

7: Evaluating, comparing and expanding models

Taylor

University of Virginia

This chapter focuses mostly on quantifying a model's predictive capabilities for the purposes of model selection and expansion.

New Notation!

- 1 f is the true model
- 2 y is the data we use to estimate our model
- 3 \tilde{y} is the future (time series) or alternative (not time series) data that we test our predictions on
- 4 $p_{\text{post}}(\tilde{y}) = p(\tilde{y} \mid y)$
- 5 $p_{\text{post}}(\theta) = p(\theta \mid y)$
- 6 $E_{\text{post}}[\cdot]$ is taken with respect to $p(\theta \mid y)$

A **scoring rule/function** $S(p, \tilde{y})$ is a function that takes

- 1 the distribution you're using to forecast p (ppd, or likelihood with estimated parameters), and
- 2 a realized value \tilde{y}

and then gives you a real-valued number/score/utility. Higher is better, although this convention isn't always followed in the literature.

Keep in mind that the realized value cannot be used to fit the data.

Examples

Example: $S(p, \tilde{y}) = -(\tilde{y} - E_p[\tilde{y}])^2$

Example: $S(p, \tilde{y}) = \log p(\tilde{y})$

Future/unseen data is unknown, so we must take the expected score under the true distribution f :

$$E_f[S(p, \tilde{y})].$$

A scoring rule is **proper** if the above expectation is minimized when $f = p$.

A scoring rule is **local** if $S(p, \tilde{y})$ only depends on $p(\tilde{y})$ (don't care about events that didn't happen).

Note, when we are dealing with a logarithmic scoring rule, $E[-2 \log p(\tilde{y})]$ is often called an **information criterion**. The book switches back and forth between dealing with expected score, and information criteria.

Examples

Example: $S(p, \tilde{y}) = -(\tilde{y} - E_p[\tilde{y}])^2$

Most common, perhaps not local or proper for non-Gaussian data.

Example: $S(p, \tilde{y}) = \log p(\tilde{y})$

Obviously local. Proper, too (homework question).

Problem

We are generally not able to evaluate the expectation because we don't know f . However, we may be able to wait for new out-of-sample data and use a Monte-Carlo approach:

$$n^{-1} \sum_{i=1}^n S(p, \tilde{y}^i) \rightarrow E_f[S(p, \tilde{y})]$$

as $n \rightarrow \infty$

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If we can afford to wait for an infinite amount of data, though, what is the point of trying to predict it?

Problem

NB: the textbook focuses on $S(p, \tilde{y}) = \log p(\tilde{y})$, and the data are iid (after conditioning on the parameter). They call the following quantity the “elppd:”

expected log pointwise predictive density

$$\begin{aligned} E_f[\log p(\tilde{y})] &= E_f \left[\log \prod_i p(\tilde{y}_i) \right] \\ &= \sum_{i=1}^n E_f [\log p(\tilde{y}_i)] \end{aligned}$$

Problem

For the moment let's use $p(\tilde{y}) = p_{\text{post}}(\tilde{y})$

The “elppd” is not obtainable because

- ① you don't know f (can't directly integrate)
- ② you don't have \tilde{y} (no Monte-Carlo)

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Using y for \tilde{y} , we can come up with a rough elppd estimate called the “lppd”

log pointwise predictive density

$$\text{lppd} = \log p_{\text{post}}(y) = \sum_{i=1}^n \log p_{\text{post}}(y_i)$$

Problem

There's also the problem that arises where we cannot evaluate

$$p_{\text{post}}(y) = \int p(y | \theta) p(\theta | y) d\theta = E_{\text{post}}[p(y | \theta)]$$

The “computed lppd” again uses y for \tilde{y} , but it also uses Monte-Carlo to sample from the posterior

log pointwise predictive density

$$\text{computed lppd} = \log \hat{p}_{\text{post}}(y) = \sum_{i=1}^n \log \left(\frac{1}{S} \sum_{j=1}^S p(y_i | \theta^j) \right)$$

A third problem

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However, we can get around this in two ways generally:

- 1 plug in the already-used y data, but then add an extra penalty term (e.g. AIC, DIC, WAIC, etc.)
- 2 Cross-Validation: split the data y , many different ways, into a train and test set; estimate and evaluate on each split.

AIC stands for “an information criterion” or “Akaike’s Information Criterion.” Let k be the number of parameters:

$$\widehat{\text{elpd}}_{\text{AIC}} = \log p(y \mid \hat{\theta}_{\text{MLE}}) - \underbrace{k}_{\text{penalty}}$$

or

$$\text{AIC} = \underbrace{-2 \log p(y \mid \hat{\theta}_{\text{MLE}})}_{\text{a deviance}} + 2k$$

We estimate $\hat{\theta}_{\text{MLE}}$ using y , and we plug y into the log likelihood.

DIC replaces the point estimate with $\hat{\theta}_{\text{Bayes}} = E[\theta | y]$, and replaces the penalty term with p_{DIC}

$$\widehat{\text{elpd}}_{\text{DIC}} = \log p(y | \hat{\theta}_{\text{Bayes}}) - p_{\text{DIC}}$$

or

$$\text{DIC} = -2 \log p(y | \hat{\theta}_{\text{Bayes}}) + 2p_{\text{DIC}}$$

The book gives two ways to estimate p_{DIC} :

- ① $p_{\text{DIC}} = 2 \left(\log p(y \mid \hat{\theta}_{\text{Bayes}}) - E_{\text{post}} [\log p(y \mid \theta)] \right)$
- ② $p_{\text{DIC alt}} = 2 \text{Var}_{\text{post}} [\log p(y \mid \theta)]$

Both of these can be approximated using samples from the posterior.

Motivation for p_{DIC}

$$\begin{aligned} & E_{\tilde{y}} \left[-2 \log p(\tilde{y} \mid \hat{\theta}_{\text{Bayes}}) \right] \\ &= -2 \log p(y \mid \hat{\theta}_{\text{Bayes}}) + E_{\tilde{y}} \left[-2 \log p(\tilde{y} \mid \hat{\theta}_{\text{Bayes}}) \right] + 2 \log p(y \mid \hat{\theta}_{\text{Bayes}}) \\ &\approx -2 \log p(y \mid \hat{\theta}_{\text{Bayes}}) + E_{\theta|y} [-2 \log p(y \mid \theta)] + 2 \log p(y \mid \hat{\theta}_{\text{Bayes}}) \\ &= -2 \log p(y \mid \hat{\theta}_{\text{Bayes}}) + p_{\text{DIC}} \end{aligned}$$

p_{WAIC} either stands for “widely applicable information criterion” or “Watanabe-Akaike information criterion.”

The book refers to it as the most “fully Bayesian” of the three, probably because it doesn’t plug in point estimates into the likelihood instead of integrating.

$$\widehat{\text{elppd}}_{\text{WAIC}} = \text{lppd} - p_{\text{WAIC}}$$

or

$$\text{WAIC} = -2\text{lppd} + 2p_{\text{WAIC}}$$

where $\text{lppd} = \sum_{i=1}^n \log \left(\frac{1}{S} \sum_{s=1}^S p(y_i | \theta^s) \right)$

Two ways to estimate

- ① $p_{\text{WAIC } 1} = 2 (\log p(y | y) - E_{\theta|y} \{\log p(y | \theta)\})$
- ② $p_{\text{WAIC } 2} = \sum_{i=1}^n \text{var}_{\text{post}}(\log p(y_i | \theta))$

Both of these can be approximated using samples from the posterior.

Motivation for p_{WAIC} :

$$\begin{aligned} & E_{\tilde{y}} [-2 \log p(\tilde{y} | y)] \\ & E_{\tilde{y}} [-2 \log E_{\theta|y}(p(\tilde{y} | \theta))] \\ &= -2 \log p(y | y) + 2 (\log p(y | y) - E_{\tilde{y}} [\log E_{\theta|y}(p(\tilde{y} | \theta))]) \\ &\approx -2 \log p(y | y) + 2 (\log p(y | y) - E_{\tilde{y}} [E_{\theta|y}(\log p(\tilde{y} | \theta))]) \\ &\approx -2 \log p(y | y) + 2 (\log p(y | y) - E_{\theta|y} [E_{\tilde{y}}(\log p(\tilde{y} | \theta))]) \\ &\approx -2 \log p(y | y) + 2 (\log p(y | y) - E_{\theta|y} [\log p(y | \theta)]) \\ &= -2 \log p(y | y) + 2 \left(\log \prod_i p(y_i | y) - E_{\theta|y} \left[\log \prod_i p(y_i | \theta) \right] \right) \\ &= -2 \log p(y | y) + 2 \sum_i (\log p(y_i | y) - E_{\theta|y} [\log p(y_i | \theta)]) \\ &= -2 \log p(y | y) + p_{\text{WAIC1}} \end{aligned}$$

Cross-Validation

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- 1 The partitions are nonrandom, test sets are disjoint
- 2 for each split/estimation/prediction, we never use a data point twice
- 3 for each split/estimation/prediction, we lose parameter estimation accuracy because each training set is smaller than the full set
- 4 however, we get to average over many prediction scores, which reduces variance
- 5 there is still a bias that we have to estimate (but it's usually smaller than AIC/DIC/WAIC/etc.)
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The logo of this QA website illustrates the idea nicely!

leave-one-out cross-validation (loo-cv) is a special case where each test set is of size 1.

This necessarily implies that each training set is of size $n - 1$, and there are n possible splits.

If this ends up being too computationally expensive, it is also possible to do **k -fold cross-validation**, which selects k splits/folds. This means the size of each test set is n/k , and the size of each training set is $n - n/k$

Cross-Validation Notation

We only discuss loo-cv...

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If this ppd isn't tractable, we can use draws from the posterior as follows:

$$p_{\text{post}(-i)}(y_i) = \frac{1}{S} \sum_{s=1}^S p(y_i \mid \theta^s)$$

where θ^s are draws from $p_{\text{post}(-i)}(\theta)$

The Bayesian loo-cv estimate for out-of-sample predictive fit is

$$\text{lppd}_{\text{loo-cv}} = \sum_{i=1}^n \log p_{\text{post}(-i)}(y_i)$$

There are also bias-corrected versions as well.

Bayes factors are another way to compare models, two at a time. You compare each model's prior predictive distribution

Bayes Factors

$$\begin{aligned} B_{2,1} &= \frac{p(y \mid H_2)}{p(y \mid H_1)} \\ &= \frac{\int p(y \mid \theta_2, H_2) p(\theta_2 \mid H_2) d\theta_2}{\int p(y \mid \theta_1, H_1) p(\theta_1 \mid H_1) d\theta_1} \end{aligned}$$

assuming $0 < p(y \mid H_i) < \infty$

NB: models do not have to be nested, and the parameters can be of varying dimension

Bayes Factors

$$B_{2,1} = \frac{p(y|H_2)}{p(y|H_1)}$$

$\log_{10}(B_{10})$	B_{10}	Evidence against H_0
0 to 1/2	1 to 3.2	Not worth more than a bare mention
1/2 to 1	3.2 to 10	Substantial
1 to 2	10 to 100	Strong
>2	>100	Decisive

From <http://www.andrew.cmu.edu/user/kk3n/simplicity/KassRaftery1995.pdf>

Bayes Factors

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$$\begin{aligned}\text{posterior odds} &= \frac{p(H_2 | y)}{p(H_1 | y)} \\ &= \frac{p(y | H_2)p(H_2)/p(y)}{p(y | H_1)p(H_1)/p(y)} && \text{(Bayes rule)} \\ &= \frac{p(y | H_2)}{p(y | H_1)} \frac{p(H_2)}{p(H_1)} \\ &= \text{Bayes factor} \times \text{prior odds}\end{aligned}$$

You should not use improper priors when you calculate Bayes factors because

$$p(y | H_1) = \int p(y | \theta_1, H_1)p(\theta_1 | H_1)d\theta_1$$

is not a density (homework question), and the normalizing constant will be ambiguous.

Even noninformative proper priors can be “biased” towards one of the hypotheses.

Consider the following example of the **Jeffreys-Lindley's paradox**:

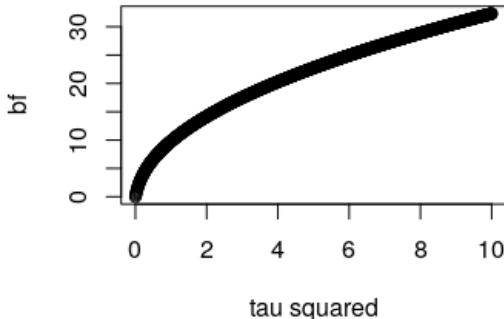
- ① $p(\bar{y} \mid \theta, H_1) = (2\pi)^{-n/2} n^{n/2} \exp \left[-\frac{n}{2} \bar{y}^2 \right]$
- ② under H_1 : $\theta = 0$ with prior probability 1
- ③ under H_2 : $p(\theta) = N(0, \tau^2)$
- ④ $p(\bar{y} \mid H_2) = [2\pi(\tau^2 + n^{-1})]^{-n/2} \exp \left[-\frac{1}{2(\tau^2 + n^{-1})} \bar{y}^2 \right]$

so

$$B_{1,2} = (n\tau^2 + 1)^{1/2} \exp \left[-\frac{\bar{y}^2}{2} \left(n - \frac{1}{(\tau^2 + n^{-1})} \right) \right]$$

Bayes Factors: The Jeffreys-Lindley's paradox

Say $\bar{y} = 1.5$ and $n = 10$. Then our p-value for the null is $2.101436e - 06$, but



Different decisions based on whether we are frequentist or Bayesian?!

Bayes Factors

If you can't derive $p(y | H_i)$, then you can resort to simulation. Notice that the joint $p(y | \theta_i, H_i)p(\theta_i | H_i)$ is an unnormalized target!

For instance, here is the justification behind importance sampling:

$$\begin{aligned} p(y | H_i) &= \int p(y | \theta_i, H_i)p(\theta_i | H_i)d\theta_i \\ &= \int \frac{p(y | \theta_i, H_i)p(\theta_i | H_i)}{q(\theta_i)}q(\theta_i)d\theta_i \\ &\leftarrow \sum_{s=1}^n \frac{p(y | \theta_i^s, H_i)p(\theta_i^s | H_i)}{q(\theta_i^s)} \end{aligned}$$

where $\theta_i^s \sim q(\theta_i)$

Bayes Factors and the “Worst Monte Carlo Method Ever”

One might be tempted to use the posterior samples, too:

$$\begin{aligned} p(y \mid H_i) &= \left[\frac{1}{p(y \mid H_i)} \int p(\theta_i \mid H_i) d\theta_i \right]^{-1} \\ &= \left[\int \frac{p(y \mid \theta_i, H_i) p(\theta_i \mid H_i)}{p(y \mid H_i) p(y \mid \theta_i, H_i)} d\theta_i \right]^{-1} \\ &= \left[\int \frac{p(\theta_i \mid y, H_i)}{p(y \mid \theta_i, H_i)} d\theta_i \right]^{-1} \\ &\leftarrow \left[\frac{1}{S} \sum_{s=1}^S \frac{1}{p(y \mid \theta_i^s, H_i)} \right]^{-1} \end{aligned}$$

where $\theta_i^s \sim p(\theta_i \mid y, H_i)$ are samples from the posterior.

However, this estimator often has infinite variance, and so it shouldn't be used.