# **ADVANCED** BAYESIAN MODELING

Bayesian Cross-Validation

Recall evaluation of a fitted model: how well it predicts new data.

Recall problem with using deviance for model evaluation:

Same data y is used both for model fitting and for estimating the expected (logarithmic) score, which makes evaluation too optimistic.

This is why criteria like DIC include a correction for effective number of parameters.

# Data Splitting

A different approach –

Split data y into two parts (preferably at random):

$$y = (y_{\mathsf{train}}, y_{\mathsf{eval}})$$

Use  $y_{\text{train}}$  to fit the model and  $y_{\text{eval}}$  to estimate its predictive accuracy (score).

#### Issues:

- Depends on which split of data is used.
- ▶ Biased evaluation because fit is based on only a subset of the data set.

#### **Cross-Validation**

**Cross-validation**: Use many different data splits, and combine the evaluation results.

**Leave-one-out cross-validation (LOO-CV)**: For n observations, use the n splits in which  $y_{\text{eval}}$  has only one observation.

This reduces evaluation bias, since  $y_{\text{train}}$  is almost the full data.

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# Bayesian Evaluation

For Bayesian models, generally assume  $y_{\rm train}$  and  $y_{\rm eval}$  are conditionally independent, then use log predictive density of  $y_{\rm eval}$  based on  $y_{\rm train}$ 

$$\log p_{\mathsf{train}}(y_{\mathsf{eval}}) = \log \int p(y_{\mathsf{eval}} \mid \theta) \, p_{\mathsf{train}}(\theta) \, d\theta$$

where  $p_{\mathsf{train}}(\theta)$  is the posterior using only  $y_{\mathsf{train}}$ .

In LOO-CV, each  $y_{\text{eval}}$  is just a  $y_i$  ( $i=1,\ldots,n$ ), and we denote the log predictive densities as

$$\log p_{\mathsf{post}(-i)}(y_i) \qquad i = 1, \dots, n$$

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# Bayesian LOO-CV

We choose the combined LOO-CV estimate to be the sum

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

for which larger values indicate better models.

Note: Resembles

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

used in WAIC.

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Note: The Monte Carlo approximation to  $\log p_{post(-i)}(y_i)$  is

$$\log\left(\frac{1}{S}\sum_{s=1}^{S}p(y_i\mid\theta^{is})\right)$$

where

$$\theta^{i1}, \ldots, \theta^{iS}$$

is a sample from the posterior when  $y_i$  is left out.

Bayesian LOO-CV needs a total of n such samples: expensive for large n.

#### Remarks (BDA3, Sec. 7.2):

- ▶ There is a correction for the remaining bias in LOO-CV (usually small if n is large).
- ▶ There is a way to define an effective number of parameters.
- ▶ Bayesian LOO-CV is asymptotically equivalent to WAIC (under some conditions).