Model assessment, selection and averaging

Part 1: cross-validation
Part 2: projection predictive inference

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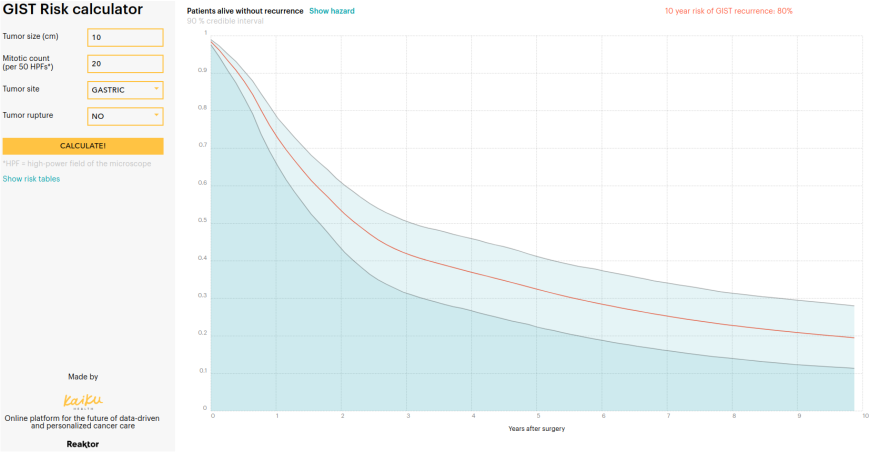
Aalto University, Finland

Slides and extra material at avehtari.github.io/masterclass/

Predicting concrete quality

Slides and extra material at avehtari.github.io/masterclass/

Predicting cancer recurrence



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Model assessment, comparison, selection and averaging

- Modeling complex phenomena with models that are much simpler than the nature (M-open)

Model assessment, comparison, selection and averaging

- Modeling complex phenomena with models that are much simpler than the nature (M-open)
- Decision theoretical approch in spirit of
  - Lindley, Box, Rubin, Bernardo & Smith, etc.

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
```

Outline

- 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

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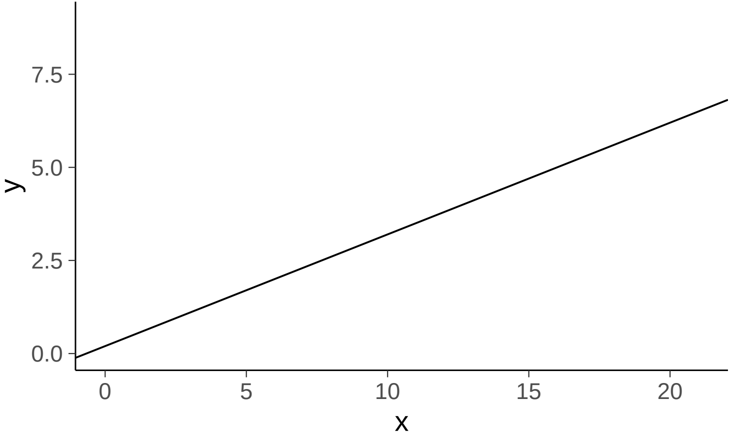
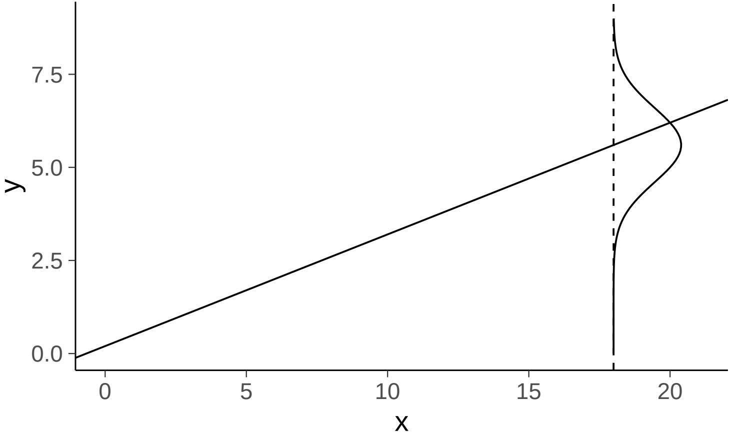
- Model averaging with Bayesian stacking
- Part 2: Projective Inference in High-dimensional Problems: Prediction and Feature Selection

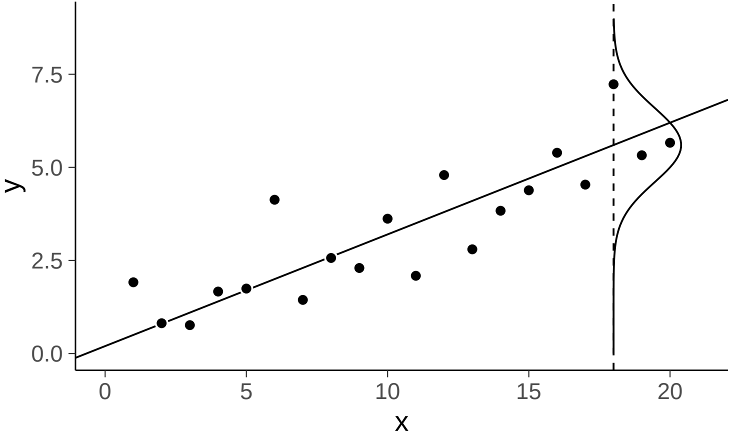
True mean y = a + bx



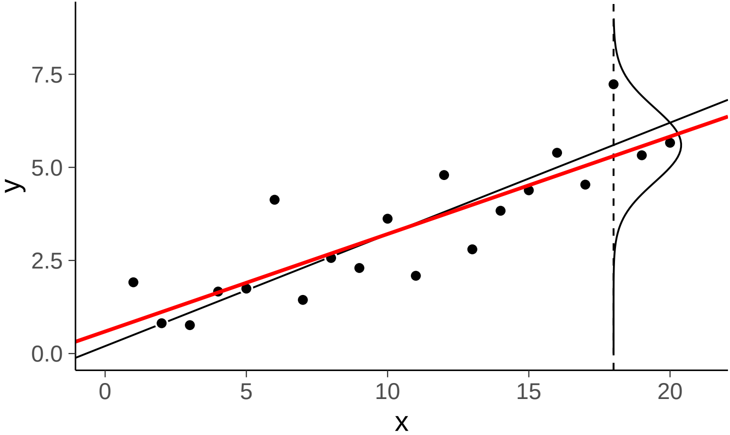
True mean and sigma



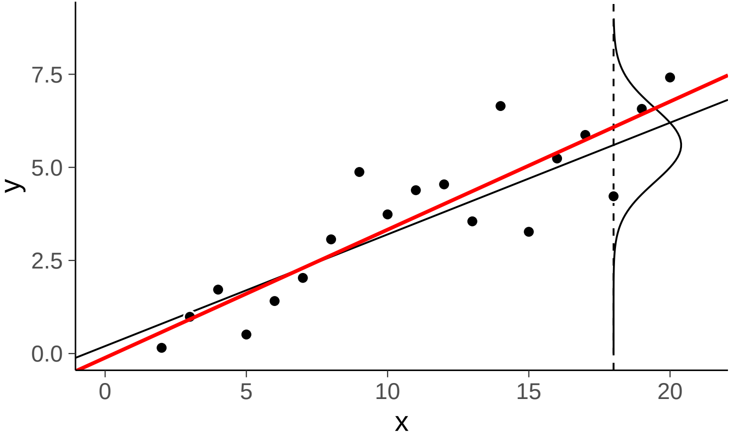
Data



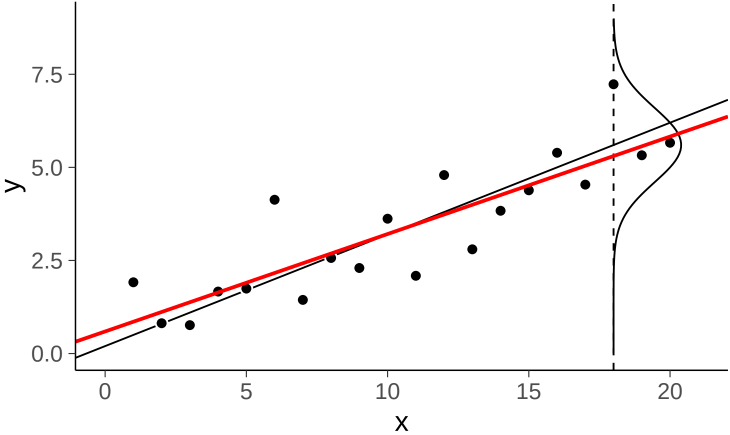
Posterior mean



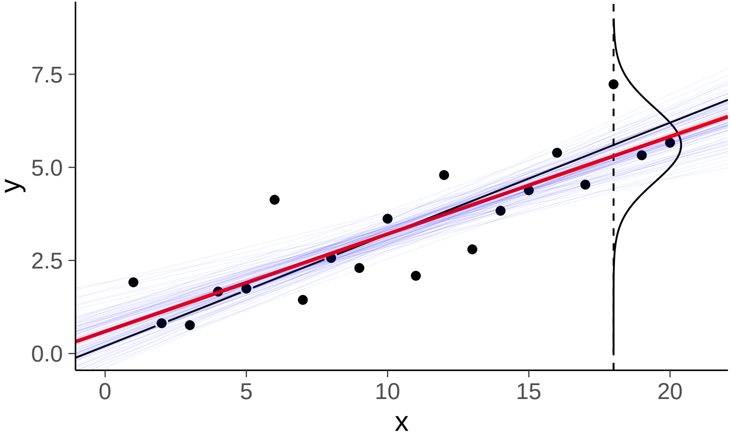
Posterior mean, alternative data realisation



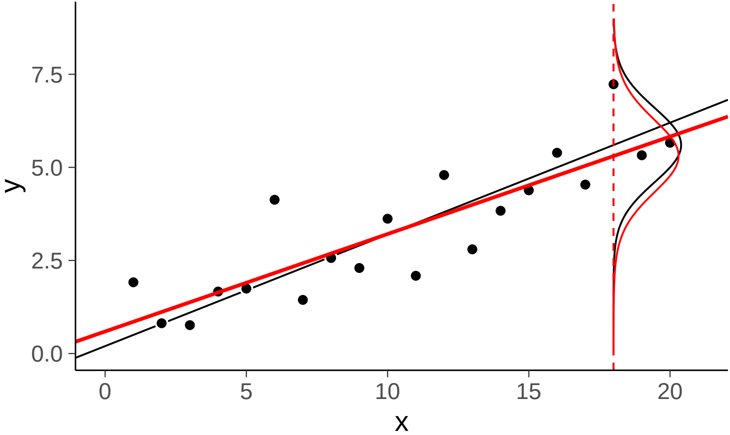
Posterior mean



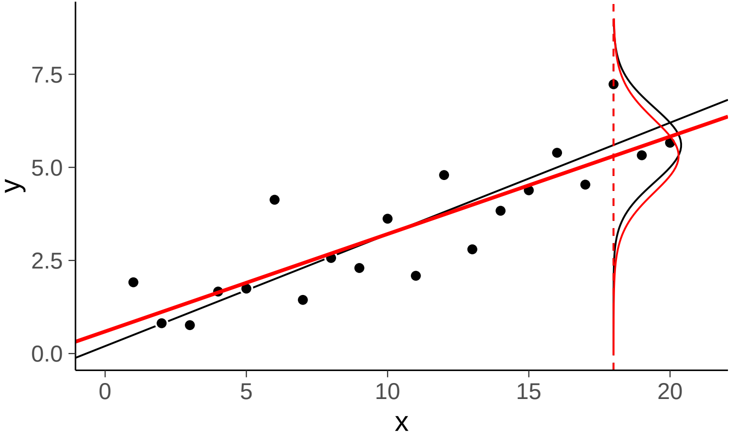
Posterior draws



Posterior predictive distribution

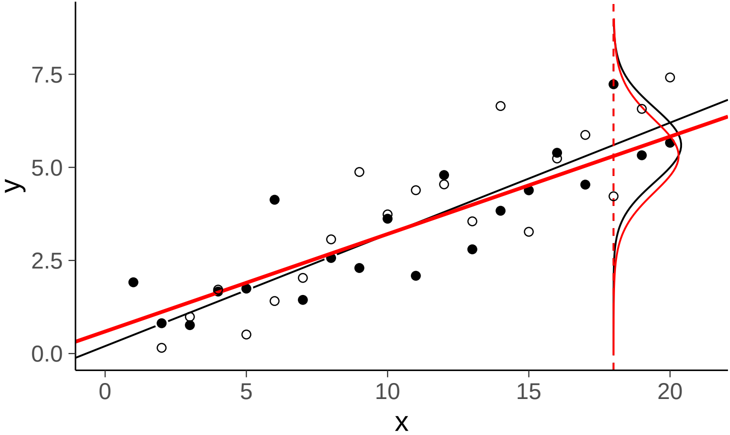


Posterior predictive distribution

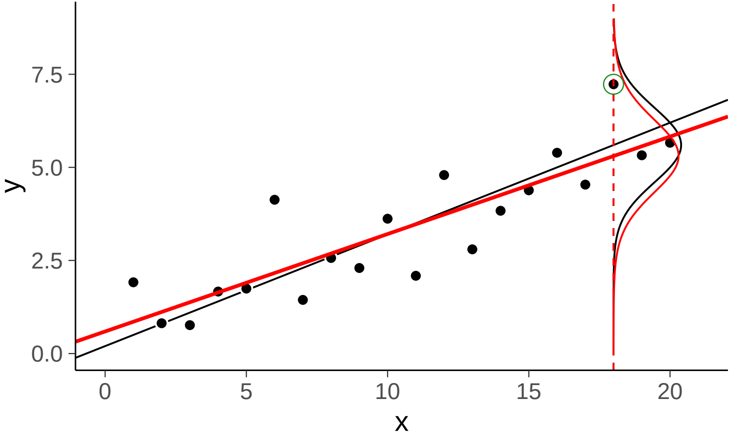


$$p(\tilde{y}|\tilde{x} = 18, x, y) = \int p(\tilde{y}|\tilde{x} = 18, \theta)p(\theta|x, y)d\theta$$

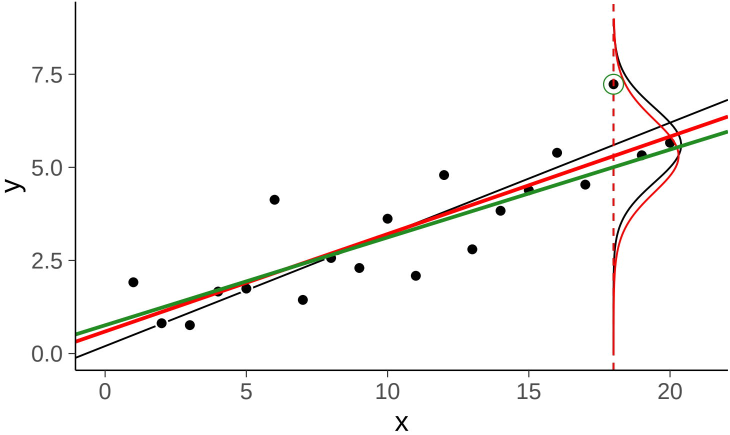
New data



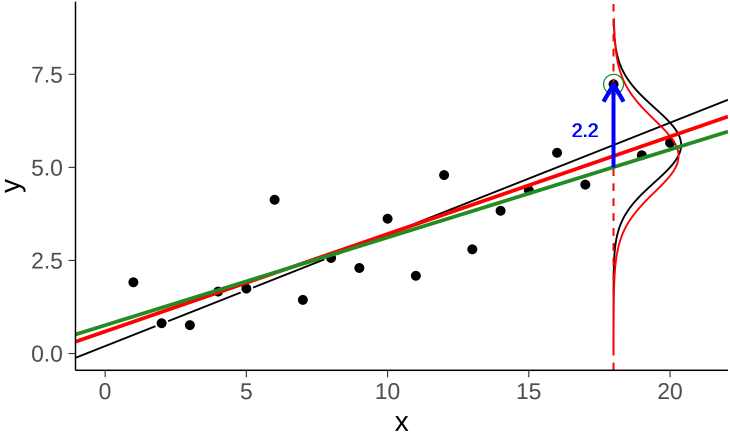
Posterior predictive distribution



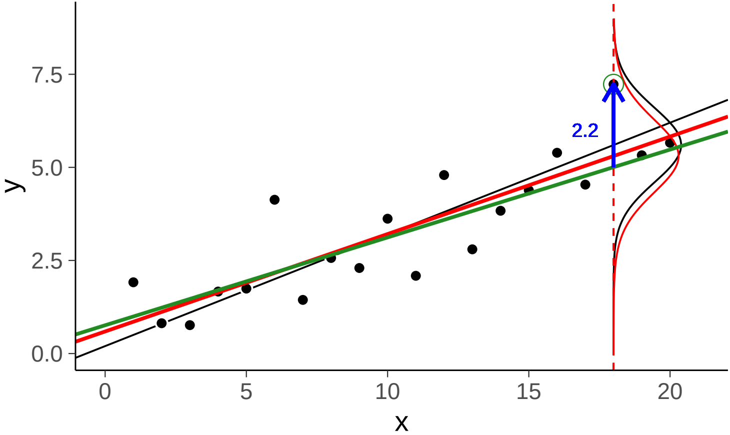
Leave−one−out mean



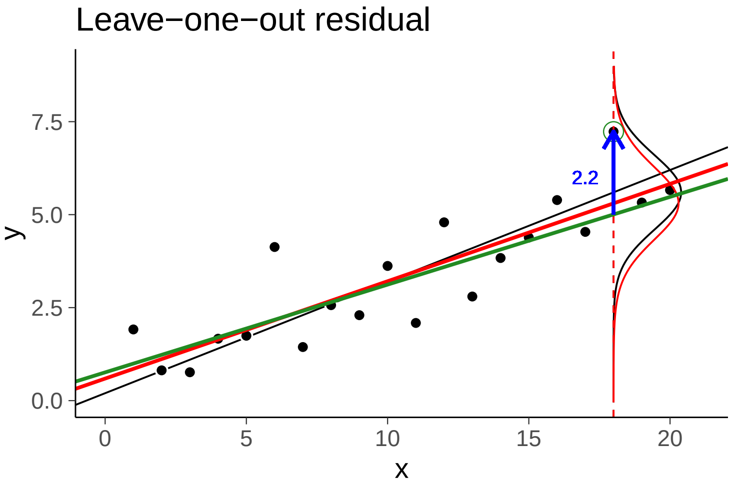
Leave−one−out residual



Leave−one−out residual

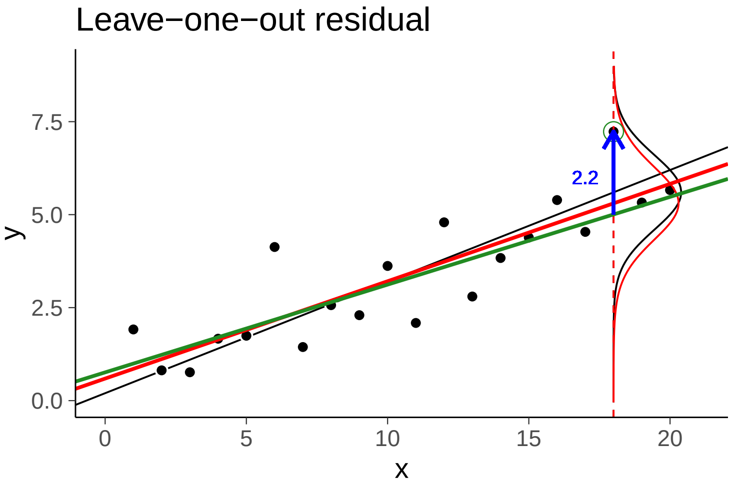


$$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$$



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

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

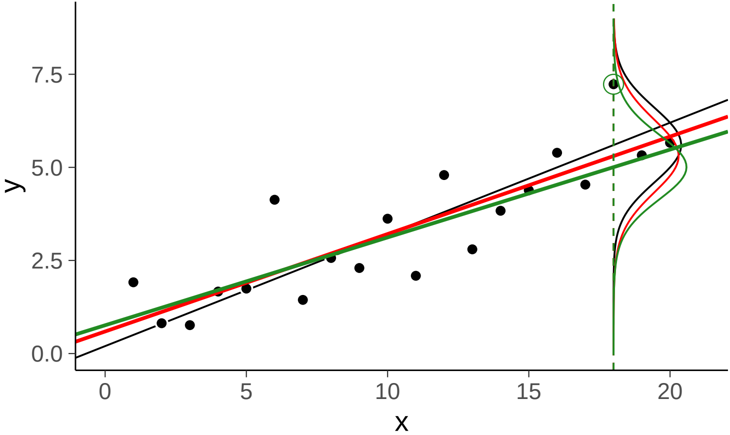


$y_{18} - E[p(\tilde{y}|\tilde{x} = 18, x_{-18}, y_{-18})]$

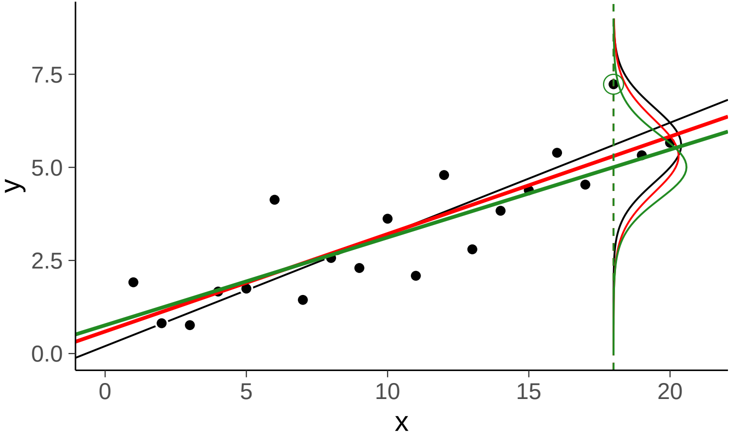
Can be use to compute, e.g., RMSE, R^2, 90% error

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

Leave−one−out predictive distribution

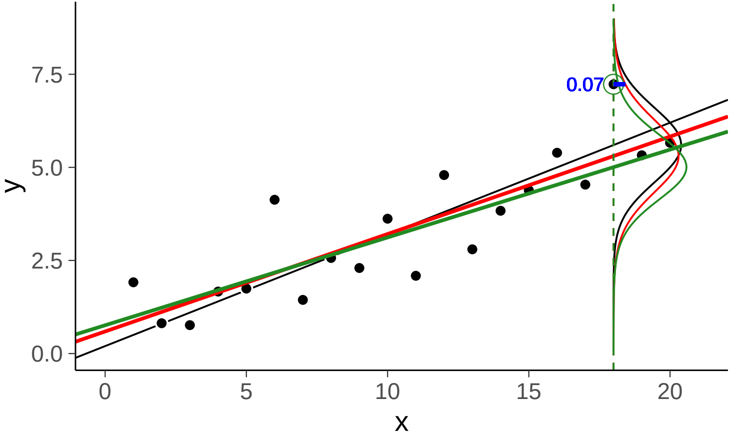


Leave−one−out predictive distribution

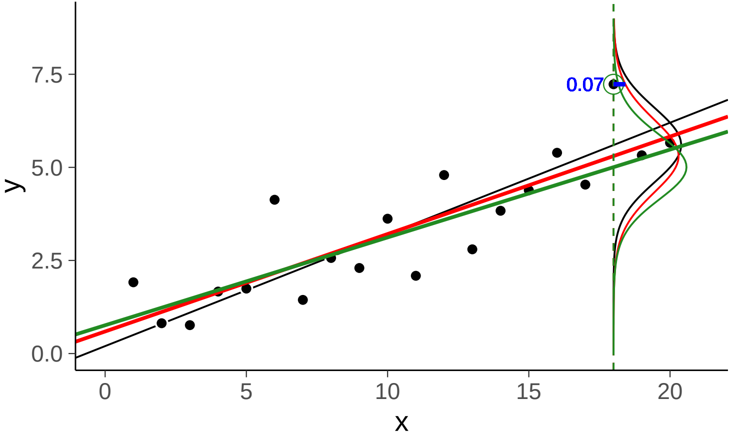


$$p(\tilde{y}|\tilde{x}=18, x_{-18}, y_{-18}) = \int p(\tilde{y}|\tilde{x}=18,\theta)p(\theta|x_{-18}, y_{-18})d\theta$$

Posterior predictive density

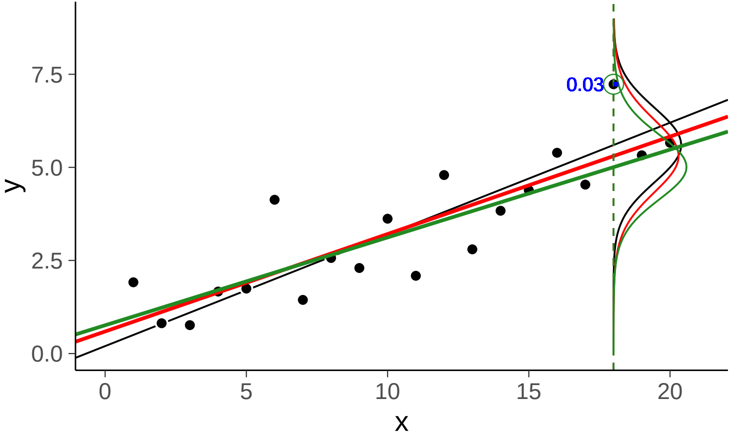


Posterior predictive density



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

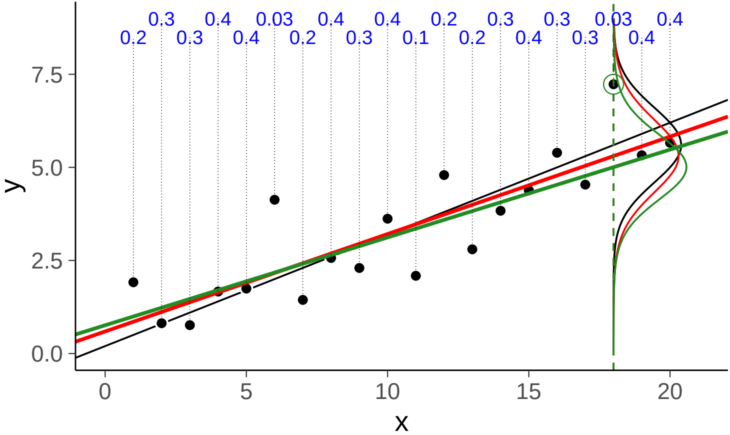
Leave−one−out predictive density



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

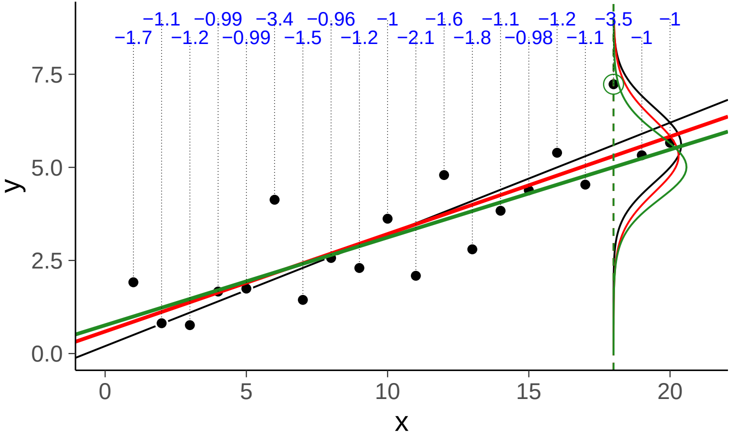
$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$

Leave−one−out predictive densities



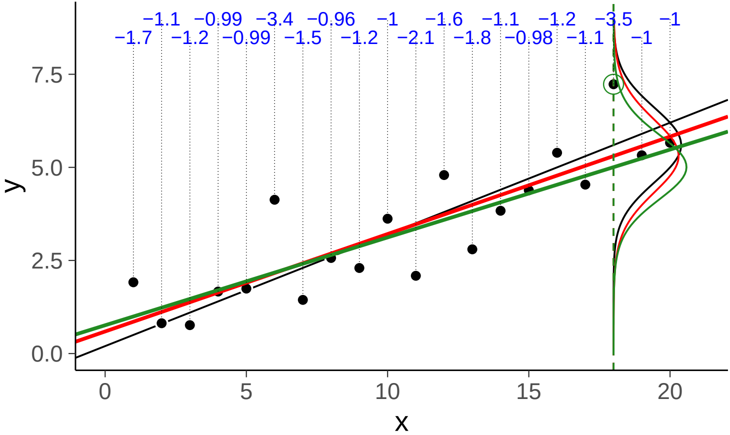
$p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$

Leave−one−out log predictive densities



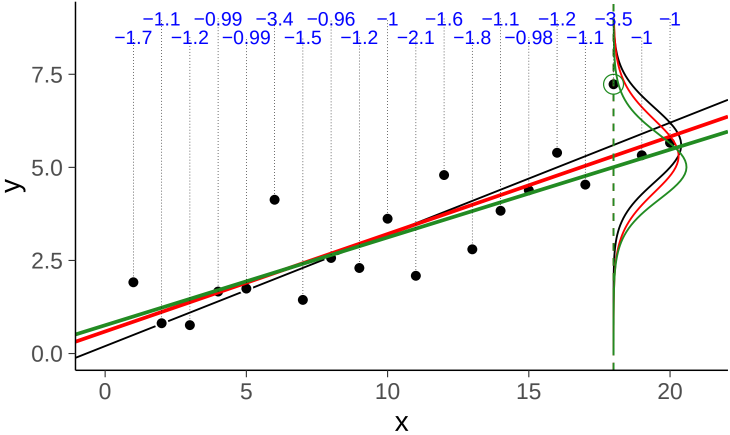
$\log p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \ldots, 20$

Leave−one−out log predictive densities

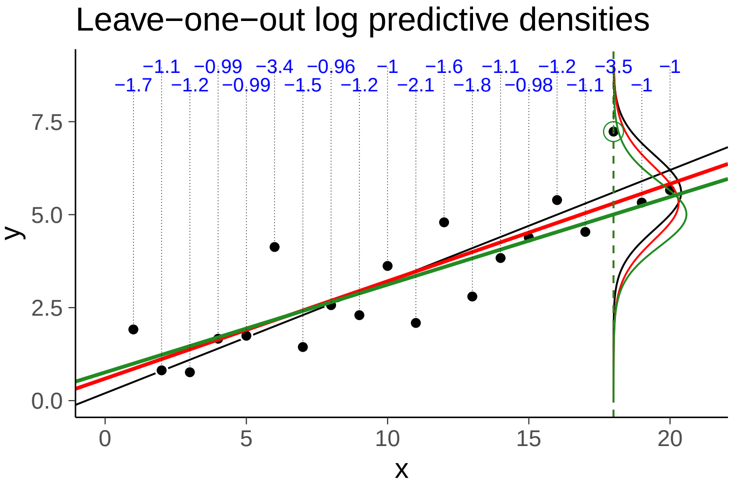


$\sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

Leave−one−out log predictive densities



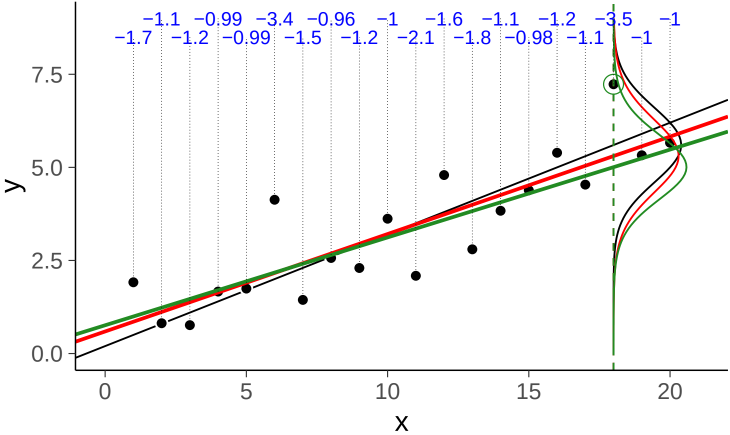
$\text{elpd\_loo} = \sum_{i=1}^{20} \log p(y_i | x_i, x_{-i}, y_{-i}) \approx -29.5$



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

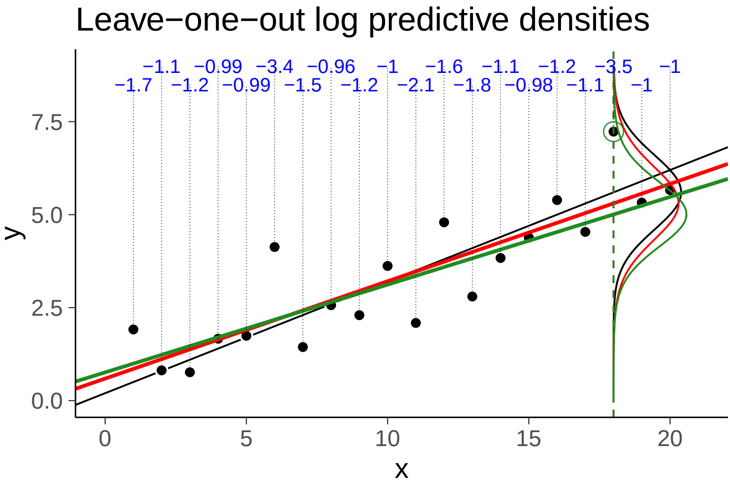
unbiased estimate of log posterior pred. density for new data

Leave−one−out log predictive densities



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

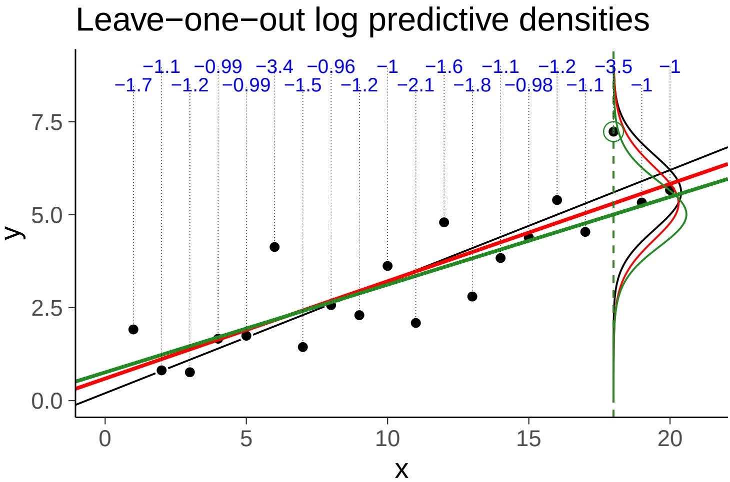
$$\text{lpd} = \sum_{i=1}^{20} \log p(y_i | x_i, x, y) \approx -26.8$$



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

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

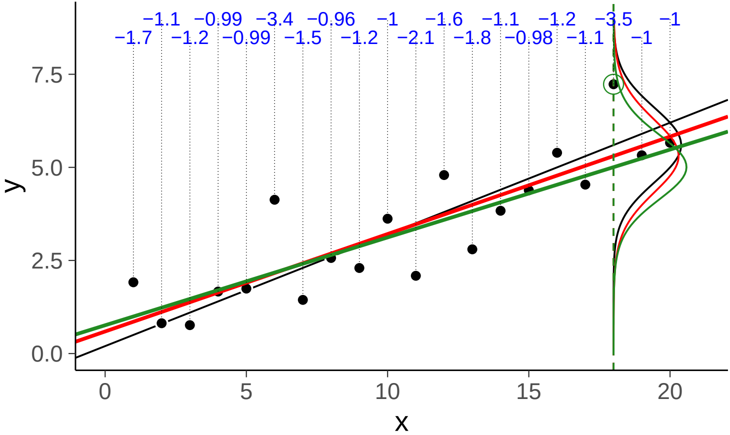
$\text{p\_loo} = \text{lpd} - \text{elpd\_loo} \approx 2.7$



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

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

Leave−one−out log predictive densities



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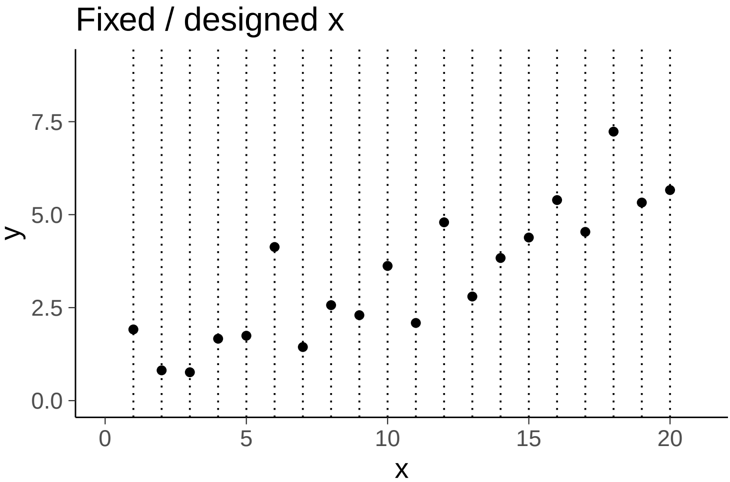
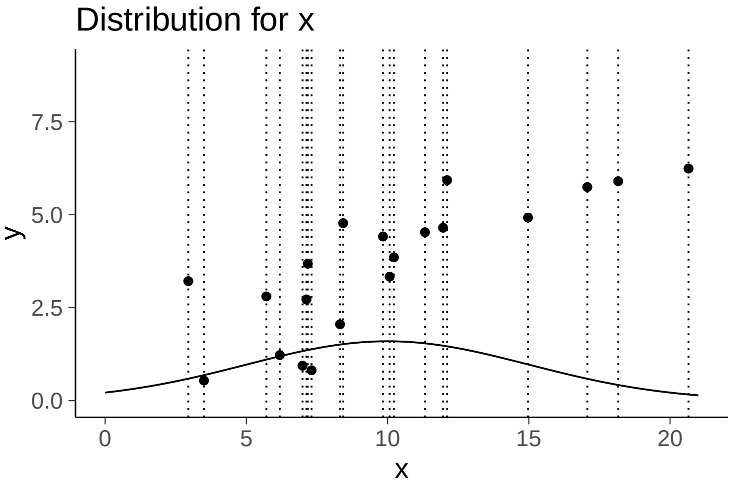
SE $= \mathrm{sd}(\log p(y_i|x_i, x_{-i}, y_{-i})) \cdot \sqrt{20} \approx 3.3$

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



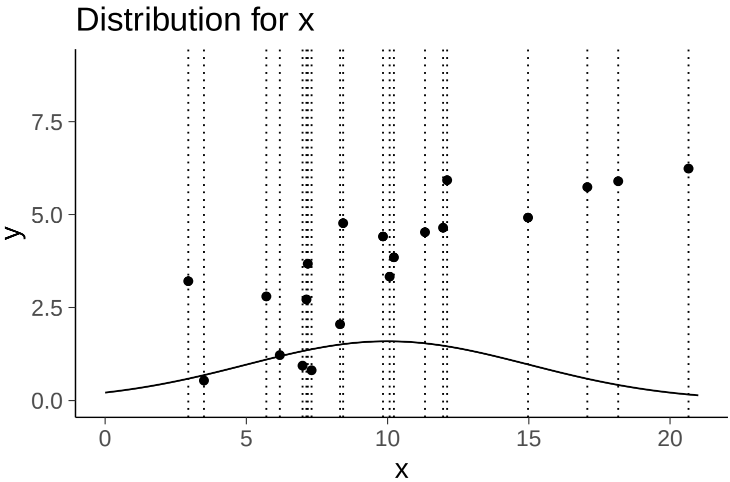
LOO is ok for fixed / designed x. SE is uncertainty about $y|x$.

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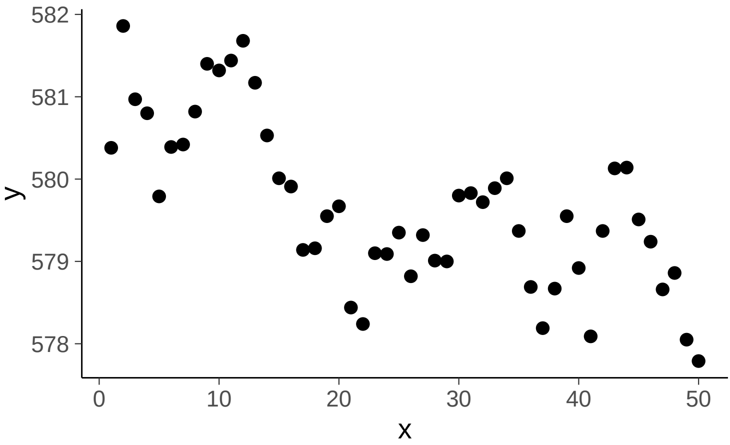
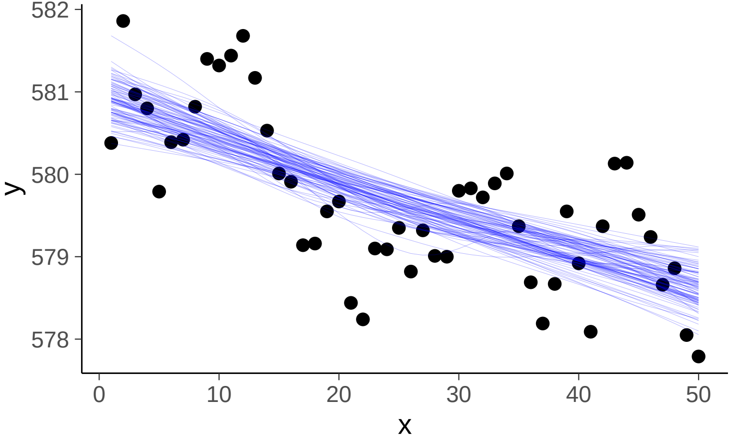
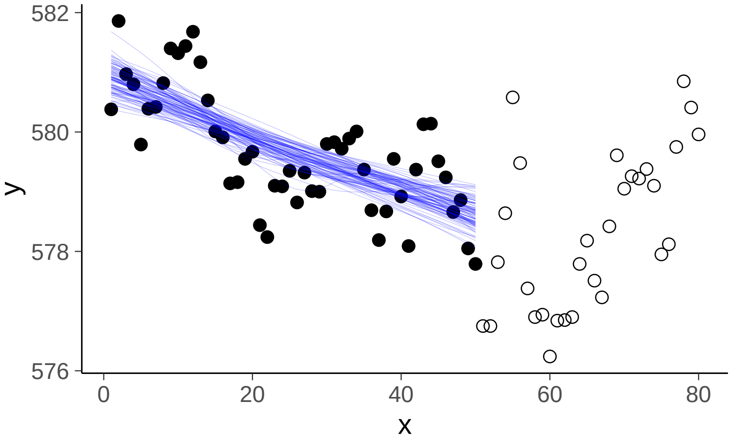
All Pareto k estimates are ok (k < 0.7).
See help('pareto-k-diagnostic') for details.
```

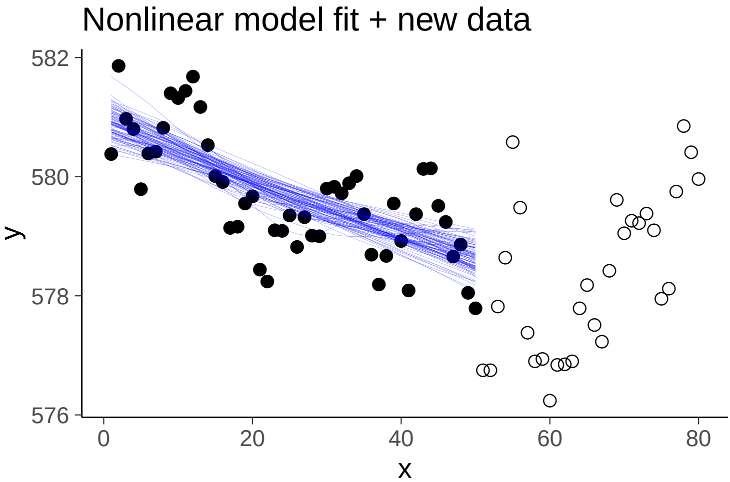

582
581
580
579
578
y
0
10
20
30
40
50
x

Nonlinear model fit

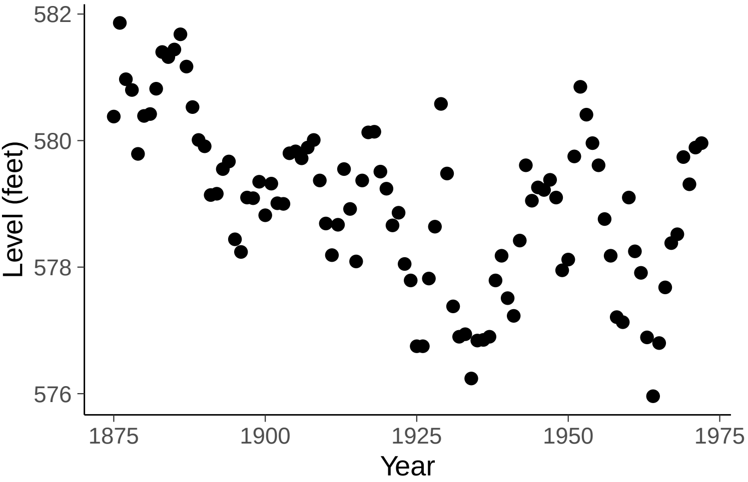


Nonlinear model fit + new data

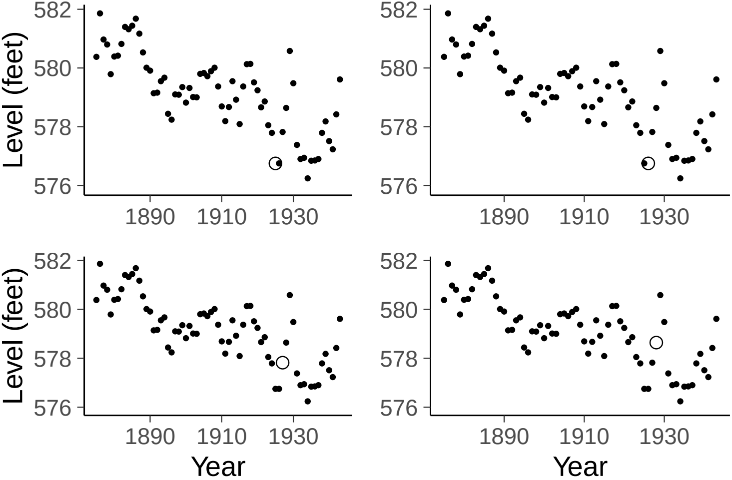




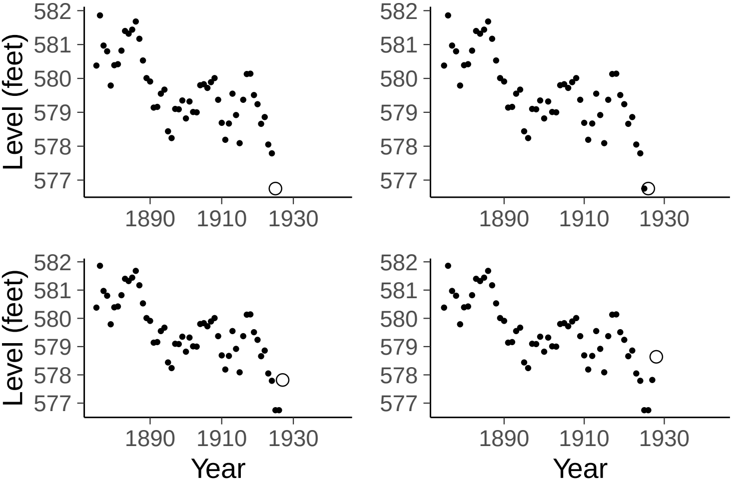
Extrapolation is more difficult



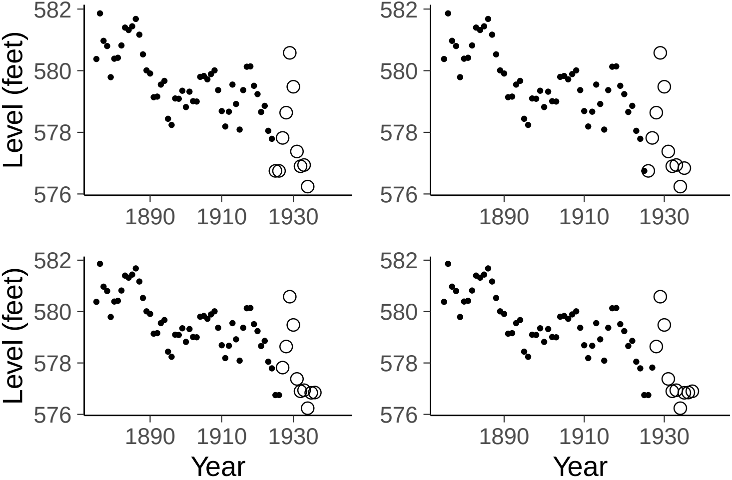
Can LOO or other cross-validation be used with time series?



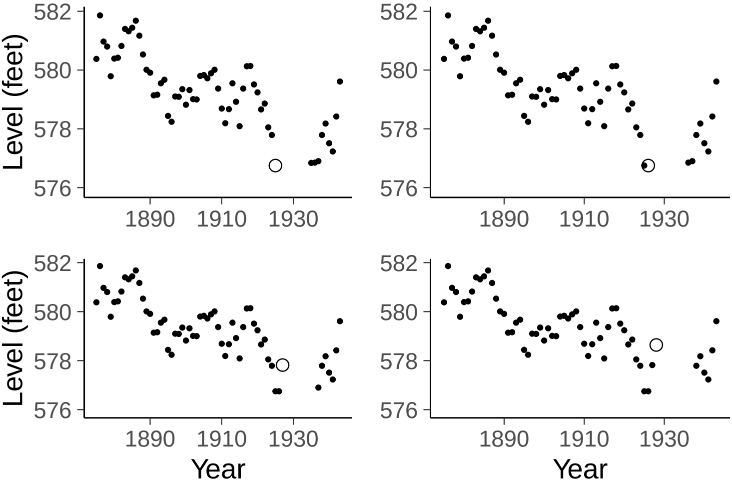
Leave-one-out cross-validation is ok for assessing conditional model



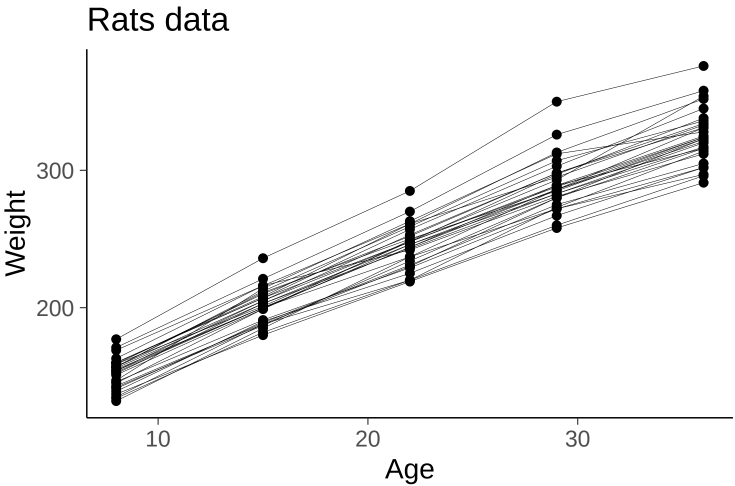
leave-future-out cross-validation is better for predicting future



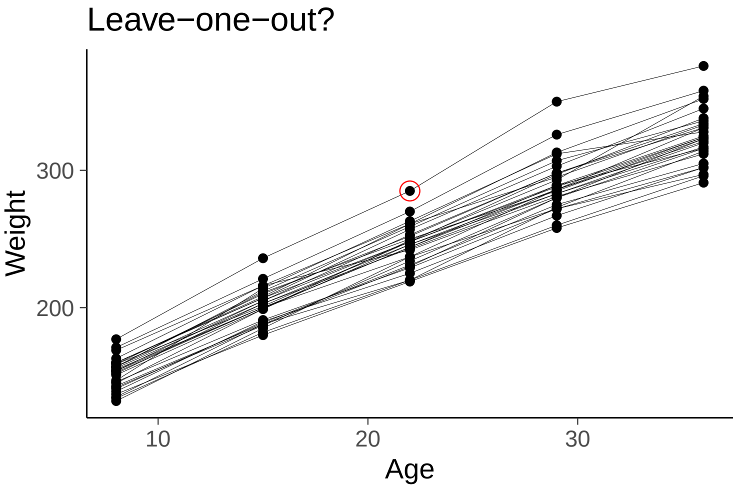
m-step-ahead cross-validation is better for predicting further future



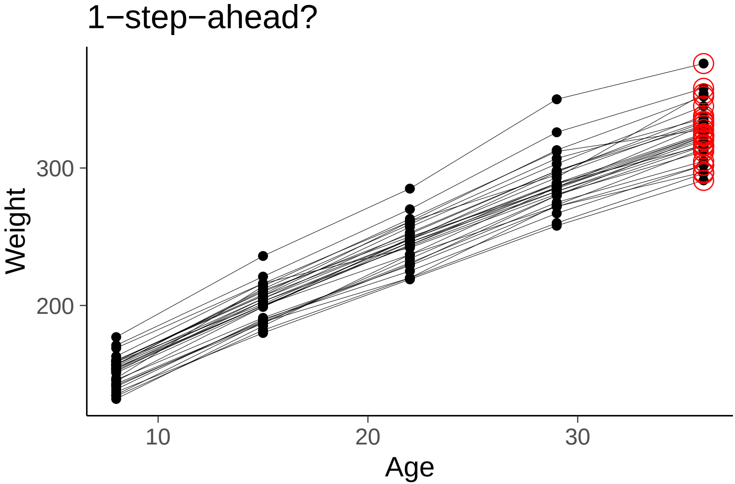
m-step-ahead leave-a-block-out cross-validation



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

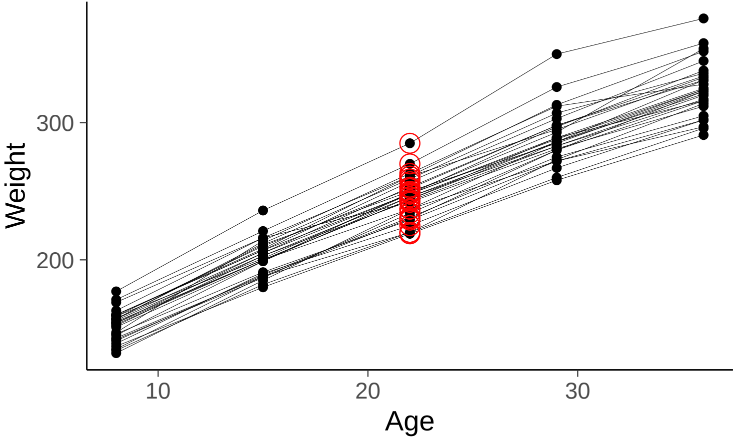


Yes!



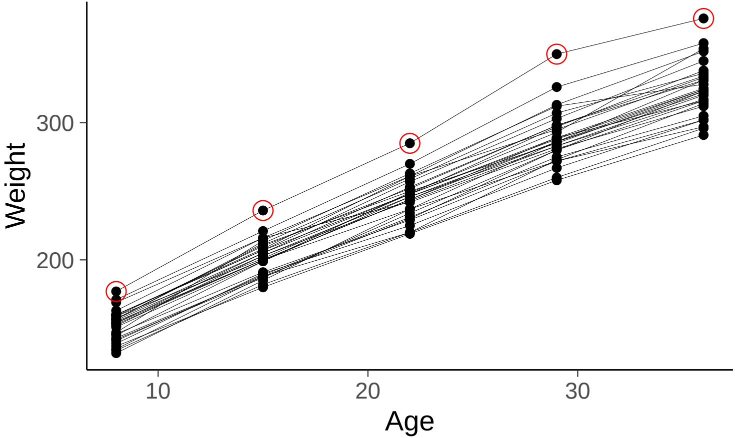
Yes!

Leave−one−time−point−out?



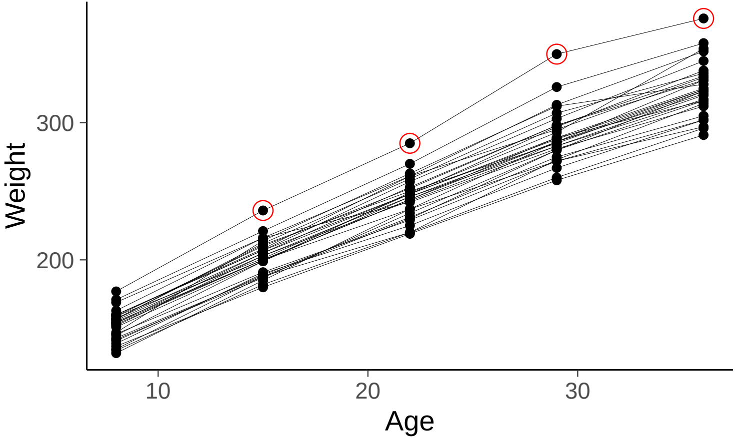
Yes!

Leave−one−rat−out?



Yes!

Predict given initial weight?



Yes!

Summary of data generating mechanisms and prediction tasks

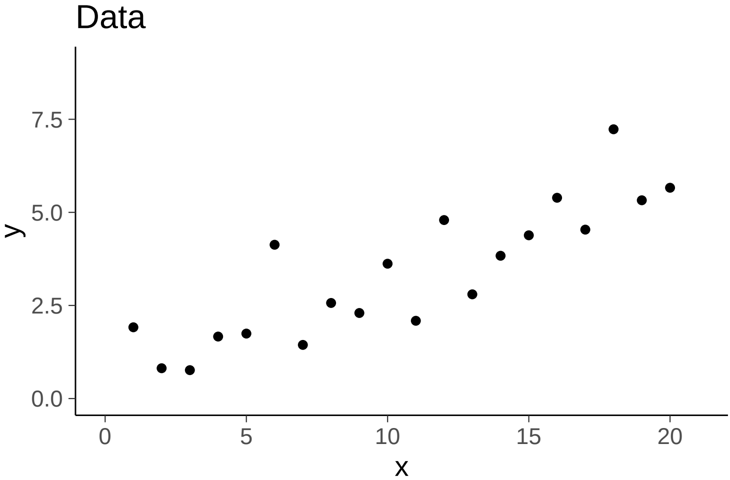
- You have to make some assumptions on data generating mechanism
- Use the knowledge of the prediction task if available
- Cross-validation can be used to analyse different parts, even if there is no clear prediction task

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

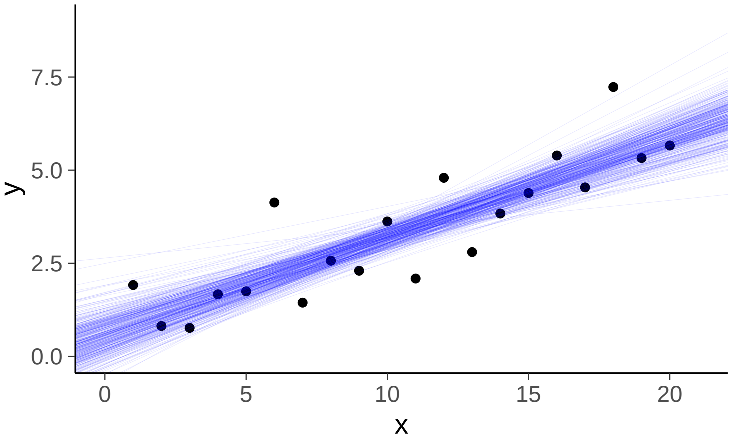
Fast cross-validation

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

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

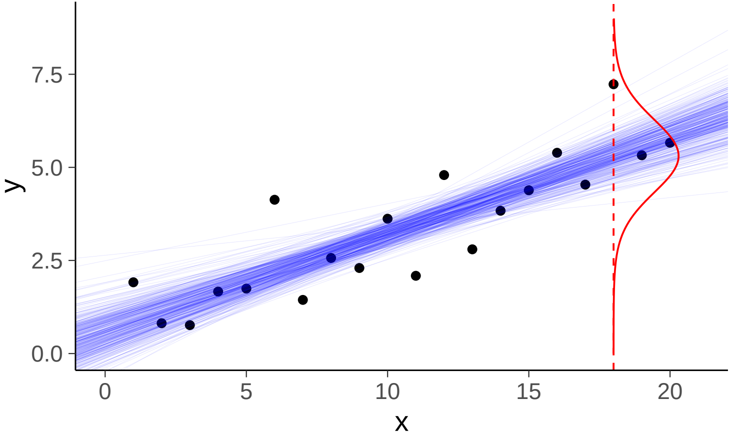

Data
y
7.5
5.0
2.5
0.0
0
5
10
15
20
x

Posterior draws



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

Posterior predictive distribution



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

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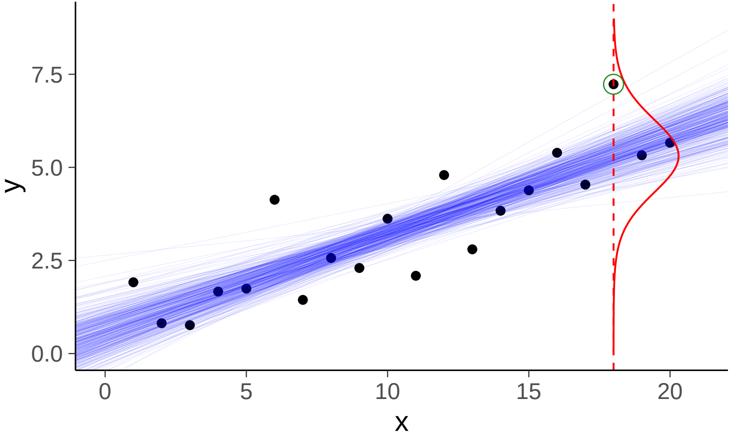

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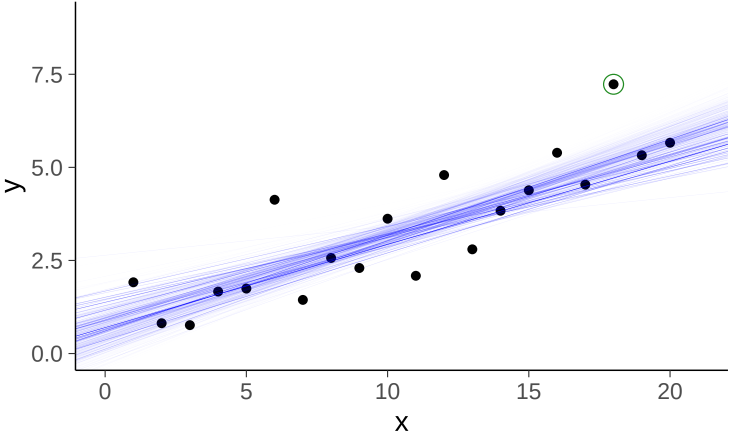
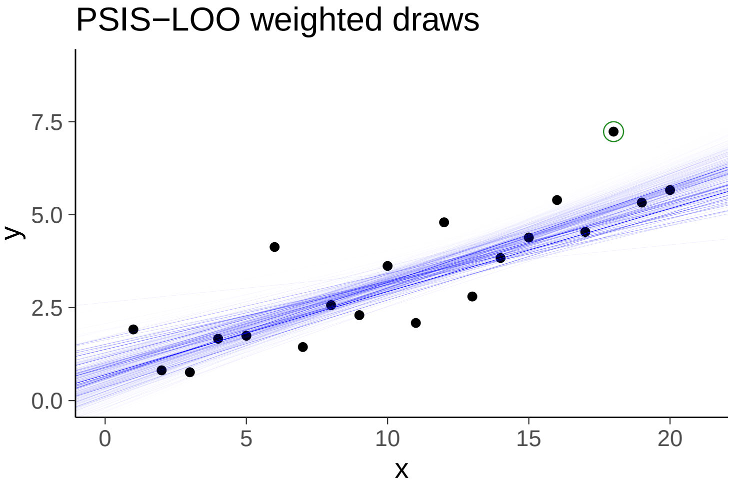
PSIS−LOO weighted draws

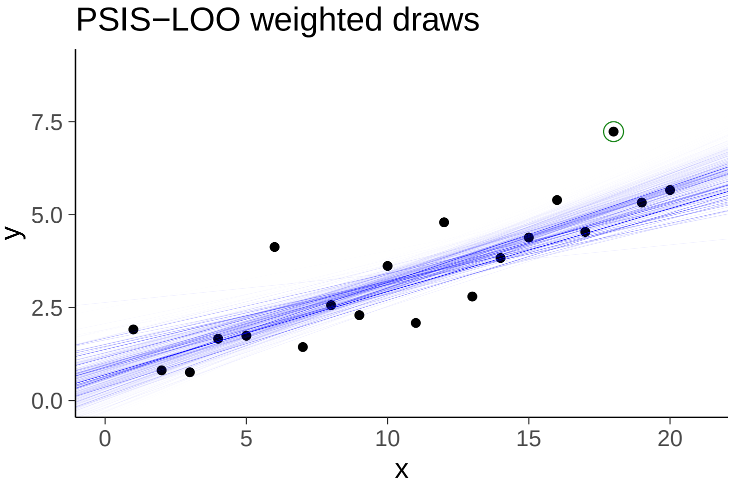


$$\theta^{(s)} \sim p(\theta|x, y)$$
$$r_i^{(s)} = p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y)$$



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

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



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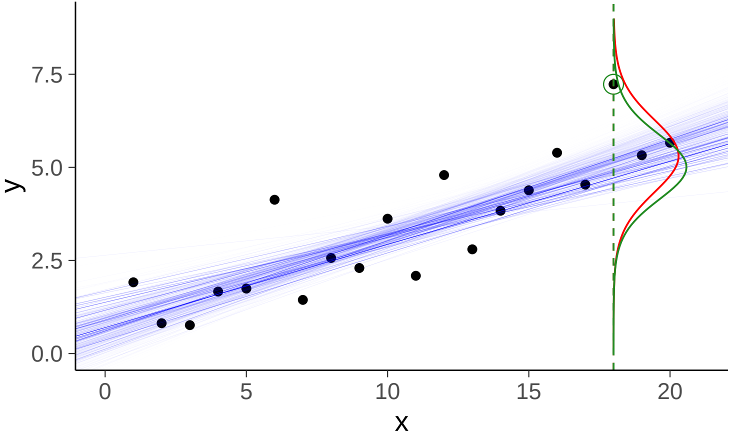
$$\log(1/p(y_i|x_i,\theta^{(s)})) = -\text{log\_lik}[i]$$

PSIS−LOO weighted predictive distribution



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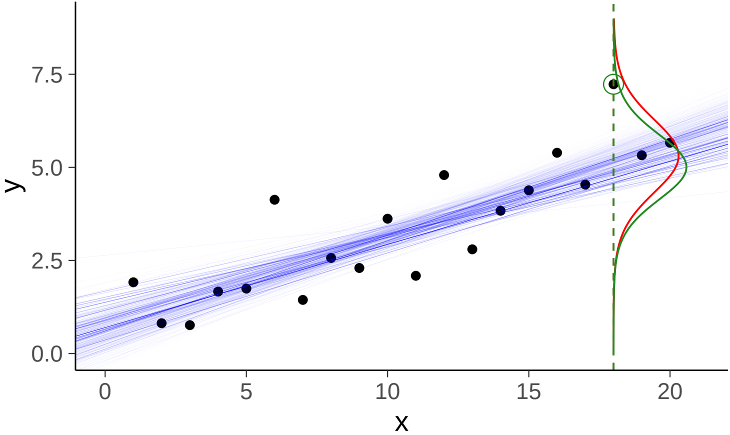

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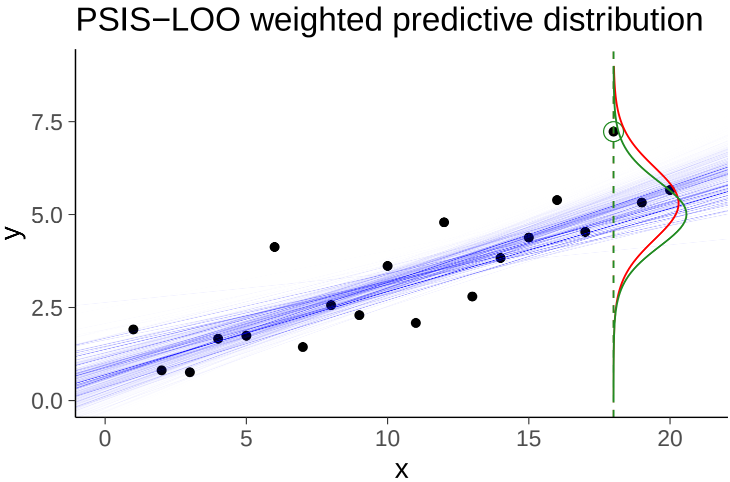

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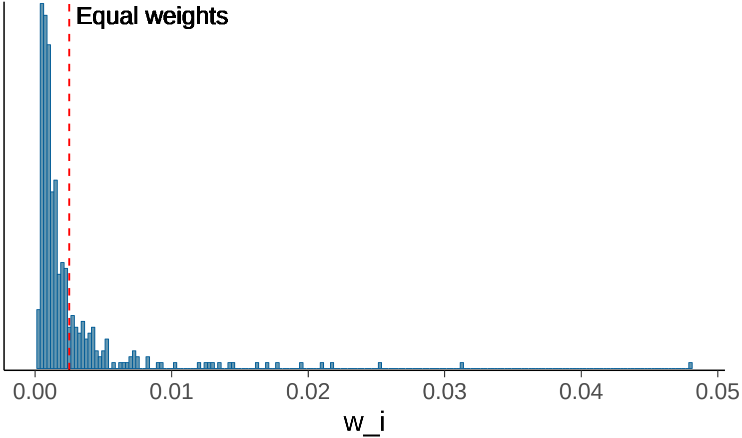
$p(y_i|x_i, x_{-i}, y_{-i}) \approx \sum_{s=1}^{S}[w_i^{(s)} p(y_i|x_i, \theta^{(s)})]$, where $w \leftarrow \text{PSIS}(r)$

400 importance weights for leave−18th−out



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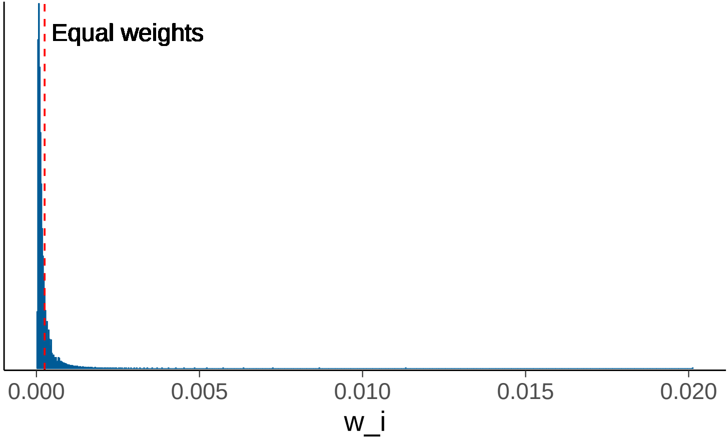

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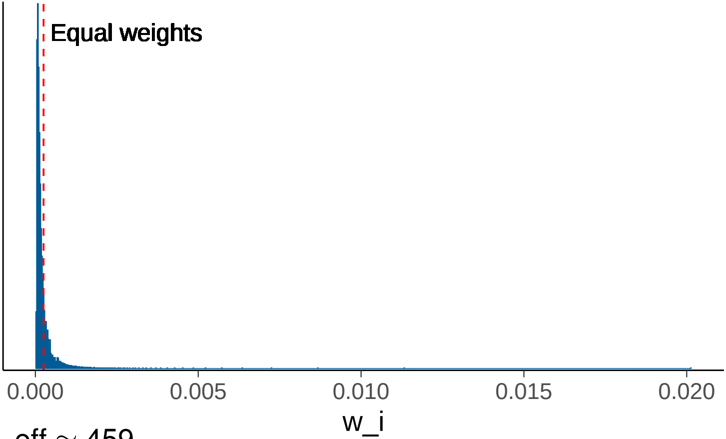
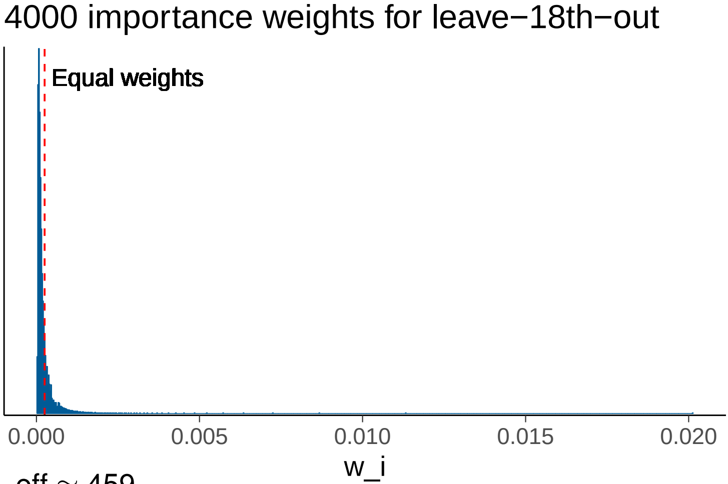


n_eff ≈ 459

see Vehtari, Gelman & Gabry (2017b)

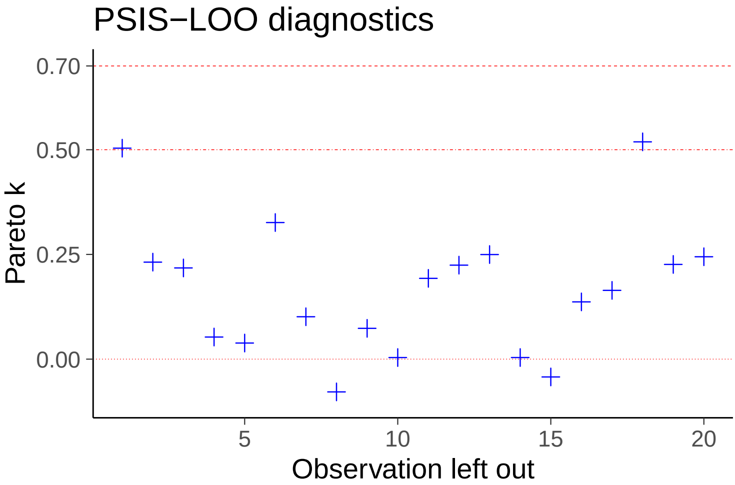


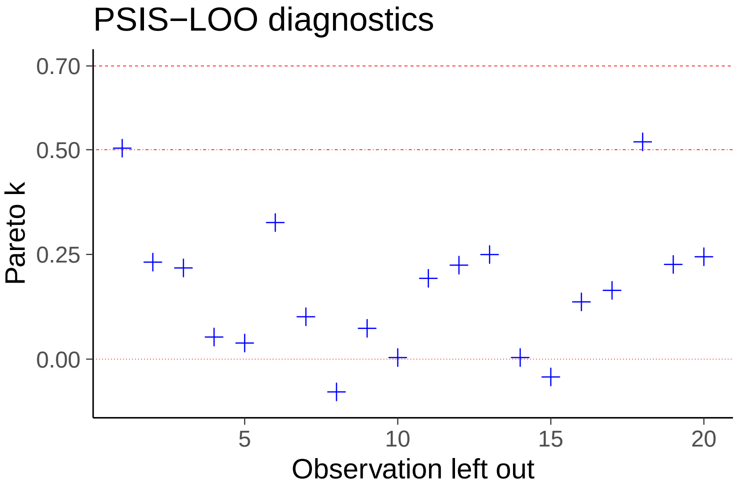
n_eff $\approx$ 459

Pareto $\hat{k} \approx 0.52$

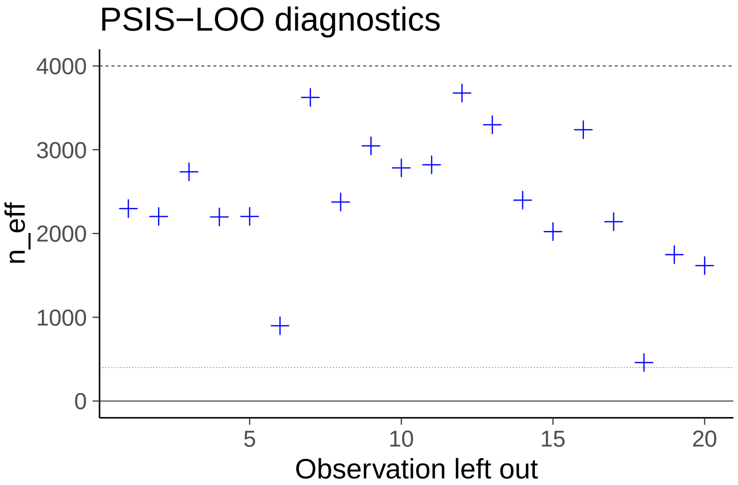
- Pareto $\hat{k}$ estimates the tail shape which determines the convergence rate of PSIS. Less than 0.7 is ok.

see Vehtari, Gelman & Gabry (2017b)


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




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



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loo package

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

         Estimate  SE
elpd_loo    -29.5 3.3
p_loo         2.7 1.0

------
Monte Carlo SE of elpd_loo is 0.1.

Pareto k diagnostic values:
                         Count Pct.    Min. n_eff
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All Pareto k estimates are ok (k < 0.7).
See help('pareto-k-diagnostic') for details.
```

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

Stan code

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

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```
...
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);
}
```

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```

- 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

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  - mc-stan.org/loo/articles/loo2-non-factorizable.html

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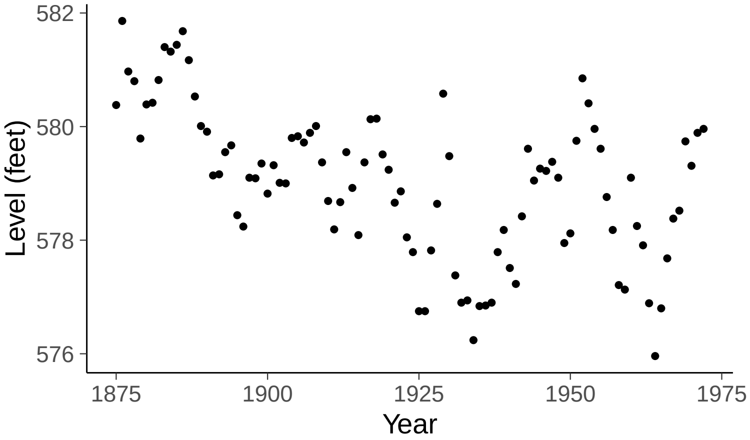
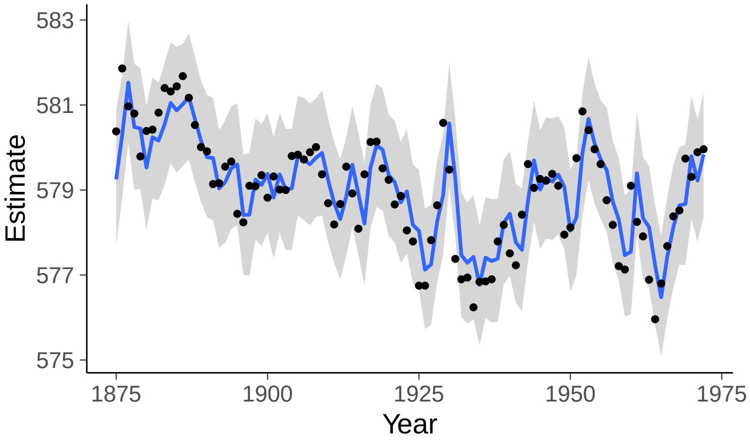
- PSIS-LOO for non-factorizable models
  - mc-stan.org/loo/articles/loo2-non-factorizable.html
- PSIS-LOO for time series
  - Approximate leave-future-out cross-validation

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

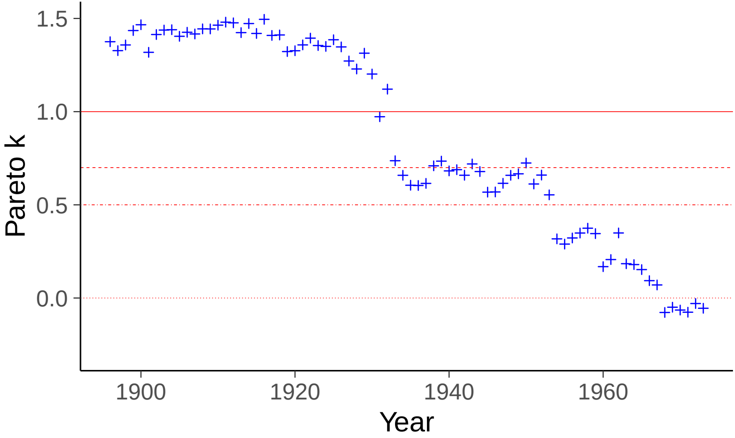
Data

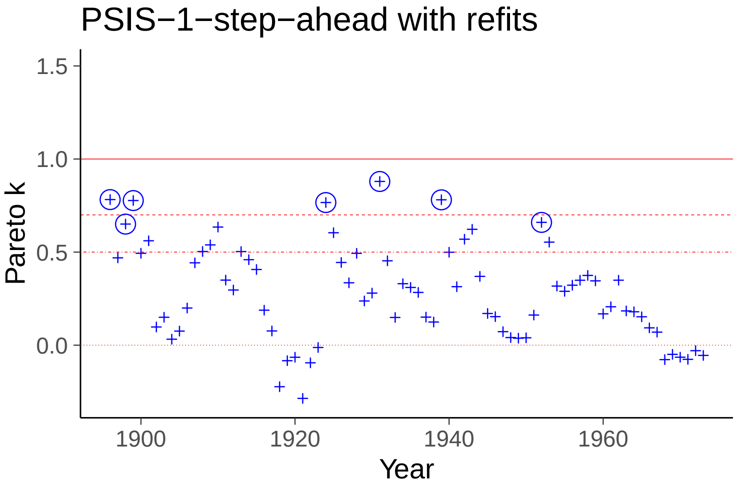


AR−2 prediction with 95% interval



PSIS−1−step−ahead



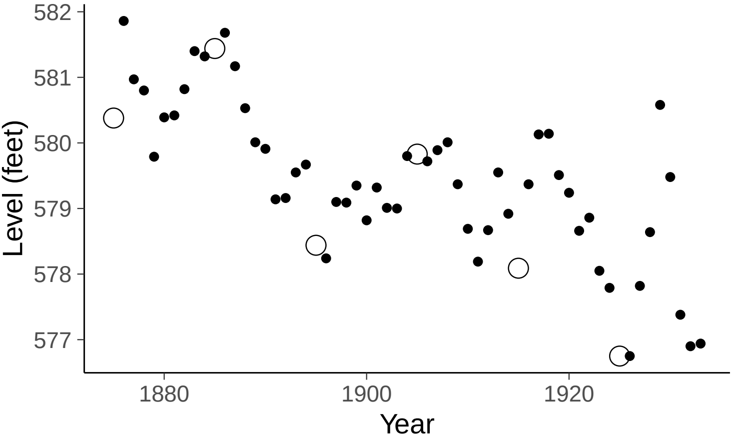


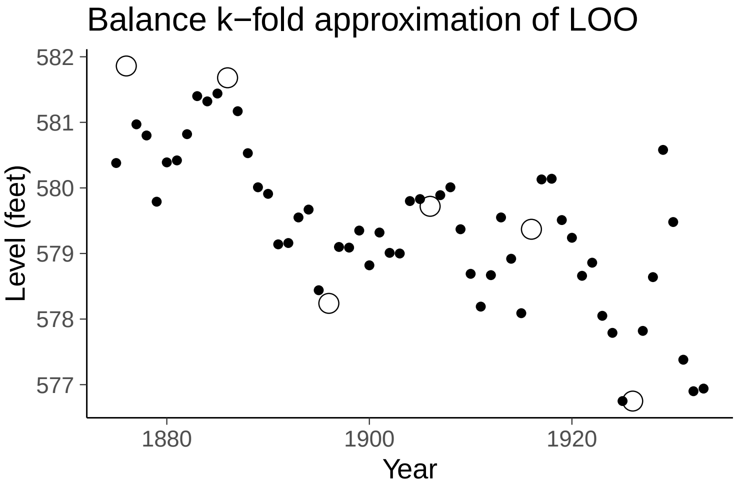
mc-stan.org/loo/articles/loo2-lfo.html

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

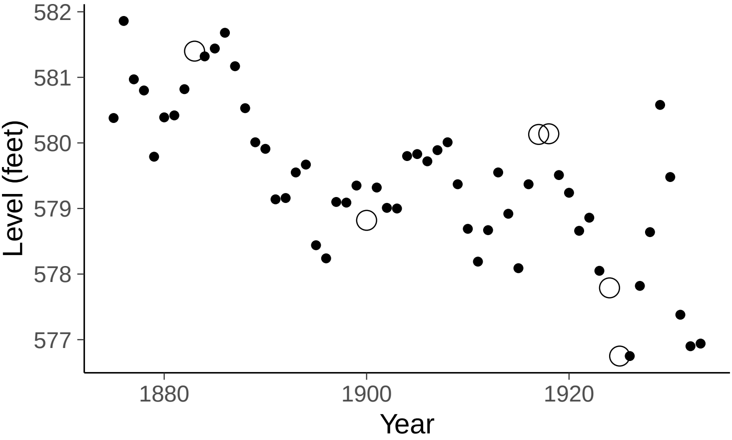
Balance k−fold approximation of LOO



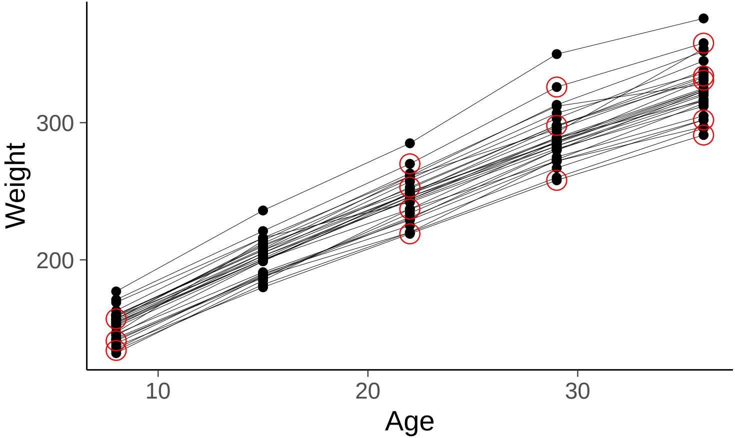


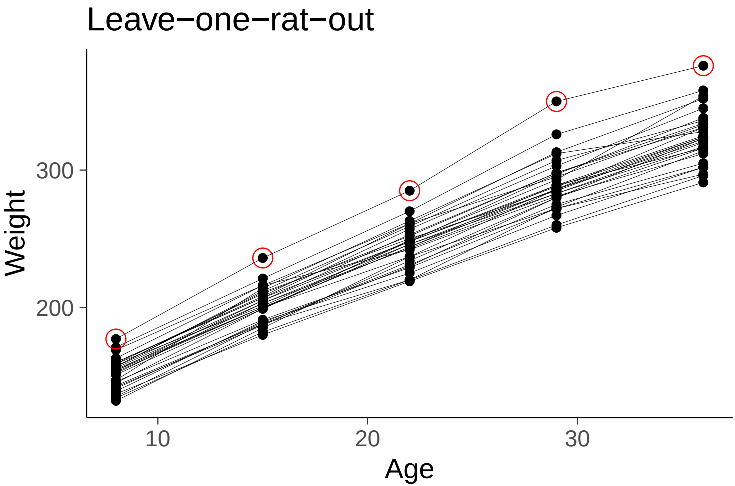
Balance k−fold approximation of LOO
582
581
580
579
578
577
Level (feet)
1880
1900
1920
Year

Random k−fold approximation of LOO



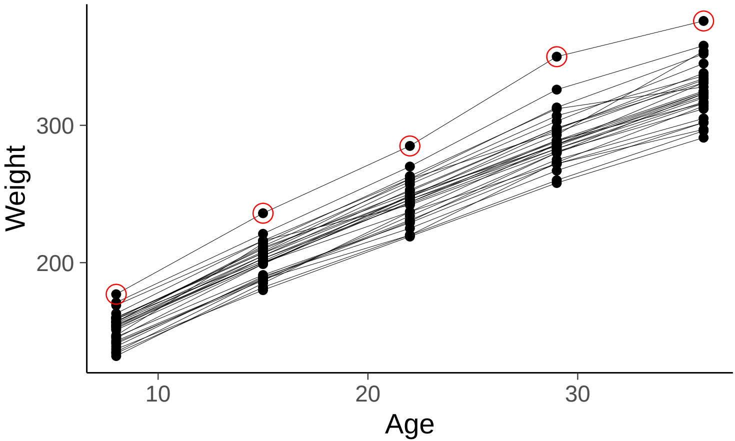
Random kfold approximation of LOO





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)

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- PSIS-LOO is more accurate

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- 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 corss-validation but starting with 0 observations

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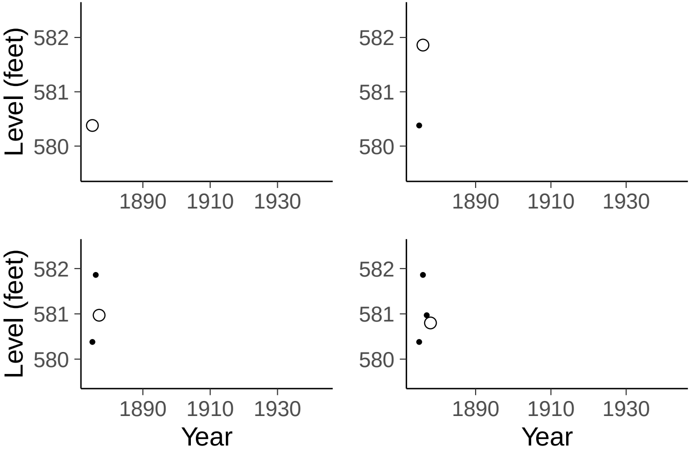

Marginal likelihood / Bayes factor

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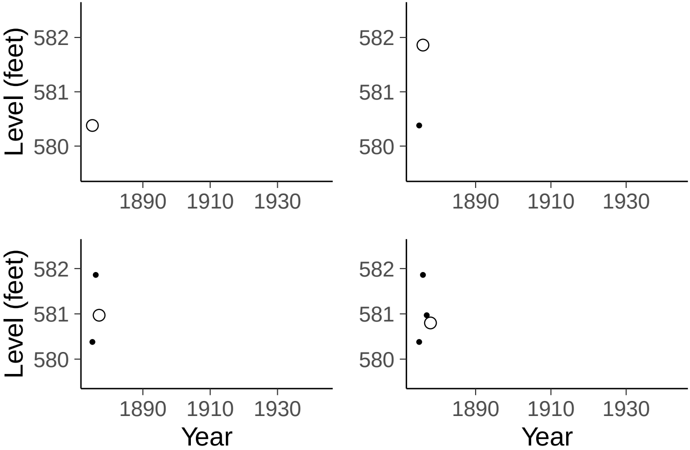

Marginal likelihood / Bayes factor

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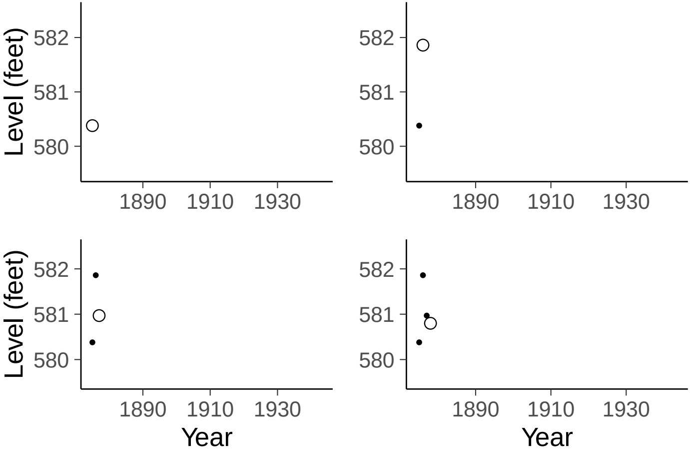

Marginal likelihood / Bayes factor

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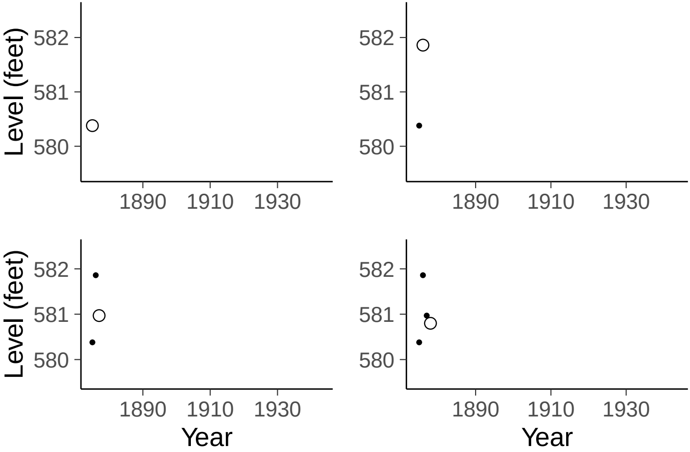

Cross-validation for model assessment

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  - 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/

Sometimes cross-validation is not needed

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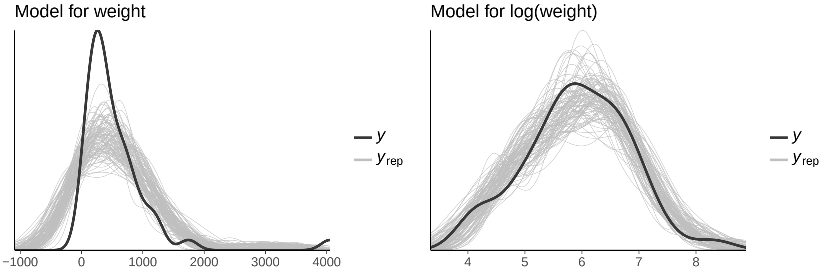
- Posterior predictive checking is often sufficient



Predicting the yields of mesquite bushes.

Gelman, Hill & Vehtari (2019): Regression and Other Stories, Chapter 11.

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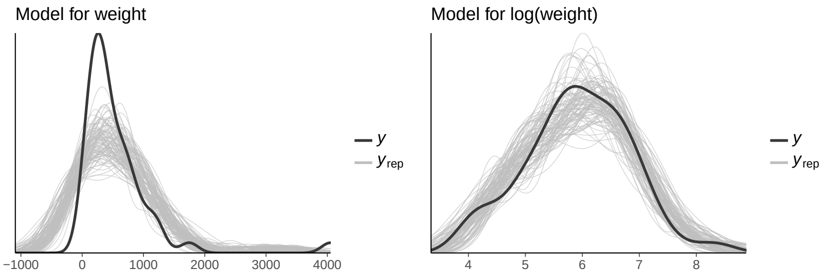

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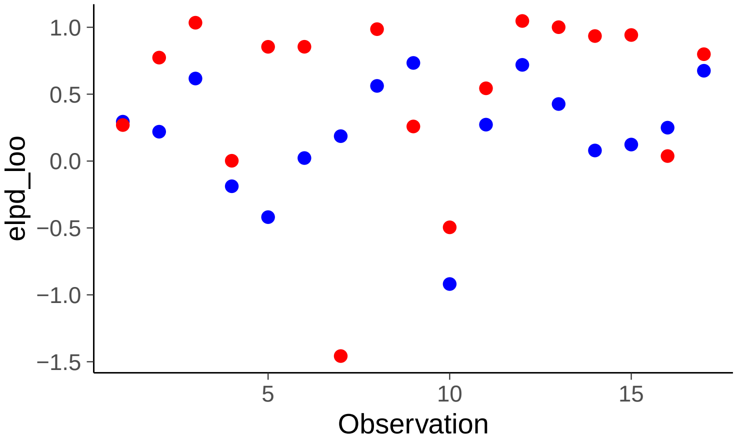
- mc-stan.org/bayesplot/articles/graphical-ppcs.html
- betanalpha.github.io/assets/case_studies/principled_bayesian_workflow.html

Model comparison

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

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

Pointwise comparison LOO models: Model 1



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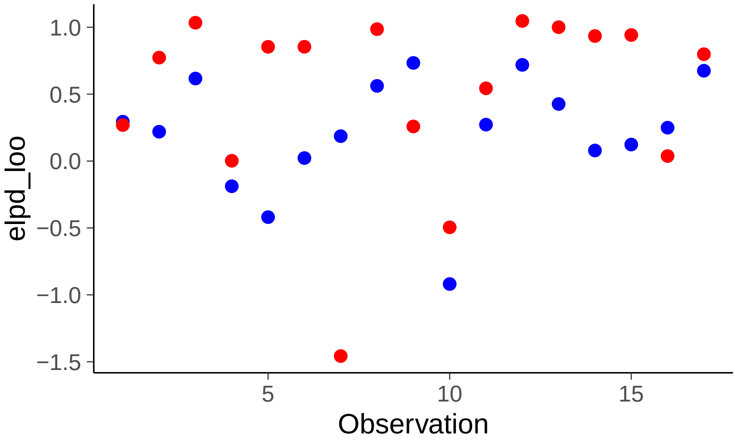
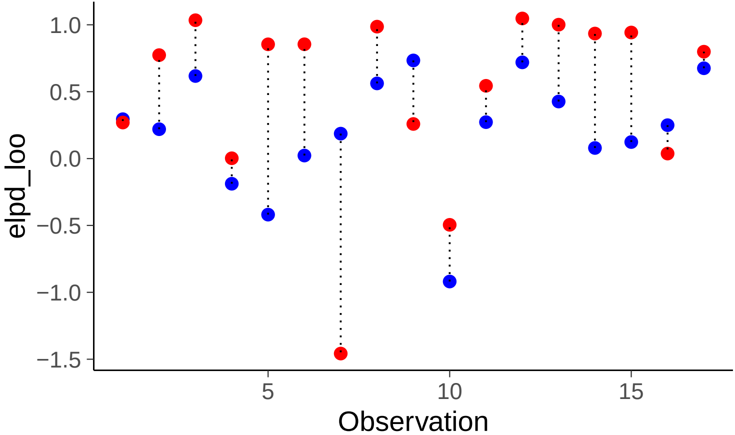


Model 1 elpd_loo $\approx$ 3.7, SE=1.8
Model 2 elpd_loo $\approx$ 8.4, SE=2.8

Pointwise comparison LOO models: Model 1



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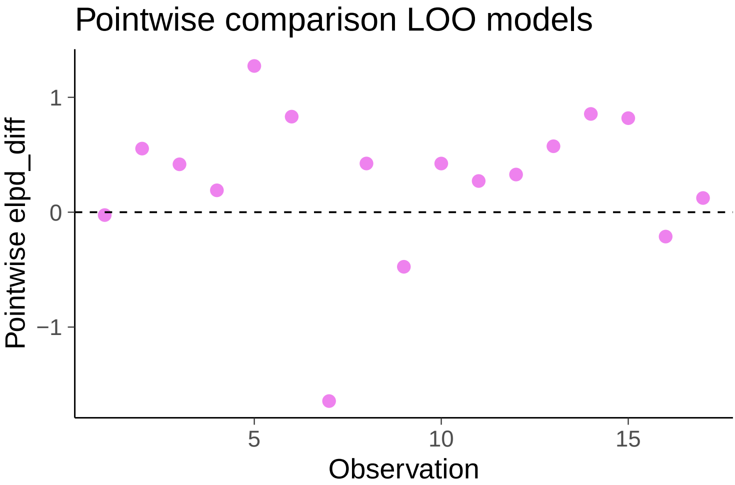
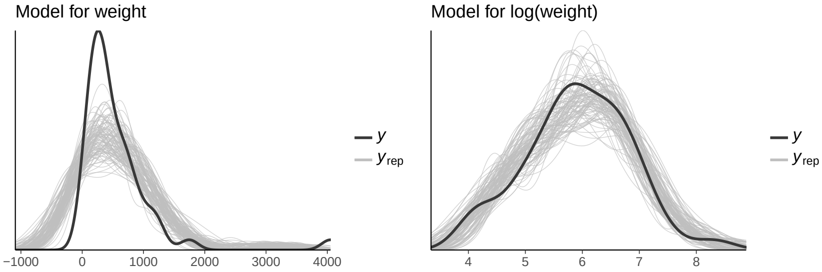



```
Model comparison:
(negative 'elpd_diff' favors 1st model, positive favors 2nd)

elpd_diff        se
      4.7       2.7
```

Sometimes cross-validation is not needed

- Posterior predictive checking is often sufficient



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  - see Vehtari & Ojanen (2012) for earlier references
  - posterior convergence rate can be slow for fully non-parametric models

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
- For fully non-parametric models you may assume that true model is included in the list of models considered (M-closed)
  - related to talk by Chris Holmes
  - see Vehtari & Ojanen (2012) for earlier references
  - posterior convergence rate can be slow for fully non-parametric models
- In nested case, often easier and more accurate to analyse posterior distribution of more complex model directly
  avehtari.github.io/modelselection/betablockers.html

What if one is not clearly better than others?

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- We define the stacking weights as the solution to the following optimization problem:

$$\max_w \frac{1}{n}\sum_{i=1}^{n} S\Big(\sum_{k=1}^{K} w_k \hat{p}(y_i|x_{-i}, y_{-i}, M_k)\Big),$$

$$s.t. \quad w_k \geq 0, \quad \sum_{k=1}^{K} w_k = 1.$$

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- Other cross-validation structures can be used, too

Gaussian mixture example

$y \sim \mathrm{N}(3.4, 1), \quad p_k = \mathrm{N}(k, 1)$ with $k = 1, \ldots, 8$

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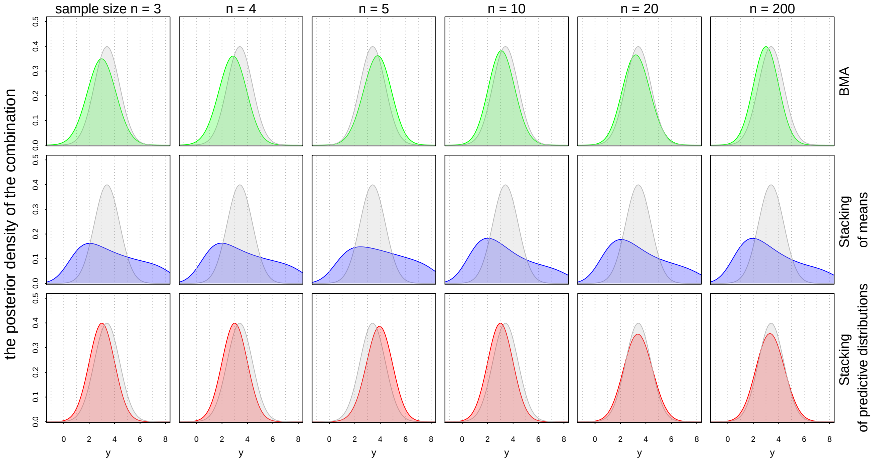
Model averaged predictive distributions



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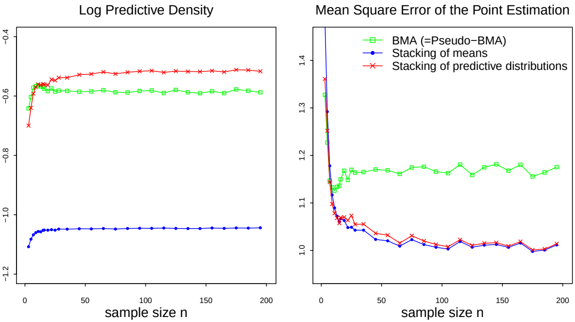
(a, b) Stacking of predictive distributions vs. BMA



(a) (b)

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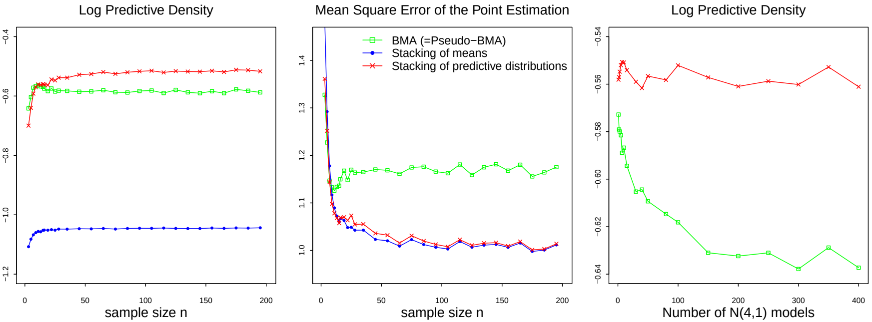

(a) (b) (c)

(c) Dilutation of prior by adding copies of $\mathrm{N}(4, 1)$ to the model space

Linear subset regression example k

$y \sim \mathrm{N}(\mu, 1), \quad \mu = \beta_1 X_1 + \ldots \beta_{15} X_{15}$

$\beta_j = \gamma\left((1_{|j-4|<h}(h - |j-4|)^2 + (1_{|j-8|<h})(h - |j-8|)^2 + (1_{|j-12|<h})(h - |j-12|)^2\right)$

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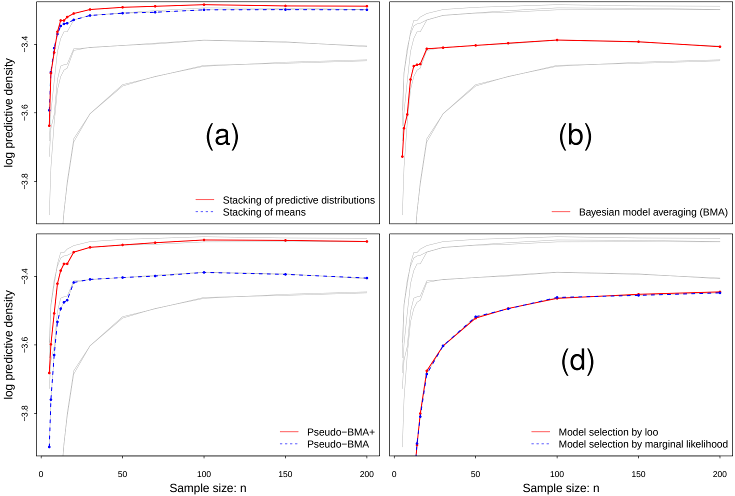

(a) Stacking, (b) BMA, (d) model selection by LOO and BF

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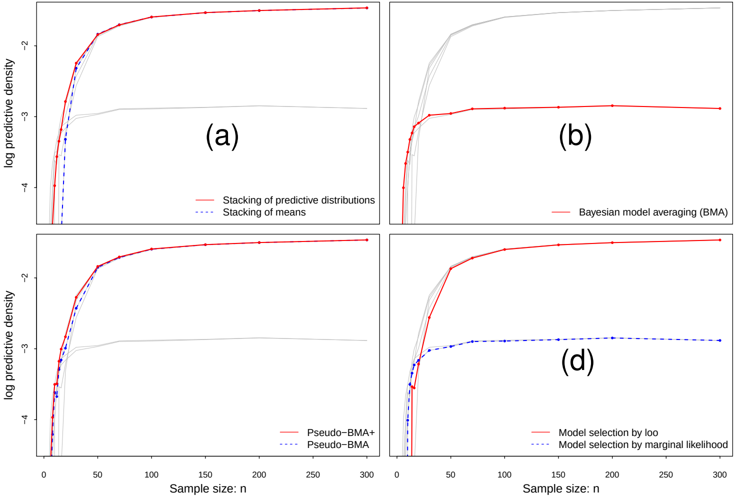

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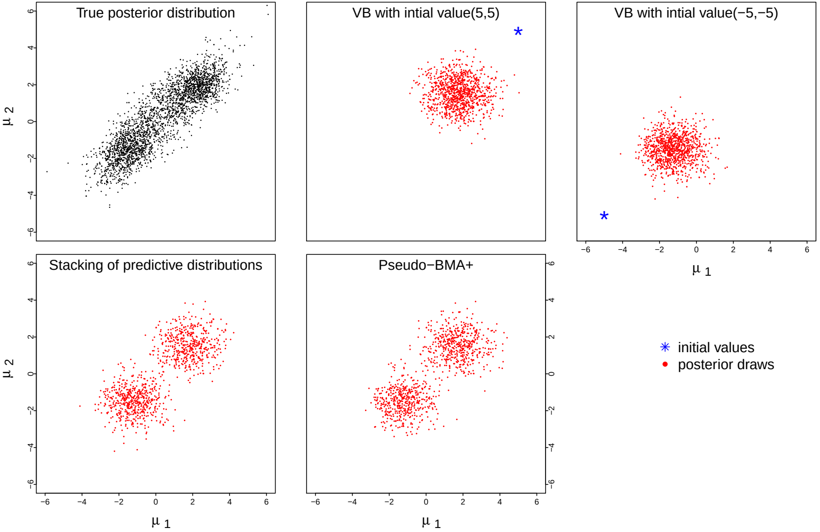
Variational multimodal example

Stacking of predictive distributions can be helpful also in case of multimodal posteriors



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Bayesian stacking

- In M-open case works better than BMA
- In M-closed case can have a better small sample performance than BMA
- Should be used only for model averaging
  - you may drop models with 0 weights
  - you shouldn't choose the model with largest weight unless it's 1
- 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

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- 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
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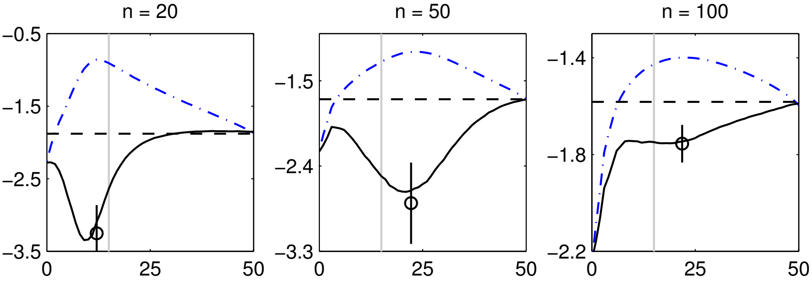
Selection induced bias in variable selection



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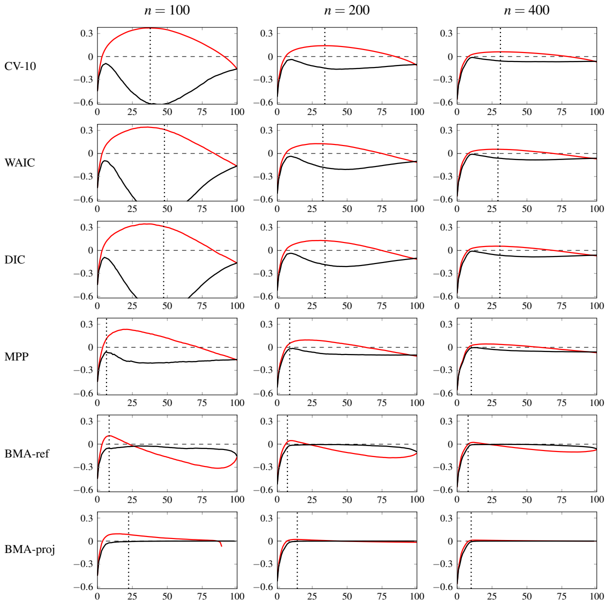

Piironen & Vehtari (2017)

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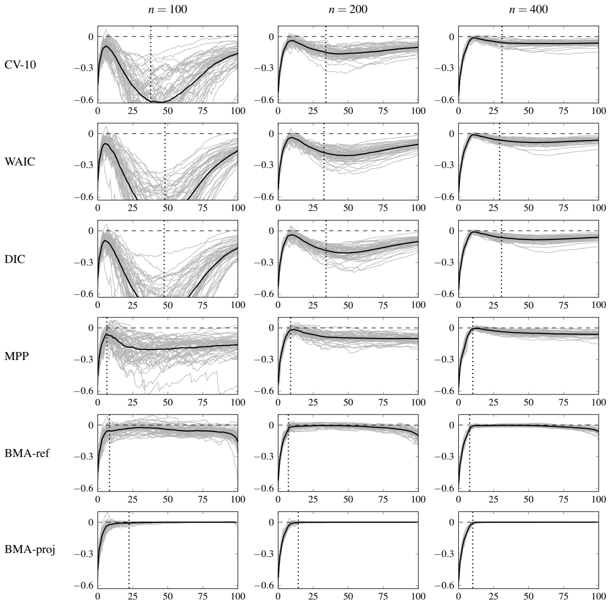

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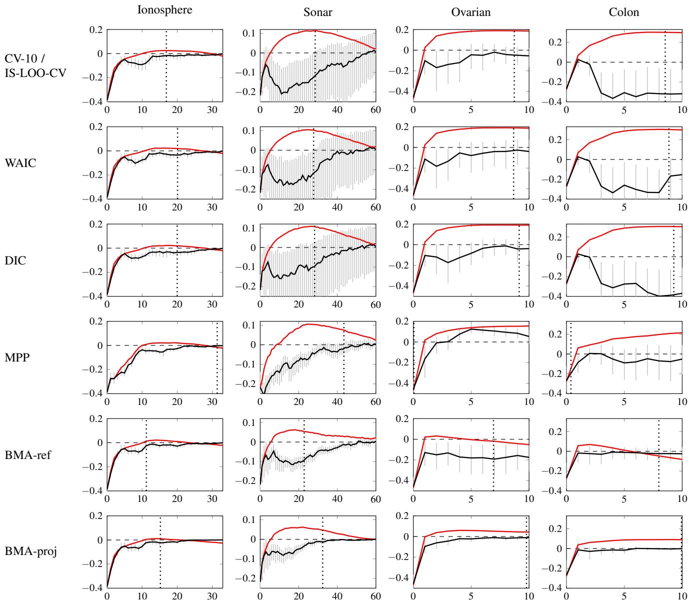

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Take-home messages (part 1)

- 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
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Part 2: Projective Inference in High-dimensional Problems: Prediction and Feature Selection

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  - could scale to bigger n and bigger p

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- The main content of this part: Two stage approach
  - Construct a best predictive model you can
    $\Rightarrow$ *reference model*
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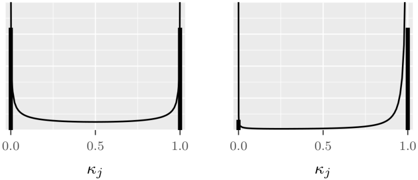
- Two options for variable selection
  - Find a minimal subset of features that yield a good predictive model
  - Identify all features that have predictive information

Regularized horseshoe prior

- Horseshoe: can be seen as continuos version of spike-and-slab with *infinite* width slab
  - no shrinkage ($\kappa_j \to 0$) allows complete separation in logistic model with $n \ll p$



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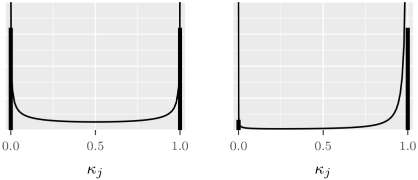
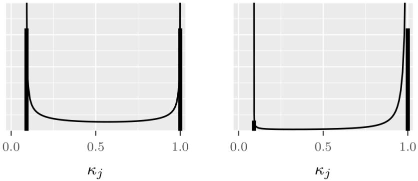


- Regularized horseshoe: adds additional *finite* width slab
  - some minimal shrinkage ($\kappa_j > 0$) for relevant features, but maintains division to relevant and non-relevant features



Regularized horseshoe

- Piironen and Vehtari (2017). Sparsity information and regularization in the horseshoe and other shrinkage priors. In Electronic Journal of Statistics, 11(2):5018-5051. Online
    - regularized horseshoe
    - how to set the prior based on the sparsity assumption

Why shrinkage priors alone do not solve the variable selection problem

- A common strategy:
  - Fit model with a shrinkage prior
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Why shrinkage priors alone do not solve the variable selection problem

- A common strategy:
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- Problems
  - Marginal posteriors are difficult with correlated features
  - How to do post-selection inference correctly?

Example

Consider data

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\begin{aligned}
f &\sim \mathrm{N}(0,1), \\
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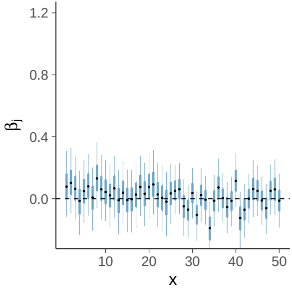
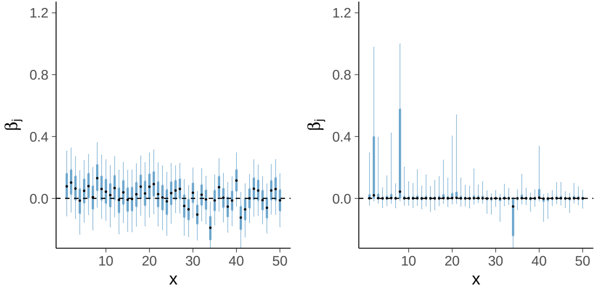
Generate one data set $\{x^{(i)}, y^{(i)}\}_{i=1}^{n}$ with $n = 50$ and $\rho = 0.8$ and assess the feature relevances

Example



A) Gaussian prior, posterior median with 50% and 90% intervals

Example



A) Gaussian prior, posterior median with 50% and 90% intervals
B) Horseshoe prior, same things

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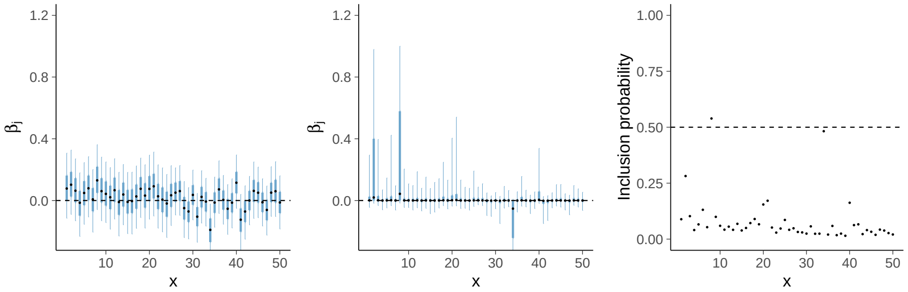
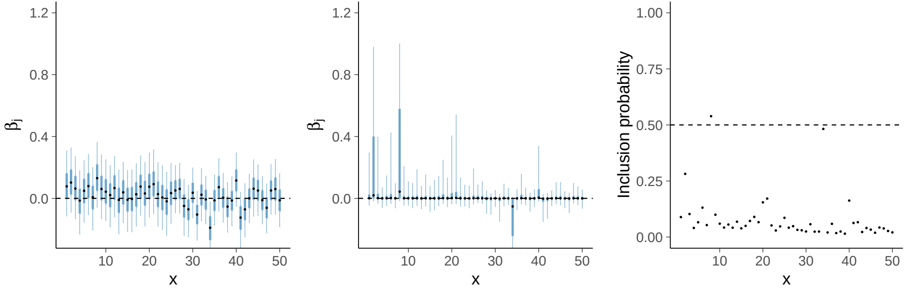


A) Gaussian prior, posterior median with 50% and 90% intervals
B) Horseshoe prior, same things
C) Spike-and-slab prior, posterior inclusion probabilities

Example



A) Gaussian prior, posterior median with 50% and 90% intervals
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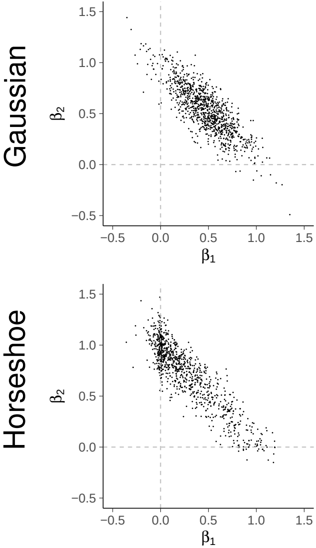
Half of the features relevant, but all marginals substantially overlapping with zero

What happens?



$p_{\text{rel}} = 2$

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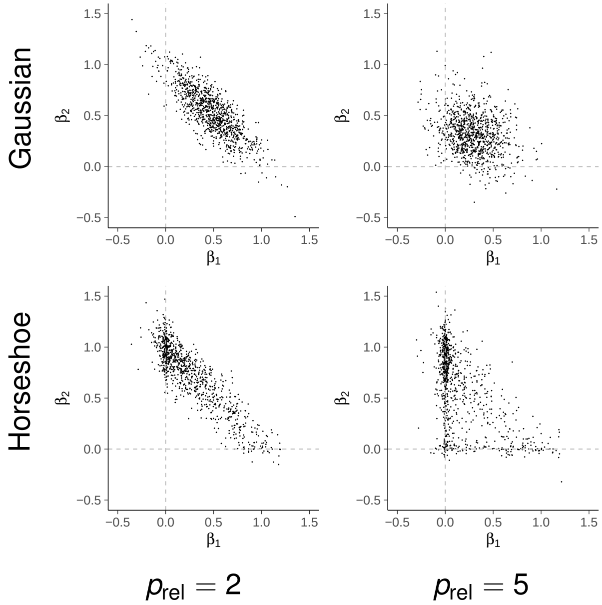

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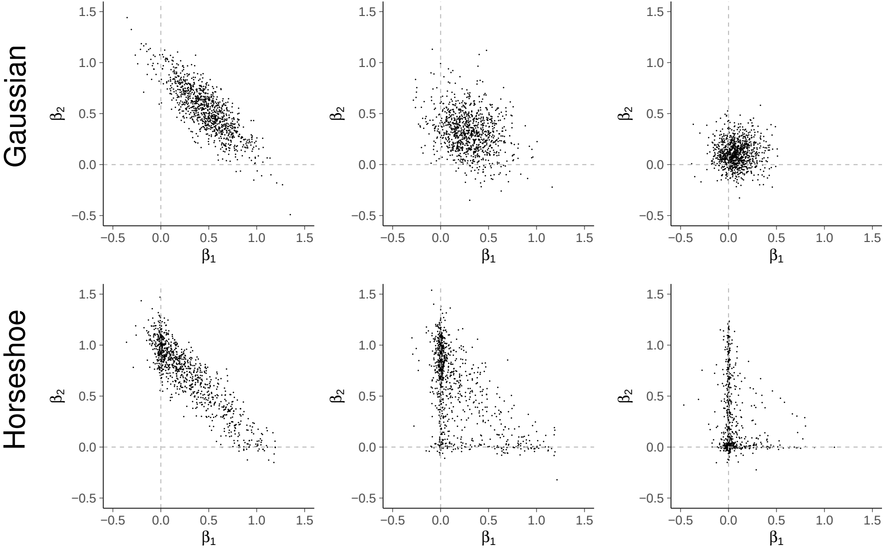

$p_{\mathrm{rel}} = 2$ $p_{\mathrm{rel}} = 5$ $p_{\mathrm{rel}} = 25$

Focus on predictive performance

- Two stage approach
  - Construct a best predictive model you can
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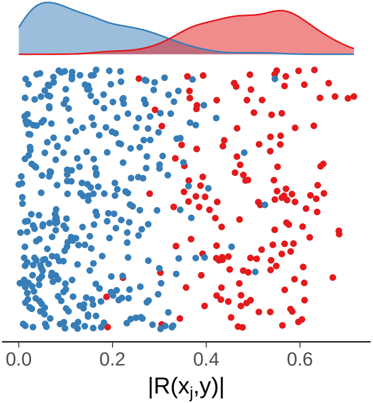
    $\Rightarrow$ *projection*
- Instead of looking at the marginals, find the minimal subset of features which have (almost) the same predictive performance as the reference model

Reference model improves variable selection

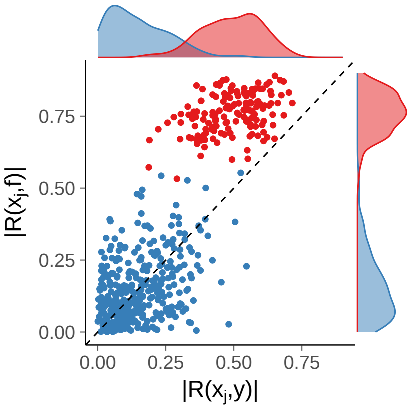
Same data generating mechanism, but
$n = 30$, $p = 500$, $p_{\text{rel}} = 150$, $\rho = 0.5$.



irrelevant x_j, relevant x_j

Sample correlation with y

Reference model improves variable selection



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A) Sample correlation with y vs. sample correlation with f

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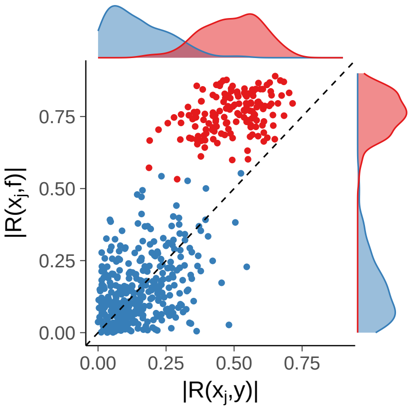

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A) Sample correlation with y vs. sample correlation with f

B) Sample correlation with y vs. sample correlation with f_*

$f_* =$ linear regression fit with 3 supervised principal components

(Iterative) Supervised Principal Components

- Dimension reduction for high dimensional small data with highly correlating features
  - dimension reduction helps to speed up later computation without discarding much information
  - supervised means that features correlating with the target are favored in construcing the principal components
- Piironen and Vehtari (2018). Iterative supervised principal components. 21st AISTATS, PMLR 84:106-114. Online.

Predictive projection, idea

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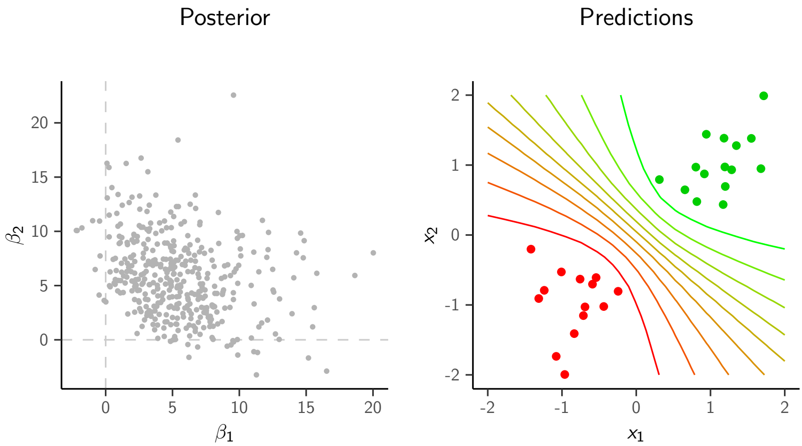
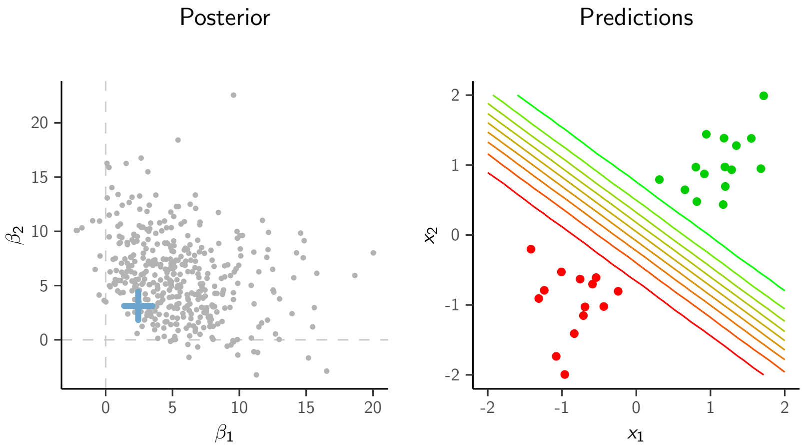
- The decision theoretic idea of conditioning the smaller model inference on the full model can be tracked to Lindley (1968)
  - draw by draw projection introduced by Goutis & Robert (1998), and Dupuis & Robert (2003)
  - see also many related references in a review by Vehtari & Ojanen (2012)

Logistic regression with two features



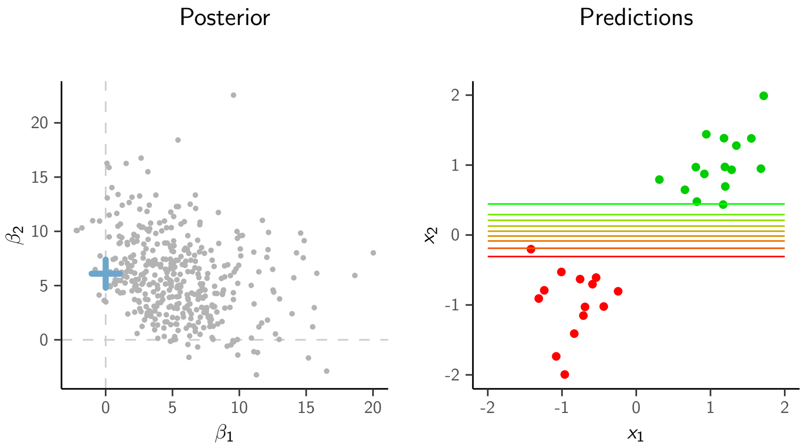
Full posterior for β_1 and β_2 and contours of predicted class probability

Logistic regression with two features



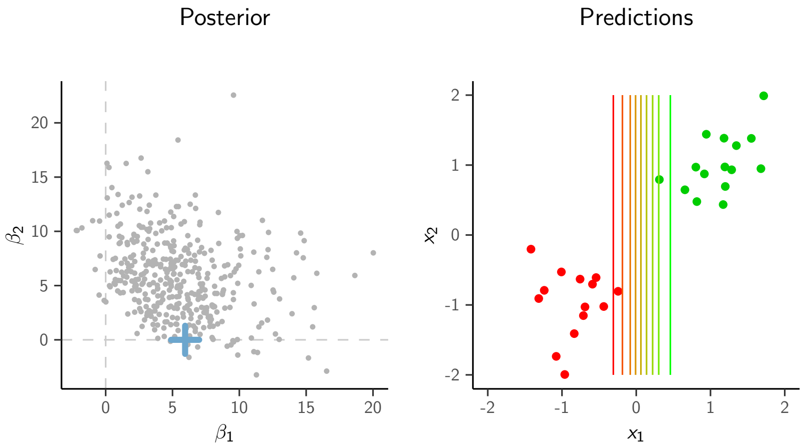
Projected point estimates for β_1 and β_2

Logistic regression with two features



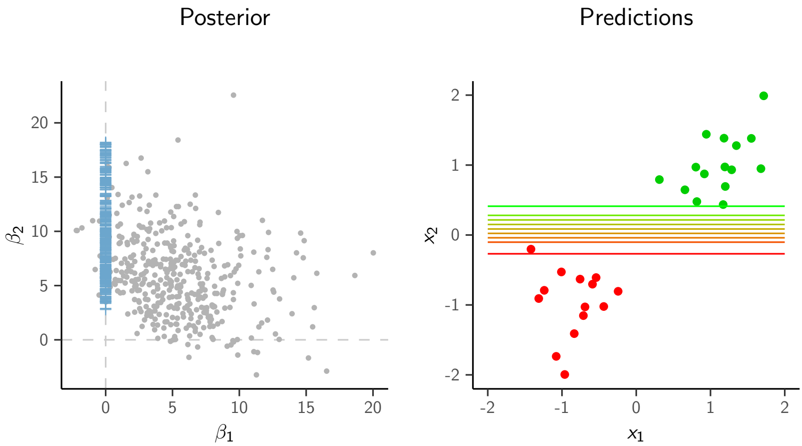
Projected point estimates, constraint $\beta_1 = 0$

Logistic regression with two features



Projected point estimates, constraint $\beta_2 = 0$

Logistic regression with two features



Draw-by-draw projection, constraint $\beta_1 = 0$

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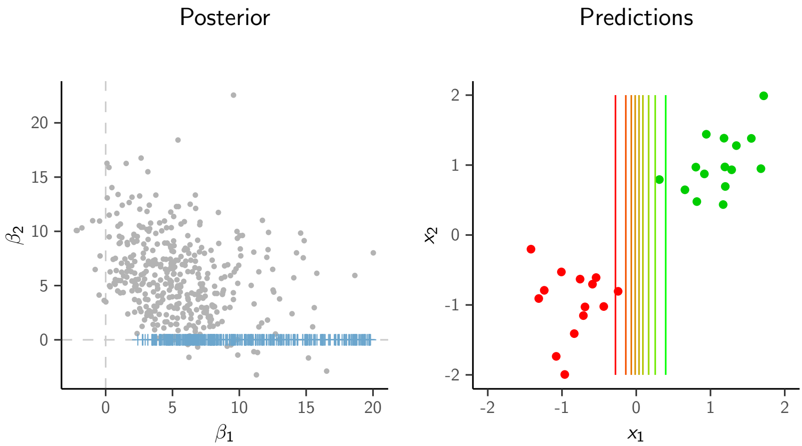

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- As the full posterior $p(\theta \mid D)$ is projected to $q(\theta)$
  - the prior is also projected and there is no need to define priors for submodels separately
  - even if we constrain some coefficients to be 0, the predictive inference is conditoned on the information related features contributed to the reference model

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- Search heuristics, e.g.
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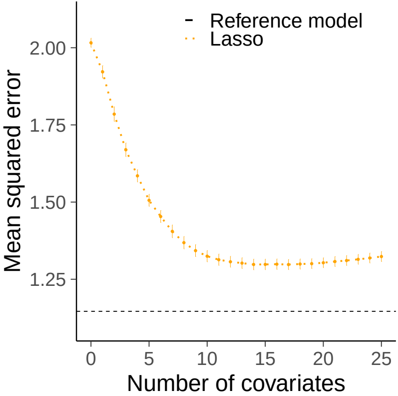
- Use cross-validation to select the appropriate model size
  - need to cross-validate over the search paths

Projective selection vs. Lasso

Same simulated regression data as before,

Â $n = 50$, $p = 500$, $p_{\text{rel}} = 150$, $\rho = 0.5$



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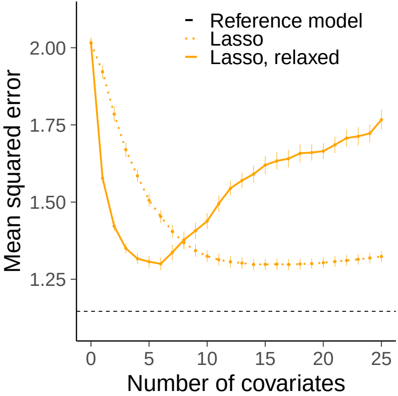

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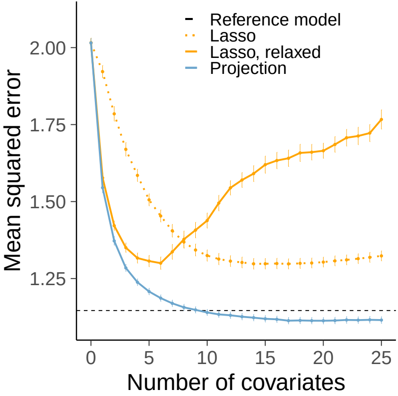

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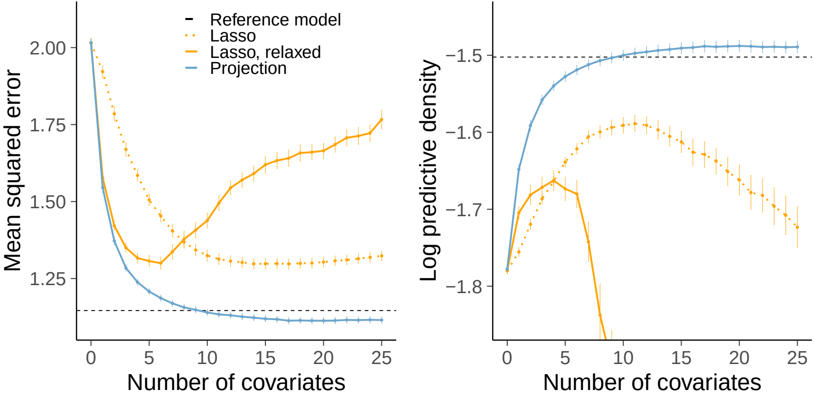
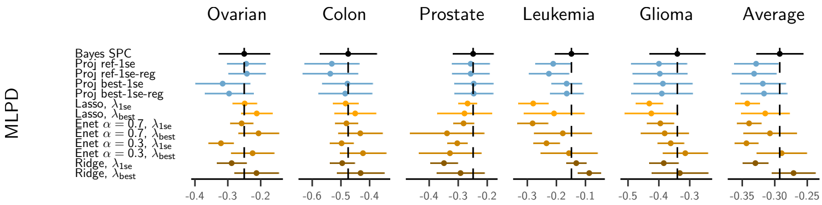


Real data benchmarks

$n = 54...102$, $p = 1536...22283$, Bayes SPC as the reference



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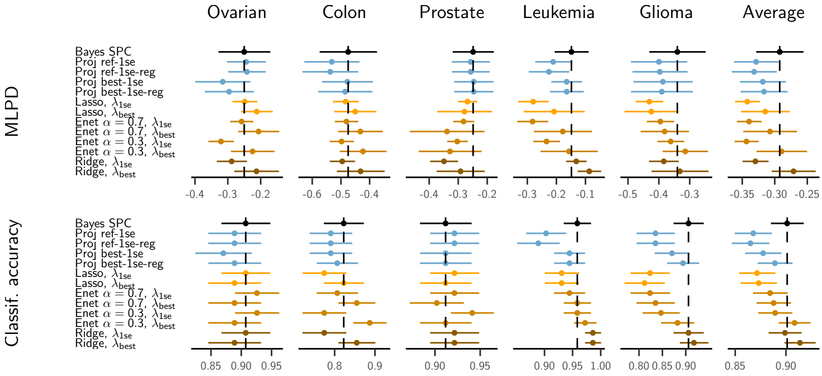

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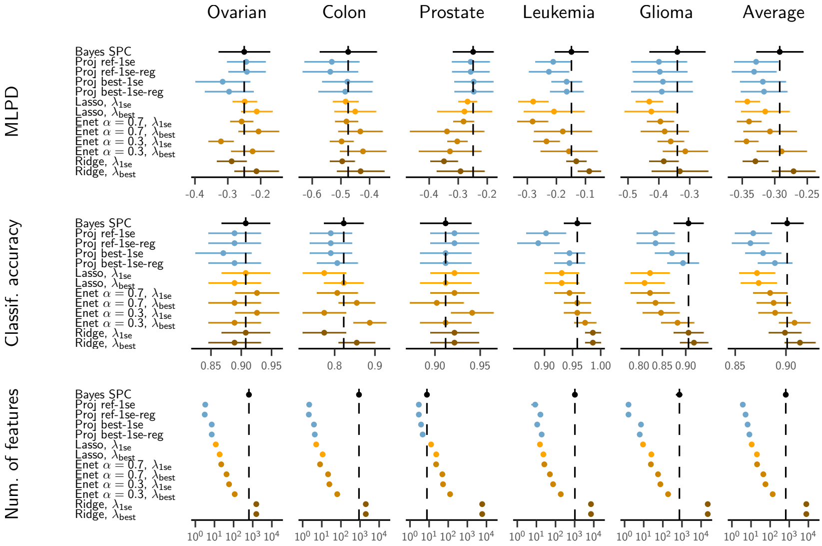
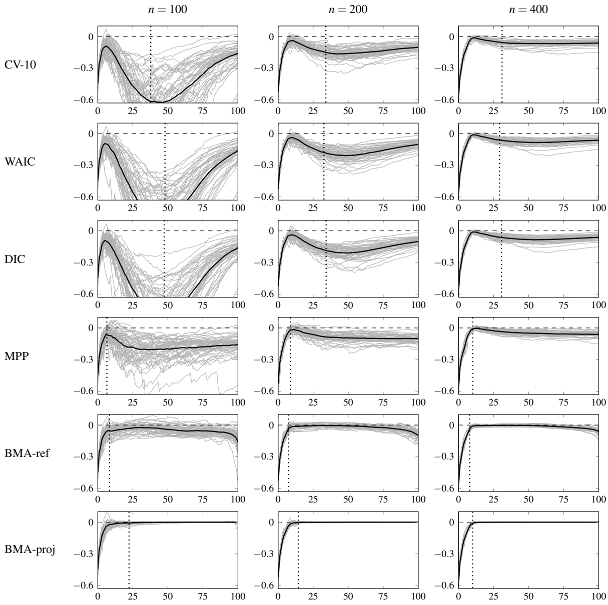


Computation time

Data set	n	p	Computation time			
			Bayes SPC	Projection	Lasso1	Lasso2
Ovarian	54	1536	30.4	3.6	1.3	0.2
Colon	62	2000	31.0	4.0	1.6	0.3
Prostate	102	5966	49.4	7.6	5.0	0.8
Leukemia	72	7129	47.0	6.3	5.6	0.7
Glioma	85	22283	95.8	14.2	15.6	2.6

Table: *Computation times:* Average computation time (in seconds) over five repeated runs. In all cases the time contains the cross-validation of the tuning parameters and/or the model size. The first result for Lasso is computed using our software (`projpred`) whereas the second result (and that of ridge) is computed using the R-package `glmnet` which is more highly optimized.

Selection induced bias in variable selection



Piironen & Vehtari (2017)

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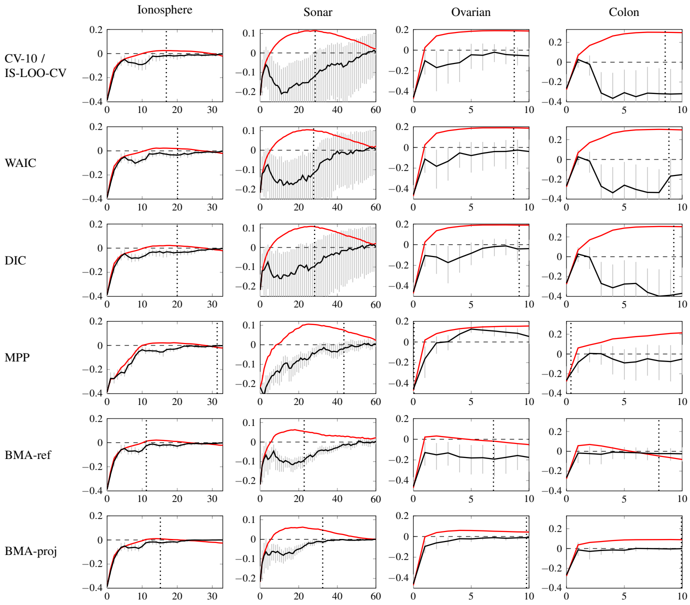

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Bodyfat: small p example of projection predictive

Predict bodyfat percentage. The reference value is obtained by immersing person in water. $n = 251$.

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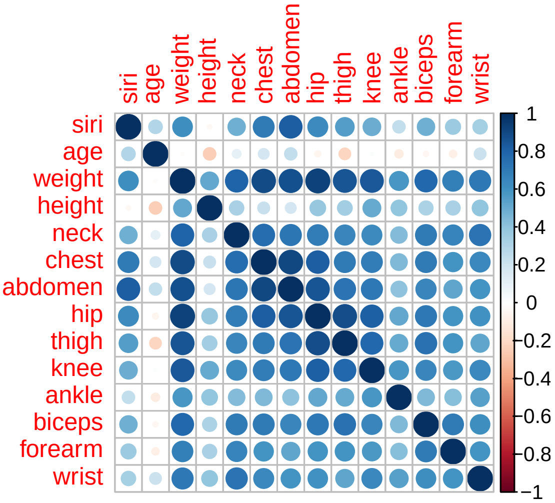
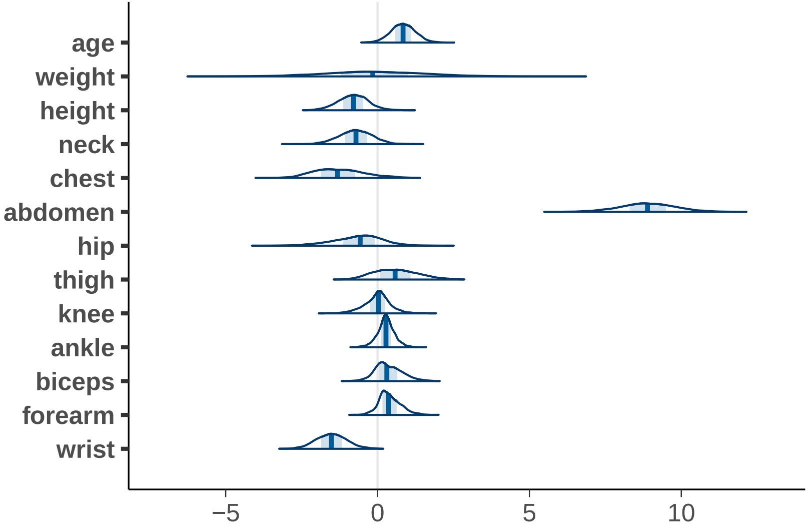


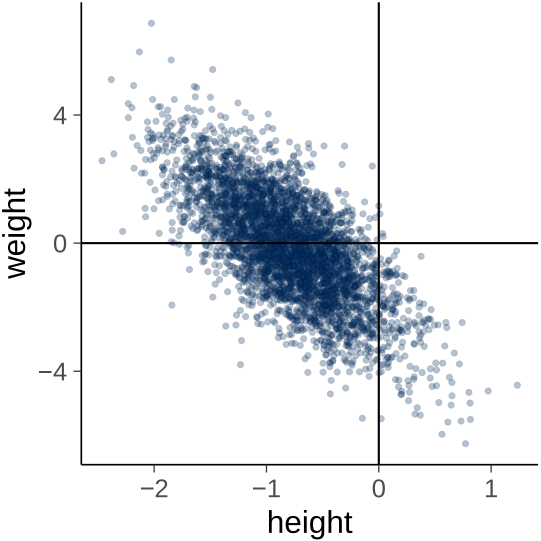
Bodyfat

Marginal posteriors of coefficients



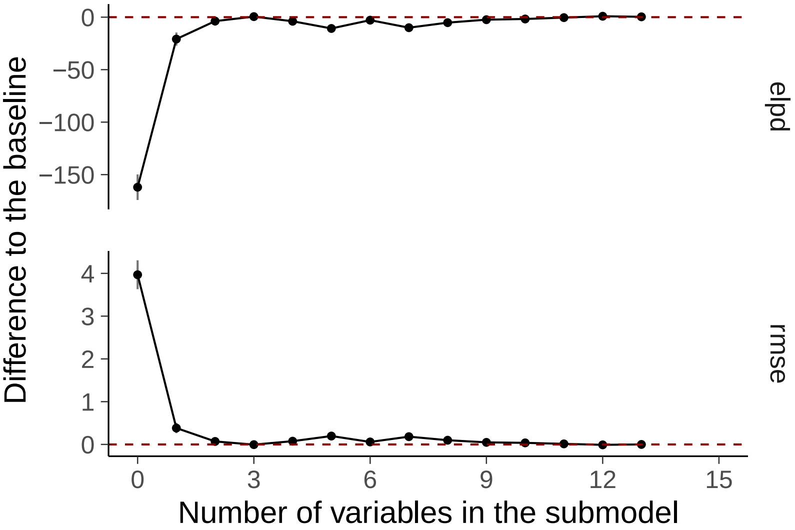
Bodyfat

Bivariate marginal of weight and height



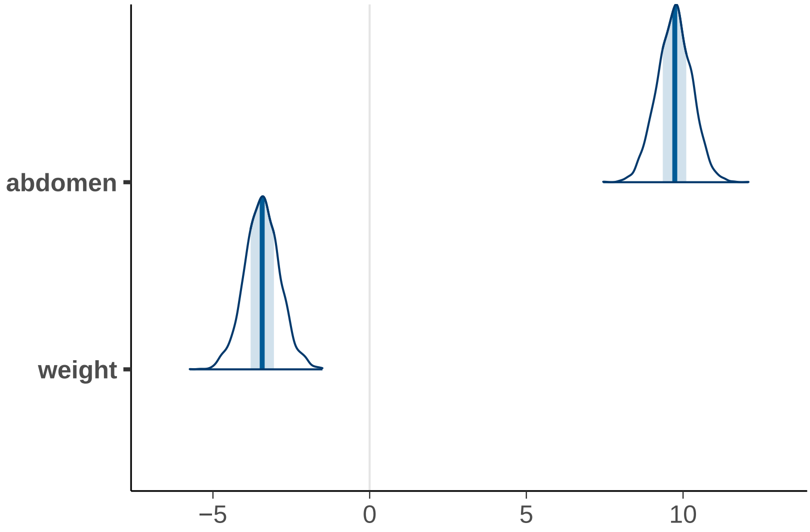
Bodyfat

The predictive performance of the full and submodels



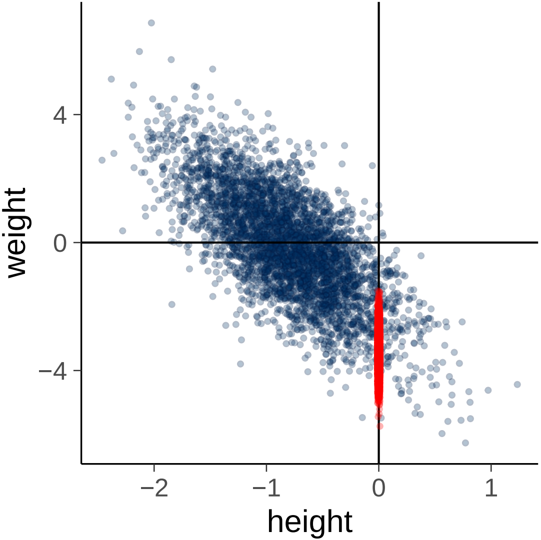
Bodyfat

Marginals of projected posterior



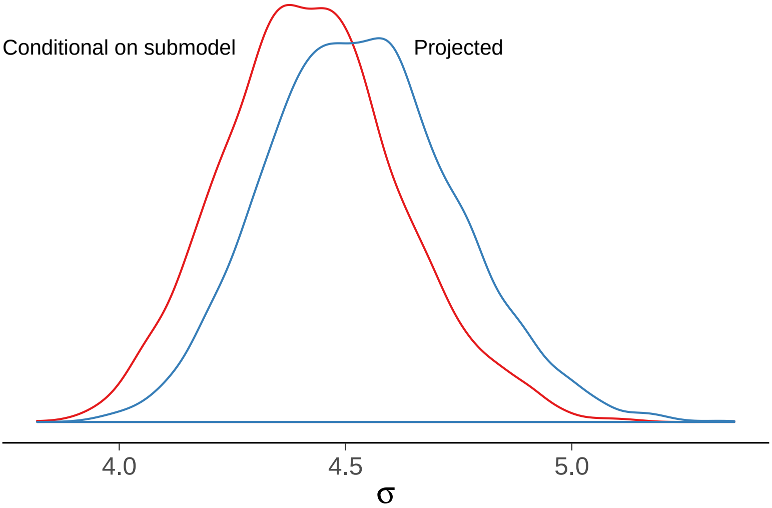
Bodyfat

Projected posterior is not just the conditional of joint



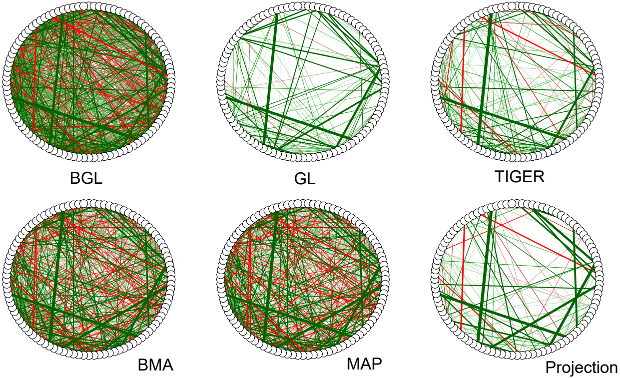
Bodyfat

Projected posterior is different than posterior conditioned only on selected features



Projection of Gaussian graphical models

- Williams, Piironen, Vehtari, Rast (2018). Bayesian estimation of Gaussian graphical models with projection predictive selection. arXiv:1801.05725



CEU genetic network. BGL: Bayesian glasso; GL: glasso; TIGER: tuning insensitive graph estimation and regression; BMA: Bayesian model averaging; MAP: Maximum a posteriori; Projection: projection predictive

More results

- More results projpred vs. Lasso and elastic net:
  Piironen, Paasiniemi, Vehtari (2018). Projective Inference in High-dimensional Problems: Prediction and Feature Selection. arXiv:1810.02406
- More results projpred vs. marginal posterior probabilities:
  Piironen and Vehtari (2017). Comparison of Bayesian predictive methods for model selection. Statistics and Computing, 27(3):711-735. doi:10.1007/s11222-016-9649-y.
- projpred for Gaussian graphical models:
  Williams, Piironen, Vehtari, Rast (2018). Bayesian estimation of Gaussian graphical models with projection predictive selection. arXiv:1801.05725
- More results for Bayes SPC:
  Piironen and Vehtari (2018). Iterative supervised principal components. 21st AISTATS, PMLR 84:106-114. Online.
- Several case studies for small to moderate dimensional ($p = 4 \ldots 100$) small data:
  Vehtari (2018). Model assesment, selection and inference after selection. https://avehtari.github.io/modelselection/

Take-home messages (part 2)

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- R-package `projpred` in CRAN and github
  https://github.com/stan-dev/projpred
  (easy to use, e.g. with RStan, RStanARM, brms)

References

References and more at avehtari.github.io/masterclass/ and avehtari.github.io/modelselection//

- Model selection tutorial at StanCon 2018 Asilomar
  - more about projection predictive variable selection
- Regularized horseshoe talk at StanCon 2018 Asilomar
- Several case studies
- References with links to open access pdfs