Section 7

Model comparisons

Model selection

- We now have many potential models in our arsenal
- For a given dataset, how do determine whether a simple model is sufficient or if we need to bring out the "big guns"?
- Is there a "right" model? Probably not
- A **statistical model** is a mathematical representation of the system that includes errors and biases in the observation process
- All models are simplifications of reality
- We want a model that is as simple as possible yet seems to fit the data reasonably well

Outline

These notes cover Chapter 5

- For model comparisons there are a finite number of candidate models and we want to select one
  - Bayes factors
  - Stochastic search variable selection
  - Cross validation
  - Deviance information criteria (DIC)
  - Watanabe-Akaike information criteria (WAIC)
- In cases where multiple models fit well, we will discuss
  - Bayesian model averaging (BMA)
- After selecting a model, we want to test whether it fits the data well
  - Posterior predictive checks

Bayes factors (BF)

- In some sense BFs are the gold standard
- Say we are comparing two models, $\mathcal{M}_1$ and $\mathcal{M}_2$
- For example, $Y \sim \text{Binomial}(n, \theta)$ and the two models are

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

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

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

- Another example,

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

Bayes factors (BF)

- This is really the same as hypothesis testing, and in fact Bayes factors are the gold standard for hypothesis testing
- As before we proceed by computing the posterior probability of the two models
- This require priors probabilities $p(\mathcal{M}_1)$ and $p(\mathcal{M}_2)$
- This is not prior on a parameter, it is a prior on the model!
- This approach permits statements such "Given the data we have observed, the quadratic model is 5 times more likely than a linear model"

Bayes factors (BF)

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

$$BF = \frac{\text{Posterior odds}}{\text{Prior odds}} = \frac{p(\mathcal{M}_2|\mathbf{Y})/p(\mathcal{M}_1|\mathbf{Y})}{p(\mathcal{M}_2)/p(\mathcal{M}_1)} = \frac{p(\mathbf{Y}|\mathcal{M}_2)}{p(\mathbf{Y}|\mathcal{M}_1)}$$

- 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

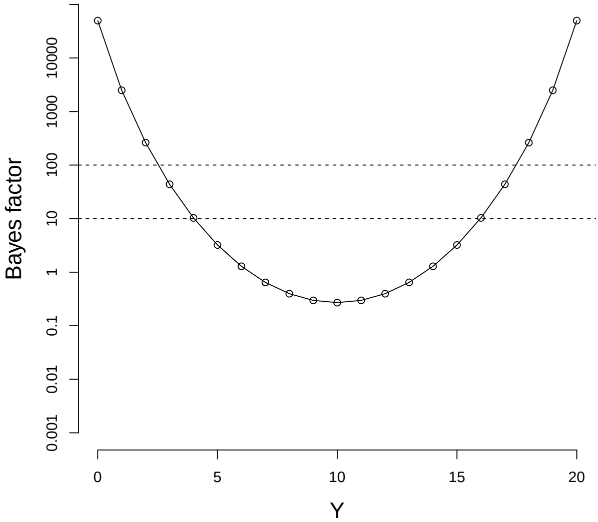
$$\mathcal{M}_1 : \theta = 0.5 \text{ and } \mathcal{M}_2 : \theta \neq 0.5$$

- $p(Y|\mathcal{M}_1)$ is just the binomial density with $\theta = 0.5$
- $\mathcal{M}_2$ involves an unknown parameter θ
- This requires a prior, say $\theta \sim \text{Beta}(a, b)$, and integration

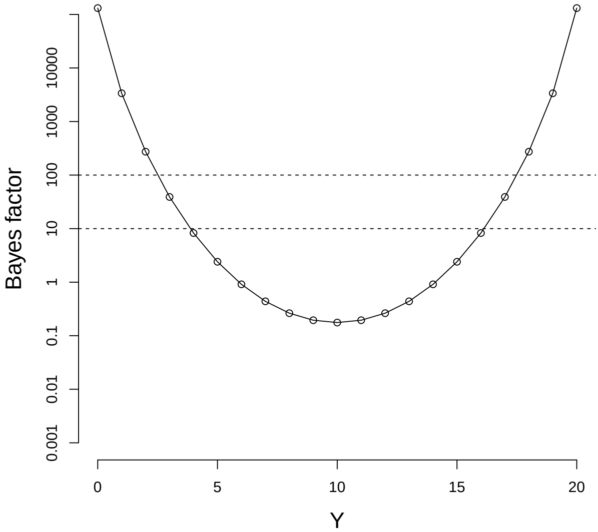
$$p(Y|\mathcal{M}_2) = \int p(Y, \theta) d\theta = \int p(Y|\theta) p(\theta) d\theta$$

- See “BF Beta-binomial” in the online derivations

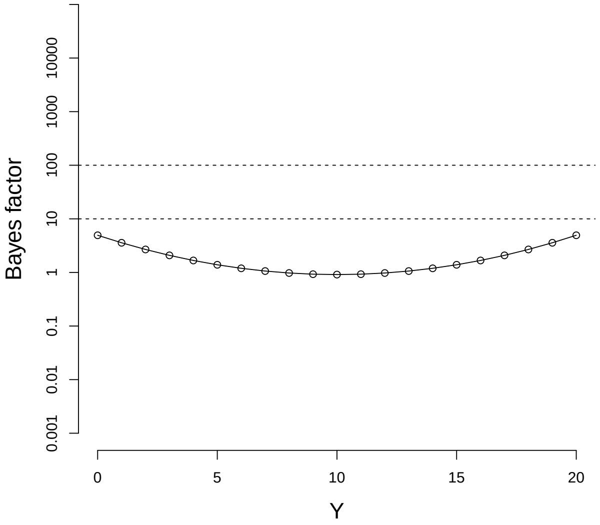
BF by Y with $n = 20$ and prior $a = 1$ and $b = 1$



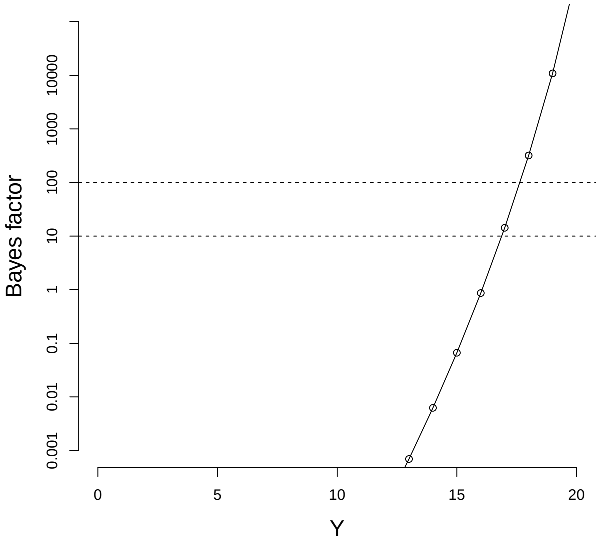
BF by Y with $n = 20$ and prior $a = 0.5$ and $b = 0.5$



BF by Y with $n = 20$ and prior $a = 50$ and $b = 50$



BF by Y with $n = 20$ and prior $a = 50$ and $b = 1$



Problems with Bayes factors

- Often hard to compute the required integrals which is only feasible for simple models
- Requires proper priors
- Can be very sensitive to priors (Lindley's paradox)
- In most cases, I prefer computing posterior intervals from the full model and testing by comparing these to the null

Computing Bayes factors using MCMC

- If models can be written as nested, then MCMC can be used to approximate model probabilities
- For example, say

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

- Both model can be written as

$$\mathrm{E}(Y) = \beta_0 + \beta_1 X + \gamma \beta_2 X^2$$

  where $\gamma \in \{0, 1\}$ indicates the model

- The prior on models becomes $\gamma \sim \text{Bernoulli}(0.5)$
- Then $\text{Prob}(\gamma = 1|\mathbf{Y}) = \text{Prob}(\mathcal{M}_2|\mathbf{Y})$ can be appoximated using MCMC

Stochastic search variable selection (SSVS)

- This is the Bayesian analog of forward/backward/stepwise variable selection
- We place a prior on all 2^p models using p variable inclusion indicators γ_j
- MCMC returns the approximate posterior probability of each model
- With large p all models will have low probability and so this requires long MCMC runs
- As with Bayesian factors, SSVS can be sensitive to priors

Model averaging

- Let's go back to the linear regression example

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

- 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

Model 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
- This is implemented in the `R` package `BMA`

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 predictions than competing models
- Advantages: Simple, intuitive, and broadly applicable
- Disadvantages: Slow because it requires several model fits and it is hard to say a difference is statistically significant

K-fold Cross validation

0 Split the data into K equally-sized groups

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

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

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

4 Measure prediction accuracy, e.g.,

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

Variants

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

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

Information criteria

- Several information criteria have been proposed that do not require fitting the model several times
- Many are functions of the **deviance**, i.e., twice the negative log likelihood

$$D(\mathbf{Y}|\theta) = -2\log[f(\mathbf{Y}|\theta)]$$

- Ideally, models will have small deviance
- However, if a model is too complex it will have small deviance between be unstable (over-fitting)
- The Akaike information criteria has a complexity penalty

$$AIC = D(\mathbf{Y}|\hat{\theta}) + 2p$$

  where $\hat{\theta}$ is the MLE
- Model with smaller *AIC* are preferred

Bayesian information criteria (BIC)

- The Bayesian information criteria is similar

$$BIC = D(\mathbf{Y}|\hat{\theta}) + \log(n)p$$

- This is motivated as an approximation to the log Bayes factor of the model compared to the null model

- However, this is only an asymptotic (large *n*) approximation

- With large *n* the prior is irrelevant, and so this is not satisfying to a subjective Bayesian

Deviance information criteria (DIC)

- *DIC* is a popular Bayesian analog of *AIC* or *BIC*
- Unlike CV, *DIC* requires only one model fit
- 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

Deviance information criteria (DIC)

- Let $\bar{D} = \mathrm{E}[D(Y|\theta)|\mathbf{Y}]$ be the posterior mean of the deviance
- Denote $\hat{\theta}$ as the posterior mean of θ
- The effective number of parameters is

$$p_D = \bar{D} - D(\mathbf{Y}|\hat{\theta})$$

- DIC can be written like AIC,

$$DIC = \bar{D} + p_D = D(\mathbf{Y}|\hat{\theta}) + 2p_D$$

- 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 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 $\theta \sim \text{Beta}(1000, 1000)$?
- In some cases p_D has a nice closed form
- A few examples are worked out in "DIC" on the online derivations

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
- *DIC* can only be used to compare models with the same likelihood

Watanabe-Akaike information criteria (WAIC)

- *WAIC* is an alternative to *DIC*
- It is motivated as an approximation to leave-one-out CV
- In the end *WAIC* has model-fit and model-complexity components
- It is used the same as *DIC* with smaller *WAIC* begin preferred
- In practice the two often give similar results, but *WAIC* is arguably more theoretically justified

Watanabe-Akaike information criteria (WAIC)

- *WAIC* is written in terms of the posterior of the likelihood rather than parameters
- Let m_i and v_i be the posterior mean and variance of
$$\log[f(Y_i|\theta)]$$
- The effective model size is $p_W = \sum_{i=1}^n v_i$
- The criteria is
$$WAIC = -2\sum_{i=1}^n m_i + 2p_W$$

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; added variable plots; etc.
- 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 then predict $Y_{new} \sim f(y|\hat{\theta})$
- This suppresses uncertainty in θ
- We would like to propagate this uncertainty through to the predictions

Posterior predictive distributions (PPD)

- We really want the PPD

$$f(Y_{new}|\mathbf{Y}) = \int f(Y_{new}, \theta|\mathbf{y})d\theta = \int f(Y_{new}|\theta)f(\theta|\mathbf{y})d\theta$$

- 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 datasets from the PPD with the identical design (same n, same $\mathbf{X}$) as the original data set

- We then define a statistic describing the dataset, e.g.,

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

- Denote the statistic for the original data set as d_0 and the statistic from simulated data set number s as d_s

- If the model is correct, then d_0 should fall in the middle of the $d_1, ..., d_S$

Posterior predictive checks

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

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

- If p is near zero or one the model doesn't fit

- This is repeated for several d to give a comprehensive evaluation of model fit