Outline

Last week

- What is cross-validation
- LOO-PIT checking
- Fast cross-validation with PSIS
- LOO model comparison and selection (elpd_diff, se)

This week

- Model comparison with LOO-CV
- When is cross-validation applicable?
- *K*-fold cross-validation
- Related methods (WAIC, *IC, BF)
- Hypothesis testing
- Potential overfitting

Student retention – Posterior predictive distributions

with tidybayes

Latent hierarchical linear model



Latent hierarchical linear model + spline



Student retention – Marginal PPC

pp_check(fit, ndraws=100)



Latent hierarchical linear model + spline



Student retention - LOO intervals

LOO predictive intervals - latent hierarchical linear



LOO predictive intervals - latent hierarchical linear + spline



Student retention – LOO-PIT checking

pp_check(fit, type = "loo_pit_qq", ndraws=4000)



LOO-PIT check - latent hierarchical linear + spline



Student retention – R^2

Latent hierarchical linear vs. latent hierarchical linear + spline

> loo_R2(fit4) |> round(digits=2)
Estimate Est.Error Q2.5 Q97.5

R2 0.92 0.02 0.88 0.95

> loo_R2(fit6) |> round(digits=2)
 Estimate Est.Error Q2.5 Q97.5
R2 0.97 0.01 0.95 0.98

 R^2 measures the goodness of the mean of the predictive distribution

Gelman, Goodrich, Gabry, and Vehtari (2019). R-squared for Bayesian regression models. *The American Statistician*, 73(3):307-309.

- information theoretical goodness of the whole distribution
- elpd = expected log predictive density (probability)
- elpd_loo = estimated with LOO predictive densities / probs $\sum_{n=1}^{N} \log p(y_i | x_i, x_{-i}, y_{-i})$

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LOO predictive intervals - latent hierarchical linear + spline

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LOO predictive intervals – latent hierarchical linear + spline

-8.4 -5.6 -2.9 -2.9 -2.8 -3.0 -4.0 -3.2 -3.9 -3.2 -3.4 -3.2 -2.9 -3.9 -3.4 -3.4 -3.2 -2.7 -2.8 -3.1 -2.5 -2.8 -2.9 -3.4 -5.4 -3.7 -3.1 -3.3 -3.5 -3.2 -3.5 -3.5 -6.6 -3.8 -3.7 -3.4 -2.5 -2.8 -2.9 -3.3

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LOO predictive intervals – latent hierarchical linear + spline

 $\begin{array}{l} -8.4 \ -5.6 \ -2.9 \ -2.9 \ -2.8 \ -3.0 \ -4.0 \ -3.2 \ -3.9 \ -3.2 \ -3.4 \ -3.2 \ -2.9 \ -3.9 \ -3.4 \ -3.4 \ -3.2 \ -2.7 \ -2.8 \ -3.1 \\ -2.5 \ -2.8 \ -2.9 \ -3.4 \ -3.4 \ -3.4 \ -3.2 \ -2.7 \ -2.8 \ -3.1 \\ -2.5 \ -2.8 \ -2.9 \ -3.4 \ -3.4 \ -3.4 \ -2.5 \ -2.8 \ -2.9 \ -3.3 \\ \sum = -141.7 \end{array}$

Latent hierarchical linear + spline

> loo(fit6)

Computed from 4000 by 40 log-likelihood matrix

	Estimate	SE			
elpd_loo	-141.7	7.2			
p_loo	10.9	2.5			

Latent hierarchical linear + spline

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 Estimate
 SE

 elpd_loo
 -141.7
 7.2

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Latent hierarchical linear

> loo(fit4)

Computed from 4000 by 40 log-likelihood matrix

	Estimate	SE
elpd_loo	-184.3	17.3
p_loo	24.3	5.8

LOO predictive intervals - latent hierarchical linear



 $-15.7 - 7.6 - 3.9 - 2.9 - 6.7 - 4.2 - 2.9 - 3.1 - 12.9 - 4.7 - 3.3 - 3.4 - 9.0 - 3.0 - 3.3 - 3.2 - 8.2 - 2.8 - 3.2 - 3.0 - 2.9 - 3.3 - 3.0 - 4.6 - 4.3 - 3.3 - 3.0 - 4.0 - 3.0 - 5.6 - 3.6 - 5.4 - 4.9 - 3.6 - 3.9 - 5.2 - 2.7 - 3.7 - 3.0 - 4.1 \sum_{i=1}^{n} = -184.3$



-2.5 -2.8 -2.9 -3.4 -5.4 -3.7 -3.1 -3.3 -3.5 -3.2 -3.5 -3.5 -6.6 -3.8 -3.7 -3.4 -2.5 -2.8 -2.9 -3.3 ∑ = -141.7 9/74





















Latent hierarchical linear + spline

> loo(fit6) Estimate SE elpd_loo -141.7 7.2 p_loo 10.9 2.5

Latent hierarchical linear

```
> loo_compare(loo(fit4), loo(fit6))
        elpd_diff se_diff
fit6        0.0        0.0
fit4 -42.6        14.3
```

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2. The models are misspecified with outliers in the data

3. The number of observations is small

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 - in nested case the skewness favors the simpler model
 - any inference with small *n* is difficult
 - if $|elpd_loo| > 4$, model is well specified, and n > 100 then the normal approximation is good

- Log score is not easily interpretable
- but is information theoretically good utility for the goodness of the whole distribution
- and thus is useful in model comparison

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 - compare to guessing uniformly from the data range [121,310] having $1/(310 121 + 1) \approx 0.5\%$ probability (log score -210)
- Interpretation in continuous case
 - can be compared to a simple reference distribution

Assumptions about the future observations Fixed / designed x



elpd_loo = $\sum_{i=1}^{20} \log p(y_i \mid x_i, x_{-i}, y_{-i}) \approx -29.5$ SE = sd(log $p(y_i \mid x_i, x_{-i}, y_{-i})$) $\cdot \sqrt{20} \approx 3.3$ LOO is ok for fixed / designed x. SE is uncertainty about $y \mid x$.

see Vehtari & Ojanen (2012) and CV-FAQ

Assumptions about the future observations Distribution for x



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Covariate shift handled with importance weighting or modelling see Vehtari & Ojanen (2012) and CV-FAQ









 Extrapolation is more difficult item<5> In high dimensional case mostly extrapolation



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 (LFO) 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!



Yes!



Yes!



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 CV-FAQ

Pareto smoothed importance sampling CV variants

- PSIS-LOO for hierarchical models
 - leave-one-group out is challenging for PSIS-LOO
 - Stan demo of the challenges and integrated LOO at https://users.aalto.fi/~ave/modelselection/roaches.html
 - see also Merkel, Furr and Rabe-Hesketh (2018)

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- PSIS-LOO for time series
 - Approximate leave-future-out cross-validation (LFO-CV) mc-stan.org/loo/articles/loo2-lfo.html

K-fold cross-validation

- K-fold cross-validation can approximate LOO
 - the same use cases as with 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











K-fold-CV code

- RStan, CmdStanR
 See vignette http://mc-stan.org/loo/articles/loo2-elpd.html
- RStanARM, brms kfold(fit)
- Alternative data divisions kfold_split_random() kfold_split_balanced() kfold_split_stratified()

looic?

> loo(fit6)

Computed from 4000 by 40 log-likelihood matrix

	Estimate	SE
elpd_loo	-141.7	7.2
p_loo	10.9	2.5
looic	283.4	14.4

Monte Carlo SE of elpd_loo is 0.1.

- loo output shows also looic
- for historical non-Bayesian reasons it's -2 * elpd_loo
 - connection to deviance and information criteria
 - you can just ignore it (I'd prefer it would not be shown)

Information criteria estimate predictive performance, too

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- TIC, NIC, RIC, PIC, BPIC, QIC, AICc, ...
- WAIC is the only Bayesian information criterion

WAIC vs PSIS-LOO

WAIC has the same target and assumptions as LOO

Vehtari, Gelman and Gabry (2017). Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC. *Statistics and Computing*, 27(5):1413–1432 Vehtari & Ojanen (2012). A survey of Bayesian predictive methods for model assessment, selection and comparison. *Statistics Surveys*, 6:142-228.

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- WAIC has the same target and assumptions as LOO
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- Multiplying by -2 doesn't give any benefit (Watanabe didn't multiply by -2)

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Bayes Factor $\frac{p(y|M_1)}{p(y|M_2)}$

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- Oelrich, Ding, Magnusson, Vehtari, and Villani (2020). When are Bayesian model probabilities overconfident? *arXiv:2003.04026*.

Predictive model selection

- Predictive model selection is most natural when the models are used for making predictions
- Predictive model selection can be also useful when the models are not directly used for prediction but for obtaining insights
 - if there is no single independent parameter to look at

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- Predictive model selection can be also useful when the models are not directly used for prediction but for obtaining insights
 - if there is no single independent parameter to look at
- Student retention
 - latent hierarchical linear vs.
 - latent hierarchical linear + spline

is a good example where predictive model selection is useful

Sometimes cross-validation is not needed

- In a simple nested case, often easier and more accurate to analyze posterior distribution of an independent parameter directly
 - instead of comparing Model 1: y ~ normal(α, σ) vs Model 2: y ~ normal(α + βx, σ) look at the posterior of β directly

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 - instead of comparing Model 1: y ~ normal(α, σ) vs Model 2: y ~ normal(α + βx, σ) look at the posterior of β directly
- Randomized control treatment studies is natural example

Common statistical tests as Bayesian models

Most common statistical tests are linear models

test	model	formula
t-test	mean of data	y ~ 1
paired <i>t</i> -test	mean of diffs	(y1 - y2) ~ 1
Pearson correl.	linear model	y ~ 1 + x
two-sample <i>t</i> -test	group means	y ~ 1 + gid
ANOVA	hier. model	y ~ 1 + (1 gid)

. . .

-

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. . .

 See longer list and illustrations (with lm) at https://lindeloev.github.io/tests-as-linear/ and

with rstanarm in Regression and other stories

Beta blockers

- An experiment was performed to estimate the effect of beta-blockers on mortality of cardiac patients
- A group of patients were *randomly* assigned to *control* and treatment groups:
 - out of 674 patients receiving the control, 39 died
 - out of 680 receiving the treatment, 22 died

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fitb1 <- brm(y | trials(N) ~ 1, family = binomial(), data = d_bin2)</pre>

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Posterior inference

- Instead of model selection, report full posterior and
 - compare to expert information
 - combine with utility/cost function



Posterior inference

- Instead of model selection, report full posterior
 - for continuous posterior there is zero probability that e.g. treatment effect is exactly zero



Posterior inference

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 - for continuous posterior we could report the probability that we know the sign of the effect



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 - more abiut decision analysis next week
- Now we look at idealized hypothesis testing

- Instead of model selection, report full posterior and
 - for continuous posterior some people compare whether posterior interval includes null case



- Equivalence testing (region of practical equivalence)
 - what is the probability that the effect is closer than ε to null, where ε is based on what is practically useful effect size



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 - for continuous posterior there is zero probability that e.g. treatment effect is exactly zero



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- Bayes factor
 - sensitive to the prior choice even when the posterior is not



with bridgesampling package, see also BDA3 13.10

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 - is there difference in predictive performance with, e.g., treatment effect fixed to zero or unknown treatment effect
 - requires posterior inference for the null model or projection from the full to null
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 Leave-one-person-out works, but is less efficient than looking at the posterior (see https://users.aalto.fi/~ave/modelselection/betablockers.html)

```
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```

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In the beta blockers example

 Leave-one-person-out works, but is less efficient than looking at the posterior (see https://users.aalto.fi/~ave/modelselection/betablockers.html)

• For another similar, but more elaborate example, see https: //users.aalto.fi/~ave/casestudies/Nabiximols/nabiximols.html

Bodyfat: many predictors

- Predict bodyfat percentage
- The reference value (siri) is obtained by immersing person in water. *n* = 251.
- Which measurements to use in the future?

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 - no model selection needed

Predictive performance based variable selection

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- Select the minimal number of covariates with similar predictive performance as the full model

Hypothesis testing and posterior dependencies

Looking at the marginal posterior $p(\beta < 0)$ can be misleading when there are many parameters

Marginal posteriors of coefficients in bodyfat example



Hypothesis testing and posterior dependencies

Looking at the marginal posterior(s) can be misleading when there are many parameters

Bivariate marginal of weight and height



Hypothesis testing and posterior dependencies

In bodyfat example, starting from full model

- BF in favor of removing weight (p=0.92)
- LOO in favor of removing weight (p=0.99)

In bodyfat example, starting from model y \sim abdomen

- BF in favor of adding weight (p=1.0)
- LOO in favor of adding weight (p=1.0)

Predictive performance based variable selection

Projection predictive variable selection selects the minimal set of variables with similar predictive performance as the full model



Projected posterior

Projection predictive variable selection selects the minimal set of variables with similar predictive performance as the full model



More about projpred in the end of the course

- Classic example is polynomial model with increasing number of components
 - overfits also with Bayesian inference and weak priors

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Simulated data by Richard McElreath

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Polynomial basis functions



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logistic regression: 30 **completely irrelevant** variables, 100 observations

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N(0,3) prior on each coefficient



N(0,3) prior on each coefficient 1 variable



N(0,3) prior on each coefficient 2 variables



N(0,3) prior on each coefficient 3 variables



N(0,3) prior on each coefficient 30 variables



N(0,3) prior on each coefficient 30 variables



A weak prior on parameters can be a strong prior on predictions that favors overfitting
$N(0, \frac{1}{\sqrt{p}})$ prior on each coefficient







 $N(0, \frac{1}{\sqrt{p}})$ prior on each coefficient 2 variables



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 $N(0, \frac{1}{\sqrt{p}})$ prior on each coefficient 30 variables



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Prior on predictions (almost) fixed when the model gets bigger

Better priors, no overfitting

logistic regression: 30 **completely irrelevant** variables, 100 observations, N(0, $\frac{1}{\sqrt{p}}$) prior



Better priors, no overfitting

logistic regression: 30 **completely irrelevant** variables, 100 observations, regularized horseshoe prior



Many weak effects, wide prior on parameters

logistic regression: 30 **weakly relevant** variables, 100 observations, N(0,3) prior



Many weak effects, better prior

logistic regression: 30 **weakly relevant** variables, 100 observations, $N(0, \frac{1}{\sqrt{p}})$ prior



Correlating variables, wide prior on parameters

logistic regression: 30 **correlating relevant** variables, 100 observations, N(0,3) prior



Correlating variables, better prior

logistic regression: 30 correlating relevant variables, 100 observations $N(0, \frac{1}{\sqrt{p}})$ prior



Implied prior on R^2

Regression and Other Stories, Section 12.7 Models for regression coefficients:

Wide prior on coefficients favors overfitting



Implied prior on R^2

Regression and Other Stories, Section 12.7 Models for regression coefficients:

Scaled prior on coefficients



Implied prior on R^2

Regression and Other Stories, Section 12.7 Models for regression coefficients:

Regularized horseshoe prior on coefficients



For example:

- scaled: many weak effects
- regularized horseshoe, R2-D2: only some relevant
- R2-D2: defined directly for R^2
- PCA-type: highly correlating variables

$p \gg n$

- With good priors, possible to have more variables than observations
- e.g. *p* = 22283, *n* = 85 demonstrated by Piironen, Paasiniemi, Vehtari (2020)

Variable selection

Variable selection

- 1. is not needed to avoid overfitting
- 2. can be used to reduce costs and improve explainability

- 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
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- Bigger problem if there is a large number of models as in covariate selection

- Variable selection with forward selection
 - start with null model
 - add the variable improving the predictive performance most
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Wide normal prior



R2D2 prior reduces overfit in model selection



R2D2 prior reduces overfit in model selection



Reminder: variable selection is not needed with good priors to get good predictive performance, but may be useful for other purposes

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- Bayesian model averaging is just the usual integration over unknowns
- Bayesian stacking may work better than BMA in case of misspecified models or small data
 - Yao, Vehtari, Simpson, and Gelman (2018). Using stacking to average Bayesian predictive distributions (with discussion). *Bayesian Analysis*, 13(3):917-1003

Cross-validation and model selection

- · Cross-validation can be used for model selection if
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 - the difference between models is clear
- Be careful if using cross-validation to choose from a large set of models
 - selection process can lead to severe overfitting
- Overfitting in selection process is not unique for cross-validation

Take-home messages

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

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