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- Introduction

Bayesian Statistics and Data Analysis
Lecture 8b

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Department of Statistics, Uppsala University
Thanks to Aki Vehtari, Aalto University

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Section 1

Introduction

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Model assessment, selection and inference after selection

1. Extra material at https://avehtari.github.io/modelselection/
   - 1.1 Videos, Slides, Notebooks, References
   - 1.2 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"

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- Introduction

Predicting concrete quality

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- Introduction

Predicting cancer recurrence

GIST Risk calculator

Tumor size (cm) 10

Mitotic count (per 50 HPFs*) 20

Tumor site GASTRIC

Tumor rupture NO

CALCULATE!

*HPF = high-power field of the microscope

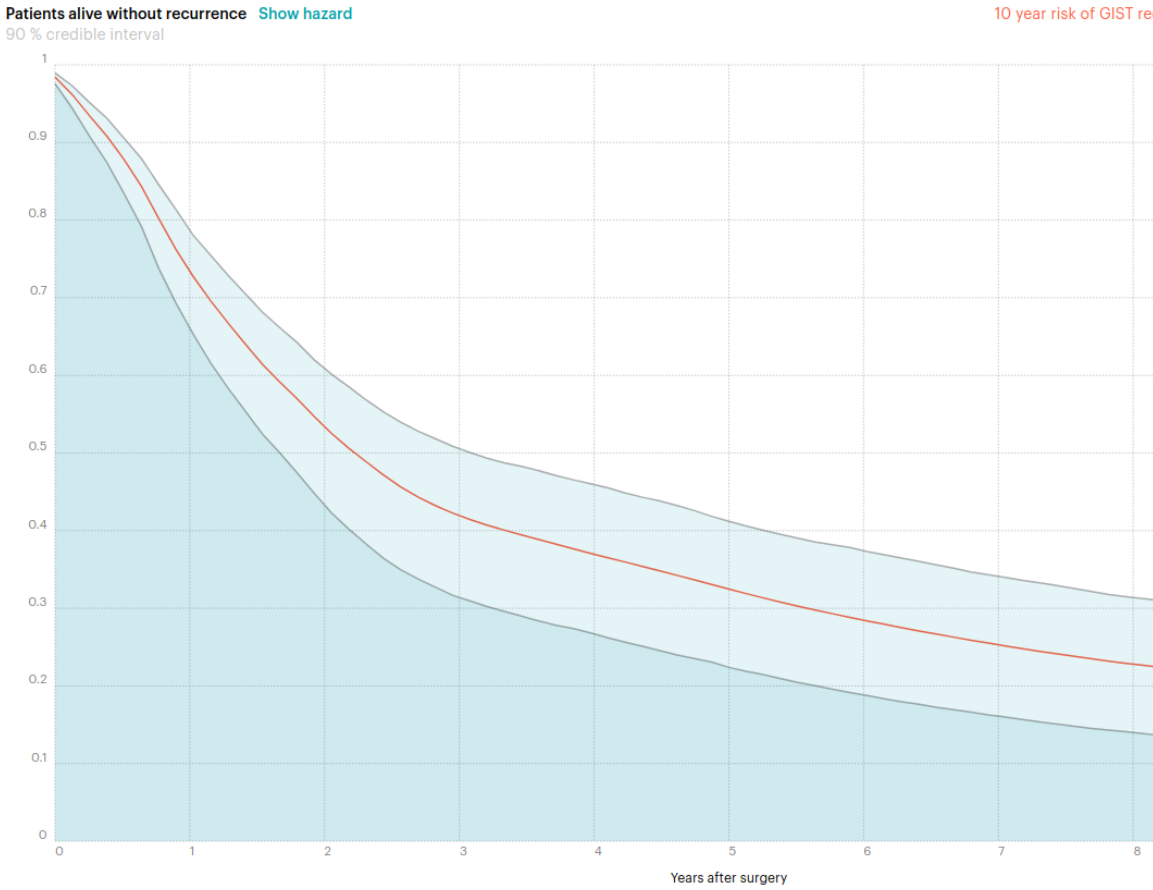
Show risk tables

Made by

kaiku HEALTH

Online platform for the future of data-driven and personalized cancer care

Reaktor



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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

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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

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

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Outline

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

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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
```

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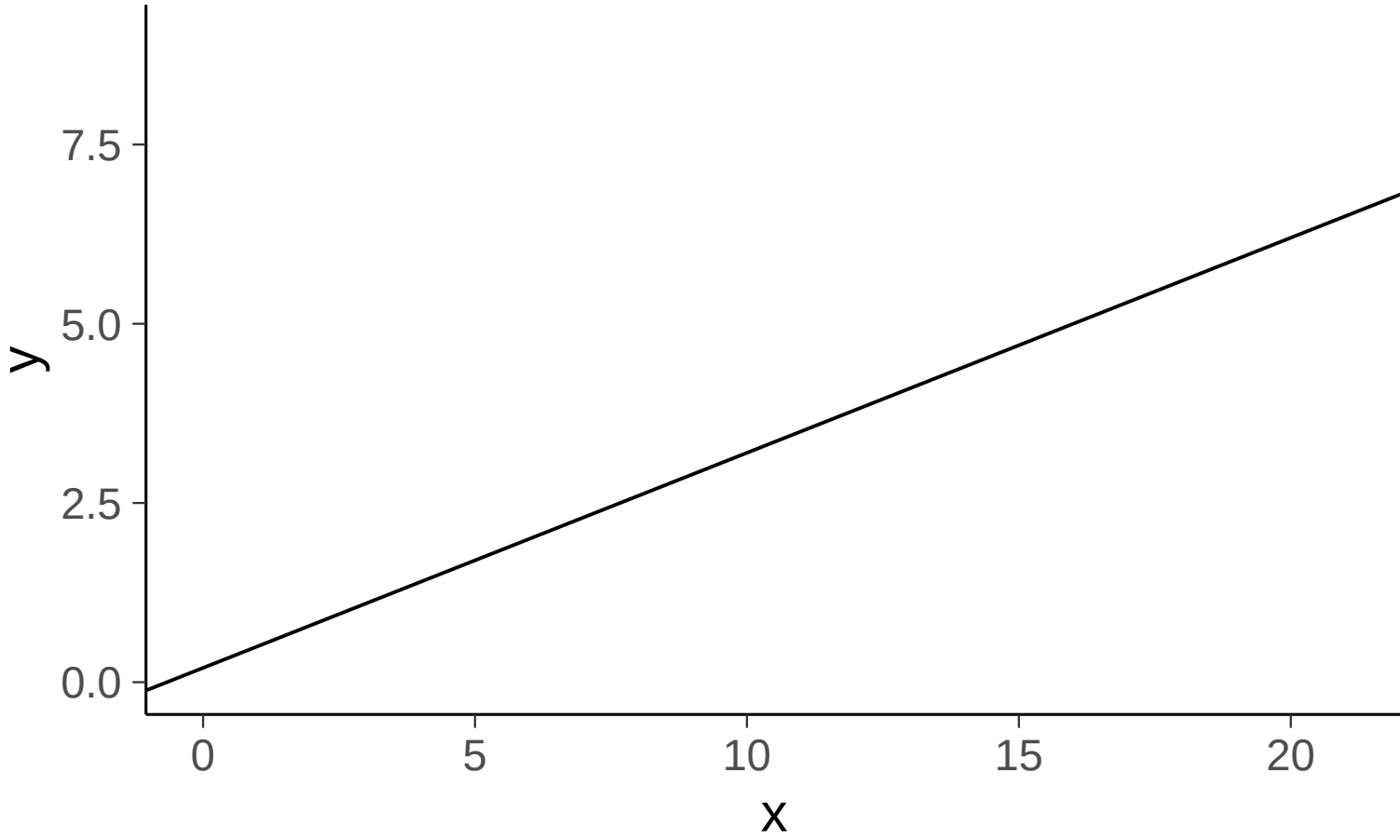
True mean y = a + bx



True mean and sigma

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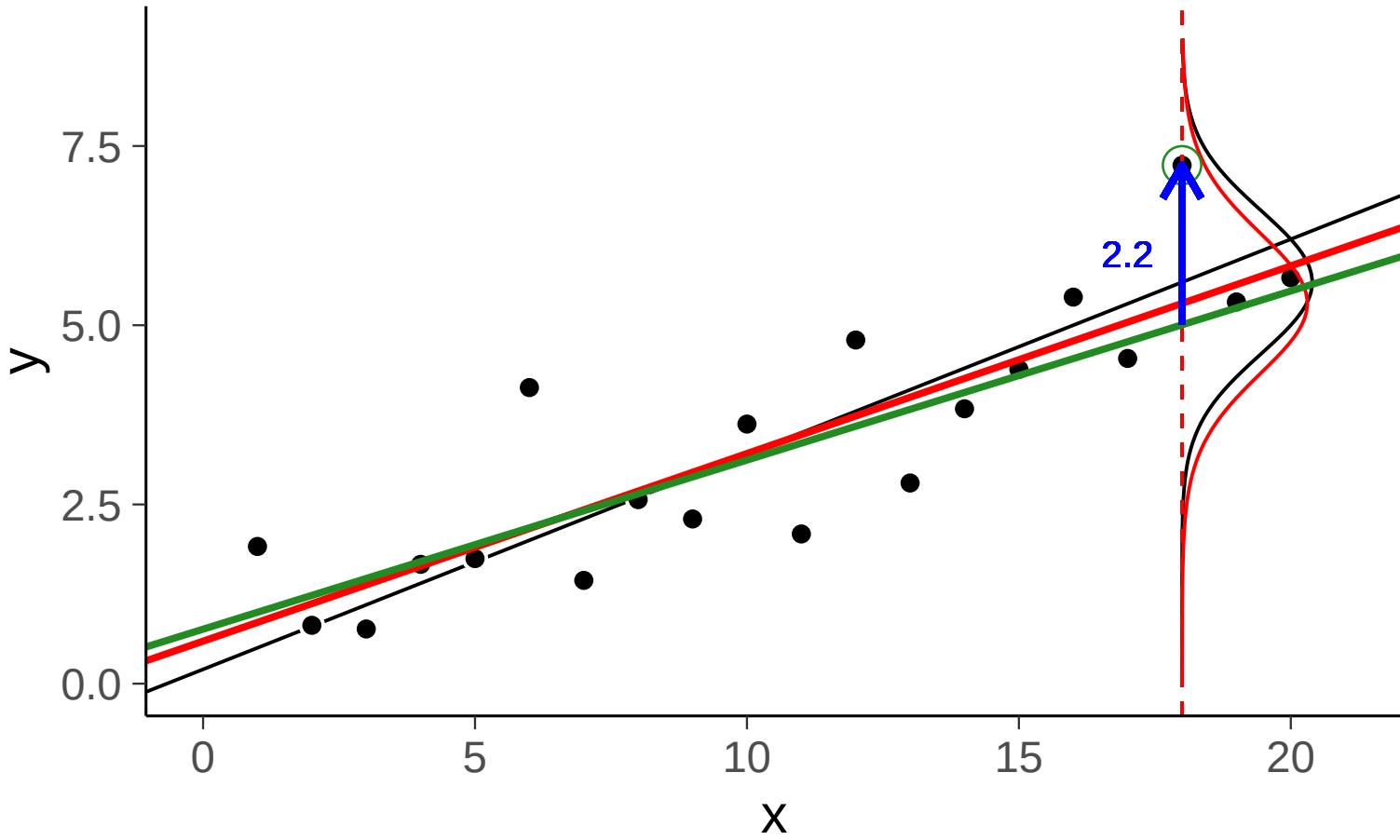
Leave−one−out residual



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

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

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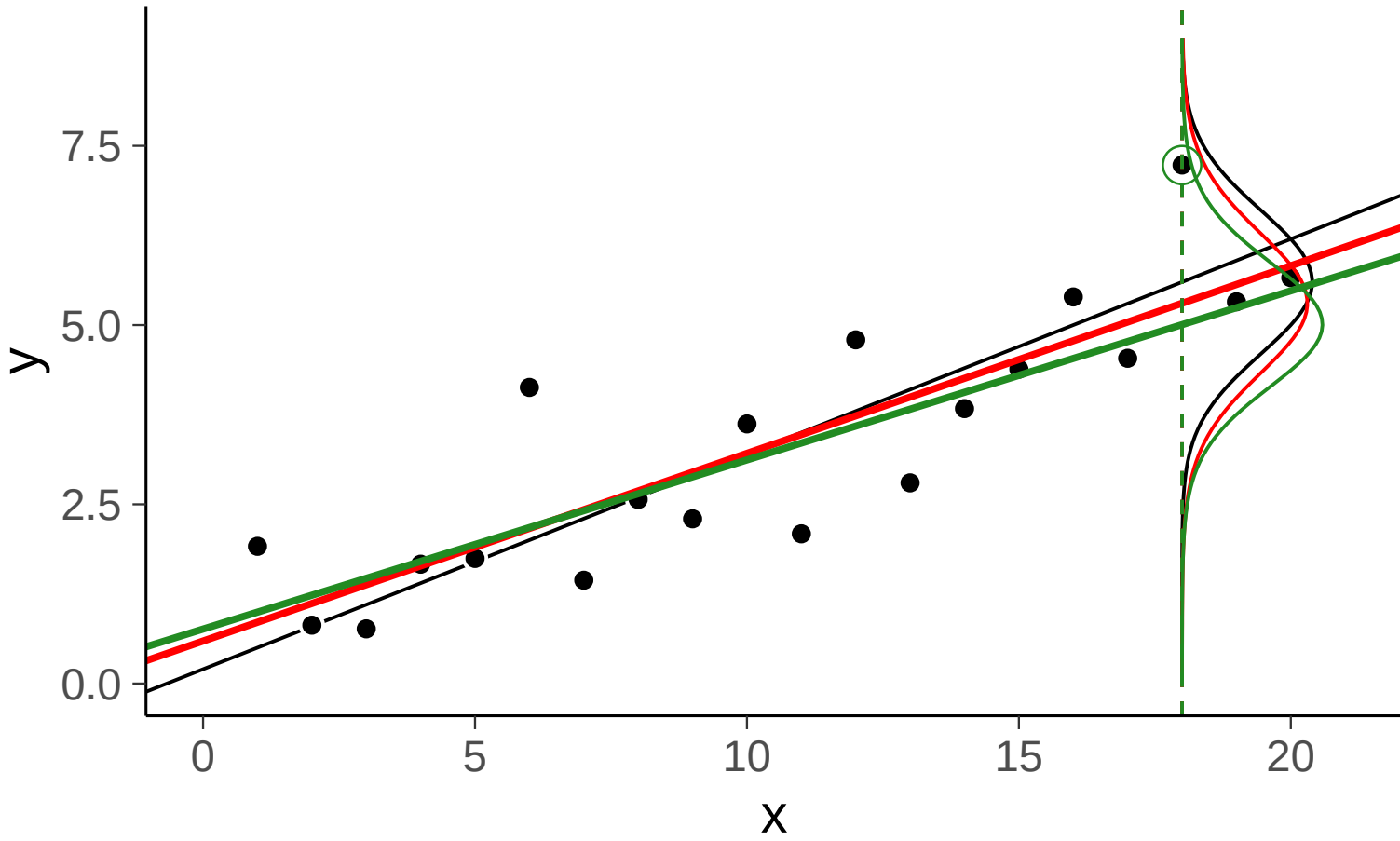
Leave−one−out predictive distribution



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

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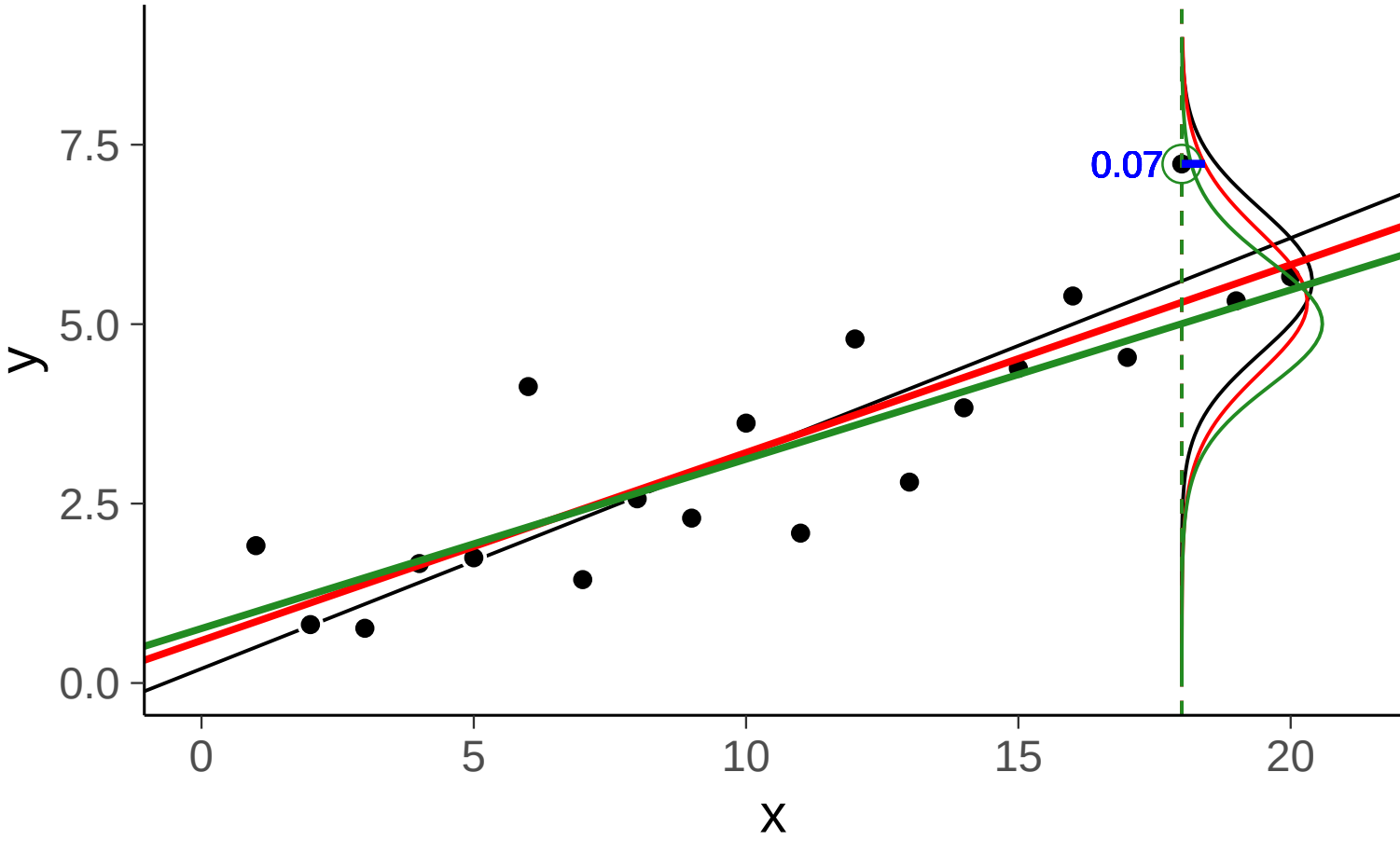
Posterior predictive density



Leave−one−out predictive density

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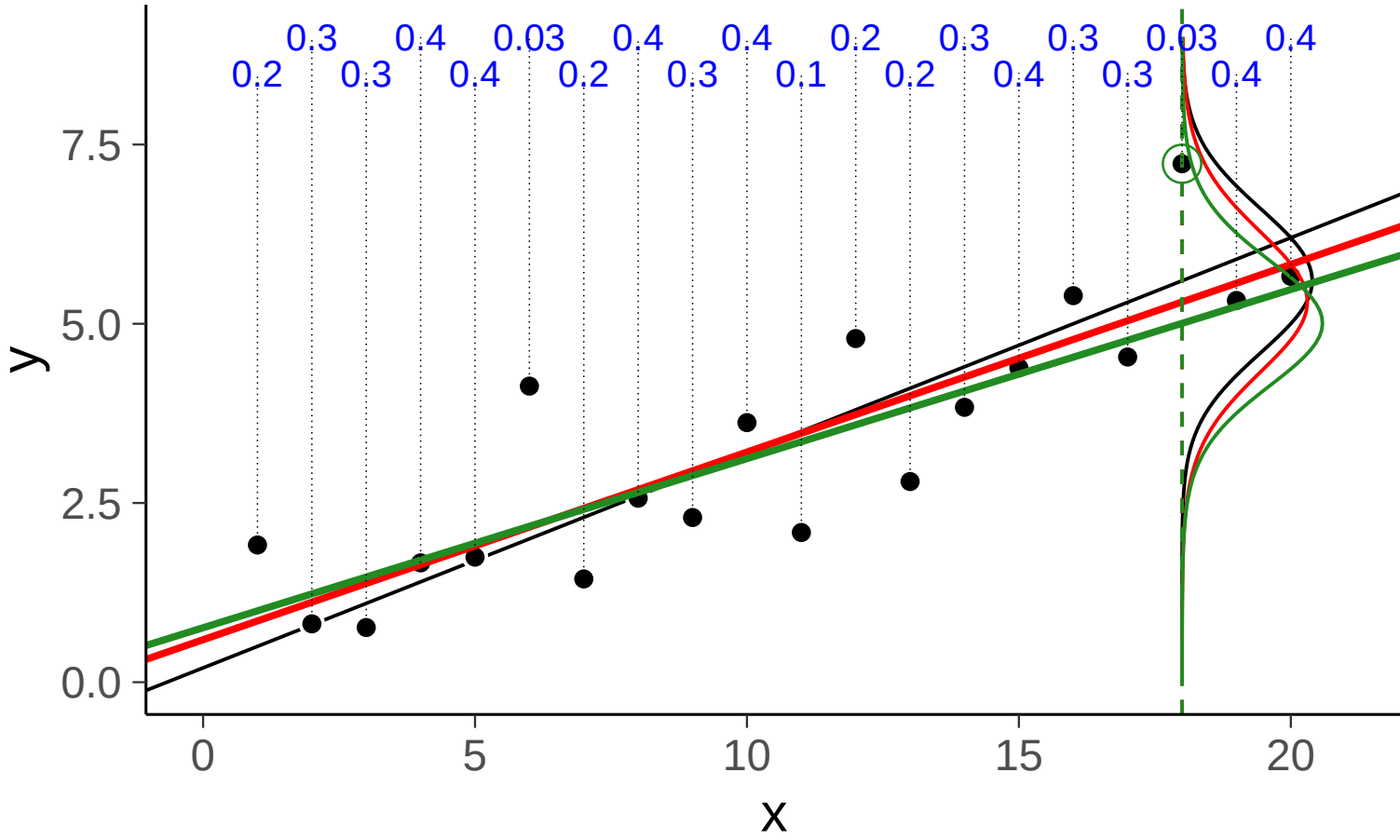
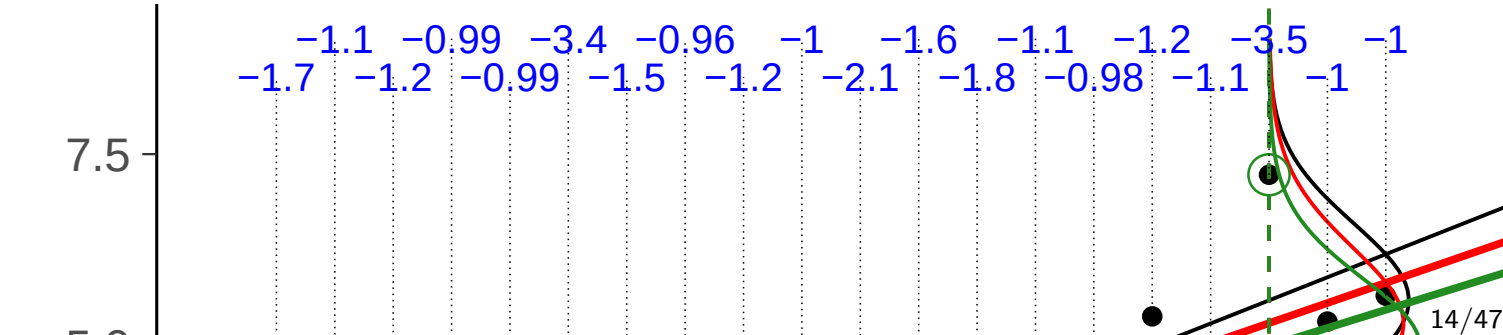
Leave−one−out predictive densities



Leave−one−out log predictive densities



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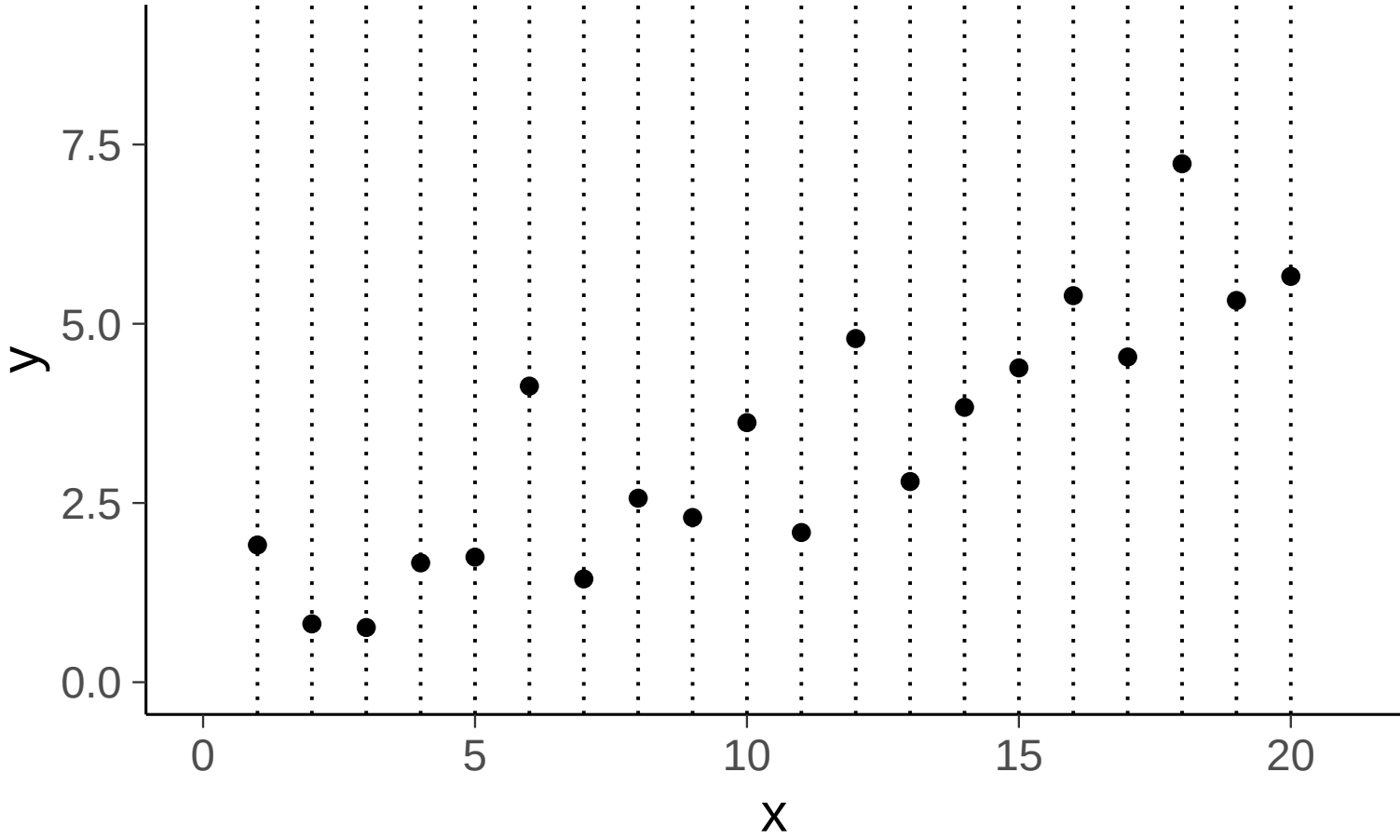
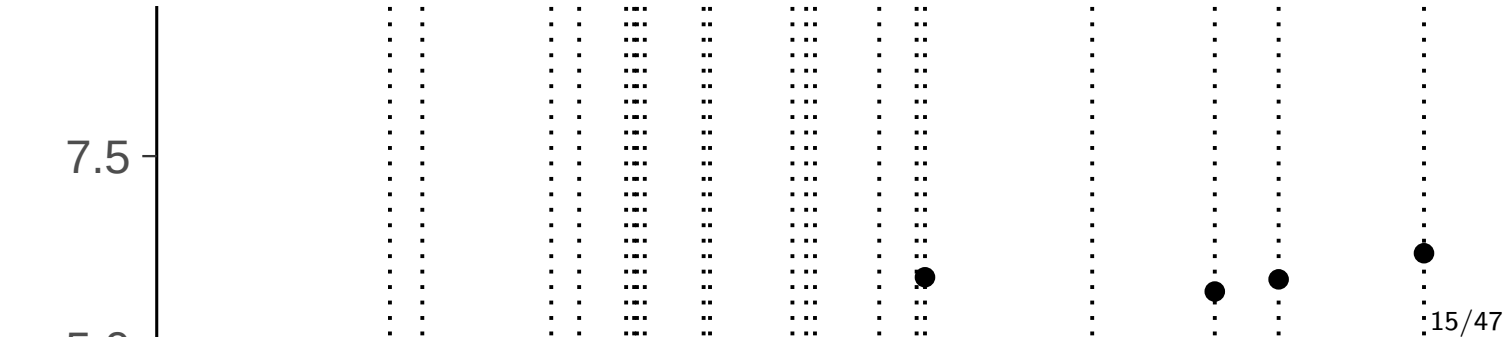
Fixed / designed x



Distribution for x



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loo package

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

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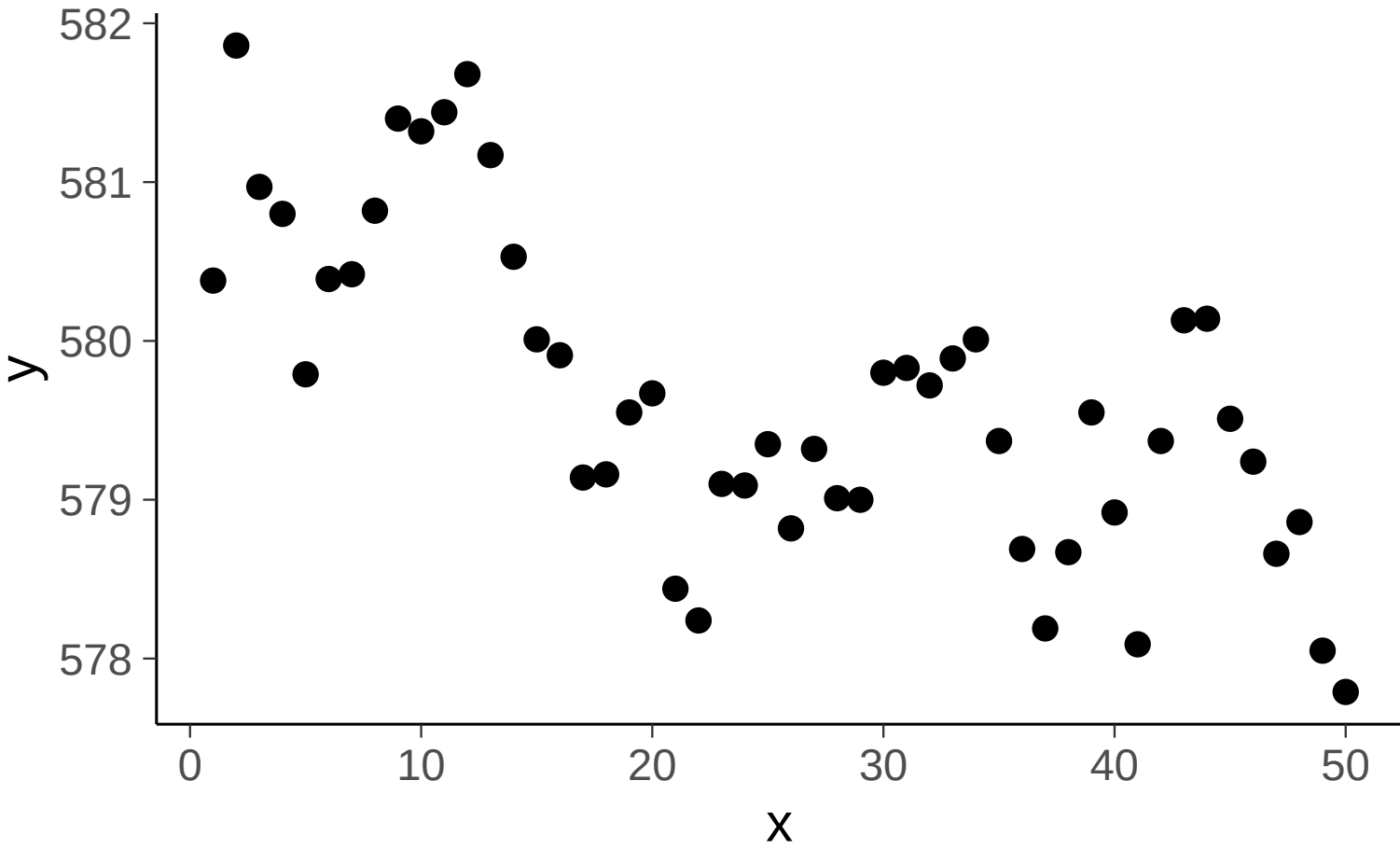
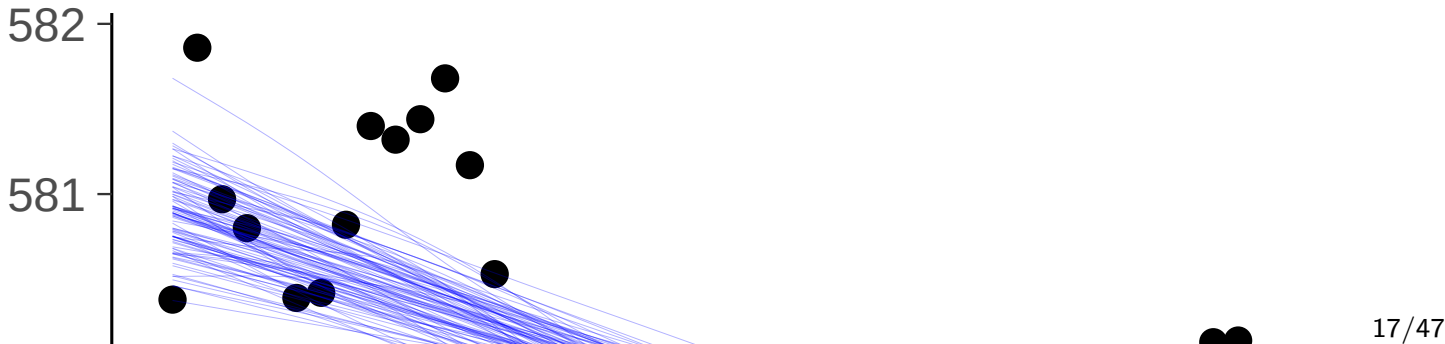


Nonlinear model fit



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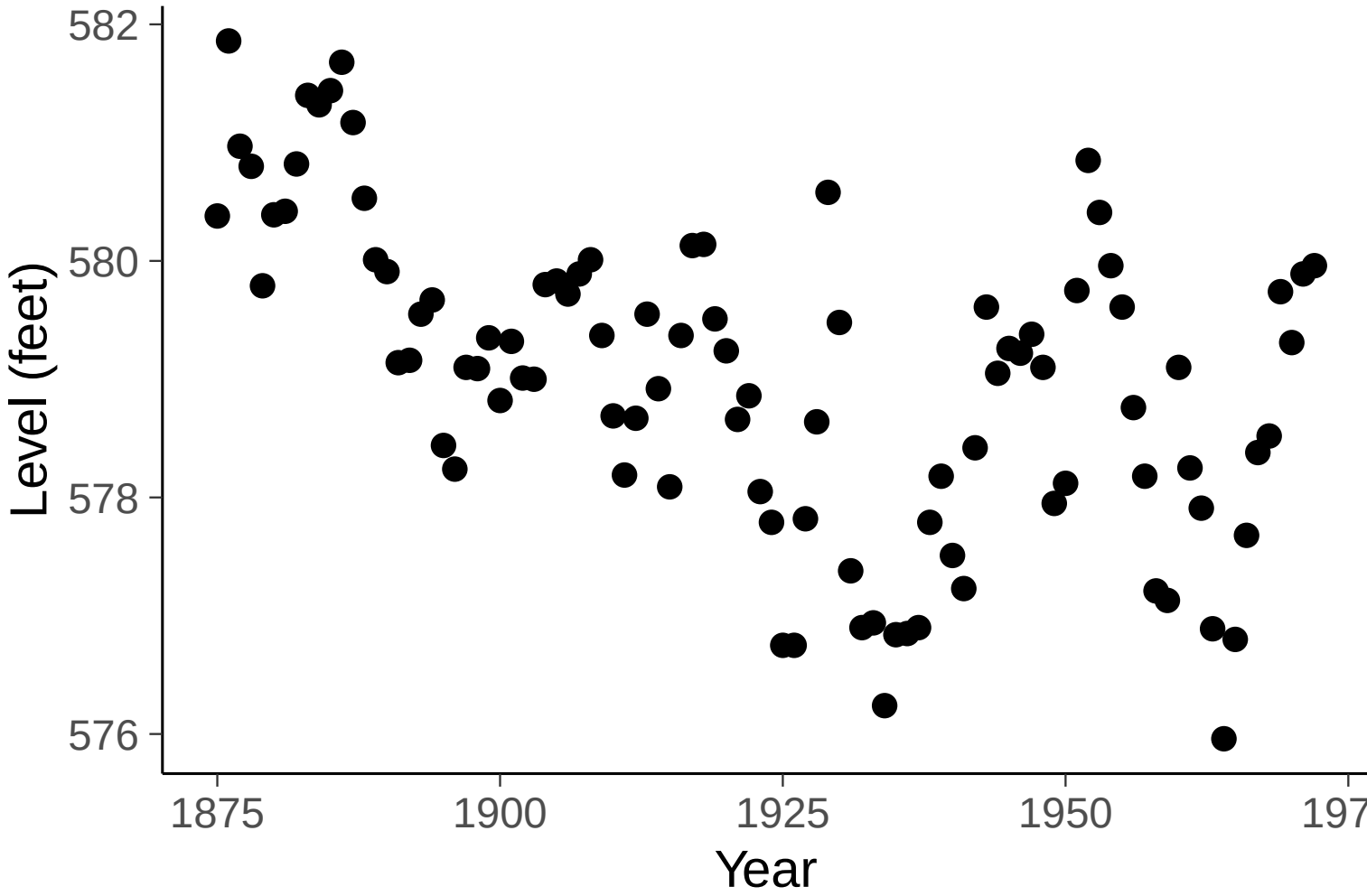

Can LOO or other cross-validation be used with time series?

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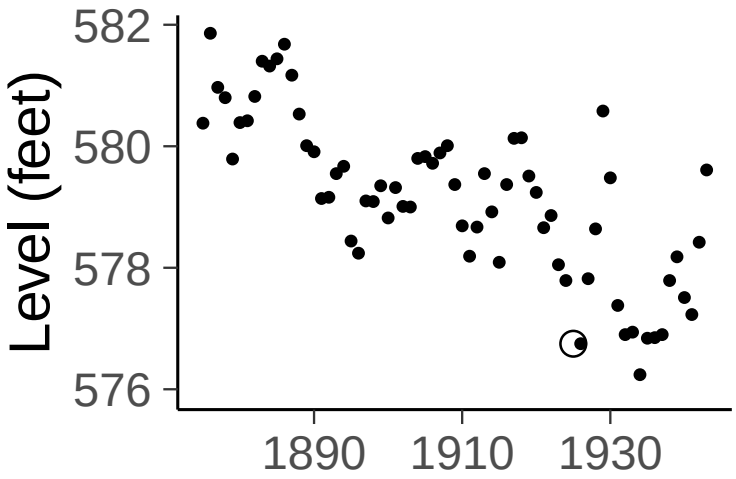

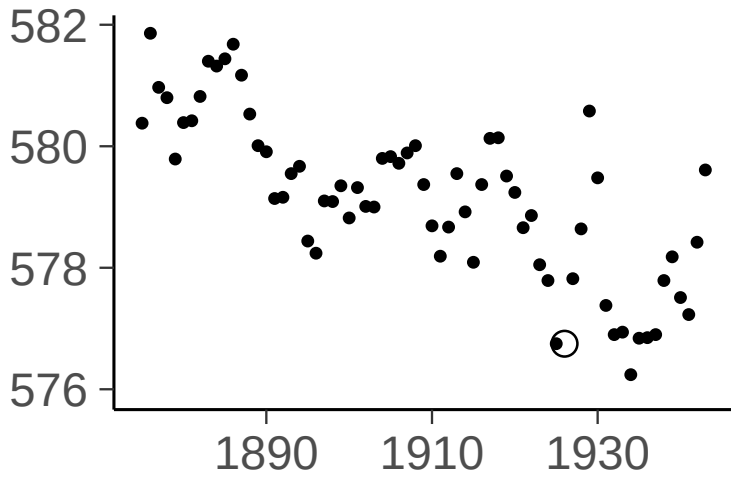

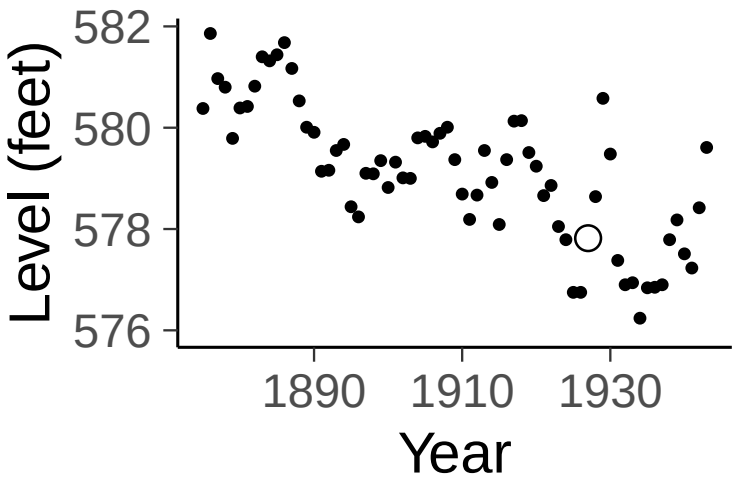

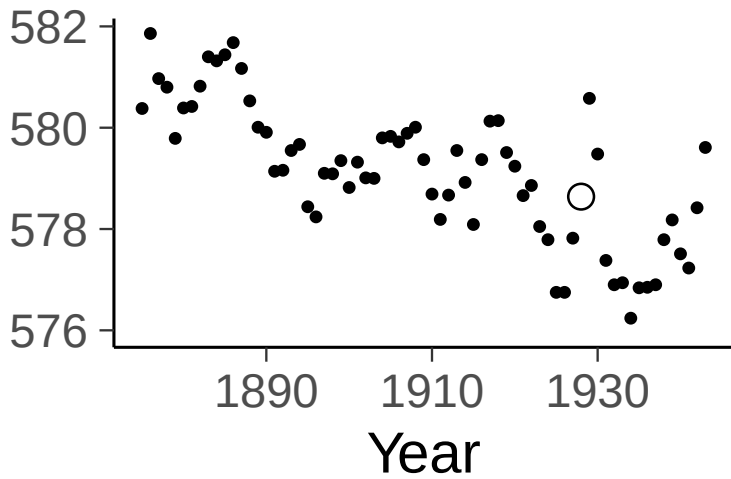

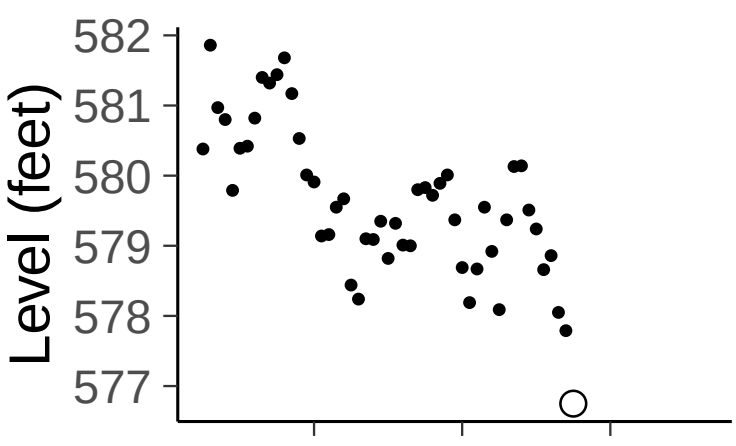

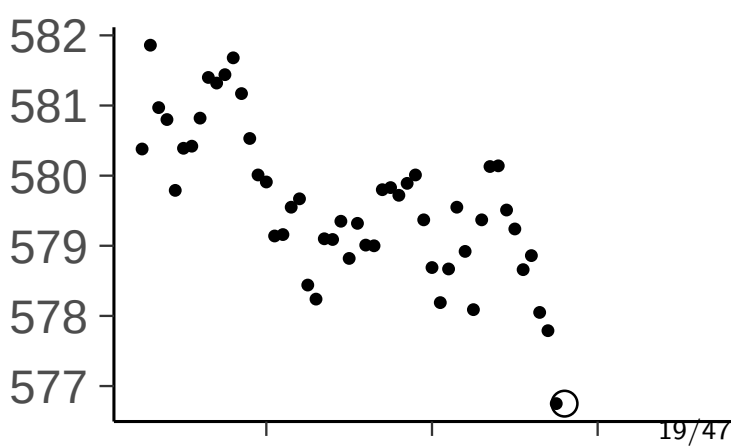

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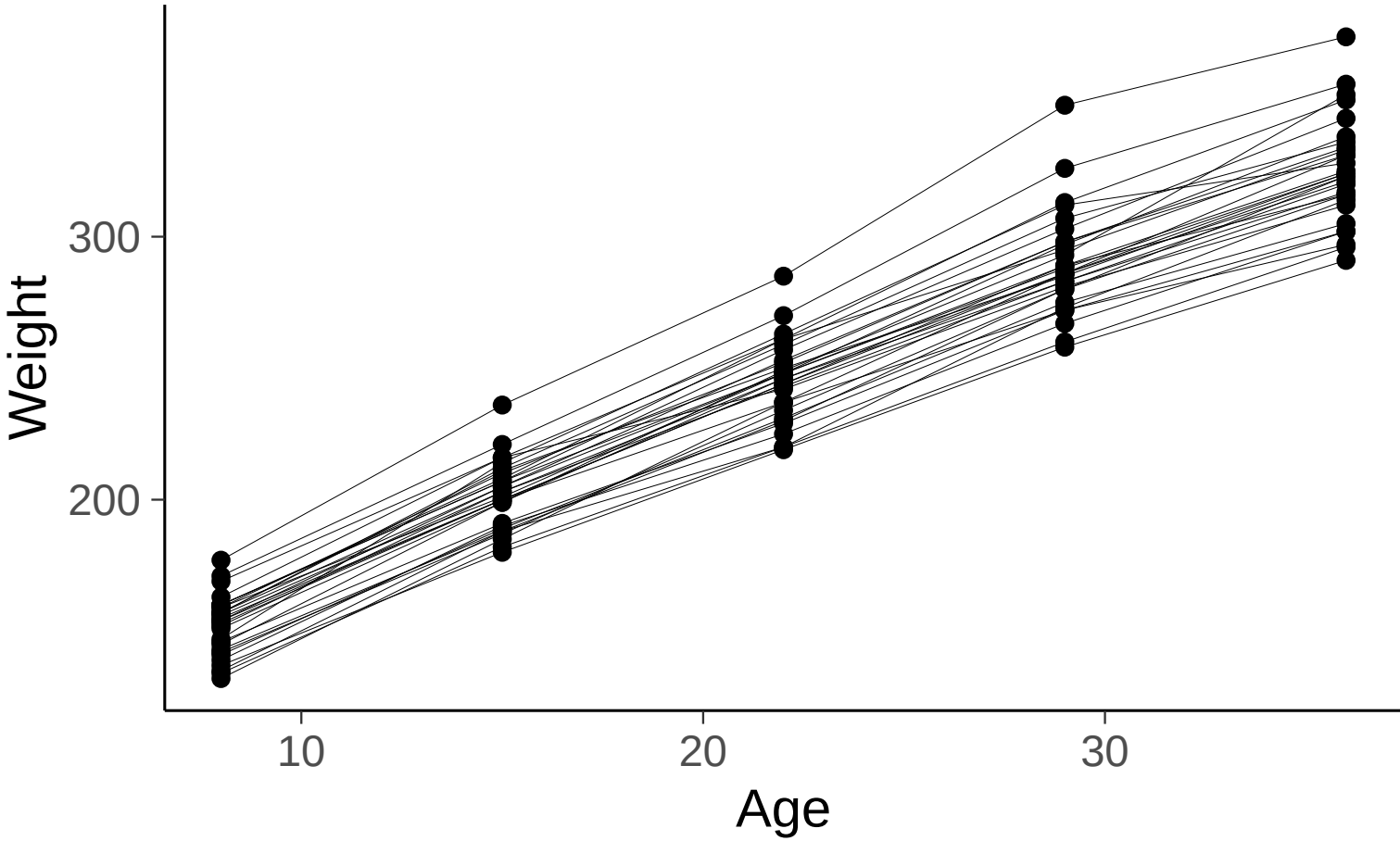
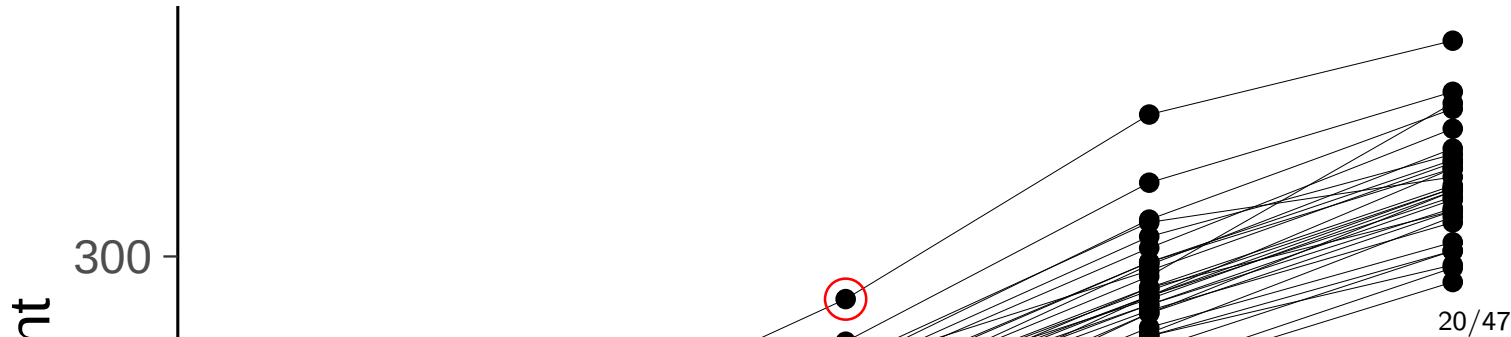
Rats data



Leave−one−out?



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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/`

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

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

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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);
}
```

1. RStanARM and BRMS compute log_lik by default

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Pareto smoothed importance sampling LOO

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

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

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

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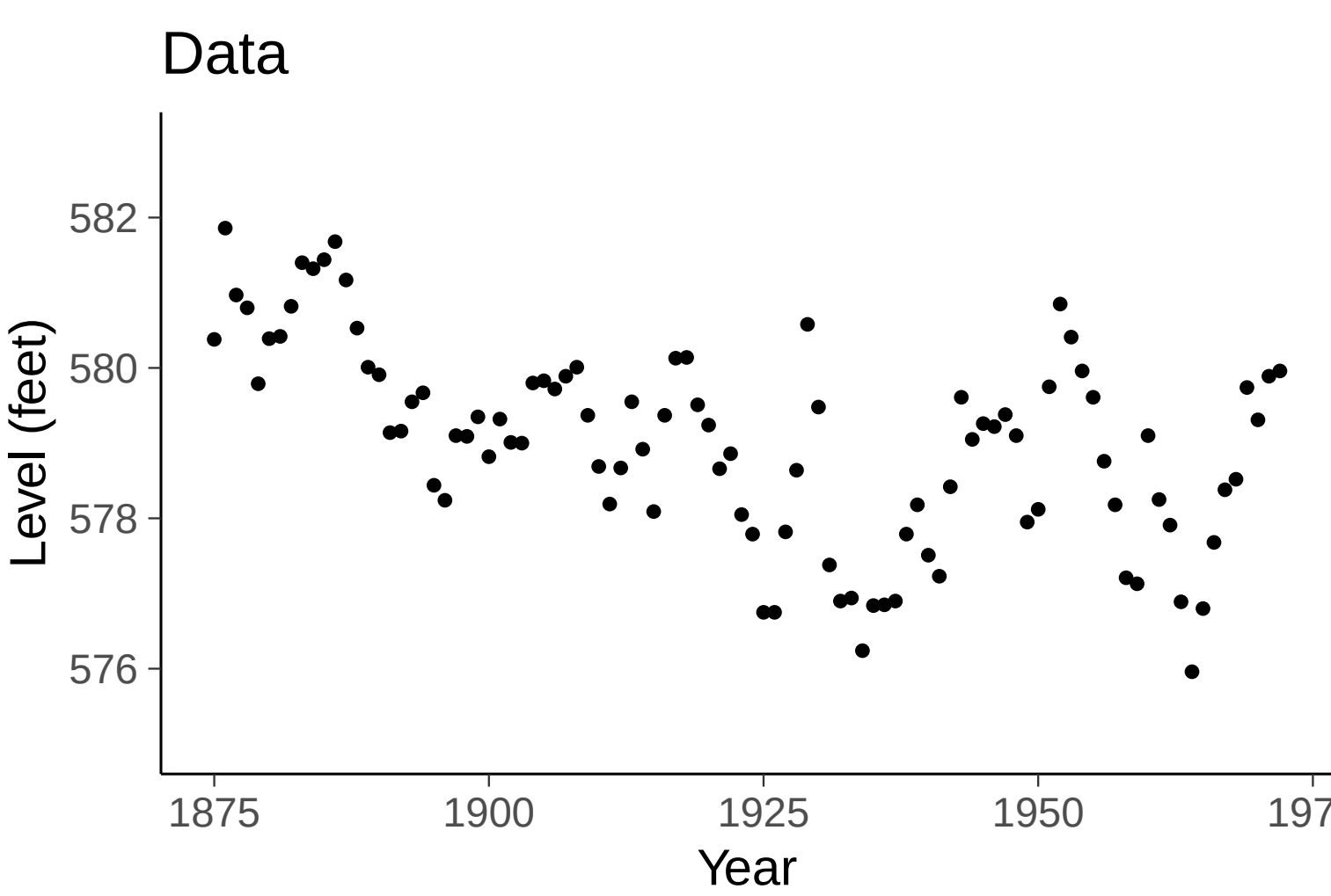

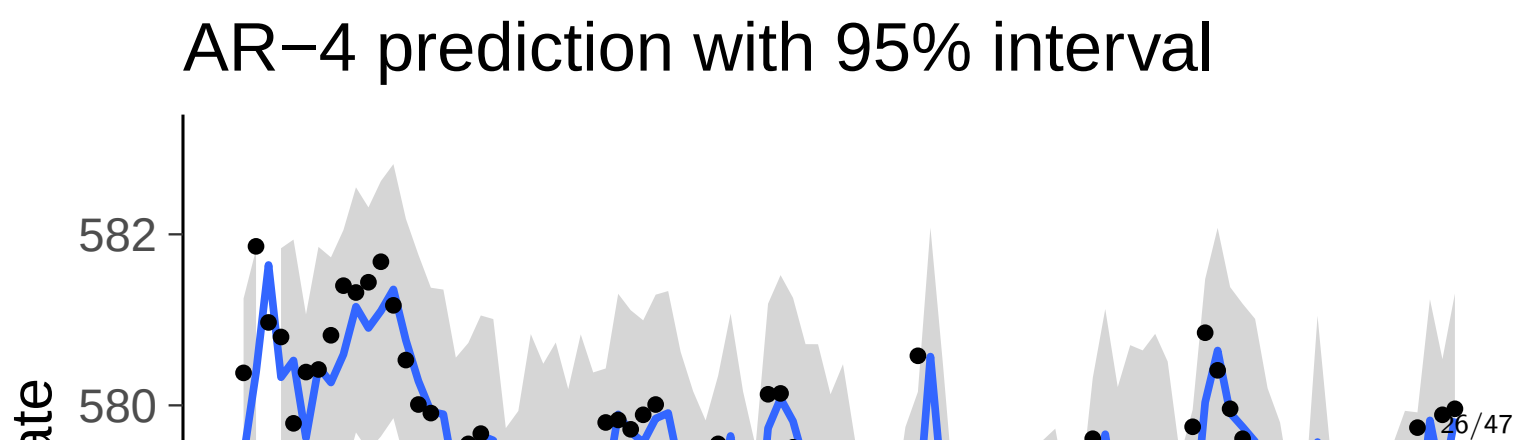

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K-fold cross-validation

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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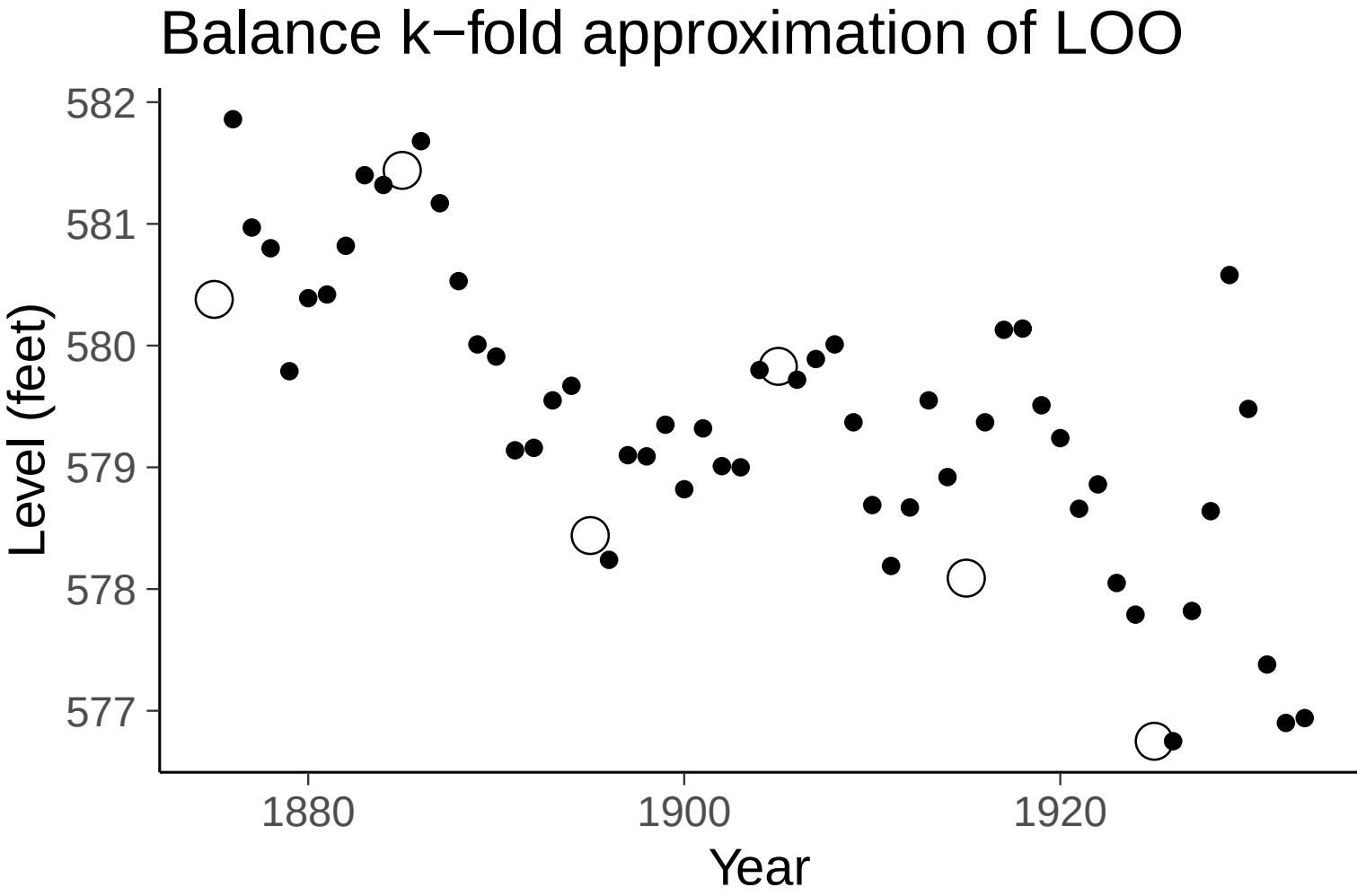

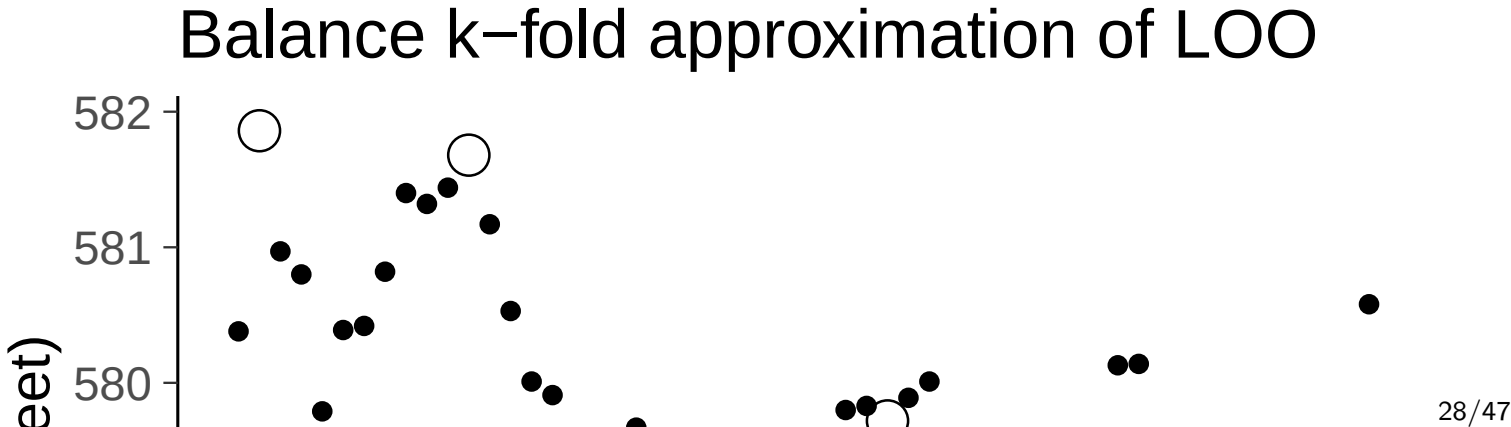

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WAIC vs PSIS-LOO

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)

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*IC

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

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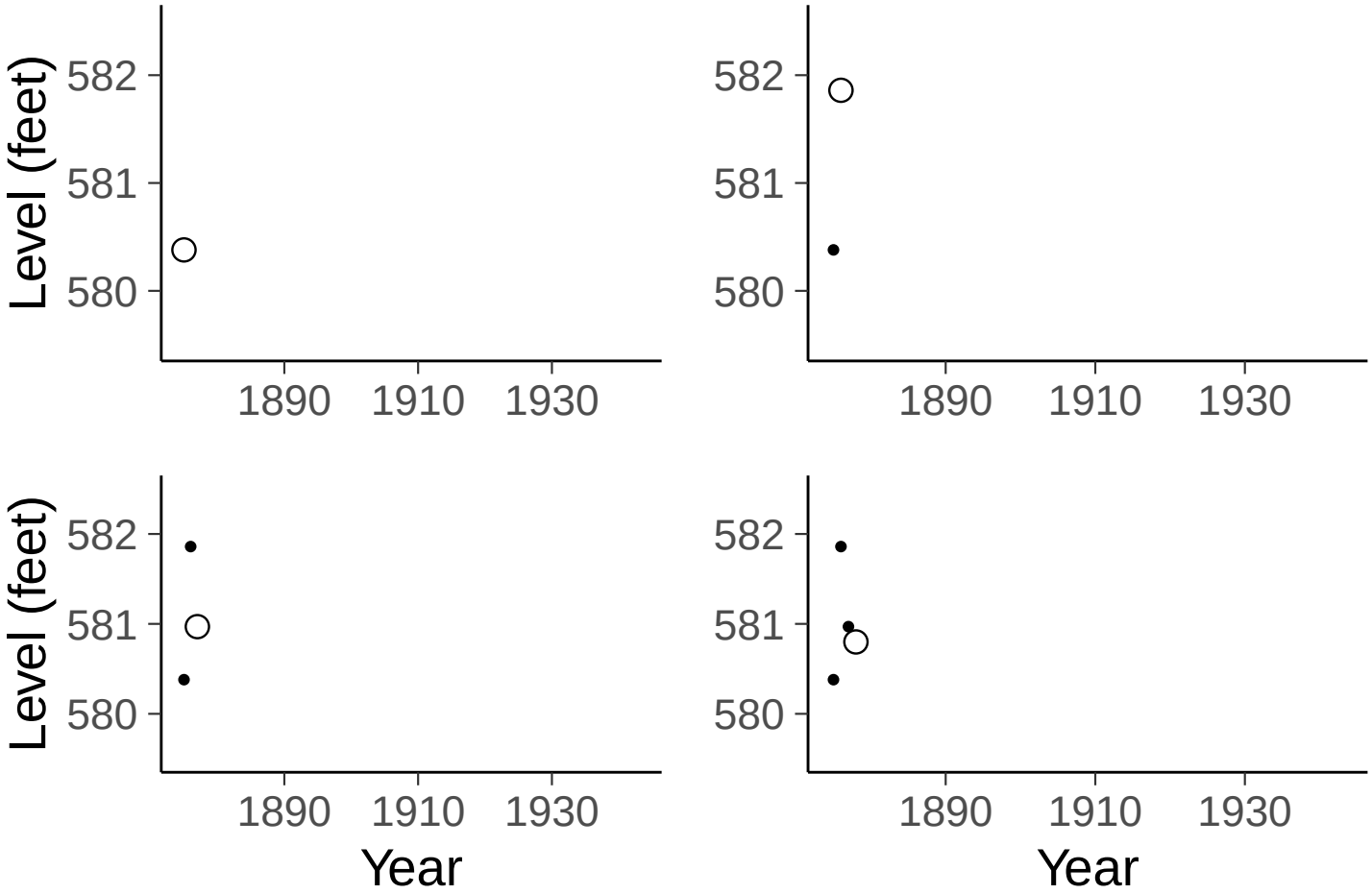
Marginal likelihood / Bayes factor

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



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Cross-validation for model assessment

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

see demos avehtari.github.io/modelselection/

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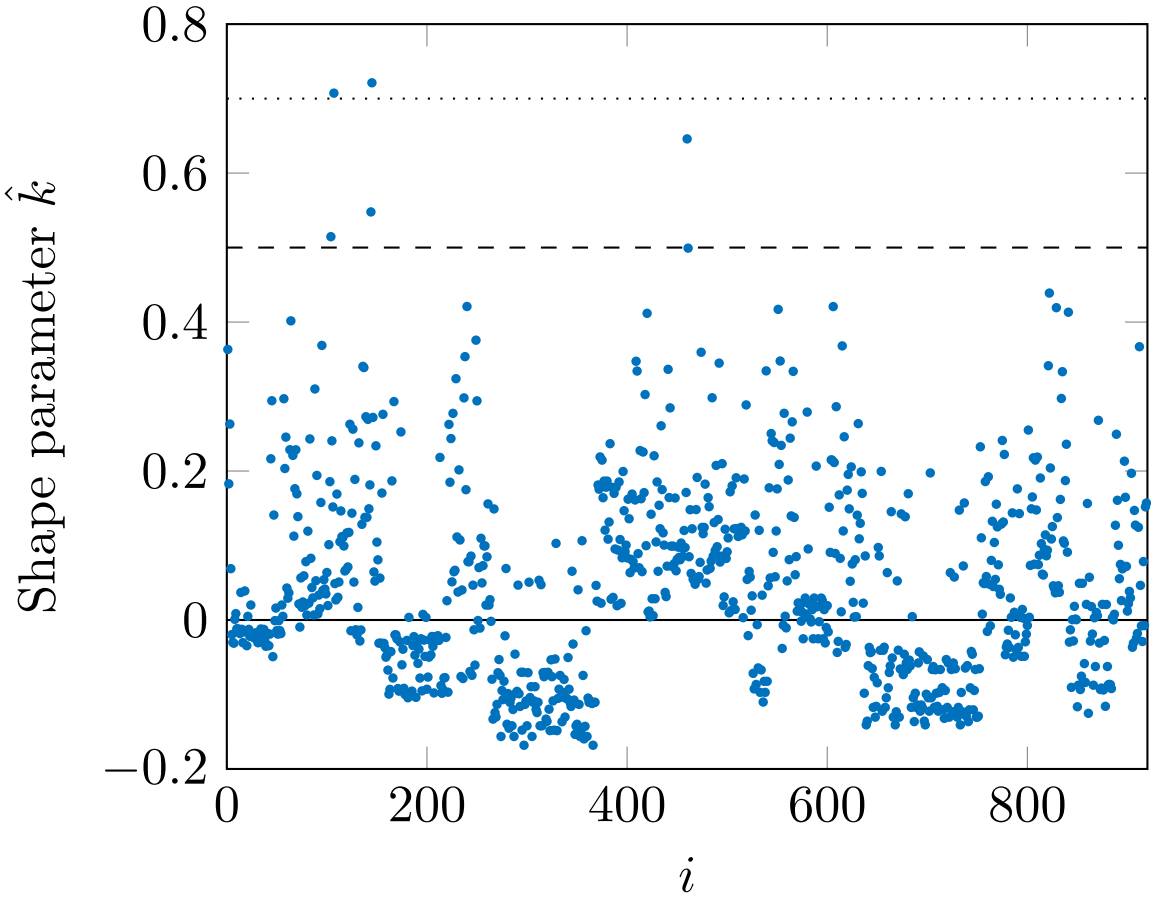
Radon example

PSIS-LOO diagnostics



see Vehtari, Gelman & Gabry (2017a)

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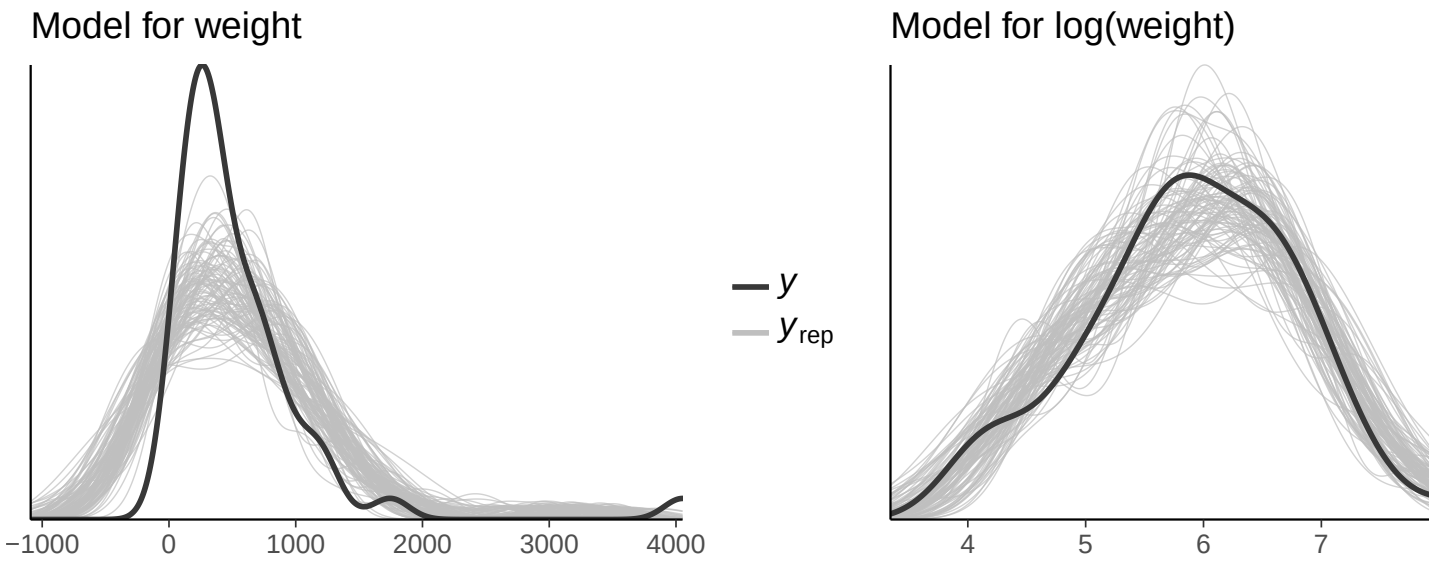
Sometimes cross-validation is not needed

1. Posterior predictive checking is often sufficient



Predicting the yields of mesquite bushes.

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

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.

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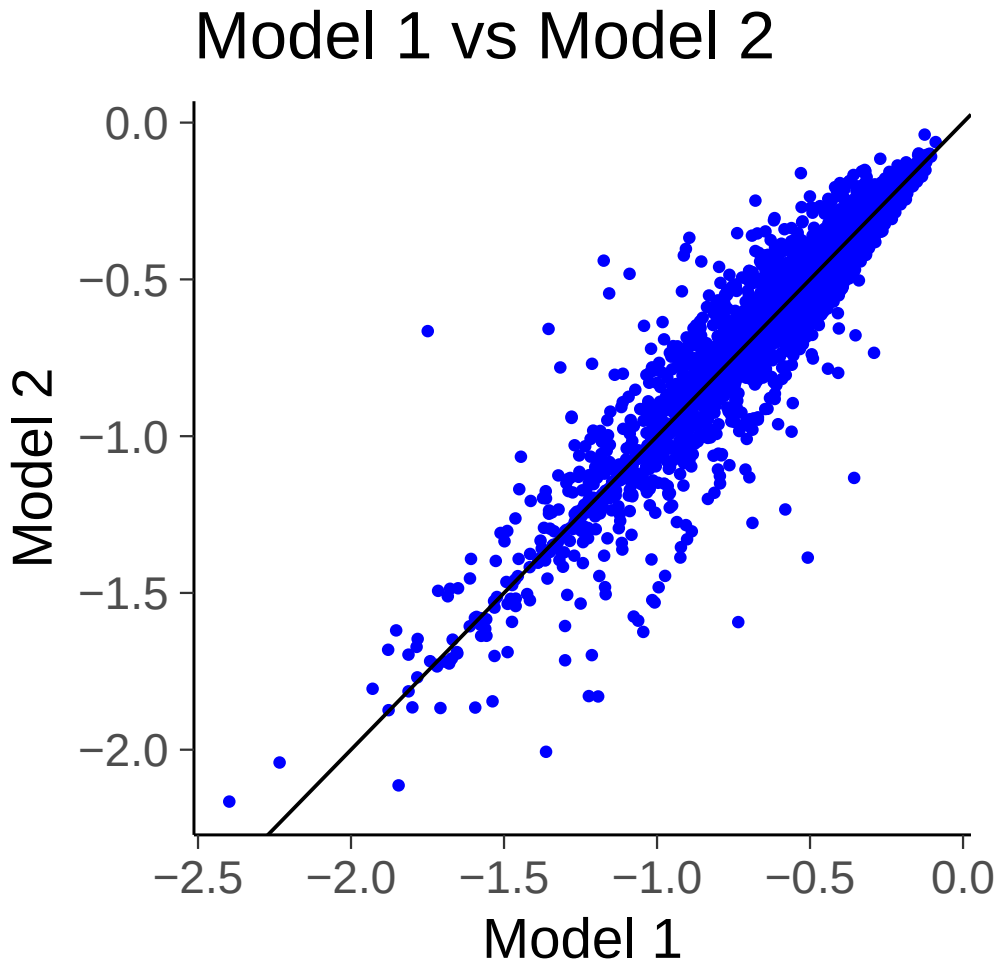
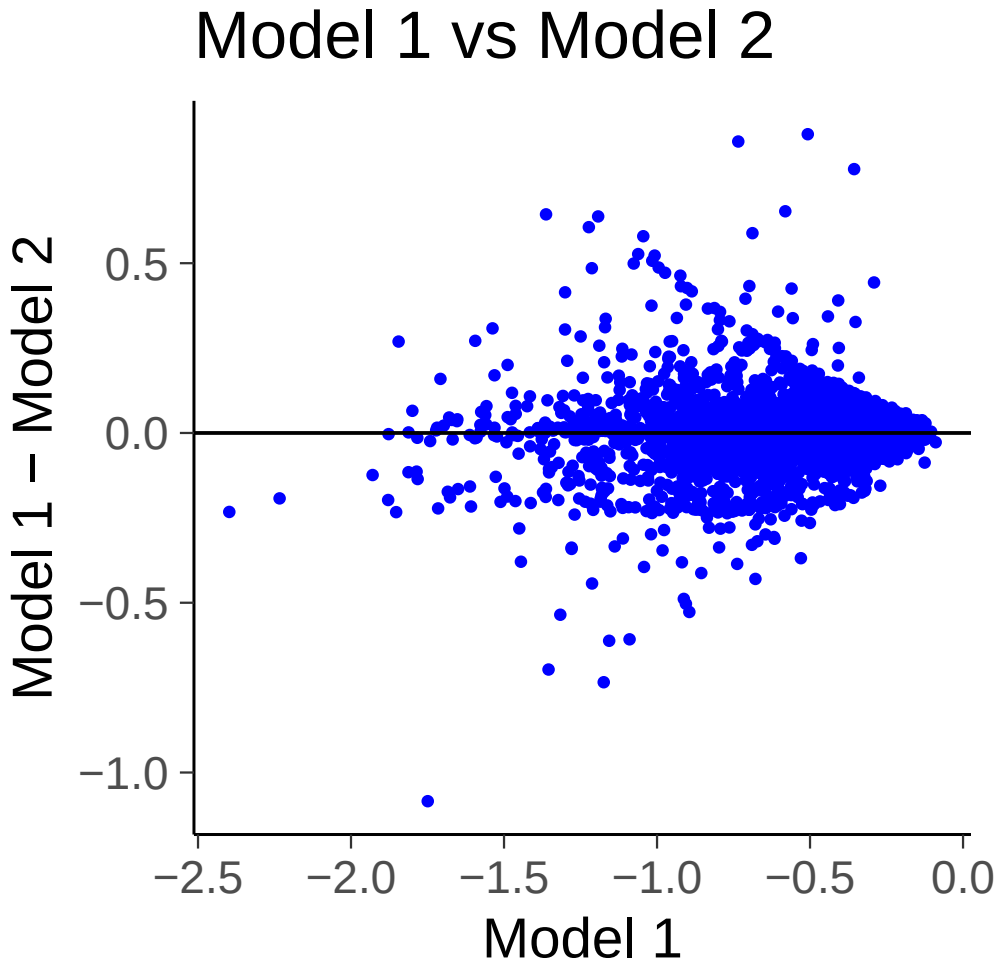
Arsenic well example – Model comparison



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

Arsenic well example – Model comparison




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

see Vehtari, Gelman & Gabry (2017a)

Arsenic well example – Model comparison

```
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       elpd_diff se_diff
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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).

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Sometimes cross-validation is not needed

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

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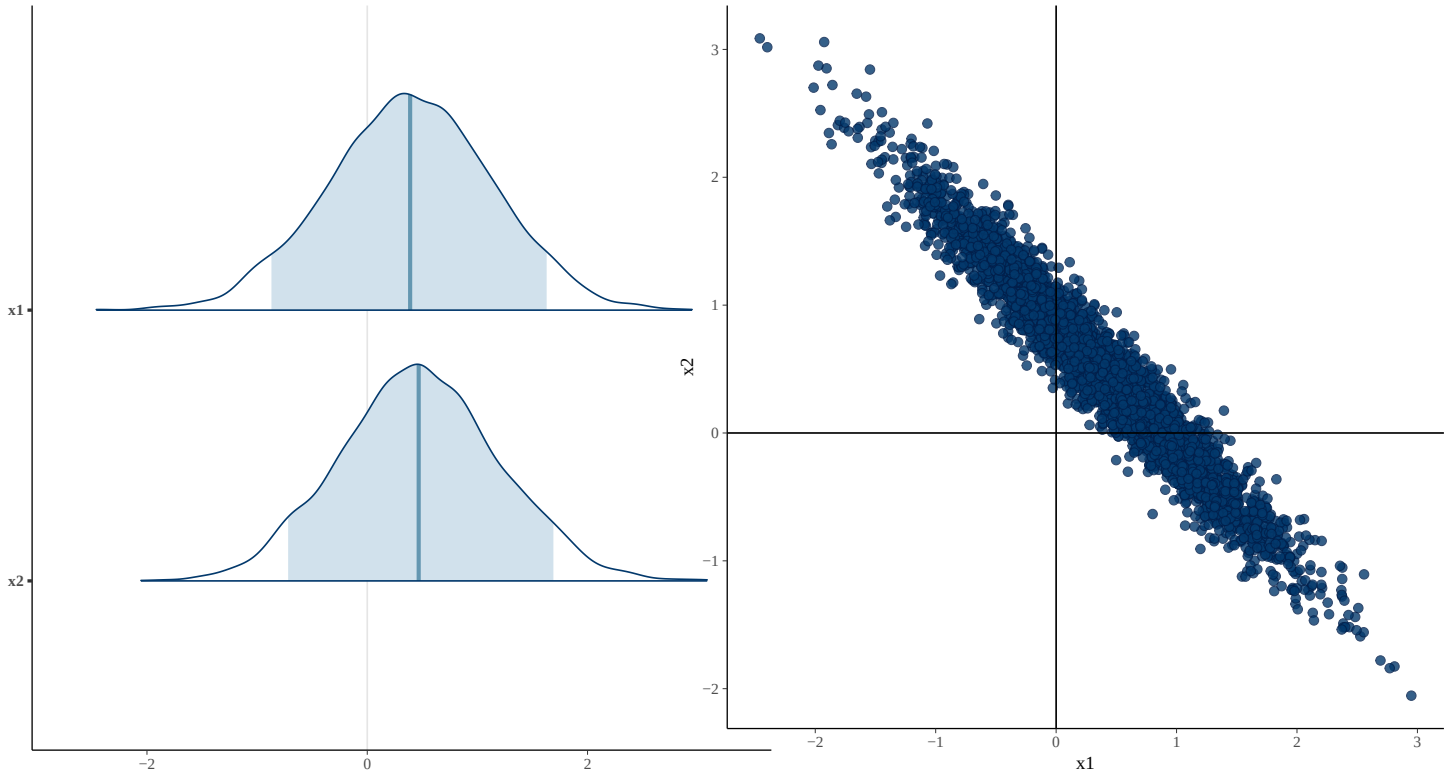
Sometimes predictive model comparison can be useful



Marginal posterior intervals Joint posterior density

rstanarm + bayesplot

see also Collinear demo

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What if one is not clearly better than others?

1. Continuous expansion including all models?
   - 1.1 and then analyse the posterior distribution directly
     avehtari.github.io/modelselection/betablockers.html
   - 1.2 sparse priors like regularized horseshoe prior instead of variable selection
     video, refs and demos at
     avehtari.github.io/modelselection/
2. Model averaging with BMA or Bayesian stacking?
   mc-stan.org/loo/articles/loo2-example.html
3. In a nested case choose simpler if assuming some cost for extra parts?
   andrewgelman.com/2018/07/26/parsimonious-principle-vs-integration-uncertainties/
4. 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

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)

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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
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

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Selection induced bias and overfitting

- Selection induced bias in cross-validation
  - same data is used to assess the performance and make the selection
  - the selected model fits more to the data
  - 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

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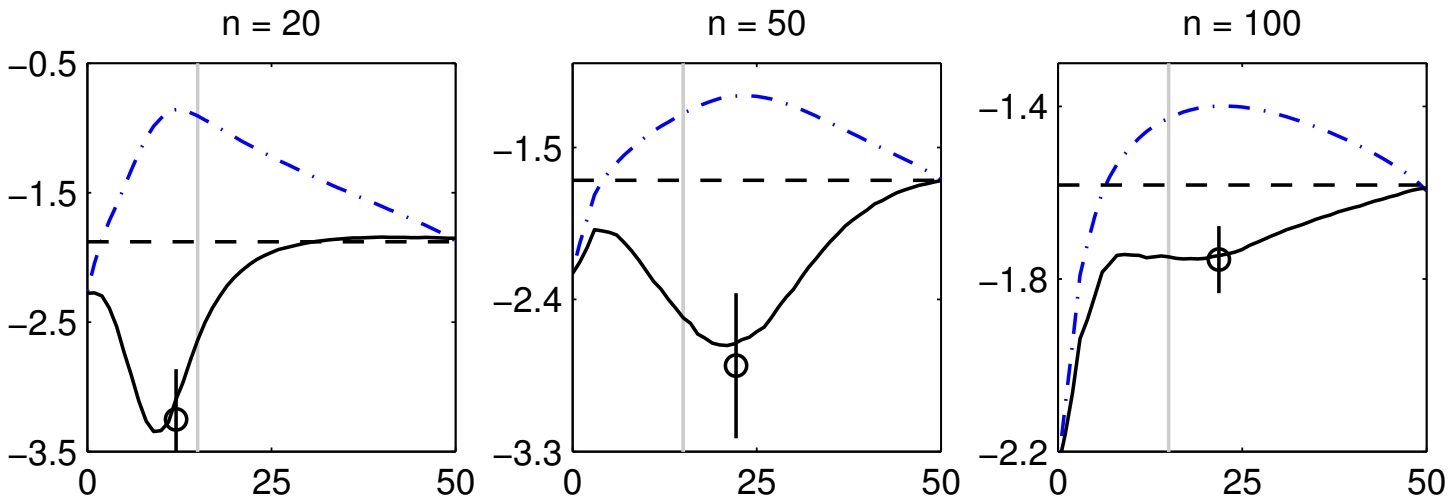
Selection induced bias in variable selection



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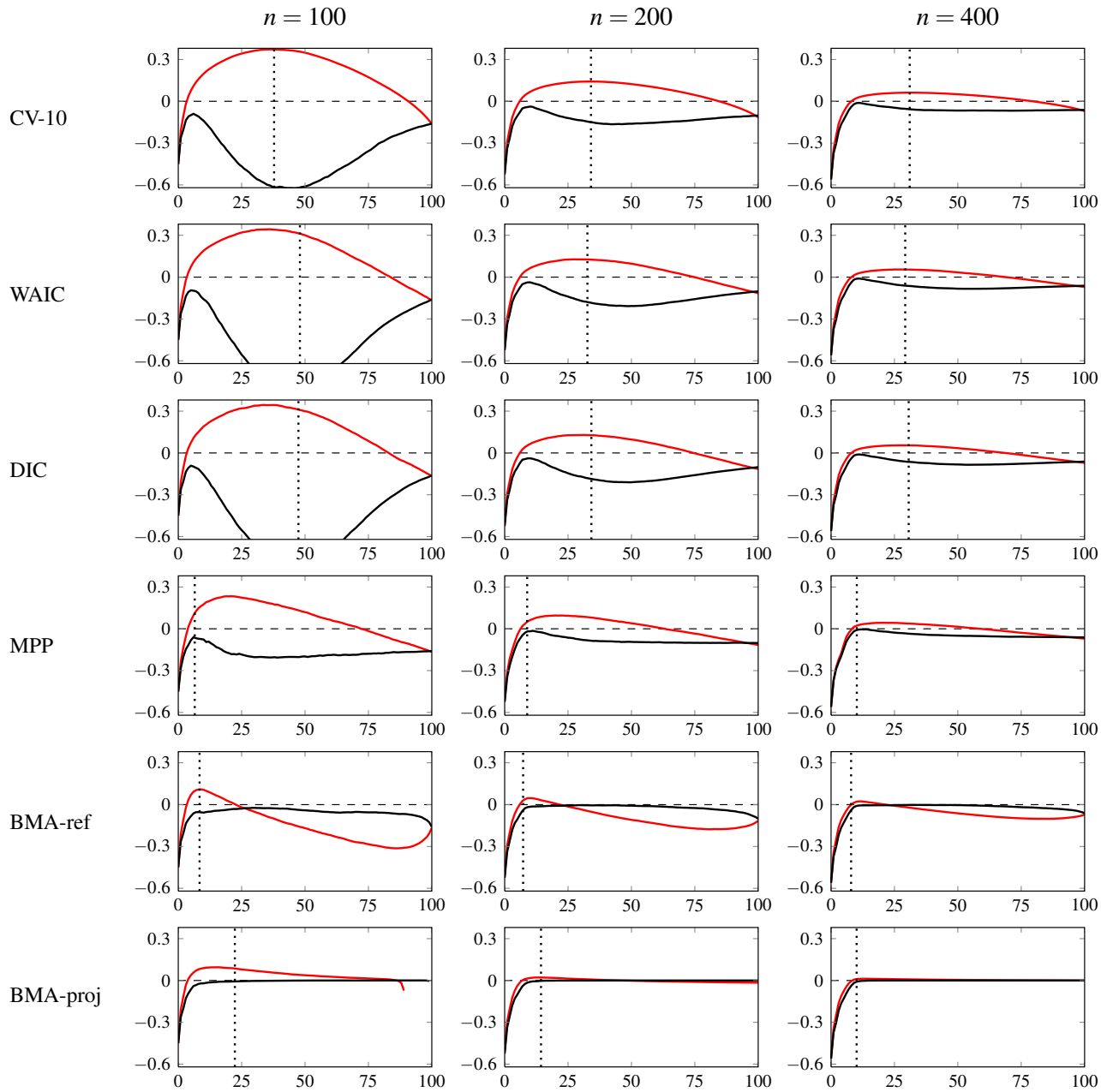
Selection induced bias in variable selection



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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