

# PREDICTIVE INFERENCE TOOLS FOR RESEARCHERS

by

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# Contents

<b>1</b>	<b>Thesis Abstract</b>	<b>4</b>
<b>2</b>	<b>Introduction: Predictive Inference</b>	<b>5</b>
2.1	Why is predictive inference important? . . . . .	5
2.2	Difference between parametric inference and predictive inference . . . . .	5
2.2.1	When is predictive inference more useful? . . . . .	5
2.2.2	When is parametric inference more useful? . . . . .	5
2.3	The Bayesian Parametric Prediction Format . . . . .	5
2.4	[Maybe] Example of Difference between results from Plug-in estimator and results using Predictive Inference . . . . .	5
<b>3</b>	<b>Chapter 1: Predictive Problems with Conjugate Priors</b>	<b>6</b>
3.1	Prediction of Future Successes: Beta-Binomial (Geisser p. 73) . . . . .	6
3.1.1	Derivation . . . . .	6
3.1.2	R Implementation . . . . .	7
3.1.3	Example . . . . .	7
3.2	Survival Time: Exponential-Gamma (Geisser p. 74) . . . . .	7
3.2.1	Derivation . . . . .	7
3.2.2	R Implementation . . . . .	9
3.2.3	Example . . . . .	9
3.3	Poisson-Gamma Model (Hoff p. 43ff) . . . . .	11
3.3.1	Derivation . . . . .	11
3.3.2	R Implementation . . . . .	15
3.3.3	Example . . . . .	15
3.4	Normal Observation with Normal-Inverse Gamma Prior . . . . .	15
3.4.1	One sample . . . . .	15
3.4.1.1	Derivation . . . . .	15
3.4.1.2	R Implementation . . . . .	15
3.4.1.3	Example . . . . .	15
3.4.2	Two samples . . . . .	15
3.4.2.1	Derivation . . . . .	15
3.4.2.2	R Implementation . . . . .	15
3.4.2.3	Example . . . . .	15
3.4.3	$k$ samples . . . . .	16
3.4.3.1	Derivation . . . . .	16
3.4.3.2	R Implementation . . . . .	16
3.4.3.3	Example . . . . .	16
3.4.3.4	Ranking Treatments . . . . .	16
<b>4</b>	<b>Chapter 2: Normal Regression with Zellner's <math>g</math>-prior</b>	<b>17</b>
4.0.0.1	Derivation . . . . .	17
4.0.0.2	R Implementation . . . . .	17
4.0.0.3	Example . . . . .	17
<b>5</b>	<b>Conclusion</b>	<b>18</b>

# 1 Thesis Abstract

- (paragraph) Statement of the thesis topic and objectives
- (paragraph) Explanation of R package

## 2 Introduction: Predictive Inference

### 2.1 Why is predictive inference important?

### 2.2 Difference between parametric inference and predictive inference

#### 2.2.1 When is predictive inference more useful?

#### 2.2.2 When is parametric inference more useful?

[examples, comparisons]

### 2.3 The Bayesian Parametric Prediction Format

[Geisser p. 49]

Let

$$f(x^{(N)}, x_{(M)} | \theta) = f(x_{(M)} | x^{(N)}, \theta) f(x^{(N)} | \theta).$$

Here  $x^{(N)}$  represents observed events and  $x_{(M)}$  are future events. We calculate

$$f(x_{(M)}, x^{(N)}) = \int f(x^{(N)}, x_{(M)} | \theta) p(\theta) d\theta$$

where  $p(\theta)$  is the prior density and

$$f(x_{(M)} | x^{(N)}) = \frac{f(x_{(M)}, x^{(N)})}{f(x^{(N)})} = \int f(x_{(M)} | \theta) p(\theta | x^{(N)}) d\theta$$

where

$$p(\theta | x^{(N)}) \propto f(x^{(N)} | \theta) p(\theta).$$

### 2.4 [Maybe] Example of Difference between results from Plug-in estimator and results using Predictive Inference

### 3 Chapter 1: Predictive Problems with Conjugate Priors

[Problems with closed-form solutions. These problems will be what the R package is designed for. Use problems from Geisser, Casella & Berger (Bayesian chapter), other sources. Regression problem—predictive distributions of models that include and exclude some predictor]

#### 3.1 Prediction of Future Successes: Beta-Binomial (Geisser p. 73)

##### 3.1.1 Derivation

Let  $X_i$  be independent binary variables with  $\Pr(X_i = 1) = \theta$ , and let  $T = \sum X_i$ . Then  $T$  has probability

$$\binom{N}{t} \theta^t (1 - \theta)^{N-t}.$$

Assume  $\theta \sim \text{Beta}(\alpha, \beta)$ , so

$$p(\theta) = \frac{\Gamma(\alpha + \beta) \theta^{\alpha-1} (1 - \theta)^{\beta-1}}{\Gamma(\alpha) \Gamma(\beta)}.$$

Then

$$p(\theta | X^{(N)}) = \frac{\Gamma(N + \alpha + \beta) \theta^{t+\alpha-1} (1 - \theta)^{N-t+\beta-1}}{\Gamma(t + \alpha) \Gamma(N - t + \beta)}$$

So for  $R = \sum_{i=1}^M X_{N+i}$  we have Beta-Binomial predictive distribution

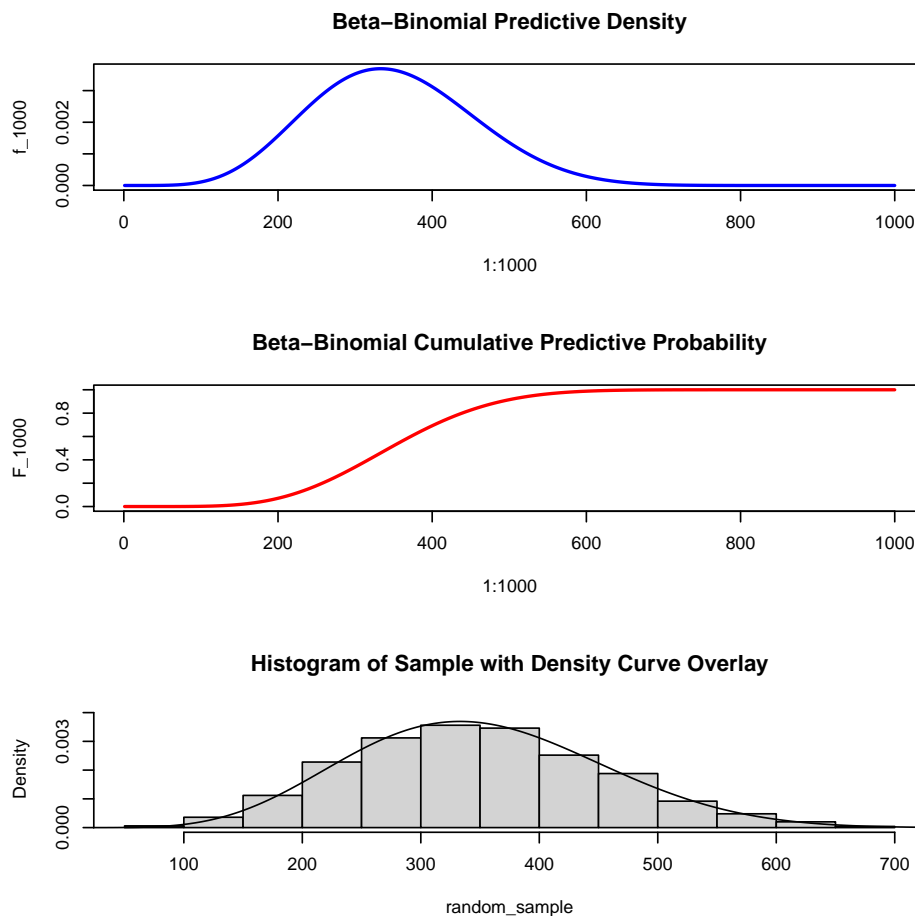
$$\begin{aligned} \Pr[R = r | t] &= \int \binom{M}{r} \theta^r (1 - \theta)^{M-r} p(\theta | X^{(N)}) d\theta \\ &= \binom{M}{r} \int \theta^r (1 - \theta)^{M-r} \frac{\Gamma(N + \alpha + \beta)}{\Gamma(t + \alpha) \Gamma(N - t + \beta)} \theta^{t+\alpha-1} (1 - \theta)^{N-t+\beta-1} d\theta \\ &= \frac{M!}{r!(M-r)!} \frac{\Gamma(N + \alpha + \beta)}{\Gamma(t + \alpha) \Gamma(N - t + \beta)} \int \theta^{r+t+\alpha-1} (1 - \theta)^{M-r+N-t+\beta-1} d\theta \\ &= \frac{\Gamma(M+1) \Gamma(N + \alpha + \beta) \Gamma(r+t+\alpha) \Gamma(M-r+N-t+\beta)}{\Gamma(r+1) \Gamma(M-r+1) \Gamma(t+\alpha) \Gamma(N-t+\beta) \Gamma(M+N+\alpha+\beta)} \end{aligned}$$

### 3.1.2 R Implementation

This result has been used to create “standard” R functions `dpredBB()`, `ppredBB()`, and `rpredBB()` for the Beta-Binomial distribution for density, cumulative probability, and random sampling, respectively (see appendix). These functions are exercised in the following example.

### 3.1.3 Example

Suppose  $t = 5$  successes have been observed out of  $N = 10$  binary events,  $\alpha = 2$  and  $\beta = 8$ . For  $M = 1000$  future observations, the figures below show the predictive distribution from `dpredBB()`, the cumulative distribution from `ppredBB()`, and a histogram of random draws from `rpredBB()`.



## 3.2 Survival Time: Exponential-Gamma (Geisser p. 74)

### 3.2.1 Derivation

Suppose  $X^{(N)} = (X^{(d)}, X^{(N-d)})$  where  $X^{(d)}$  represents copies fully observed from an exponential survival time density

$$f(x|\theta) = \theta e^{-\theta x}$$

and  $X^{(N-d)}$  represents copies censored at  $x_{d+1}, \dots, x_N$ , respectively. Hence

$$L(\theta) \propto \theta^d e^{-\theta N\bar{x}}$$

when  $N\bar{x} = \sum_{i=1}^N x_i$ , as shown below.

The usual exponential likelihood is used for the fully observed copies, whereas for the censored copies we need  $\Pr(x > \theta) = 1 - \Pr(x \leq \theta) = 1 - F(x|\theta) = 1 - (1 - e^{-\theta x}) = e^{-\theta x}$ . Thus the overall likelihood is

$$L(\theta|x) = \prod_{i=1}^d \theta e^{-\theta x_i} \prod_{i=d+1}^N e^{-\theta x_i} = \theta^d e^{-\theta N\bar{x}}$$

Assuming a Gamma( $\delta, \gamma$ ) prior for  $\theta$ ,

$$p(\theta) = \frac{\gamma^\delta \theta^{\delta-1} e^{-\gamma\theta}}{\Gamma(\delta)}$$

we obtain the posterior

$$\begin{aligned} p(\theta|X^{(N)}) &= \frac{p(x^{(N)}|\theta) p(\theta)}{\int p(X^{(N)}|\theta) p(\theta) d\theta} \\ &= \frac{\theta^d e^{-\theta N\bar{x}} \cdot \frac{\gamma^\delta \theta^{\delta-1} e^{-\gamma\theta}}{\Gamma(\delta)}}{\int \left( \theta^d e^{-\theta N\bar{x}} \cdot \frac{\gamma^\delta \theta^{\delta-1} e^{-\gamma\theta}}{\Gamma(\delta)} \right) d\theta} \\ &= \frac{\cancel{\frac{\gamma^\delta}{\Gamma(\delta)}} (\theta^{d+\delta-1} e^{-\theta(\gamma+N\bar{x})})}{\cancel{\frac{\gamma^\delta}{\Gamma(\delta)}} \int (\theta^{d+\delta-1} e^{-\theta(\gamma+N\bar{x})}) d\theta} \\ &= \frac{\frac{(\gamma+N\bar{x})^{d+\delta}}{\Gamma(d+\delta)} (\theta^{d+\delta-1} e^{-\theta(\gamma+N\bar{x})})}{\cancel{\frac{(\gamma+N\bar{x})^{d+\delta}}{\Gamma(d+\delta)}} \int \cancel{(\theta^{d+\delta-1} e^{-\theta(\gamma+N\bar{x})})} d\theta} \\ &= \frac{(\gamma+N\bar{x})^{d+\delta} \theta^{d+\delta-1} e^{-\theta(\gamma+N\bar{x})}}{\Gamma(d+\delta)} \end{aligned}$$

with the Gamma( $d+\delta, \gamma+N\bar{x}$ ) density in the next to last step integrating to 1.

Thus the survival time predictive probability is



$$\begin{aligned}
P(X = x|\theta, X^{(N)}) &= \int p(\theta|X^{(N)}) p(x|\theta) d\theta \\
&= \int \frac{(\gamma + N\bar{x})^{d+\delta} \theta^{d+\delta-1} e^{-\theta(\gamma+N\bar{x})}}{\Gamma(d+\delta)} \cdot \theta e^{-\theta x} d\theta \\
&= (d+\delta)(\gamma + N\bar{x})^{d+\delta} \int \frac{\theta^{(d+\delta+1)-1} e^{-\theta(\gamma+N\bar{x}+x)}}{(d+\delta)\Gamma(d+\delta)} d\theta \\
&= \frac{(d+\delta)(\gamma + N\bar{x})^{d+\delta}}{(\gamma + N\bar{x} + x)^{d+\delta+1}} \int \frac{(\gamma + N\bar{x} + x)^{d+\delta+1} \theta^{(d+\delta+1)-1} e^{-\theta(\gamma+N\bar{x}+x)}}{\Gamma(d+\delta+1)} d\theta \\
&= \frac{(d+\delta)(\gamma + N\bar{x})^{d+\delta}}{(\gamma + N\bar{x} + x)^{d+\delta+1}}
\end{aligned}$$

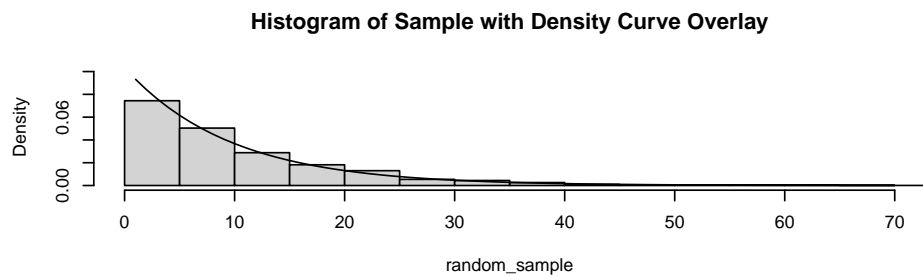
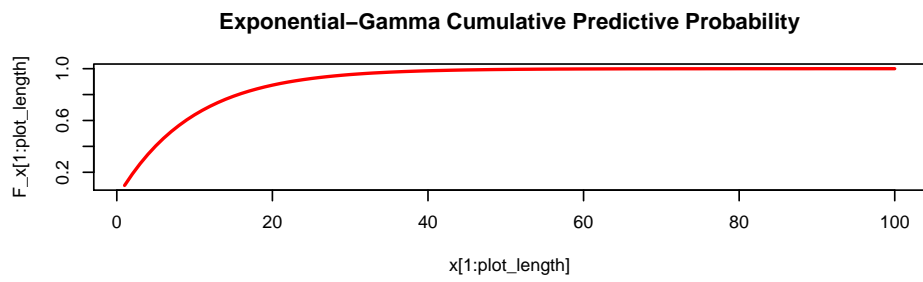
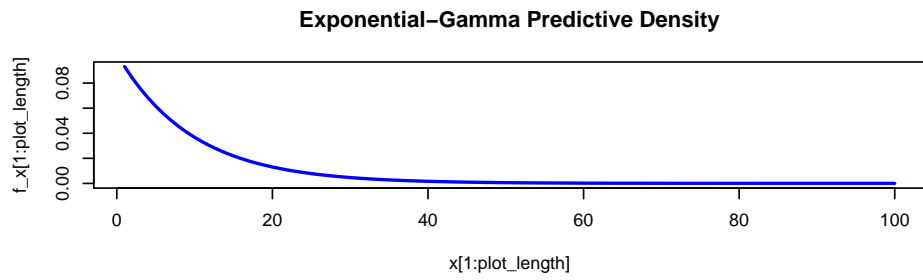
(simplifying by constructing a  $\text{Gamma}(d + \delta + 1, \gamma + N\bar{x} + x)$  density in the final integrand.)

### 3.2.2 R Implementation

This result has been used to create standard format R functions `dpredEG()`, `ppredEG()`, and `rpredEG()` for the Gamma-Exponential distribution for density, cumulative probability, and random sampling, respectively (see appendix). These functions are exercised in the following example.

### 3.2.3 Example

Suppose  $d = 800$  out of  $N = 1000$  copies have been observed, and the remaining 200 censored. Say  $\delta = 20$ ,  $\gamma = 5$ , and we are interested in the number of survivors out of  $M = 1000$  future observations. The figures below illustrate the predictive probability using `dpredEG()` and `rpredEG()`, along with a histogram of a random sample taken using `rpredEG()`.



### 3.3 Poisson-Gamma Model (Hoff p. 43ff)

#### 3.3.1 Derivation

[using Hoff's notation and variable names below. Should I convert this to Geisser's  $x^{(N)}, x_{(M)}$  convention for uniformity throughout my thesis?]

Suppose  $Y_1, \dots, Y_n | \theta \stackrel{i.i.d.}{\sim} \text{Poisson}(\theta)$  with Gamma prior  $\theta \sim \text{Gamma}(\alpha, \beta)$ . That is,

$$\begin{aligned} P(Y_1 = y_1, \dots, Y_n = y_n | \theta) &= \prod_{i=1}^n p(y_i | \theta) \\ &= \prod_{i=1}^n \frac{1}{y_i!} \theta^{y_i} e^{-\theta} \\ &= \left( \prod_{i=1}^n \frac{1}{y_i!} \right) \theta^{\sum y_i} e^{-n\theta} \\ &= c(y_1, \dots, y_n) \theta^{\sum y_i} e^{-n\theta} \end{aligned}$$

and

$$p(\theta) = \frac{\beta^\alpha}{\Gamma(\alpha)} \theta^{\alpha-1} e^{-\beta\theta}, \theta, \alpha, \beta > 0.$$

Then we have posterior distribution

$$\begin{aligned} p(\theta | y_1, \dots, y_n) &= \frac{p(y_1, \dots, y_n | \theta) p(\theta)}{\int_{\theta} p(y_1, \dots, y_n | \theta) p(\theta)} \\ &= \frac{p(y_1, \dots, y_n | \theta) p(\theta)}{p(y_1, \dots, y_n)} \\ &= \frac{1}{p(y_1, \dots, y_n)} \theta^{\sum y_i} e^{-n\theta} \frac{\beta^\alpha}{\Gamma(\alpha)} \theta^{\alpha-1} e^{-\beta\theta} \\ &= C(y_1, \dots, y_n, \alpha, \beta) \theta^{\alpha + \sum y_i - 1} e^{-(\beta + n)\theta} \\ &\sim \text{Gamma}\left(\alpha + \sum y_i, \beta + n\right). \end{aligned}$$

Here

$$\begin{aligned}
C(y_1, \dots, y_n, \alpha, \beta) &= \frac{1}{p(y_1, \dots, y_n)} \cdot \frac{\beta^\alpha}{\Gamma(\alpha)} \\
&= \frac{1}{\int_\theta p(y_1, \dots, y_n | \theta) p(\theta)} \cdot \frac{\beta^\alpha}{\Gamma(\alpha)} \\
&= \frac{1}{\int_\theta \left( \prod \frac{1}{y_i!} \right) \theta^{\sum y_i} e^{-n\theta} \left( \frac{\beta^\alpha}{\Gamma(\alpha)} \right) \theta^{\alpha-1} e^{-\beta\theta} \cancel{\left( \frac{\beta^\alpha}{\Gamma(\alpha)} \right)}} \cdot \left( \frac{\beta^\alpha}{\Gamma(\alpha)} \right) \\
&= \frac{1}{\left( \prod \frac{1}{y_i!} \right) \frac{\Gamma(\alpha + \sum y_i)}{(\beta + n)^{\alpha + \sum y_i}} \int_\theta \frac{(\beta + n)^{\alpha + \sum y_i}}{\Gamma(\alpha + \sum y_i)} \theta^{\sum y_i + \alpha - 1} e^{-(\beta + n)\theta}} \\
&= \frac{\prod_{i=1}^n y_i! (\beta + n)^{\alpha + \sum y_i}}{\Gamma(\alpha + \sum y_i)}
\end{aligned}$$

Call this constant  $C_n$  (for  $n$  observations).

Note that an additional observation  $y_{n+1} = \tilde{y}$  the constant becomes

$$C_{n+1} = \frac{\prod_{i=1}^{n+1} y_i! (\beta + n + 1)^{\alpha + \sum_{i=1}^{n+1} y_i}}{\Gamma(\alpha + \sum_{i=1}^{n+1} y_i)}.$$

Also note that the marginal joint distribution of  $k$  observations is

$$p(\tilde{y} | y_1, \dots, y_k) = \frac{1}{C_k} \frac{\beta^\alpha}{\Gamma(\alpha)}.$$

For future observation  $\tilde{y}$ , then, we compute predictive distribution

$$\begin{aligned}
p(\tilde{y}|y_1, \dots, y_n) &= \frac{p(y_1, \dots, y_n, \tilde{y})}{p(y_1, \dots, y_n)} = \frac{p(y_1, \dots, y_{n+1})}{p(y_1, \dots, y_n)} = \frac{\frac{1}{C_{n+1}} \frac{\beta^\alpha}{\Gamma(\alpha)}}{\frac{1}{C_n} \frac{\beta^\alpha}{\Gamma(\alpha)}} = \frac{C_n}{C_{n+1}} \\
&= \frac{\frac{\prod_{i=1}^n y_i! (\beta + n)^{\alpha + \sum_{i=1}^n y_i}}{\Gamma(\alpha + \sum_{i=1}^n y_i)}}{\frac{\prod_{i=1}^{n+1} y_i! (\beta + n + 1)^{\alpha + \sum_{i=1}^{n+1} y_i}}{\Gamma(\alpha + \sum_{i=1}^{n+1} y_i)}} \\
&= \frac{\Gamma(\alpha + \sum_{i=1}^{n+1} y_i) (\beta + n)^{\alpha + \sum_{i=1}^n y_i}}{(y_{n+1}!) \Gamma(\alpha + \sum_{i=1}^n y_i) (\beta + n + 1)^{\alpha + \sum_{i=1}^{n+1} y_i}} \\
&= \frac{\Gamma(\alpha + \sum_{i=1}^n y_i + \tilde{y}) (\beta + n)^{\alpha + \sum_{i=1}^n y_i}}{(\tilde{y}!) \Gamma(\alpha + \sum_{i=1}^n y_i) (\beta + n + 1)^{\alpha + \sum_{i=1}^n y_i + \tilde{y}}} \\
&= \frac{\Gamma(\alpha + \sum y_i + \tilde{y})}{\Gamma(\tilde{y} + 1) \Gamma(\alpha + \sum y_i)} \cdot \left( \frac{\beta + n}{\beta + n + 1} \right)^{\alpha + \sum y_i} \cdot \left( \frac{1}{\beta + n + 1} \right)^{\tilde{y}}
\end{aligned}$$

This is a negative binomial distribution:  $\tilde{y} \sim NB(\alpha + \sum y_i, \beta + n)$ .

---

$$\theta \sim NB(\alpha, \beta) \Rightarrow p(\theta) = \binom{\theta + \alpha - 1}{\alpha - 1} \left( \frac{\beta}{\beta + 1} \right)^\alpha \left( \frac{1}{\beta + 1} \right)^\theta$$

so

$$\begin{aligned}
\tilde{y} \sim NB(\alpha + \sum y_i, \beta + n) &\Rightarrow p(\tilde{y}) = \binom{\tilde{y} + \alpha + \sum y_i - 1}{\alpha + \sum y_i - 1} \left( \frac{\beta + n}{\beta + n + 1} \right)^{\alpha + \sum y_i} \left( \frac{1}{\beta + n + 1} \right)^{\tilde{y}} \\
&= \frac{(\alpha + \sum y_i + \tilde{y} - 1)!}{(\alpha + \sum y_i - 1)! (\tilde{y})!} \left( \frac{\beta + n}{\beta + n + 1} \right)^{\alpha + \sum y_i} \left( \frac{1}{\beta + n + 1} \right)^{\tilde{y}} \\
&= \frac{\Gamma(\alpha + \sum y_i + \tilde{y})}{\Gamma(\alpha + \sum y_i) \Gamma(\tilde{y} + 1)} \left( \frac{\beta + n}{\beta + n + 1} \right)^{\alpha + \sum y_i} \left( \frac{1}{\beta + n + 1} \right)^{\tilde{y}}
\end{aligned}$$


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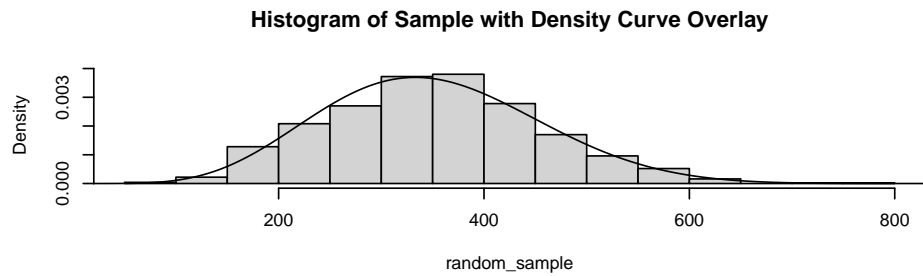
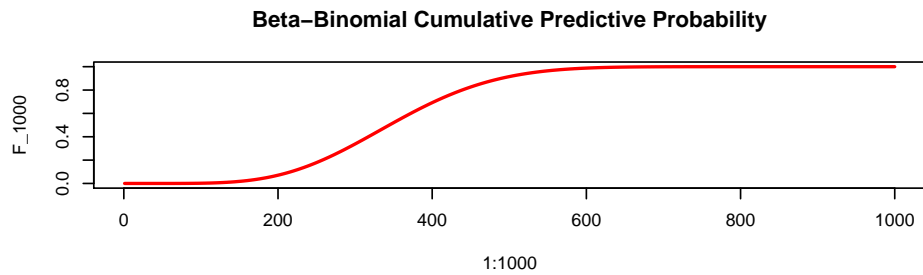
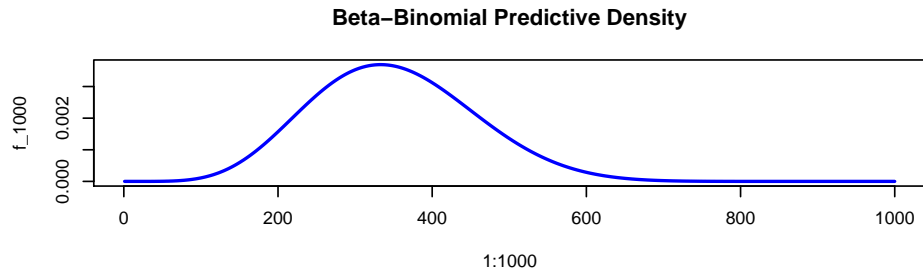
[This is the result in Hoff. The straightforward derivation below is off by a constant multiple. Need to figure out what went awry.]

$$\begin{aligned}
p(\tilde{y}|y_1, \dots, y_n) &= \int_0^\infty p(\tilde{y}|\theta, y_1, \dots, y_n) p(\theta|y_1, \dots, y_n) d\theta \\
&= \int p(\tilde{y}|\theta) p(\theta|y_1, \dots, y_n) d\theta \\
&= C \int \left( \frac{1}{\tilde{y}!} \theta^{\tilde{y}} e^{-\theta} \right) \theta^{\alpha + \sum y_i - 1} e^{-(\beta + n)\theta} d\theta \\
&= \frac{C}{\tilde{y}!} \int \theta^{\tilde{y} + \alpha + \sum y_i - 1} e^{-(\beta + n + 1)\theta} d\theta \\
&= \frac{C \Gamma(\tilde{y} + \alpha + \sum y_i)}{\Gamma(\tilde{y} + 1) (\beta + n + 1)^{\tilde{y} + \alpha + \sum y_i}} \int \frac{(\beta + n + 1)^{\tilde{y} + \alpha + \sum y_i}}{\Gamma(\tilde{y} + \alpha + \sum y_i)} \theta^{\tilde{y} + \alpha + \sum y_i - 1} e^{-(\beta + n + 1)\theta} d\theta \\
&= C \cdot \frac{\Gamma(\tilde{y} + \alpha + \sum y_i)}{\Gamma(\tilde{y} + 1) (\beta + n + 1)^{\tilde{y} + \alpha + \sum y_i}} \\
&= \frac{\prod_{i=1}^n y_i! (\beta + n)^{\alpha + \sum y_i}}{\Gamma(\alpha + \sum y_i)} \cdot \frac{\Gamma(\tilde{y} + \alpha + \sum y_i)}{\Gamma(\tilde{y} + 1) (\beta + n + 1)^{\tilde{y} + \alpha + \sum y_i}} \\
&= \prod_{i=1}^n y_i! \cdot \frac{\Gamma(\tilde{y} + \alpha + \sum y_i)}{\Gamma(\tilde{y} + 1) \Gamma(\alpha + \sum y_i)} \cdot \left( \frac{\beta + n}{\beta + n + 1} \right)^{\alpha + \sum y_i} \cdot \left( \frac{1}{\beta + n + 1} \right)^{\tilde{y}}
\end{aligned}$$

Hoff p.47:

- $b$  is interpreted as the number of prior observations
- $a$  is interpreted as the sum of counts from  $b$  prior observations

Hoff p. 49 (Birth rate example):  $a = 2, b = 1$ .



### 3.3.2 R Implementation

### 3.3.3 Example

## 3.4 Normal Observation with Normal-Inverse Gamma Prior

### 3.4.1 One sample

#### 3.4.1.1 Derivation

#### 3.4.1.2 R Implementation

#### 3.4.1.3 Example

### 3.4.2 Two samples

#### 3.4.2.1 Derivation

#### 3.4.2.2 R Implementation

#### 3.4.2.3 Example

### **3.4.3   $k$ samples**

#### **3.4.3.1   Derivation**

#### **3.4.3.2   R Implementation**

#### **3.4.3.3   Example**

#### **3.4.3.4   Ranking Treatments**



## 4 Chapter 2: Normal Regression with Zellner's $g$ -prior

### 4.0.0.1 Derivation

### 4.0.0.2 R Implementation

### 4.0.0.3 Example

## 5 Conclusion