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)

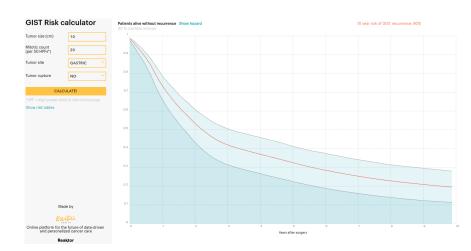
Model assessment, selection and inference after selection

- 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



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

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 - external validation
- Expected predictive performance
 - approximates the external validation

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

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- 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

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

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

Stan and loo package

Computed from 4000 by 20 log-likelihood matrix

Monte Carlo SE of elpd_loo is 0.1.

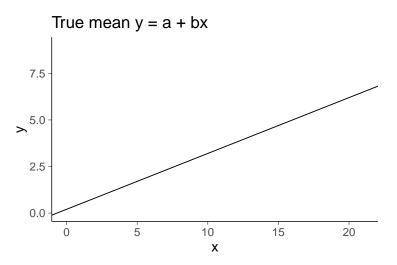
Pareto k diagnostic values:

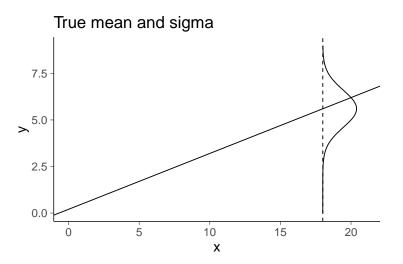
| | | | Count | Pct. | Min. | n_eff |
|-----------|------|------------|-------|-------|---------|-------|
| (-Inf, 0) | 0.5] | (good) | 18 | 90.0% | 899 | |
| (0.5, 0 | 0.7] | (ok) | 2 | 10.0% | 459 | |
| (0.7, | 1] | (bad) | 0 | 0.0% | < NA > | |
| (1, I | nf) | (very bad) | 0 | 0.0% | <NA $>$ | |
| | | | | | | |

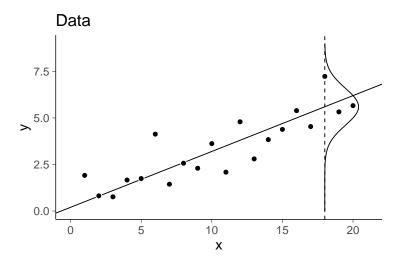
All Pareto k estimates are ok (k < 0.7). See help('pareto-k-diagnostic') for details.

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

$$\begin{array}{ccc} \text{elpd_diff} & \text{se} \\ -0.2 & 0.1 \end{array}$$

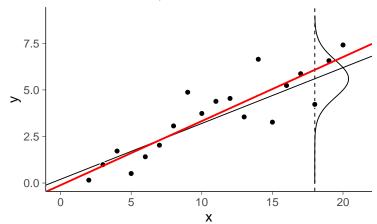




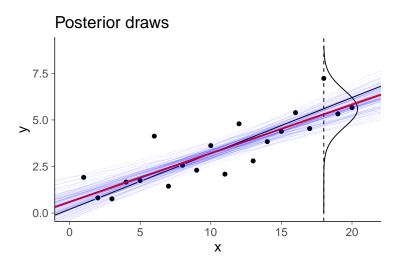


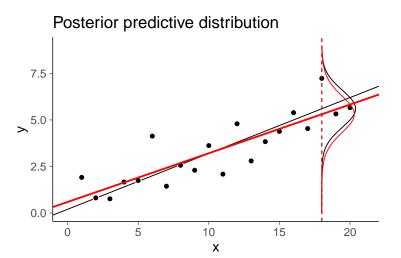


Posterior mean, alternative data realisation

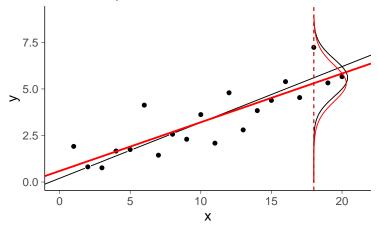




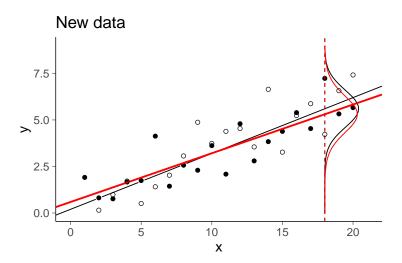


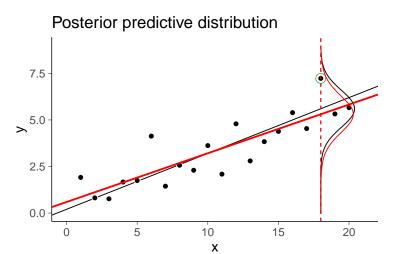


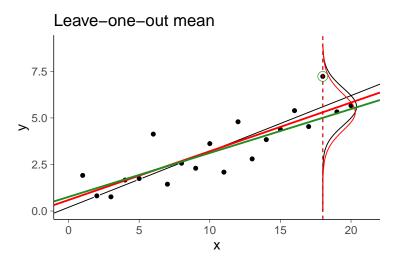
Posterior predictive distribution

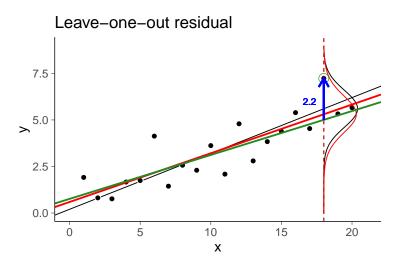


$$p(\tilde{y}|\tilde{x}=18,x,y)=\int p(\tilde{y}|\tilde{x}=18,\theta)p(\theta|x,y)d\theta$$

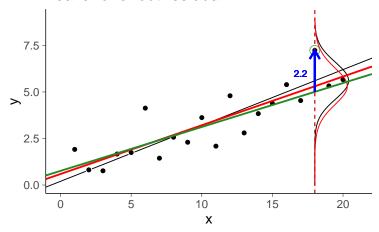






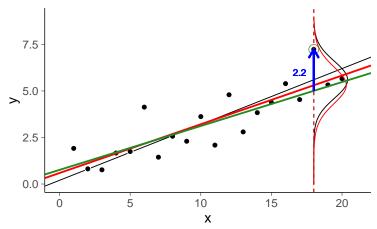


Leave-one-out residual



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

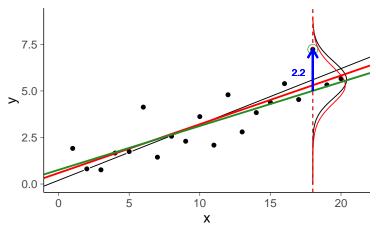
Leave-one-out residual



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

Can be use to compute, e.g., RMSE, R², 90% error

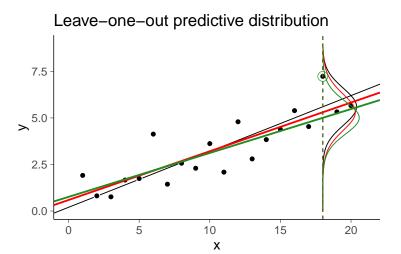
Leave-one-out residual



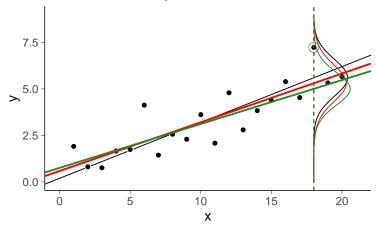
$$y_{18} - E[p(\tilde{y}|\tilde{x}=18, x_{-18}, y_{-18})]$$

Can be use to compute, e.g., RMSE, R², 90% error

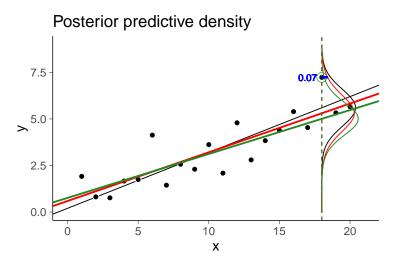
See LOO-R² at avehtari.github.io/bayes_R2/bayes_R2.html



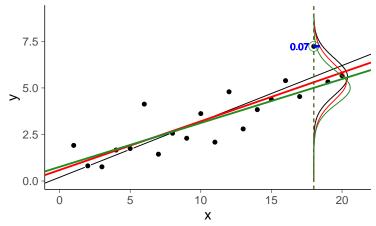
Leave-one-out predictive distribution



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

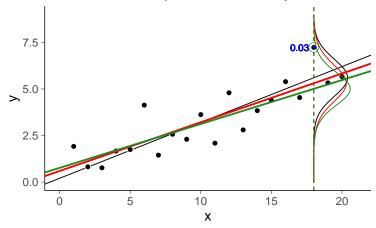


Posterior predictive density



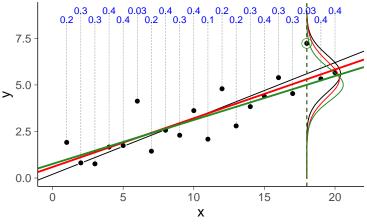
$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$$

Leave-one-out predictive density



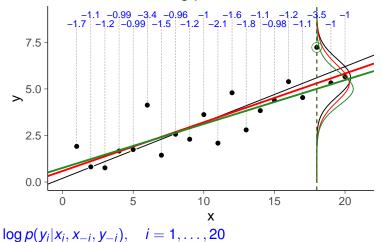
$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x, y) \approx 0.07$$
$$p(\tilde{y} = y_{18} | \tilde{x} = 18, x_{-18}, y_{-18}) \approx 0.03$$

Leave-one-out predictive densities

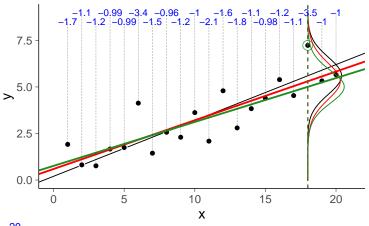


$$p(y_i|x_i, x_{-i}, y_{-i}), \quad i = 1, \dots, 20$$

Leave-one-out log predictive densities

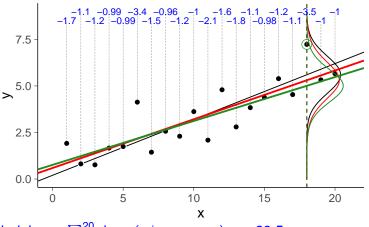


Leave–one–out log predictive densities



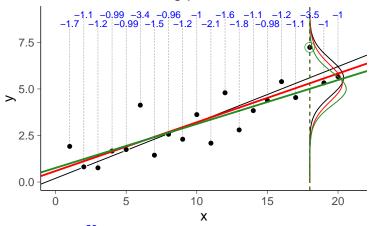
 $\sum_{i=1}^{20} \log p(y_i|x_i, x_{-i}, y_{-i}) \approx -29.5$

Leave-one-out log predictive densities



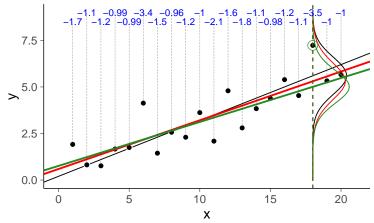
elpd_loo = $\sum_{i=1}^{20} \log p(y_i|x_i,x_{-i},y_{-i}) \approx -29.5$

Leave–one–out log predictive densities



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

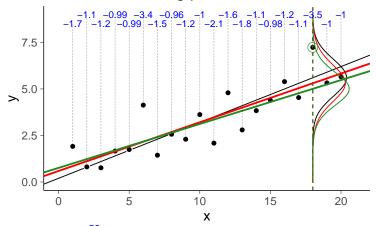
Leave–one–out log predictive densities



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

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

Leave–one–out log predictive densities

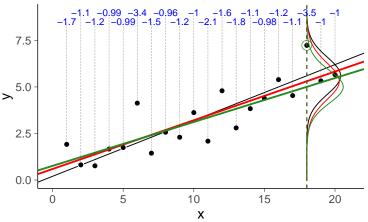


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$$p_loo = lpd - elpd_loo \approx 2.7$$

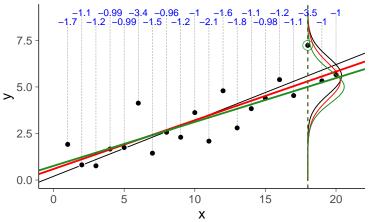
Leave–one–out log predictive densities



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

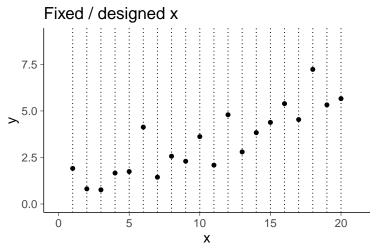
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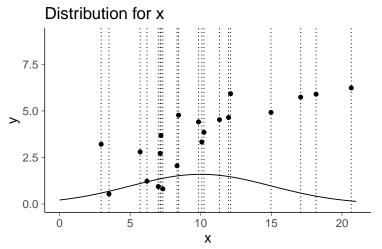
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see Vehtari, Gelman & Gabry (2017a) and Vehtari & Ojanen (2012) for more



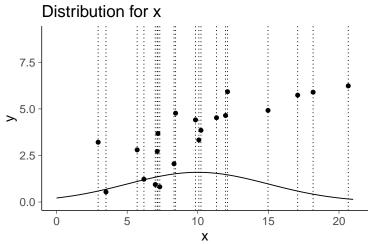
LOO is ok for fixed / designed x. SE is uncertainty about y|x.

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/

100 package

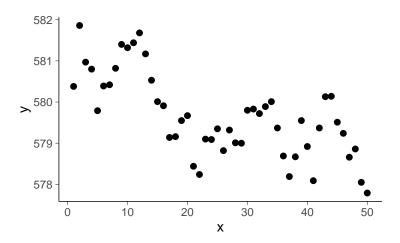
Computed from 4000 by 20 log-likelihood matrix

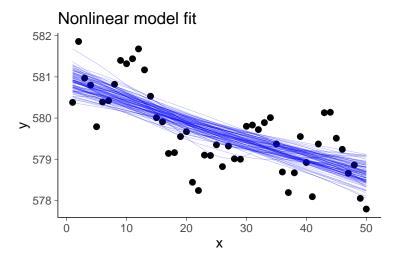
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Pareto k diagnostic values:

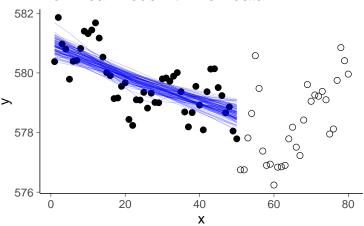
| | | | Count | Pct. | Min. | n_eff |
|------------|------|-----------|-------|-------|-----------|-------|
| (-Inf, | 0.5] | (good) | 18 | 90.0% | 899 | |
| (0.5, 0.5) | 0.7] | (ok) | 2 | 10.0% | 459 | |
| (0.7 | , 1] | (bad) | 0 | 0.0% | <NA $>$ | |
| (1, | Inf) | (very bad |) 0 | 0.0% | <na></na> | |

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

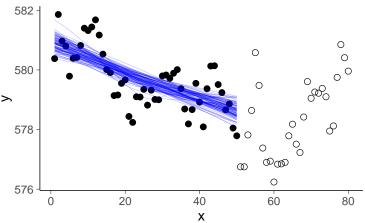




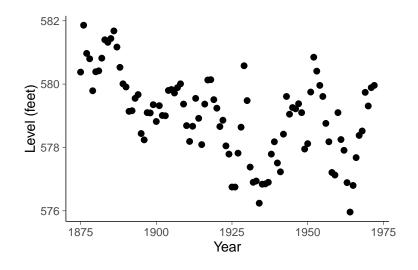
Nonlinear model fit + new data



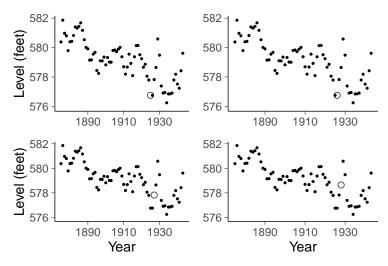
Nonlinear model fit + new data



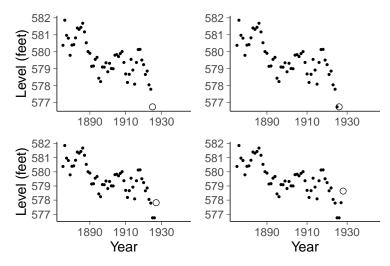
Extrapolation is more difficult



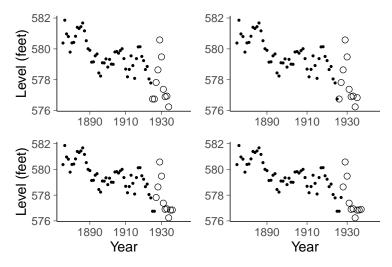
Can LOO or other cross-validation be used with time series?



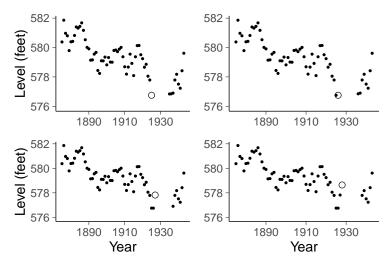
Leave-one-out cross-validation is ok for assessing conditional model



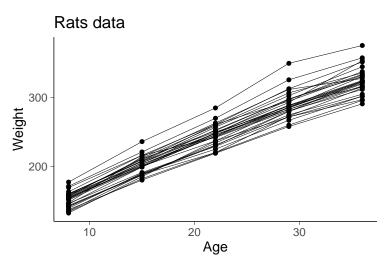
Leave-future-out cross-validation is better for predicting future



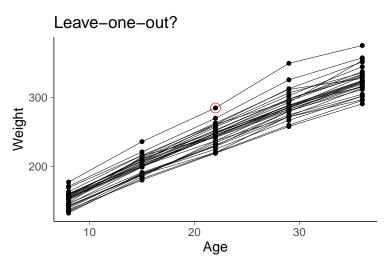
m-step-ahead cross-validation is better for predicting further future

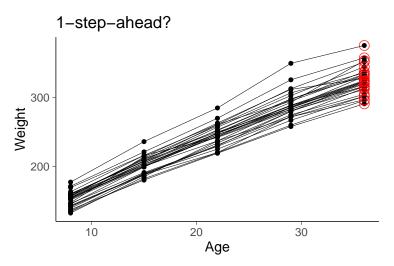


m-step-ahead leave-a-block-out cross-validation

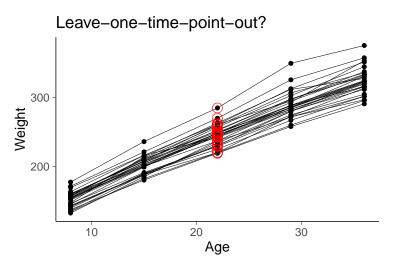


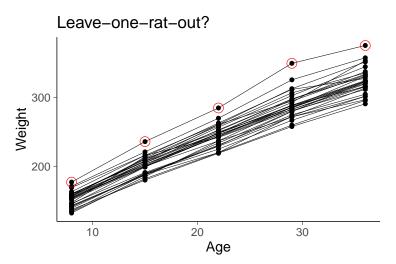
Can LOO or other cross-validation be used with hierarchical data?

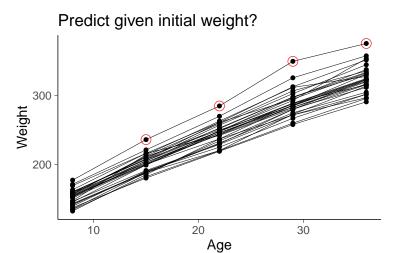




Yes!







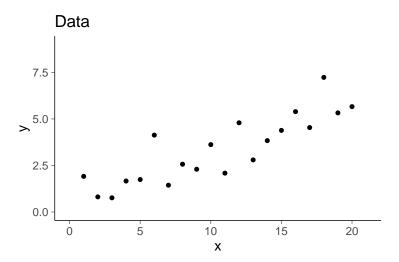
Summary of data generating mechanisms and prediction tasks

- 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/

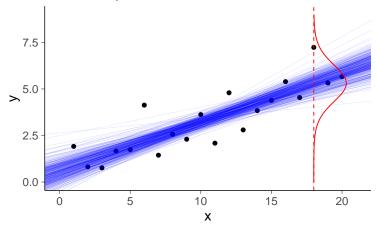
Fast cross-validation

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



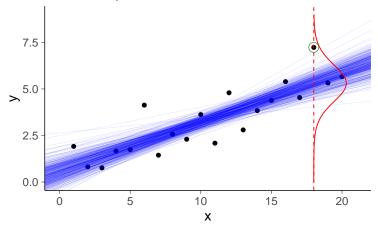
Posterior draws 7.5 > 5.0 2.5 0.0 10 15 20 5 Χ $\theta^{(s)} \sim p(\theta|x,y)$

Posterior predictive distribution



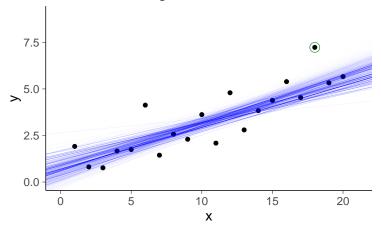
$$\theta^{(s)} \sim p(\theta|x,y), \quad p(\tilde{y}|\tilde{x},x,y) \approx \tfrac{1}{S} \textstyle \sum_{s=1}^S p(\tilde{y}|\tilde{x},\theta^{(s)})$$

Posterior predictive distribution



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

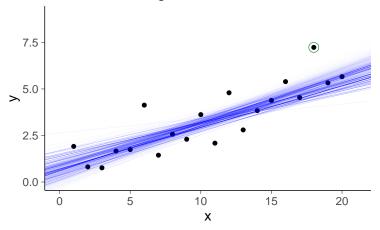
PSIS-LOO weighted draws



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

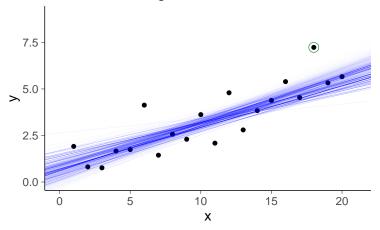
$$r_i^{(s)} = p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y)$$

PSIS-LOO weighted draws



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

PSIS-LOO weighted draws

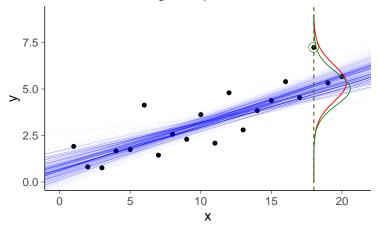


$$\theta^{(s)} \sim p(\theta|x, y)$$

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

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

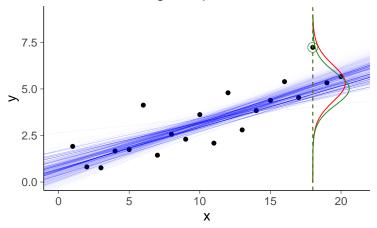
PSIS-LOO weighted predictive distribution



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

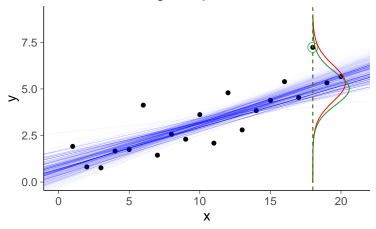
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PSIS-LOO weighted predictive distribution



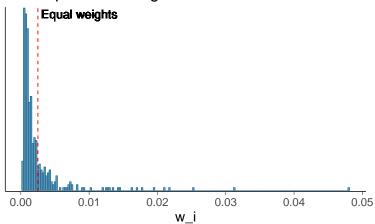
$$\begin{aligned} \theta^{(s)} &\sim p(\theta|x, y) \\ r_i^{(s)} &= p(\theta^{(s)}|x_{-i}, y_{-i})/p(\theta^{(s)}|x, y) \propto 1/p(y_i|x_i, \theta^{(s)}) \\ p(y_i|x_i, x_{-i}, y_{-i}) &\approx \sum_{s=1}^{S} [w_i^{(s)} p(y_i|x_i, \theta^{(s)})] \end{aligned}$$

PSIS-LOO weighted predictive distribution

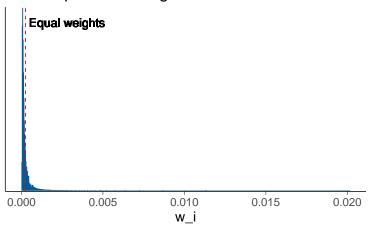


$$\begin{split} & \theta^{(s)} \sim p(\theta|x,y) \\ & r_i^{(s)} = p(\theta^{(s)}|x_{-i},y_{-i})/p(\theta^{(s)}|x,y) \propto 1/p(y_i|x_i,\theta^{(s)}) \\ & p(y_i|x_i,x_{-i},y_{-i}) \approx \sum_{s=1}^S [w_i^{(s)}p(y_i|x_i,\theta^{(s)})], \text{ where } w \leftarrow \text{PSIS}(r) \end{split}$$

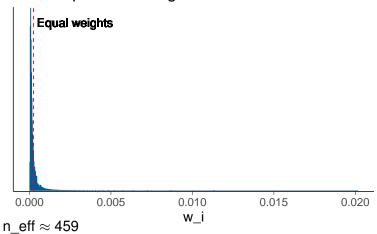
400 importance weights for leave-18th-out



4000 importance weights for leave-18th-out

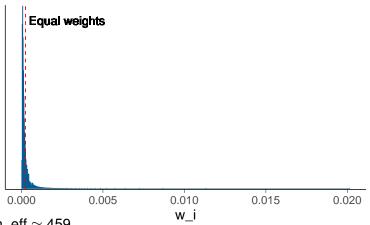


4000 importance weights for leave-18th-out



see Vehtari, Gelman & Gabry (2017b)

4000 importance weights for leave-18th-out

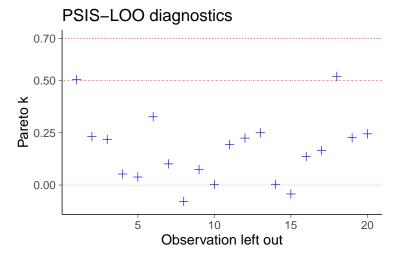


 $n_eff \approx 459$

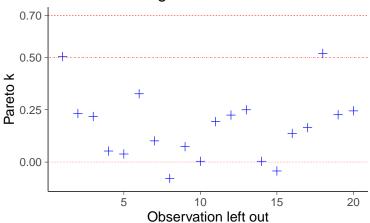
Pareto $\hat{k} \approx 0.52$

- 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)



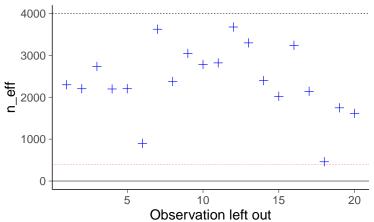
PSIS-LOO diagnostics



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_eft |
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100 package

Computed from 4000 by 20 log-likelihood matrix

Monte Carlo SE of elpd_loo is 0.1.

Pareto k diagnostic values:

| | | Coun | t Pct. | Mın. | n_eff |
|-------------|-----------|------|--------|-----------|-------|
| (-Inf, 0.5] | 5] (good) | 18 | 90.0% | 899 | |
| (0.5, 0.7 | 7] (ok) | 2 | 10.0% | 459 | |
| (0.7, -1) | 1] (bad) | 0 | 0.0% | <na></na> | |
| (1, Inf | (very ba | d) 0 | 0.0% | <na></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

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

Stan code

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\log(r_i^{(s)}) = \log(1/p(y_i|x_i, \theta^{(s)})) = -\log |\mathbf{lik}[i]|
model {
  alpha ~ normal(pmualpha, psalpha);
  beta ~ normal(pmubeta, psbeta);
  y ~ normal(mu, sigma);
generated quantities {
  vector[N] log lik;
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RStanARM and BRMS compute log_lik by default

Pareto smoothed importance sampling LOO

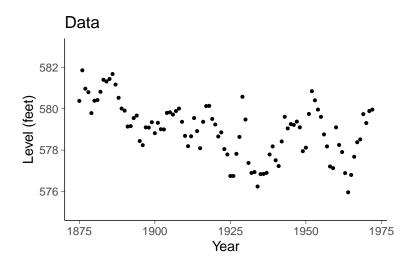
- PSIS-LOO for hierarchical models
 - leave-one-group out is challenging for PSIS-LOO see Merkel, Furr and Rabe-Hesketh (2018) for an approach using quadrature integration

Pareto smoothed importance sampling LOO

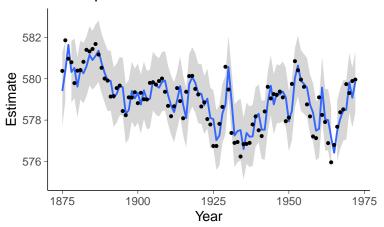
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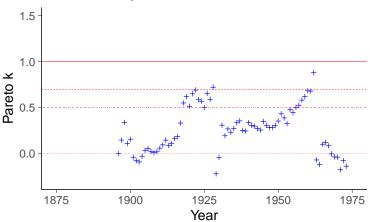
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 - mc-stan.org/loo/articles/loo2-non-factorizable.html
- PSIS-LOO for time series
 - Approximate leave-future-out cross-validation mc-stan.org/loo/articles/loo2-lfo.html



AR-4 prediction with 95% interval

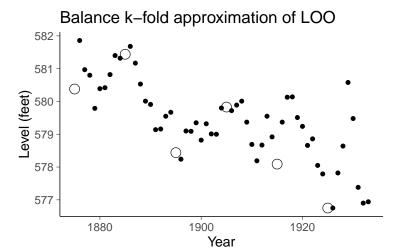


PSIS-1-step-ahead with refits

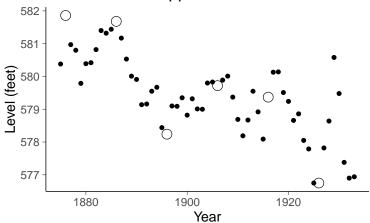


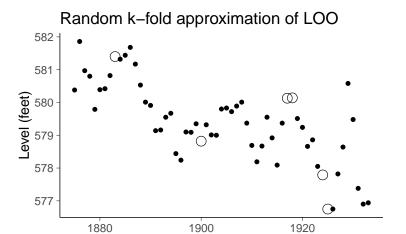
K-fold cross-validation

- 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

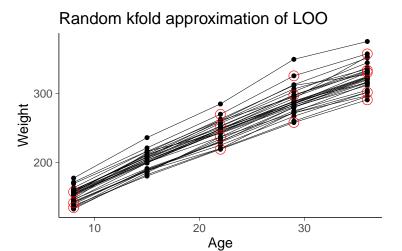


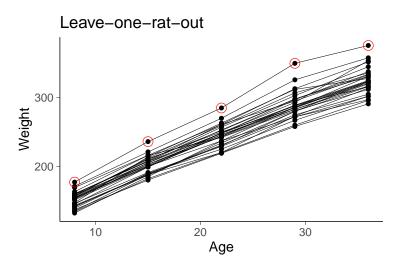
Balance k–fold approximation of LOO

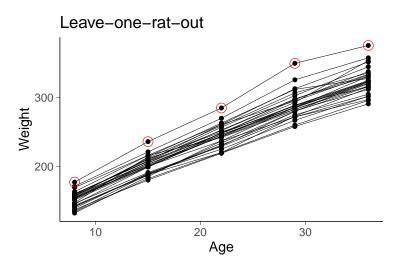




Year







kfold_split_random()
kfold_split_balanced()
kfold_split_stratified()

WAIC has same assumptions as LOO

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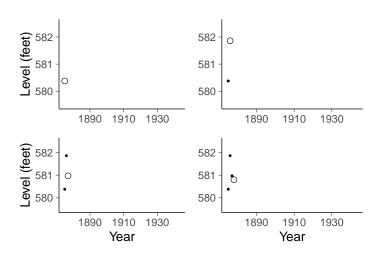
- WAIC has same assumptions as LOO
- PSIS-LOO is more accurate
- PSIS-LOO has much better diagnostics
- LOO makes the prediction assumption more clear, which helps if K-fold-CV is needed instead
- Multiplying by -2 doesn't give any benefit (Watanabe didn't multiply by -2)

*IC

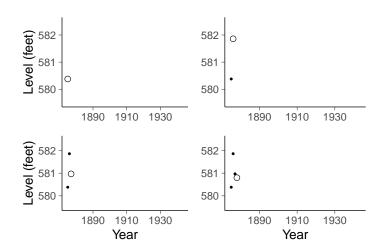
- AIC uses maximum likelihood estimate for prediction
- DIC uses posterior mean for prediction
- BIC is an approximation for marginal likelihood
- TIC, NIC, RIC, PIC, BPIC, QIC, AICc, ...

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

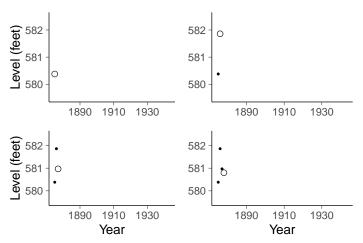
 Like leave-future-out 1-step-ahead cross-validation but starting with 0 observations



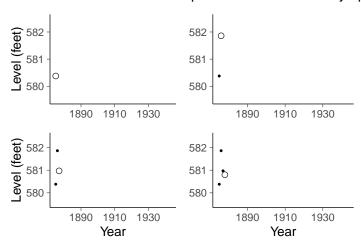
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 - unstable in case of misspecified models also asymptotically



Cross-validation for model assessment

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

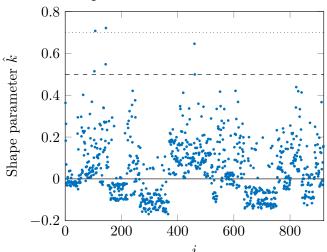
Cross-validation for model assessment

- 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/

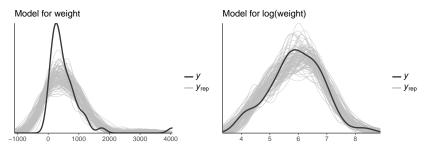
Radon example

PSIS-LOO diagnostics



see Vehtari, Gelman & Gabry (2017a)

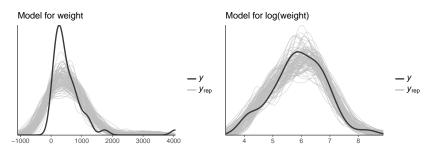
Posterior predictive checking is often sufficient



Predicting the yields of mesquite bushes.

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

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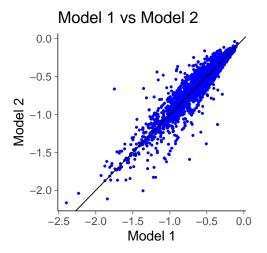
- BDA3, Chapter 6
- Gabry, Simpson, Vehtari, Betancourt, Gelman (2019). Visualization in Bayesian workflow. JRSS A, https://doi.org/10.1111/rssa.12378
- mc-stan.org/bayesplot/articles/graphical-ppcs.html
- betanalpha.github.io/assets/case_studies/principled_bayesian_ workflow.html

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

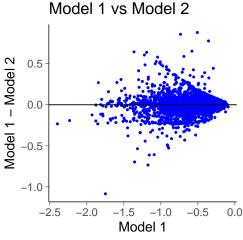
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Arsenic well example – Model comparison



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

Arsenic well example – Model comparison



Arsenic well example – Model comparison

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).

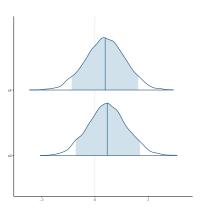
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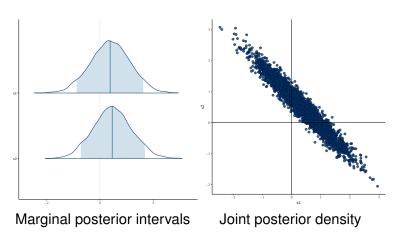
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- In nested case, often easier and more accurate to analyse posterior distribution of more complex model directly avehtari.github.io/modelselection/betablockers.html

Sometimes predictive model comparison can be useful



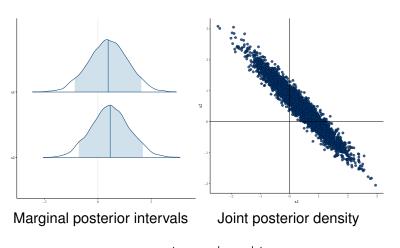
Marginal posterior intervals

Sometimes predictive model comparison can be useful



rstanarm + bayesplot

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rstanarm + bayesplot

- Continuous expansion including all models?
 - and then analyse the posterior distribution directly avehtari.github.io/modelselection/betablockers.html
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Model averaging

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Model averaging

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- 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

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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
 - the selected model fits more to the data
 - the CV estimate for the selected model is biased
 - recognized already, e.g., by Stone (1974)

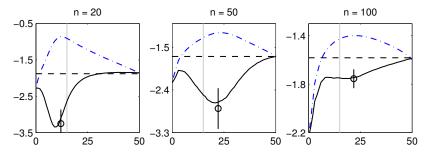
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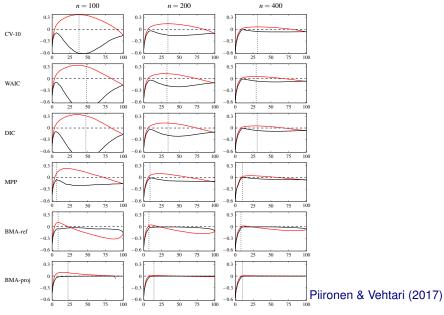
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- Performance of the selection process itself can be assessed using two level cross-validation, but it does not help choosing better models
- Bigger problem if there is a large number of models as in covariate selection

Selection induced bias in variable selection



Selection induced bias in variable selection



- 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
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