

# 6: Model Checking

Taylor

University of Virginia

# Introduction

Now we finally admit some of the uncertainty we have about our choices of likelihood and prior distribution. Instead of asking “is our model true,” we ask “are our inferences being substantially affected by the model’s deficiencies?”

We are either making inferences on unobservable  $\theta$  with  $p(\theta | y)$ , or \*potentially\* observable data with  $p(\tilde{y} | y)$ . This means it’s generally easier to check inferences on the latter!

# Notation Clarification

There is now a difference between  $y^{\text{rep}}$  and  $\tilde{y}$ !

- ①  $y$ : the data we have observed and have made inferences using
- ②  $y^{\text{rep}}$ : data simulated from the posterior predictive distribution (ppd)
- ③  $\tilde{y}$ : actual future data, possibly coming from the true model we aren't using
- ④  $p(y^{\text{rep}} \mid y)$  our “working” ppd that we are examining and are unsure about

# External Validation

The gold standard for evaluating the posterior predictive distribution is **external validation**, which is when you compare actual future data  $\tilde{y}$  with your predictions coming from  $p(y^{\text{rep}} \mid y)$ .

In general, we might want to predict  $T(\tilde{y})$ , where  $T$  is some arbitrary test function of a new data (set)  $\tilde{y}$ .

In a time series context: predict, wait for new data to arrive, compare.

In a non-time series context: predict, wait for new data to be collected, compare.

# Posterior Predictive Checks

When we can't/won't wait for new data to arrive, we can use our existing data set  $y$  by calculating a **posterior predictive p-value**  $p_B$ .

$$p_B = P(T(y^{\text{rep}}) > T(y) \mid y) = \int_{\{T(y^{\text{rep}}): T(y^{\text{rep}}) > T(y)\}} p(y^{\text{rep}} \mid y) dy^{\text{rep}}.$$

- ① if  $p_B = .5$ , the median of  $p(T(y^{\text{rep}}) \mid y)$  is exactly equal to  $T(y)$ .
- ② if  $p_B > .5$ , the median of  $p(T(y^{\text{rep}}) \mid y)$  is greater than  $T(y)$ .
- ③ if  $p_B < .5$ , the median of  $p(T(y^{\text{rep}}) \mid y)$  is less than  $T(y)$

# Posterior Predictive Checks

$p_B = .5$  does not prove your model is good!

- ① Maybe you're overfitting. Remember, you're using the data twice.
- ② Maybe you're using an "easy" test function (e.g. a sufficient statistic).
- ③ Maybe it does poorly for other test functions.

We can extend this a bit further:

$$p_B = P(T(y^{\text{rep}}, \theta) > T(y, \theta) \mid y) = \iint_A p(y^{\text{rep}}, \theta \mid y) dy^{\text{rep}} d\theta$$

where  $A = \{T(y^{\text{rep}}, \theta) : T(y^{\text{rep}}, \theta) > T(y, \theta)\}$

# Posterior Predictive Checks

When we can't/won't evaluate this integral, we can use Monte Carlo!

$$\begin{aligned} p_B &= \iint_A p(y^{\text{rep}}, \theta \mid y) dy^{\text{rep}} d\theta \\ &= E[\mathbf{1}((y^{\text{rep}}, \theta) \in A) \mid y] \\ &\leftarrow S^{-1} \sum_{i=1}^S \mathbf{1}((y^{i,\text{rep}}, \theta^i) \in A) \end{aligned}$$

where

If we can't simulate directly from the ppd, then we can do the following.

For  $i = 1, \dots, S$

- ① Simulate  $\theta^i \sim p(\theta \mid y)$
- ② Simulate  $y^{i,\text{rep}} \sim p(y \mid \theta^i)$
- ③ Count up the number of times  $(y^{i,\text{rep}}, \theta^i) \in A$
- ④ Divide that number by  $S$



NB: I try to use superscripts for draws, and subscripts for indexes in a particular data set.

Example:  $y^{i,\text{rep}}$  is the  $i$ th replicated data set

Example:  $y_i$  is the  $i$ th element of one data set

# Example: Speed of Light Measurements

A histogram of real/observed/historical  $y$

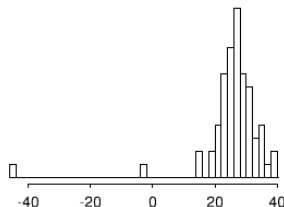


Figure 3.1 *Histogram of Simon Newcomb's measurements for estimating the speed of light, from Stigler (1977). The data are recorded as deviations from 24,800 nanoseconds.*

# Example: Speed of Light Measurements

- ①  $y$ : 66 univariate measurements
- ②  $p(y \mid \mu, \sigma^2) = \prod_{i=1}^{66} \text{Normal}(y_i \mid \mu, \sigma^2)$
- ③  $p(\mu, \sigma^2) \propto \sigma^{-2}$
- ④  $j = 1, \dots, 20$  simulations
- ⑤ each  $y^{i,\text{rep}}$  is a data set of size 66 simulated from the ppd

# Example: Speed of Light Measurements

Let's simulate a data set  $y^{\text{rep}} \sim p(y^{\text{rep}} | y)$

Recall from chapter 3:

$$y_i^{\text{rep}} | y \sim t_{n-1}(\bar{y}, s^2(1 + 1/n)).$$

```
n <- length(y)
s <- sd(y)
my <- mean(y)
sampt20 <- replicate(20, rt(n, n-1)*sqrt(1+1/n)*s+my) %>%
  as.data.frame()
dim(sampt20)
[1]    66 20
```

http:

[//avehtari.github.io/BDA\\_R\\_demos/demos\\_ch6/demo6\\_1.html](https://avehtari.github.io/BDA_R_demos/demos_ch6/demo6_1.html)

# Example: Speed of Light Measurements

Each one of these simulated data sets produces one univariate  $T(y^{\text{rep}})$

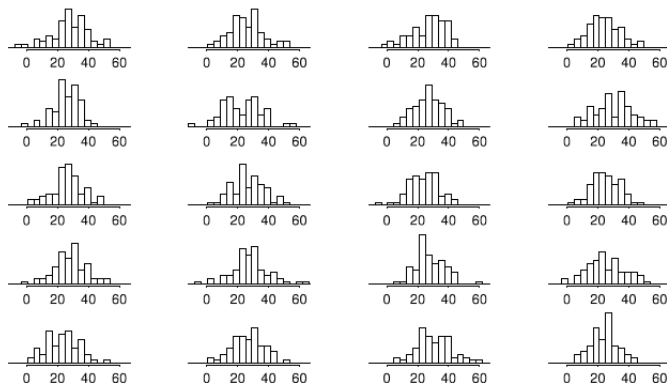


Figure 6.2 *Twenty replications,  $y^{\text{rep}}$ , of the speed of light data from the posterior predictive distribution,  $p(y^{\text{rep}}|y)$ ; compare to observed data,  $y$ , in Figure 3.1. Each histogram displays the result of drawing 66 independent values  $\tilde{y}_i$  from a common normal distribution with mean and variance  $(\mu, \sigma^2)$  drawn from the posterior distribution,  $p(\mu, \sigma^2|y)$ , under the normal model.*

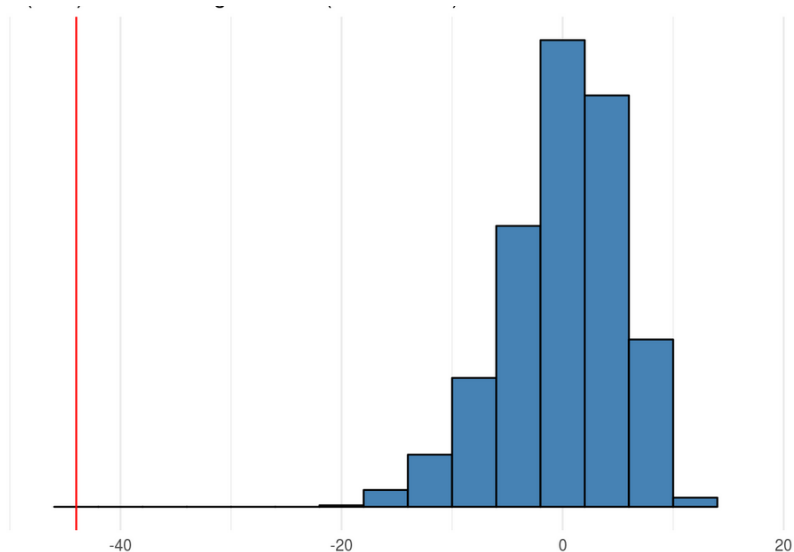
## Example: Speed of Light Measurements

Let  $T(y^{j,\text{rep}}) = \min(y_1^{j,\text{rep}}, \dots, y_n^{j,\text{rep}})$  and  $T(y) = \min(y_1, \dots, y_n)$ . Then

$$P(T(y^{\text{rep}}) > T(y) \mid y) \approx 1000^{-1} \sum_{j=1}^{1000} \mathbf{1}(T(y^{j,\text{rep}}) > T(y))$$

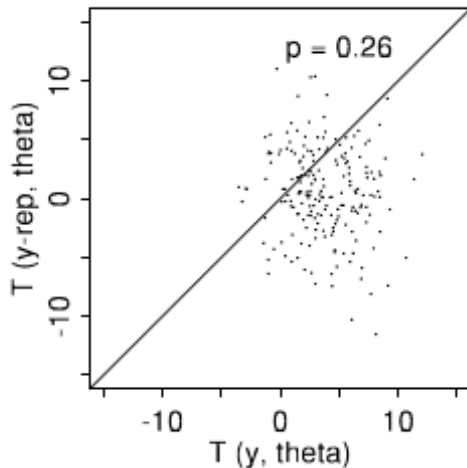
```
sampt1000 <- replicate(1000, rt(n, n-1)*sqrt(1+1/n)*s+my) %>%  
  as.data.frame()  
mean(sapply(sampt1000, min) > min(y))  
[1] 1
```

# Example: Speed of Light Measurements



## Example: Speed of Light Measurements

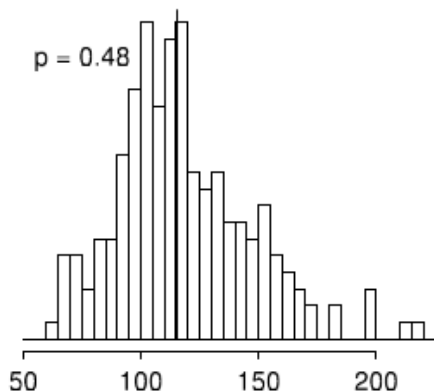
Let  $T(y, \theta) = |y_{(61)} - \theta| - |y_{(6)} - \theta|$





# Example: Speed of Light Measurements

Let  $T(y) = (n - 1)^{-1} \sum_{i=1}^n (y_i - \bar{y})^2$



Bayesian sufficiency implies “predictive sufficiency”

$$P(T(y^{\text{rep}}) > T(y) \mid y) = P(T(y^{\text{rep}}) > T(y) \mid \bar{y}, T(y))$$

## Example 2: Are our Bernoulli rvs Correlated?

From chapter 2:

- 1  $y_1, \dots, y_n \mid \theta \stackrel{\text{iid}}{\sim} \text{Bernoulli}(\theta)$
- 2  $\theta \sim \text{Uniform}(0, 1)$
- 3  $\theta \mid y \sim \text{Beta}(\sum_i y_i + 1, n - \sum_i y_i + 1)$

## Example 2: Are our Bernoulli rvs Correlated?

From chapter 2:

- 1  $y_1, \dots, y_n \mid \theta \stackrel{\text{iid}}{\sim} \text{Bernoulli}(\theta)$
- 2  $\theta \sim \text{Uniform}(0, 1)$
- 3  $\theta \mid y \sim \text{Beta}(\sum_i y_i + 1, n - \sum_i y_i + 1)$

$$y = (1, 1, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0)$$

## Example 2: Are our Bernoulli rvs Correlated?

From chapter 2:

- 1  $y_1, \dots, y_n \mid \theta \stackrel{\text{iid}}{\sim} \text{Bernoulli}(\theta)$
- 2  $\theta \sim \text{Uniform}(0, 1)$
- 3  $\theta \mid y \sim \text{Beta}(\sum_i y_i + 1, n - \sum_i y_i + 1)$

$$y = (1, 1, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 0)$$

Let  $T(y^{\text{rep}}) = \sum_{i=2}^n |y_i^{\text{rep}} - y_{i-1}^{\text{rep}}|$  be the number of switches.  
Note that  $T(y) = 3$

## Example 2: Are our Bernoulli rvs Correlated?

Problem:  $p(y^{\text{rep}} \mid y)$  is not closed-form.

For  $i = 1, \dots, 10^4$ :

- 1 draw  $\theta^i \sim p(\theta \mid y)$
- 2 draw  $y^{i,\text{rep}} \sim p(y \mid \theta^i) = \prod_{j=1}^n \text{Bernoulli}(\theta)$
- 3 return  $T(y^{\text{rep}})$

## Example 2: Are our Bernoulli rvs Correlated?

Problem:  $p(y^{\text{rep}} | y)$  is not closed-form.

For  $i = 1, \dots, 10^4$ :

- 1 draw  $\theta^i \sim p(\theta | y)$
- 2 draw  $y^{i,\text{rep}} \sim p(y | \theta^i) = \prod_{j=1}^n \text{Bernoulli}(\theta)$
- 3 return  $T(y^{\text{rep}})$

```
n <- length(y)
s <- sum(y)
rb <- function(s, n) {
  p <- rbeta(1, s+1, n-s+1)
  yr <- rbinom(n, 1, p)
  sum(diff(yr) != 0) + 0.0
}
Tyr <- data.frame(x = replicate(10000, rb(s, n)))
```

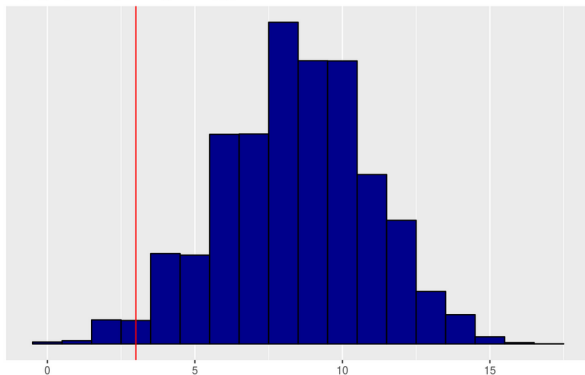
http:

[//avehtari.github.io/BDA\\_R\\_demos/demos\\_ch6/demo6\\_2.html](http://avehtari.github.io/BDA_R_demos/demos_ch6/demo6_2.html)

## Example 2: Are our Bernoulli rvs Correlated?

$$P(T(y^{\text{rep}}) > T(y) \mid y) \approx .97$$

Binomial example - number of changes?  
 $\Pr(T(y^{\text{rep}}, \theta) \leq T(y, \theta) \mid y) = 0.03$



# p-values and u-values

If  $\theta$  is perfectly estimated,

$$P(T(y^{\text{rep}}) > T(y) \mid y) = P(T(y^{\text{rep}}) > T(y) \mid \theta, y) \sim \text{Uniform}(0, 1)$$

This is related to the “CDF transformation.” For  $X, \tilde{X} \mid \theta \stackrel{\text{iid}}{\sim} F$ :

$$F_X(X) = P(X \leq x \mid \tilde{X} = x, \theta) \sim \text{Uniform}(0, 1)$$

In our case, they are saying that

$$P(T(y^{\text{rep}}) > T(y) \mid y) = P(T(y^{\text{rep}}) > T(y) \mid \theta, y),$$

or in other words

$$P(T(y^{\text{rep}}) \leq T(y) \mid y) = P(T(y^{\text{rep}}) \leq T(y) \mid \theta, y)$$



They say, generally  $P(T(y^{\text{rep}}) \leq T(y) \mid \theta, y)$  is “stochastically more variable” than  $P(T(y^{\text{rep}}) \leq T(y) \mid y)$ .

One thing the authors \*could\* mean is that these conditional probabilities are **convex ordered**.

Random variables  $X$  and  $Y$  are convex-ordered if, for any convex function  $u$ ,

$$E[u(X)] \leq E[u(Y)].$$

Conditional probabilities are convex ordered when one conditions on less than another (homework question).

# A Nice Graphic (the old book cover)

The next slide's picture plots predictions and real data from a psychological study.

$y = \{y_{i,j,k}\}$  is an array of binary variables, with

- ①  $i = 1, \dots, 6$  denoting the person
- ②  $j = 1, \dots, 15$  denoting which reaction (which row)
- ③  $k = 1, \dots, 23$  situation (which column)

# A Nice Graphic (the old book cover)

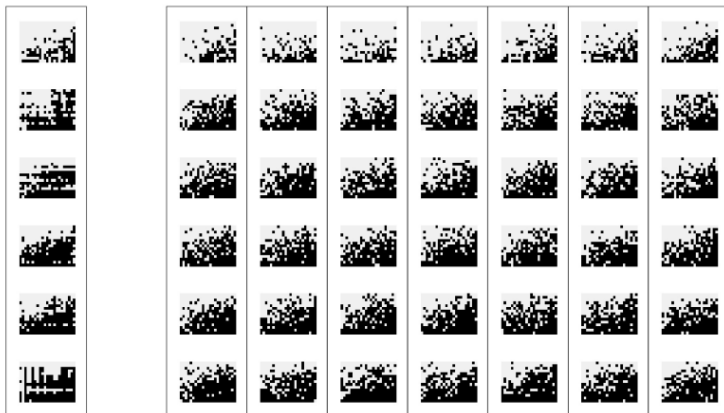


Figure 6.7 Left column displays observed data  $y$  (a  $15 \times 23$  array of binary responses from each of 6 persons); right columns display seven replicated datasets  $y^{\text{rep}}$  from a fitted logistic regression model. A misfit of model to data is apparent: the data show strong row and column patterns for individual persons (for example, the nearly white row near the middle of the last person's data) that do not appear in the replicates. (To make such patterns clearer, the indexes of the observed and each replicated dataset have been arranged in increasing order of average response.)

## Without Sorting

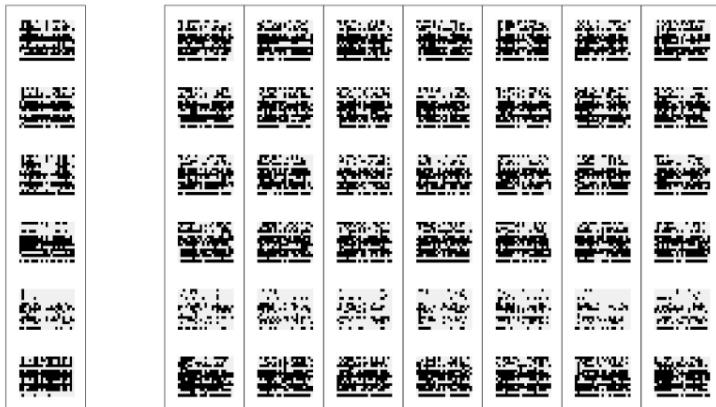


Figure 6.8 Redisplay of Figure 6.7 without ordering the rows, columns, and persons in order of increasing response. Once again, the left column shows the observed data and the right columns show replicated datasets from the model. Without the ordering, it is difficult to notice the discrepancies between data and model, which are easily apparent in Figure 6.7.