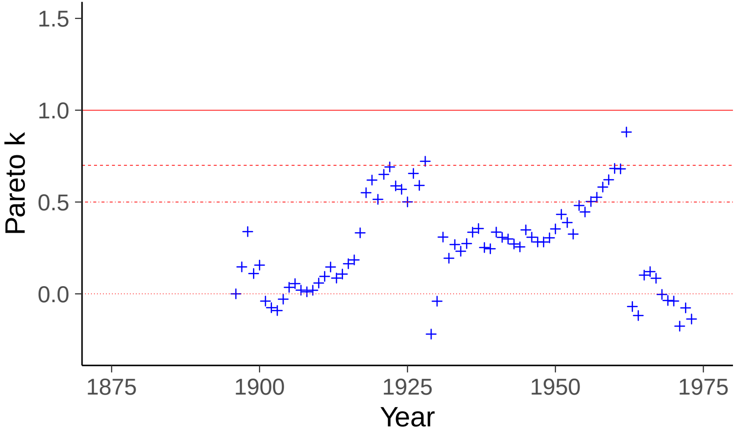
Data



AR−4 prediction with 95% interval



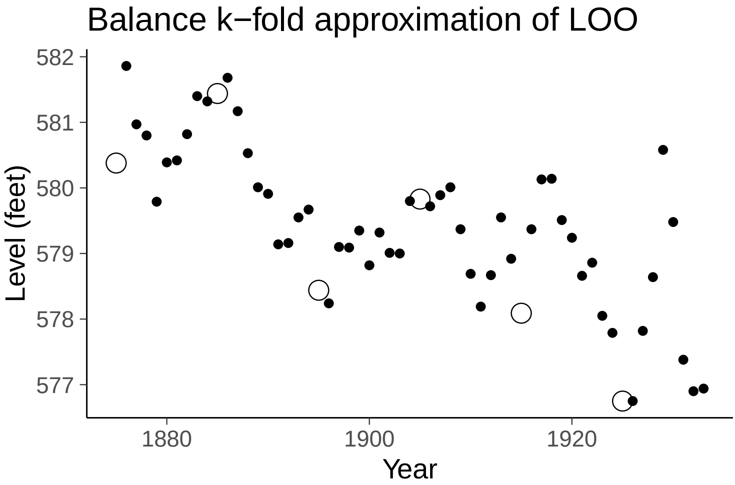
PSIS−1−step−ahead with refits



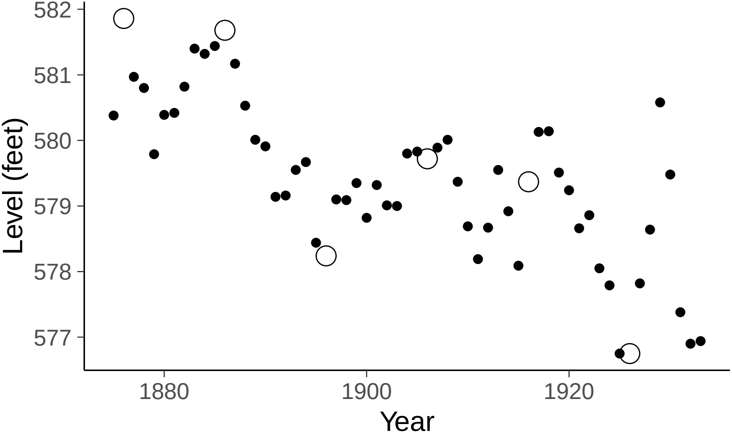
mc-stan.org/loo/articles/loo2-lfo.html

K-fold cross-validation

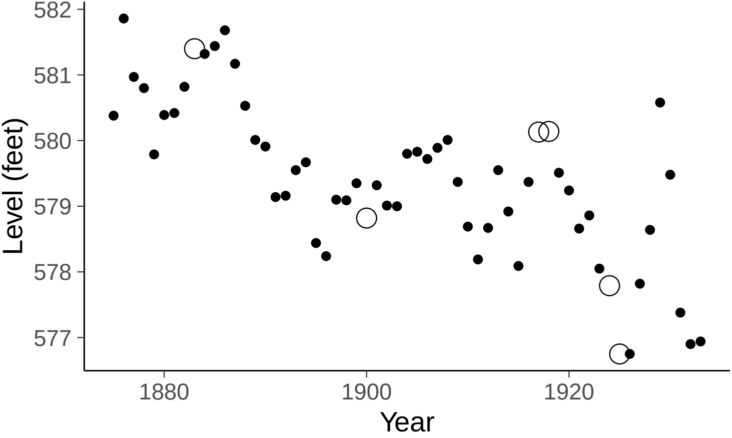
- K-fold cross-validation can approximate LOO
  - all uses for LOO
- K-fold cross-validation can be used for hierarchical models
  - good for leave-one-group-out
- K-fold cross-validation can be used for time series
  - with leave-block-out


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

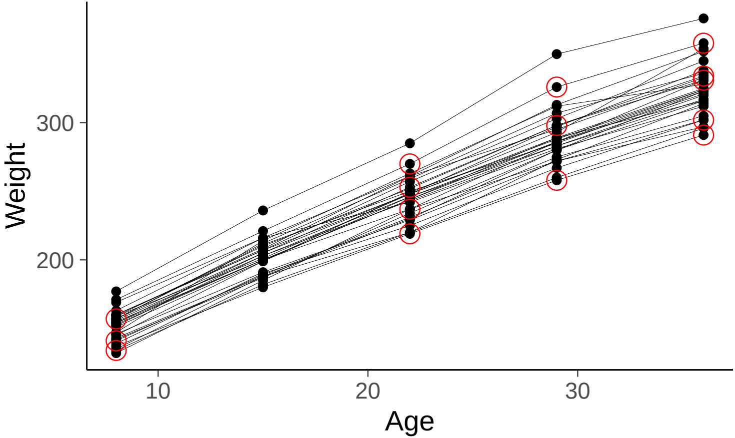
Balance k−fold approximation of LOO

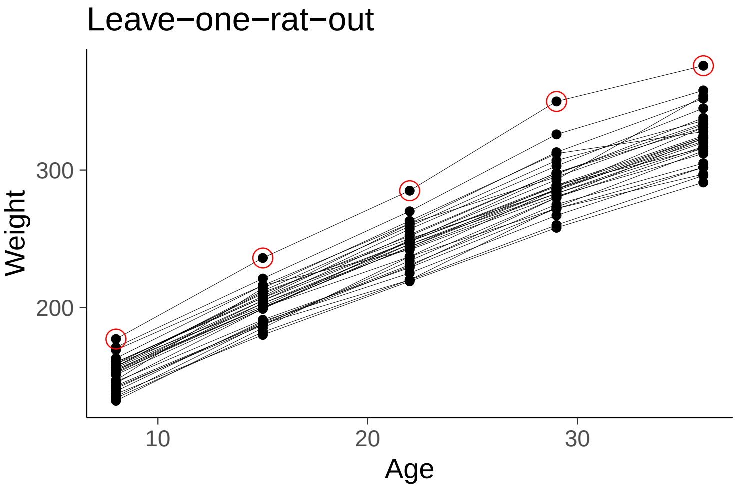


Random k−fold approximation of LOO



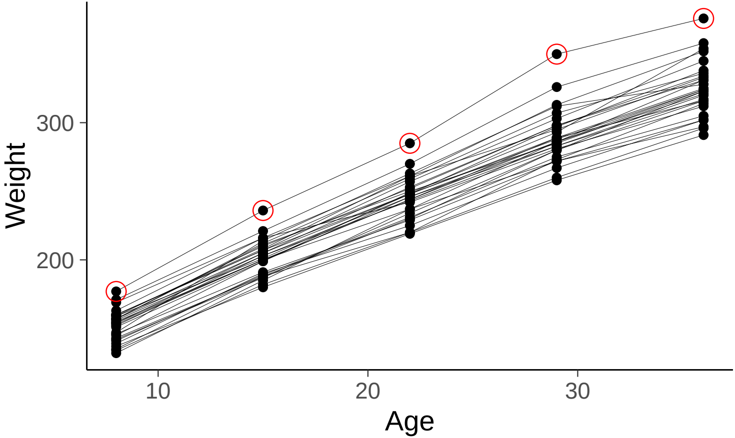
Random kfold approximation of LOO





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

Leave−one−rat−out



kfold_split_random()

kfold_split_balanced()

kfold_split_stratified()

WAIC vs PSIS-LOO

see Vehtari, Gelman & Gabry (2017a)

WAIC vs PSIS-LOO

- WAIC has same assumptions as LOO

see Vehtari, Gelman & Gabry (2017a)

WAIC vs PSIS-LOO

- WAIC has same assumptions as LOO
- PSIS-LOO is more accurate

see Vehtari, Gelman & Gabry (2017a)

WAIC vs PSIS-LOO

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

see Vehtari, Gelman & Gabry (2017a)

WAIC vs PSIS-LOO

- WAIC has same assumptions as LOO
- PSIS-LOO is more accurate
- PSIS-LOO has much better diagnostics
- LOO makes the prediction assumption more clear, which helps if K-fold-CV is needed instead

see Vehtari, Gelman & Gabry (2017a)

WAIC vs PSIS-LOO

- WAIC has same assumptions as LOO
- PSIS-LOO is more accurate
- PSIS-LOO has much better diagnostics
- LOO makes the prediction assumption more clear, which helps if K-fold-CV is needed instead
- Multiplying by -2 doesn't give any benefit (Watanabe didn't multiply by -2)

see Vehtari, Gelman & Gabry (2017a)

*IC

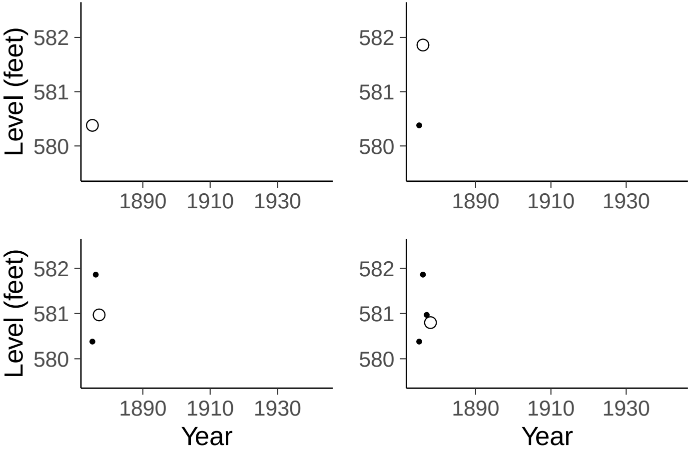
- AIC uses maximum likelihood estimate for prediction
- DIC uses posterior mean for prediction
- BIC is an approximation for marginal likelihood
- TIC, NIC, RIC, PIC, BPIC, QIC, AICc, ...

Marginal likelihood / Bayes factor

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

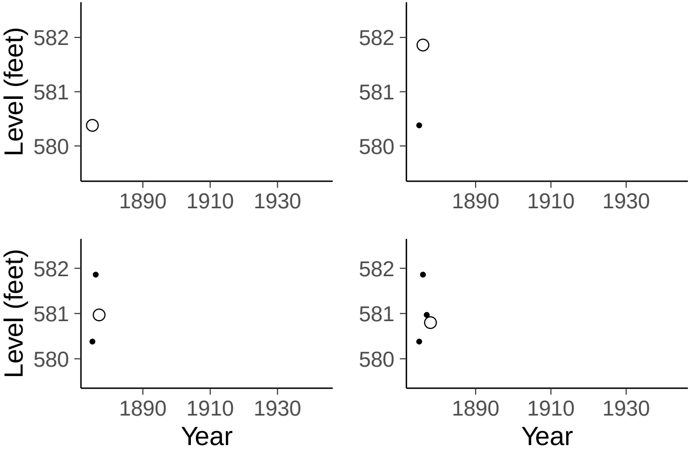
Marginal likelihood / Bayes factor

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



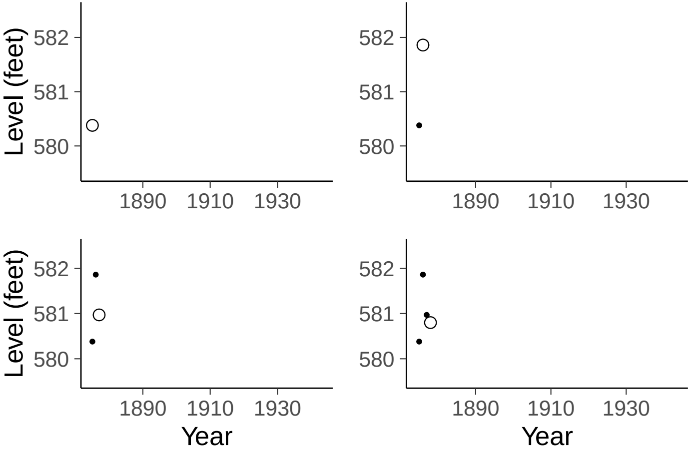
Marginal likelihood / Bayes factor

- Like leave-future-out 1-step-ahead cross-validation but starting with 0 observations
  - which makes it very sensitive to prior



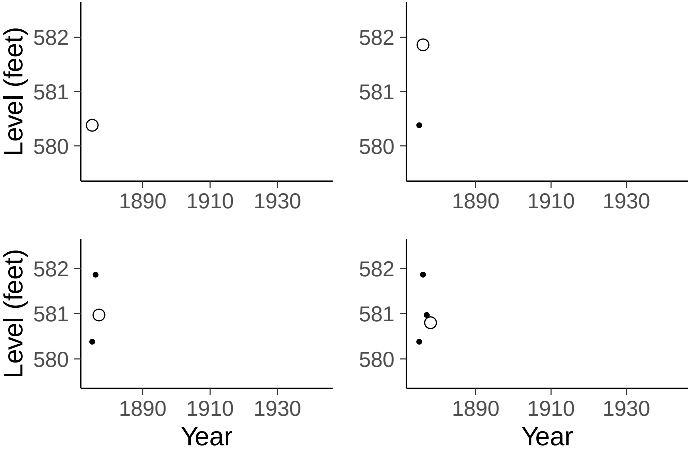
Marginal likelihood / Bayes factor

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



Marginal likelihood / Bayes factor

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



Cross-validation for model assessment

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

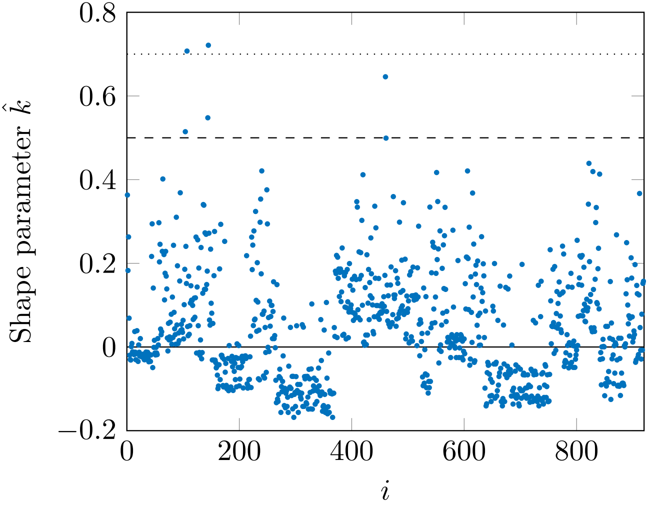
Cross-validation for model assessment

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

see demos avehtari.github.io/modelselection/

Radon example

PSIS-LOO diagnostics

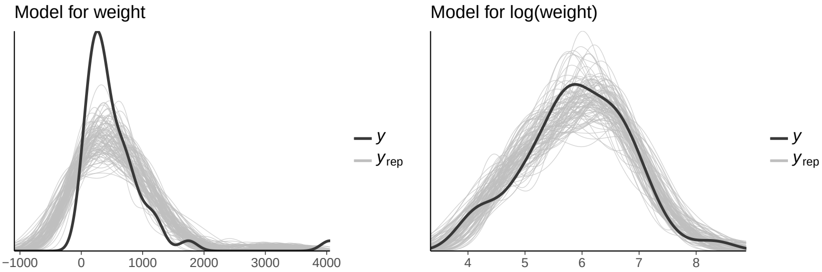


see Vehtari, Gelman & Gabry (2017a)

Sometimes cross-validation is not needed

Sometimes cross-validation is not needed

- Posterior predictive checking is often sufficient

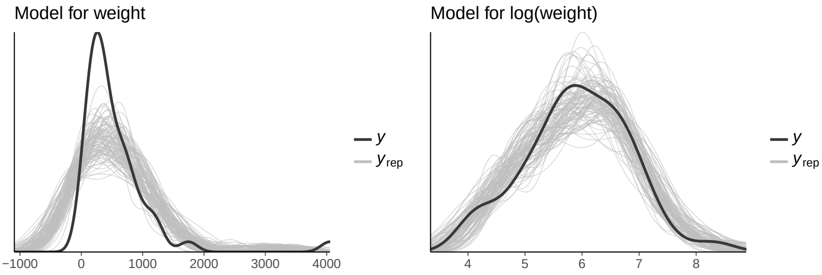


Predicting the yields of mesquite bushes.

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

Sometimes cross-validation is not needed

- Posterior predictive checking is often sufficient



Predicting the yields of mesquite bushes.

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

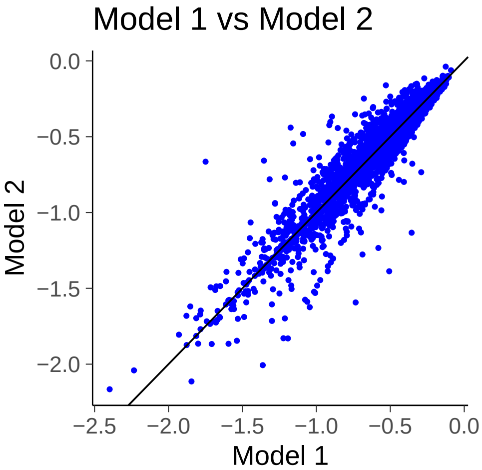
- BDA3, Chapter 6
- Gabry, Simpson, Vehtari, Betancourt, Gelman (2019). Visualization in Bayesian workflow. JRSS A, https://doi.org/10.1111/rssa.12378
- mc-stan.org/bayesplot/articles/graphical-ppcs.html
- betanalpha.github.io/assets/case_studies/principled_bayesian_workflow.html

Arsenic well example – Model comparison

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

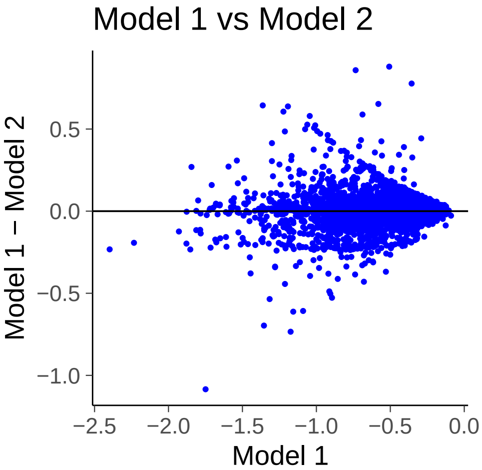
Gelman, Hill & Vehtari (2020): Regression and Other Stories, Chapter 13.

Arsenic well example – Model comparison



Model 1 elpd_loo $\approx$ -1952, SE=16
Model 2 elpd_loo $\approx$ -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

```
> loo_compare(model1, model2)
       elpd_diff se_diff
model2   0.0        0.0
model1 -14.4        6.1
```

`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).

Sometimes cross-validation is not needed

- For some very simple cases you may assume that true model is included in the list of models considered (M-closed)

Sometimes cross-validation is not needed

- For some very simple cases you may assume that true model is included in the list of models considered (M-closed)
  - see predictive model selection in M-closed case by San Martini and Spezzaferri (1984)

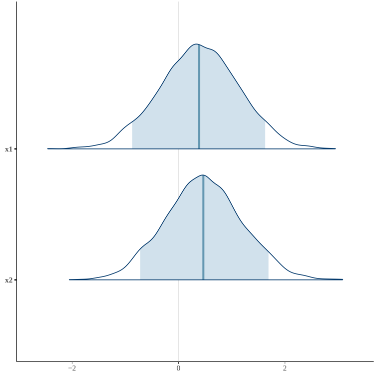
Sometimes cross-validation is not needed

- For some very simple cases you may assume that true model is included in the list of models considered (*M*-closed)
  - see predictive model selection in *M*-closed case by San Martini and Spezzaferri (1984)
  - but you should not force your design of experiment or analysis to stay in the simplified world

Sometimes cross-validation is not needed

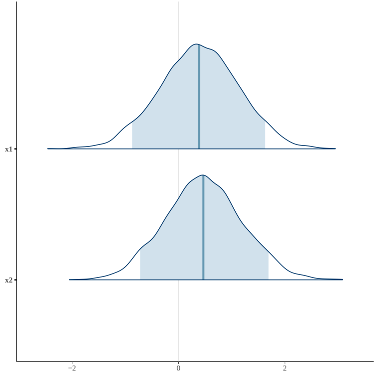
- For some very simple cases you may assume that true model is included in the list of models considered (M-closed)
  - see predictive model selection in M-closed case by San Martini and Spezzaferri (1984)
  - but you should not force your design of experiment or analysis to stay in the simplified world
- 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

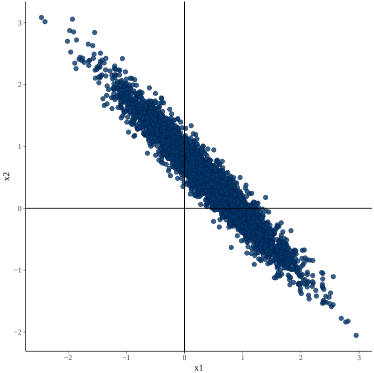


Marginal posterior intervals

Sometimes predictive model comparison can be useful



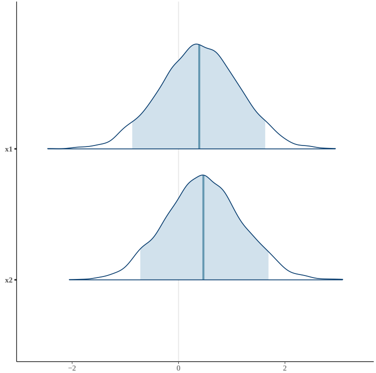
Marginal posterior intervals

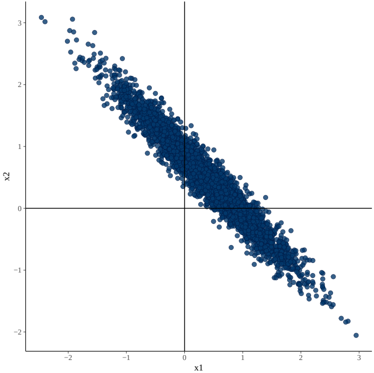


Joint posterior density

rstanarm + bayesplot

Sometimes predictive model comparison can be useful





Marginal posterior intervals   Joint posterior density

rstanarm + bayesplot

see also Collinear demo

What if one is not clearly better than others?

What if one is not clearly better than others?

- Continuous expansion including all models?
  - and then analyse the posterior distribution directly
    avehtari.github.io/modelselection/betablockers.html
  - sparse priors like regularized horseshoe prior instead of variable selection
    video, refs and demos at avehtari.github.io/modelselection/

What if one is not clearly better than others?

- Continuous expansion including all models?
  - and then analyse the posterior distribution directly
    avehtari.github.io/modelselection/betablockers.html
  - sparse priors like regularized horseshoe prior instead of variable selection
    video, refs and demos at avehtari.github.io/modelselection/
- Model averaging with BMA or Bayesian stacking?
  mc-stan.org/loo/articles/loo2-example.html

What if one is not clearly better than others?

- Continuous expansion including all models?
  - and then analyse the posterior distribution directly
    avehtari.github.io/modelselection/betablockers.html
  - sparse priors like regularized horseshoe prior instead of variable selection
    video, refs and demos at avehtari.github.io/modelselection/
- Model averaging with BMA or Bayesian stacking?
  mc-stan.org/loo/articles/loo2-example.html
- In a nested case choose simpler if assuming some cost for extra parts?
  andrewgelman.com/2018/07/26/
  parsimonious-principle-vs-integration-uncertainties/

What if one is not clearly better than others?

- Continuous expansion including all models?
  - and then analyse the posterior distribution directly
    avehtari.github.io/modelselection/betablockers.html
  - sparse priors like regularized horseshoe prior instead of variable selection
    video, refs and demos at avehtari.github.io/modelselection/
- Model averaging with BMA or Bayesian stacking?
  mc-stan.org/loo/articles/loo2-example.html
- In a nested case choose simpler if assuming some cost for extra parts?
  andrewgelman.com/2018/07/26/
  parsimonious-principle-vs-integration-uncertainties/
- In a nested case choose more complex if you want to take into account all the uncertainties.
  andrewgelman.com/2018/07/26/
  parsimonious-principle-vs-integration-uncertainties/

Model averaging

- Prefer continuous model expansion

Model averaging

- Prefer continuous model expansion
- If needed integrate over the model space = model averaging

Model averaging

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

Cross-validation and model selection

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

Cross-validation and model selection

- Cross-validation can be used for model selection if
  - small number of models
  - the difference between models is clear
- Do not use cross-validation to choose from a large set of models
  - selection process leads to overfitting

Cross-validation and model selection

- Cross-validation can be used for model selection if
  - small number of models
  - the difference between models is clear
- Do not use cross-validation to choose from a large set of models
  - selection process leads to overfitting
- Overfitting in selection process is not unique for cross-validation

Selection induced bias and overfitting

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

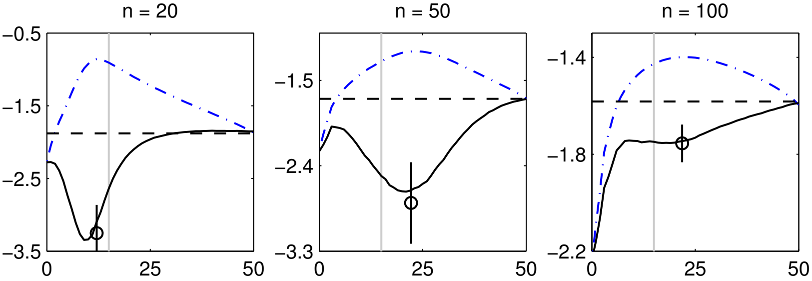
Selection induced bias and overfitting

- Selection induced bias in cross-validation
  - same data is used to assess the performance and make the selection
  - the selected model fits more to the data
  - the CV estimate for the selected model is biased
  - recognized already, e.g., by Stone (1974)
- Performance of the selection process itself can be assessed using two level cross-validation, but it does not help choosing better models

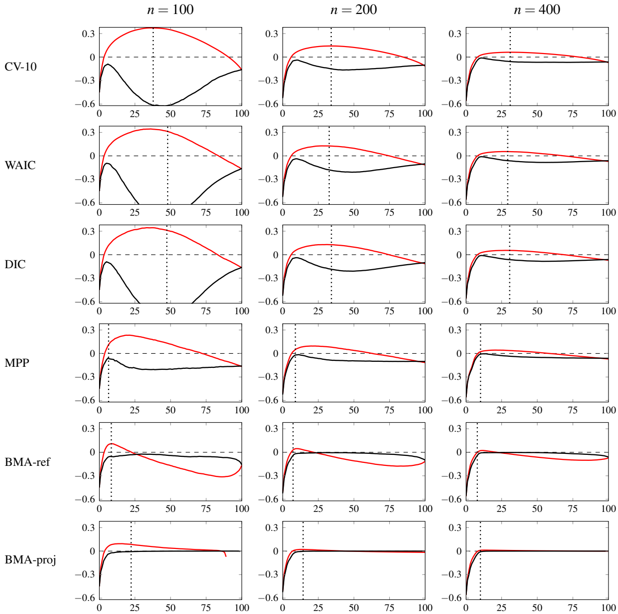
Selection induced bias and overfitting

- Selection induced bias in cross-validation
  - same data is used to assess the performance and make the selection
  - the selected model fits more to the data
  - the CV estimate for the selected model is biased
  - recognized already, e.g., by Stone (1974)
- Performance of the selection process itself can be assessed using two level cross-validation, but it does not help choosing better models
- Bigger problem if there is a large number of models as in covariate selection

Selection induced bias in variable selection



Selection induced bias in variable selection



Piironen & Vehtari (2017)

Take-home messages

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

Take-home messages

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

Take-home messages

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

Take-home messages

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

Take-home messages

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