STA 365: Applied Bayesian Statistics

Boris Babic
Assistant Professor, University of Toronto

Week 11A: Model Assessment

Objectives

- We will study methods for model comparisons and checking for model adequacy
- For model comparisons there are a finite number of candidate models and we want to select one
  - Bayes factors
  - Cross validation
  - Deviance information criteria (DIC)
- In cases where multiple models fit well, we can consider
  - Bayesian model averaging (BMA)
- After selecting a model, we want to test whether it fits the data well
  - Posterior predictive checks

Food and Drug Administration

- FDA recommends you investigate all assumptions important to your analysis.
- You may summarize this comparison using a Bayesian p-value (Gelman et al., 1996, 2004), the predictive probability that a statistic is equal to or more extreme than that observed under the assumptions of the model.
- You may also assess model checking and fit by Bayesian deviance measures, such as the Deviance Information Criterion as described in Spiegelhalter et al. (2002).
- Alternatively, two models may be compared using Bayes factors.

Bayes factors (BF)

- Consider two models: $\mathcal{M}_1$ and $\mathcal{M}_2$
- For example, $Y \sim \text{Binomial}(n, \theta)$ and the two models are

$$\mathcal{M}_1 : \theta = 0.5 \qquad \text{and} \qquad \mathcal{M}_2 : \theta \neq 0.5$$

- Another example, $Y_1, Y_2, \ldots, Y_n$ is a time series and

$$\mathcal{M}_1 : \text{Cor}(Y_{t+1}, Y_t) = 0, \qquad \text{and} \qquad \mathcal{M}_2 : \text{Cor}(Y_{t+1}, Y_t) > 0$$

- Another example,

$$\mathcal{M}_1 : \text{E}(Y) = \beta_0 + \beta_1 X, \qquad \text{and} \qquad \mathcal{M}_2 : \text{E}(Y) = \beta_0 + \beta_1 X + \beta_2 X^2.$$

Bayes factors (BF)

- This is similar to hypothesis testing
- As before we proceed by computing the posterior probabilities of the two models
- This requires prior probabilities $\pi(\mathcal{M}_1)$ and $\pi(\mathcal{M}_2)$ on the model
- This is different than the priors for parameters
- We can make the probabilistic statement that the "with the prior knowledge, the quadratic model is five times more likely than a linear model"

Bayes factors (BF)

- The Bayes factor for model 2 compared to model 1 is

$$BF = \frac{\text{Posterior odds}}{\text{Prior odds}} = \frac{\pi(\mathcal{M}_2 \mid Y)/\pi(\mathcal{M}_2 \mid Y)}{\pi(\mathcal{M}_2)/\pi(\mathcal{M}_1)} = \frac{\pi(Y \mid \mathcal{M}_2)}{\pi(Y \mid \mathcal{M}_1)}.$$

- Rule of thumb: BF > 10 is strong evidence for $\mathcal{M}_2$
- Rule of thumb: BF > 100 is decisive evidence for $\mathcal{M}_2$
- In linear regression, BIC approximates the BF comparing a model to the null model

Example

- $Y \sim \text{Binomial}(n, \theta)$ with

$$\mathcal{M}_1 : \theta = \theta_0, \qquad \mathcal{M}_2 : \theta \neq \theta_0$$

- $\pi(Y \mid \mathcal{M}_1)$ is just the binomial density with $\theta = \theta_0$.

$$\pi(Y \mid \mathcal{M}_1) = \binom{n}{Y} \theta_0^Y (1 - \theta_0)^{n-Y}$$

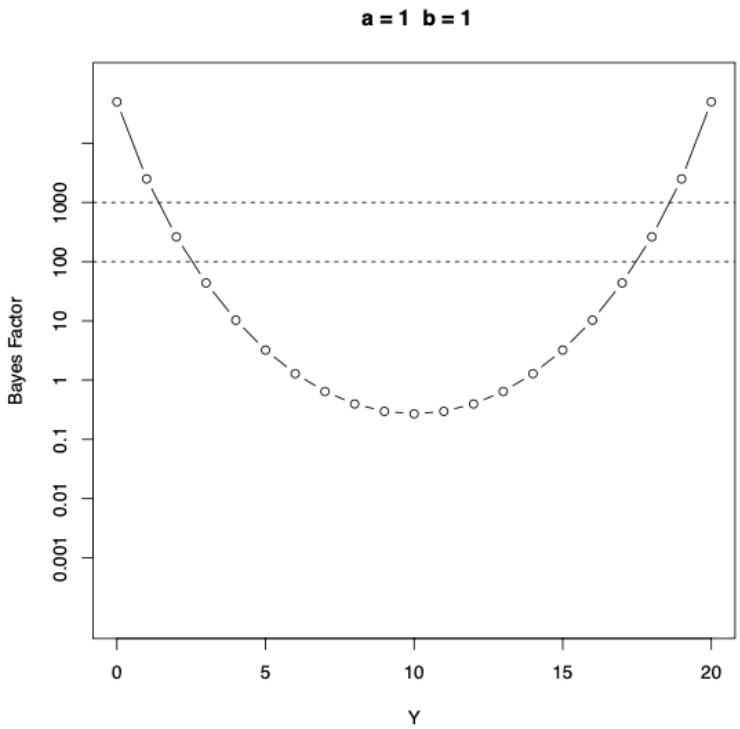
- M_2 involves an unknown parameter θ.
- This requires a prior, say $\theta \sim \text{Beta}(a, b)$, and integration

$$\pi(Y \mid \mathcal{M}_2) = \int \pi(Y, \theta) d\theta = \binom{n}{Y} \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \frac{\Gamma(Y+a)\Gamma(n-Y+b)}{\Gamma(n+a+b)}.$$

- The BF is

$$\text{BF}(\mathcal{M}_2 \mid \mathcal{M}_1) = \frac{\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \frac{\Gamma(Y+a)\Gamma(n-Y+b)}{\Gamma(n+a+b)}}{\theta_0^Y (1 - \theta_0)^{n-Y}}$$

Example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0.01
0.1
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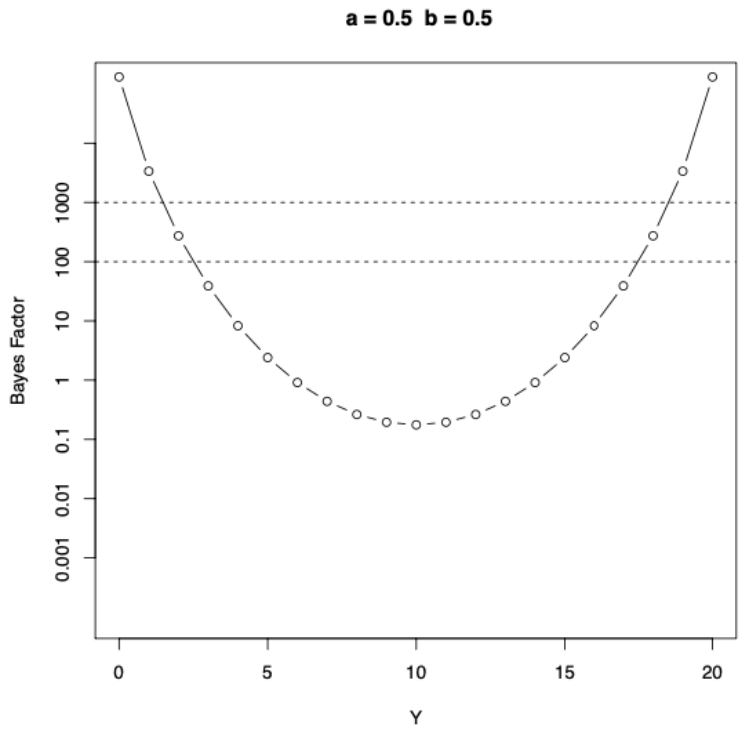
10
100
1000
0
5
10
15
20
Y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Bayes Factor
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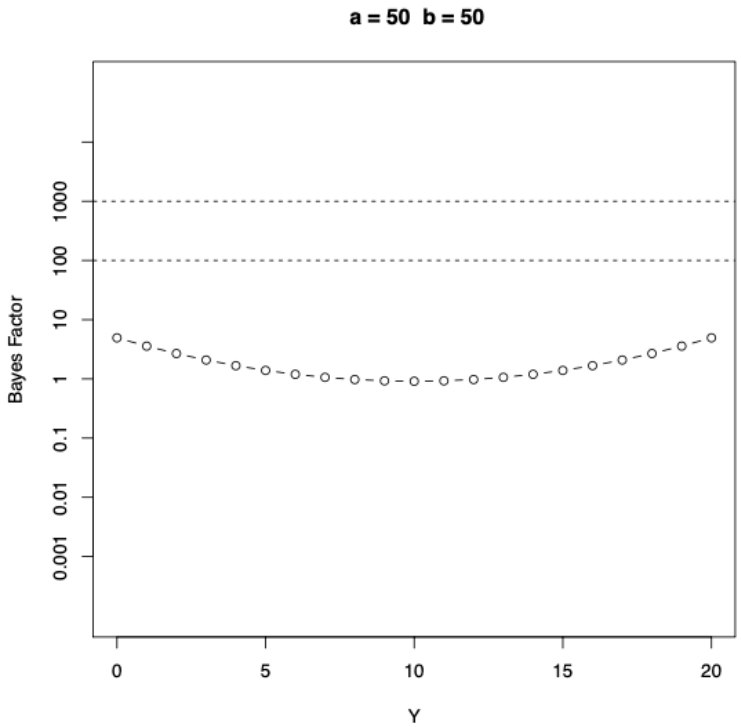
Example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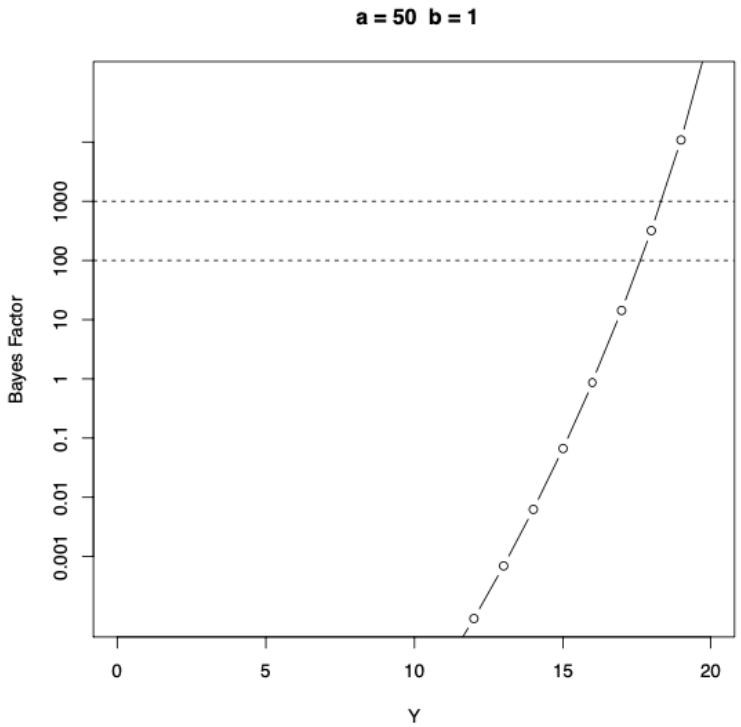
a = 50 b = 1
Bayes Factor
0.001
0.01
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Limits of Bayes Factors

- Often required intractable integral computation for complex model
  - Monte Carlo method?
- Requires proper prior specifications
- Can be sensitive to prior specifications (Lindley's paradox)
- In some scenarios, we can consider Bayesian model averaging

Bayesian Modle Averaging

- Consider the linear regression example

$$\mathcal{M}_1 : \mathrm{E}(Y) = \beta_0 + \beta_1 X \text{ v.s. } \mathcal{M}_2 : \mathrm{E}(Y) = \beta_0 + \beta_1 X + \beta_2 X^2$$

- Say we have fit both models and found that both are about equally likely, but that $\mathcal{M}_1$ is slightly preferred
- For prediction, $\hat{Y}$, we could simply take the prediction that comes from fitting $\mathcal{M}_1$
- But the prediction from $\mathcal{M}_2$ is likely different and nearly as accurate
- Also, taking the prediction from $\mathcal{M}_1$ suppresses our uncertainty about the form of the model

Bayesian Modle Averaging

- Let $\hat{Y}_k$ be the prediction from model $\mathcal{M}_k$ for $k = 1, 2$
- The model averaged predictor is

$$\hat{Y} = w\hat{Y}_1 + (1 - w)\hat{Y}_2$$

- It can be shown that the optimal weight w is the posterior probability of $\mathcal{M}_1$.
- Averaging adds stability
- In linear regression with p predictors the prediction is a weighted average of 2^p possible models
- We can implement this by introducing latent indicators.

Cross Validation

- Another very common approach is cross validation
- This is exactly the same procedure used in classical statistics
- This operates under the assumption that the "true" model likely produces better out-of-sample prediction than competing models
- Pros: conceptually simple, intuitive, and broadly applicable
- Cons:
  - Slow because it requires several model fits (can we do better?)
  - it is hard to say a difference is statistically significant.

K-Fold Cross Validation

Step 0: Split the data into K equally-sized groups

Step 1: Set aside group k as test set and fit the model to the remaining $K-1$ groups

Step 2: Make predictions for the test set k based on the model fit to the training data

Step 3: Repeat steps 1 and 2 for $k = 1, \ldots, K$ giving a predicted value $\hat{Y}_i$ for all n observations

Step 4: Measure prediction accuracy, e.g.,

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2.$$

Variants

- Usually K is either 5 or 10
- $K = n$ is called "leave-one-out" cross-validation, which is great but slow
- The predictive value $\hat{Y}_i$ can be either the posterior predictive mean or median
- Mean squared error (MSE) can be replaced with Mean absolute deviation

$$\text{MAD} = \frac{1}{n} \sum_{i=1}^{n} |Y_i - \hat{Y}_i|.$$

DIC

- DIC is a popular Bayesian analog of AIC and BIC
- Unlike CV, DIC requires only one model fit to the entire dataset
- Unlike BF, it can be applied to complex models
- However, proceed with caution
- DIC really only applies when the posterior is approximately normal, and will give misleading results when the posterior far from normality, e.g. bimodal
- DIC is also criticized for selecting overly-complex models

DIC

- Recall $\text{DIC} = \bar{D} + p_D$ where
  - $\bar{D} = \text{E}(-2 \log \pi(Y \mid \theta))$ is the posterior mean of the deviance
  - p_D is the effective number of parameters
- Models with small $\bar{D}$ fit the data well
- Models with small p_D are simple
- We prefer models that are simple and fit well, so we select the model with the smallest DIC

DIC

- The effective number of parameters is a useful measure of model complexity
- Intuitively, if there are p parameters and we have uninformative priors then $p_D \approx p$
- However, $p_D << p$ if there are strong priors
- For example, how many free degrees of freedom do we have with $\theta \sim \text{Beta}(1, 1)$ versus $\theta \sim \text{Beta}(1000, 1000)$

DIC

- As with AIC or BIC, we compute DIC for all models under consideration and select the one with smallest DIC
- Rule of thumb:a difference of DIC of less than 5 is not definitive and a difference greater than 10 is substantial
- As with AIC or BIC, the actual value is meaningless, only differences are relevant

Posterior Predictive Checks

- After comparing a few models, we settle on the one that seems to fit the best
- Given this model, we then verify it is adequate
- The usual residual checks are appropriate here: qq-plots
- A uniquely Bayesian diagnostic is the posterior predictive check
- This leads to the Bayesian p-value

Posterior Predictive Distributions

- Before discussing posterior predictive checks, let's review Bayesian prediction in general
- The plug-in approach would fix the parameters θ at the posterior mean $\hat{\theta}$ and the predict $y_{\text{new}} \sim f(y \mid \hat{\theta})$
- This suppresses uncertainty in θ
- We would like to propagate this uncertainty through to the prediction

Posterior Predictive Distributions

- We really want to PPD

$$\pi(y_{\text{new}} \mid Y) = \int \pi(y_{\text{new}}, \theta \mid Y) d\theta = \int \pi(y_{\text{new}} \mid \theta) \pi(\theta \mid Y) d\theta.$$

- MCMC easily produces draws from this distribution
- To make S draws from the PPD, for each of the S MCMC draws of θ we draw a y_{new}.
- This gives draws from the PPD and clearly accounts for uncertainty in θ.

Posterior Predictive Checks

- Posterior predictive checks sample many data sets from the PPD with the identical design (same n, same X) as the original dataset
- We then define a statistic describing the dataset, e.g.,

$$d(Y) = \max\{Y_1, \ldots, Y_n\}$$

- Denote by d_0 the statistic for the original data set and by d_s the statistic from the simulated data set s.
- If the model is correct, then d_0 should fall in the middle of the $d_1, \ldots, d_S$.

Posterior Predictive Checks

- A measure of how extreme the observed data is relative to this sampling distribution is the Bayesian p-value

$$p = \sum_{s=1}^{S} I(d_s > d_0)$$

- If p is near zero or one the model does not fit

Sensitivity Analysis

- Sensitivity analysis: It is typically the case that more than one reasonable probability model can provide an adequate fit to the data in a scientific problem. The basic question of a sensitivity analysis is: how much do posterior inferences change when other reasonable probability models are used in place of the present model? Other reasonable models may differ substantially from the present model in the prior specification, the sampling distribution, or in what information is included (for example, predictor variables in a regression). It is possible that the present model provides an adequate fit to the data, but that posterior inferences differ under plausible alternative models.
- Judging model flaws by their practical implications: We do not like to ask, 'Is our model true or false?', since probability models in most data analyses will not be perfectly true. Even the coin tosses and die rolls ubiquitous in probability theory texts are not truly exchangeable. The more relevant question is, 'Do the model's deficiencies have a noticeable effect on the substantive inferences?'

Sensitivity Analysis

- External validation: We can check a model by external validation using the model to make predictions about future data.
- Posterior predictive checking: If the model fits, then replicated data generated under the model should look similar to observed data. To put it another way, the observed data should look plausible under the posterior predictive distribution. This is really a self-consistency check: an observed discrepancy can be due to model misfit or chance.
- Our basic technique for checking the fit of a model to data is to draw simulated values from the joint posterior predictive distribution of replicated data and compare these samples to the observed data. Any systematic differences between the simulations and the data indicate potential failings of the model.