Bayesian Compromise Estimators

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Introduction

- The common form of a statistical analysis is given by the following two steps:
  - Select the best model
  - Apply the model as if it was the truth/the best overall
- The first step usually relies on either
  - model selection criteria (WAIC/*IC/CV), often data driven, or
  - scientific theory.
- However, it is quite easy to criticize the model selection step. For example:
  - Model selection can be unstable. Small changes of input data may yield radically different model choice.
  - Very different models can have similar performance overall. Then, discriminating between them is often difficult.
- What are the possible consequences? Poor generalizability and inference.
  - Unstable selection means the model may perform badly with out-of-sample data.
  - Ad-hoc choices between similar models may yield sub-optimal selection.
  - Model selection uncertainty not properly represented in final analysis
- Compromise modeling is one way of dealing with the issue. Particularly good at countering poor generalizability.

Compromise Modeling – General Idea

Suppose that φ is some quantity of interest, and that

- There are K candidate models under consideration, and
- Each candidate model produces φ_k as and approximation of φ.

Then, compromise modeling entails us a weighted average of the candidates,

$$\bar{\varphi} = \sum_{k=1}^{K} w_k \varphi_k,$$

as the final approximation of φ. Here w_k are model specific weights that can be estimated to suit the purpose of the analysis.

Example: Variable Selection in Linear Regression

Let $\mathbf{y} = (y_1, \ldots, y_n)^T$ be a vector of (continuous) outcomes and $\mathbf{X}$ be a matrix of covariates to use in linear regression.

Problem: Which subset $\mathbf{X}_k \subset \mathbf{X}$ of variables gives the best regression model?

Common solution: Use some off-the-shelf procedure to chose "optimal" subset.

Alternative solution: Consider several different subsets, and combine their information by a weighted average. For example,

- If φ is the posterior predictive distribution, $\bar{\varphi} = \sum_k w_k \cdot p(\tilde{\mathbf{y}}|\mathbf{y}, \mathbf{X}_k)$,
- If φ is the posterior predictive mean, $\bar{\varphi} = \sum_k w_k \cdot E[\tilde{\mathbf{y}}|\mathbf{y}, \mathbf{X}_k]$.

Note that both $p(\tilde{\mathbf{y}}|\mathbf{y}, \mathbf{X}_k)$ and $E[\tilde{\mathbf{y}}|\mathbf{y}, \mathbf{X}_k]$ are derived as usual. The new step in this procedure is finding suitable weights $w_1, \ldots, w_K$. In Bayesian theory, Bayesian model averaging and Bayesian stacking are the prominent ways of doing so.

Bayesian Model Averaging

Bayesian model averaging (BMA) is concerned with $\varphi = p(\Delta|D)$, where

- Δ could be a new observation, $\tilde{\mathbf{y}}$, or a vector of regression coefficients, , and
- D is the data.

The BMA posterior probability for Δ is given as

$$p(\Delta|D) = \sum_{k=1}^{K} p(\Delta|M_k, D) \cdot p(M_k|D).$$

Here, M_k denotes the k:th candidate model, and

- $p(\Delta|M_k, D)$ is the posterior probability for Δ given model k.
- $p(M_k|D)$ is the posterior probability of the model M_k.

Compare to the compromise posterior predictive on last slide, and note that $w_k = p(M_k|D)$ shows how to weight each model.

Problems in Practice

- Posterior distributions of advanced models can be hard (impossible) to find. For BMA, this amounts to
  - The usual difficulty of finding $p(\Delta|M_k, D)$, and
  - The additional step of finding the model posterior, $p(M_k|D)$. In particular, computing the integrated likelihood.
- Some simple problems have analytical solutions (see e.g. Raftery, Madigan, and Hoeting 1997 for a linear regression example).
- MCMC Model Composition (MCMCMC) simplifies things by generating a Markov chain that moves through the model space (I think it can be applied using the `BMA` package).
- Another issue of BMA has to do with the behavior of the weights in large samples. To discuss this, some further notation has to be introduced.

$\mathcal{M}$-open and $\mathcal{M}$-closed

To formalize the last drawback of BMA, and to motivate the use of Bayesian stacking, the properties of the candidate models employed need to be considered. Thus, let $\mathcal{M} = \{M_1, \dots, M_K\}$ be the set of candidate models. Then

- $\mathcal{M}$-closed means the true data generating model is included in $\mathcal{M}$, although it is not known which of the candidates it is, while
- $\mathcal{M}$-complete means that the true model is *not* in $\mathcal{M}$, but we still use $\mathcal{M}$ since the true model may be too complicated in terms of computations, interpretations, etc.
- $\mathcal{M}$-open means that the true model is *not* in $\mathcal{M}$, and there is no knowledge of how to specify an explicit form of the true model.

It is known that, as $n \to \infty$, the BMA weight of the candidate closest to the true model (in terms of KL divergence) tends to 1. That is,

- For $\mathcal{M}$-closed, this is great since BMA will chose the true model.
- For $\mathcal{M}$-complete/open, BMA clearly selects the wrong model.

I would argue that $\mathcal{M}$-complete/open is more realistic. So what to do?

Bayesian Stacking

Some preliminaries: Let

- $\mathbf{w} = (w_1, \dots, w_k)^T$, and suppose it belongs to some set $\mathcal{W}$, and
- $S(P, Q)$ be a scoring rule, measuring the similarity of two distributions P and Q.

Then, Bayesian stacking weights are given by

$$\mathbf{w}^* = \underset{\mathbf{w} \in \mathcal{W}}{\operatorname{argmax}} \; S\left(\sum_{k=1}^{K} w_k p(\tilde{\mathbf{y}} | \mathbf{y}, M_k), p_{\mathsf{true}}(\tilde{\mathbf{y}} | \mathbf{y}) \right).$$

That is, $\mathbf{w}^*$ is the weight vector that maximizes the similarity between the stacked posterior predictive and the true posterior predictive distribution

Bayesian Stacking

Of course, $p_{\text{true}}(\tilde{\mathbf{y}}|\mathbf{y})$ is not known, and some kind of empirical approximation is required. One way of estimating $\mathbf{w}^*$ is using leave-one-out cross-validation.

- Clyde and Iversen (2013) introduce it in Bayesian setting,
- Le and Clarke (2017) theoretically motivate use of CV for weight estimation,
- Yao et al. (2018) use general scoring rules.

Using the weight vector estimated by cross-validation, the stack is given by

$$\sum_{k=1}^{K} w_k^* p(\tilde{\mathbf{y}}|\mathbf{y}, M_k),$$

which is very similar to the *frequentist jackknife model averaging*.

Scoring Rules

For Bayesian stacking, it is common to use either

- The $\log$ score, $LS(P, y) = \log[p(y)]$, or
- The *energy* score, $ES(P, y) = \frac{1}{2} E_P \|Y - Y'\|^\beta - \mathbb{E}_p \|Y - y\|^\beta$. Here, Y and Y' both follow P independently. $\beta = 2$ is common in practice.

The major difference is that stacking using the $\log$ score gives a stacked posterior *distribution*, while stacking using the $\beta = 2$ energy score gives a stacked posterior *mean*.

Depending on the objective of the analysis, either approach may be suitable.

Example Using `rstanarm` and `loo`

`loo::stacking_weights` gives $\log$-score weights. See stylized example below.

```
library("rstanarm"); library("loo")

# Fitting the candidate models
cand1 <- stan_glm(y ~ X1, data = df)
cand2 <- stan_glm(y ~ X1 + X2, data = df)
cand2 <- stan_glm(y ~ X1 + X2 + X3, data = df)

# LOO-CV approximation
loo1 <- loo(cand1); loo2 <- loo(cand2); loo3 <- loo(cand3)

# Pointwise LOO ELPD
lpd_point <- cbind(loo1$pointwise[,"elpd_loo"],
                   loo2$pointwise[,"elpd_loo"],
                   loo3$pointwise[,"elpd_loo"])
stacking_weights(lpd_point) # Estimates the weights
```

An example using real data is given in the enclosed `R` script.

Research Example

Ongoing work aims to evaluate Bayesian stacking using frequentist asymptotics. In particular, the focus is to establish the *oracle property*

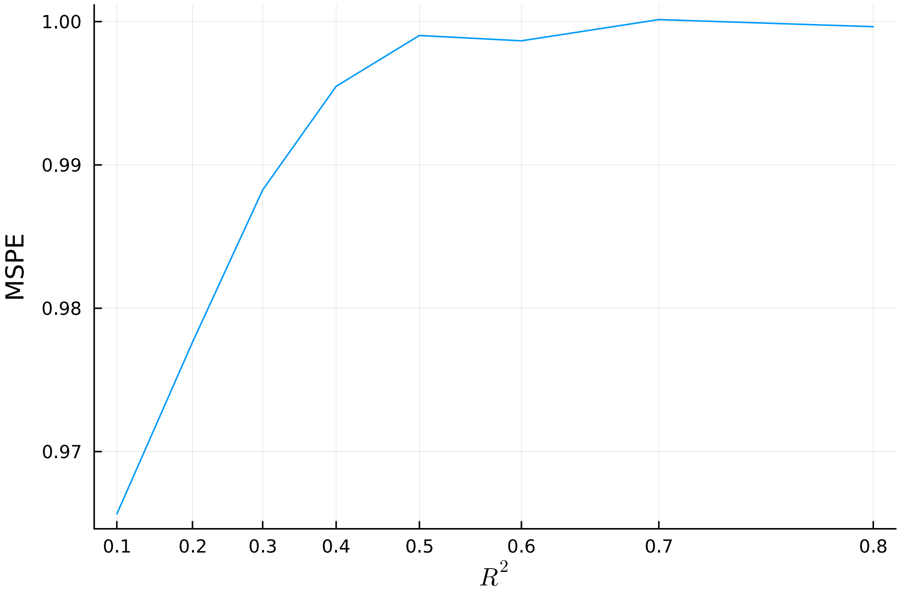
$$\frac{\|\mathbf{y} - \sum_k w_k^* E[\mathbf{y}|M_k]\|^2}{\inf_{\mathbf{w}\in\mathcal{W}} \|\mathbf{y} - \sum_k w_k E[\mathbf{y}|M_k]\|^2} \xrightarrow{p} 1.$$

This means that no candidate, nor any other average using the same candidates and weights from $\mathcal{W}$, provides smaller asymptotic error than Bayesian stacking.

To date, the oracle has been established for Bayesian stacking of linear regression models using $\mathcal{N}(\mathbf{0}, \mathbf{S})$, as the prior for β, where $\mathbf{S} > 0$ is symmetric.

The results of a simulation are given on the next slide. The curve gives the ratio of the Bayesian stacking squared error to the squared error of the best candidate.

Research Example



References

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