Model selection and cross validation

FW 891

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Christopher Cahill

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Quantitative Fisheries Center
MICHIGAN STATE UNIVERSITY

Purpose

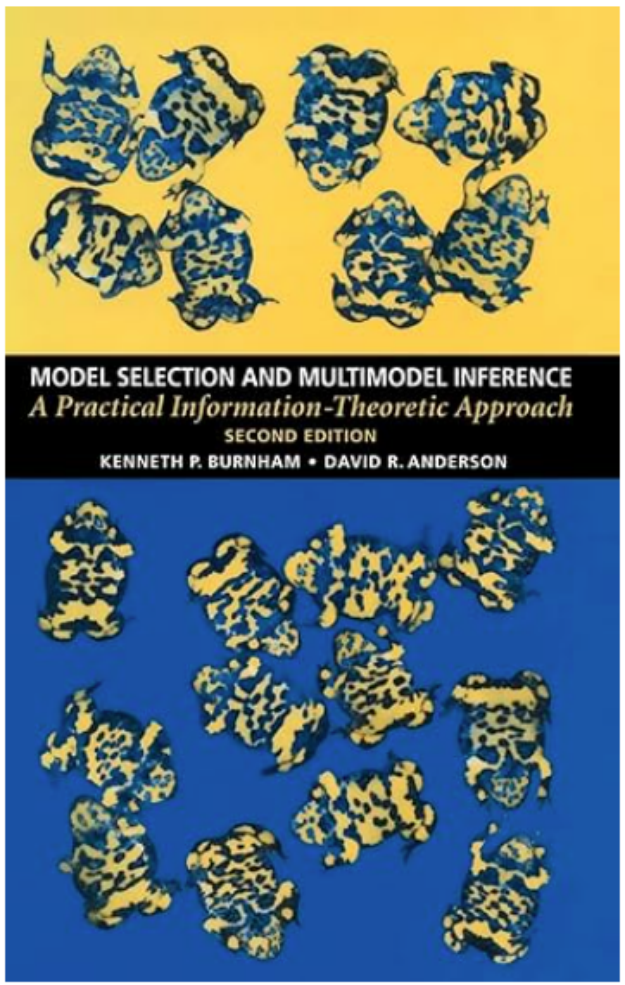
- Goal
- A philosophical preface to model selection
- k-fold and loo cross validation
- Performance criteria
- Challenges
- Approximate methods to loo cross validation
- R and Stan demo on how to implement these ideas

Useful reference on cross validation in Stan:

https://users.aalto.fi/~ave/CV-FAQ.html

TLDR: Model selection is hard and requires careful thought

Model selection: are we stuck between the devil and the deep blue sea?



Burnham and Anderson 1998; Navarro 2018; Bolker 2023

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- *The deep blue sea*: addressing scientific questions
- A question well worth pondering that I have no intention of answering:
  - Are scientific model selection questions addressable with statistical tools?

Navarro 2018; Bolker 2023

With that in mind

Arthur Schopenhauer the philosophy Bunny peering into the inferential abyss

Introduction

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Vehtari et al. 2019

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  - Select a single model from multiple candidates
  - Combine the predictions of multiple models

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- Leave one out (LOO) cross validation represents the limit of K-fold cross validation, where K equals number of data points

Some measures of predictive accuracy

Mean Square Error (MSE)

$$\frac{1}{n}\sum_{i=1}^{n}\left(y_i - \mathrm{E}\left(y_i \mid \theta\right)\right)^2$$

- y_i is data point i
- θ represent fitted model parameters
- proportional to MSE if model is normal with constant variance
- Easy to compute and understand, but less appropriate for non-normal models

Gelman et al. 2014; Vehtari et al. 2016

Expected log pointwise predictive density (elpd)

- Consider data $y_1, \ldots, y_n$ modeled as independent given parameters θ
- Also suppose we have a prior distribution $p(\theta)$ yielding a posterior $p(\theta \mid y)$
- And a posterior predictive distribution $p(\tilde{y} \mid y) = \int p\left(\tilde{y}_i \mid \theta\right) p(\theta \mid y) d\theta$

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$$\begin{aligned} \text{elpd} &= \text{expected log pointwise predictive density for a new dataset} \\ &= \sum_{i=1}^{n} \log \left(\frac{1}{S} \sum_{s=1}^{S} p\left(y_i \mid \theta^s\right) \right). \end{aligned}$$

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- where θ^s represent posterior simulations from $s = 1, \ldots, s$

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Roberts et al. 2017

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- Ecological data are commonly correlated in space, time, groups, or even phylogenetic structure
  - Dependency in groups, space, or time
- Many strategies we can use depending on our prediction task

Roberts et al. 2017

Cross validation and LOO have many limitations

Some known issues

- Computationally demanding

Gelman et al. 2013; Vehtari 2023

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- What does cross validation tell you?

Gelman et al. 2013; Vehtari 2023

How do you view the world?

M-closed vs. M-open worlds

Navarro 2019

Approximate methods for calculating elpd (sneakery)

Approximate cross validation

- Vehtari et al. (2016; 2017) introduced a method that approximates the evaluations of leave-one-out cross validation inexpensively using only the data point log likelihoods of a single model fit

Vehtari et al. 2016; 2017

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- Pareto-smoothed importance sampling (PSIS-LOO) allows us to compute an approximation to LOO without re-fitting the model many times

Vehtari et al. 2016; 2017

Importance sampling LOO

- Since we are Bayesian, we have samples from a posterior
- Approximate the likelihood our model would give some datum if we hadn't observed that datum:

$$\int p\left(y_1 \mid \theta\right) d\theta$$

- Since we are working with samples we move from an integral to an average over samples:

$$\frac{1}{S} \sum_s p\left(y_1 \mid \theta_s\right)$$

Vehtari et al. 2016; 2017

Importance sampling LOO

- Now we want to reweight the posterior samples as thought y_1 wasn't observed:

$$\frac{1}{\sum_s w_s} \sum_s w_s p\left(y_1 \mid \theta_s\right)$$

- The weighting we will use:

$$\frac{1}{p\left(y_1 \mid \theta_s\right)}$$

Vehtari et al. 2016; 2017

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The Pareto part

- It turns out that importance sampling is very noisy, and the sampling weights have very heavy tails
- We need to smooth out the tails so that a single datum doesn't dominate our adjusted posterior
- Turns out the upper tail of the importance weights fits a generalized Pareto distribution nicely and we can use this to smooth out our weights w_s

Vehtari et al. 2016; 2017

PSIS-LOO implementation

- If all of that overwhelms you…

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PSIS-LOO implementation

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- There are packages and functions that help you do this
- They have a lot of diagnostics to tell you when they think they are going wrong

Vehtari et al. 2016; 2017

To the R and Stan code

References

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