PREDICTIVE INFERENCE TOOLS FOR RESEARCHERS

by

Voyze G. Harris III

Copyright © Voyze G. Harris III 2021

A Thesis Submitted to the Faculty of the

STATISTICS AND DATA SCIENCE GRADUATE INTERDISCIPLINARY PROGRAM

In Partial Fulfillment of the Requirements For the Degree of

MASTER OF SCIENCE

In the Graduate College

THE UNIVERSITY OF ARIZONA

2021

THE UNIVERSITY OF ARIZONA GRADUATE COLLEGE

As members of the Master's Committee, we certify that we have read the thesis prepared by Voyze Gabriel Harris III, titled [Enter Thesis Title] and recommend that it be accepted as fulfilling the dissertation requirement for the Master's Degree.

	Date:
Dr. Dean Billheimer	
	Date:
Dr. Edward Bedrick	
	Date:
Dr. Walter Piegorsch	
Final approval and acceptance of this thesis is contingent upon the car final copies of the thesis to the Graduate College.	ndidate's submission of the
I hereby certify that I have read this thesis prepared under my direction	on and recommend that it be
accepted as fulfilling the Master's requirement.	
	Date:
Dr. Dean Billheimer Master's Thesis Committee Chair	
Biostatistics	
ARI701	VA

Contents

1	Thesis Abstract					
2	Intr	oductio	n: Predic	etive Inference		
	2.1	Why is	s predicti	ve inference important?		
	2.2	Differe	nce betwe	een parametric inference and predictive inference		
		2.2.1	When is	predictive inference more useful?		
		2.2.2	When is	parametric inference more useful?		
	2.3			arametric Prediction Format		
	2.4		•	le of Difference between results from Plug-in estimator and		
		-	-	edictive Inference		
3 Chapter 1: Predictive Problems with Conjugate Priors				ve Problems with Conjugate Priors		
	3.1	_		iture Successes: Beta-Binomial (Geisser p. 73)		
		3.1.1		on		
		3.1.2		mentation		
		3.1.3		2		
	3.2			Exponential-Gamma (Geisser p. 74)		
	J. <u>2</u>	3.2.1		on		
		3.2.2		mentation		
		3.2.3		2		
	3.3	Poisson-Gamma Model (Hoff p. 43ff)				
	0.0	3.3.1				
		3.3.2		mentation		
		3.3.3		2		
	3.4		_	ation with Normal-Inverse Gamma Prior		
	5.4	3.4.1		aple		
		0.4.1	3.4.1.1	Derivation		
			3.4.1.2	R Implementation		
			3.4.1.3	Example		
		3.4.2		•		
		5.4.2	3.4.2.1	aples		
			•	Derivation		
				R Implementation		
		9 4 9	3.4.2.3	Example		
		3.4.3	k sample			
			3.4.3.1	Derivation		
			3.4.3.2	R Implementation		
			3.4.3.3	Example		
			3.4.3.4	Ranking Treatments		
4	Cha	pter 2:	Normal 1	Regression with Zellner's g-prior		
			4.0.0.1	Derivation		
			4.0.0.2	R Implementation		
			4.0.0.3	Example		
5	Con	clusion				

1 Thesis Abstract

- \bullet (paragraph) Statement of the thesis topic and objectives
- \bullet (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

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

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

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

where

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

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

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

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

$$\Pr[R = r|t] = \int \binom{M}{r} \theta^r (1-\theta)^{M-r} p\left(\theta|X^{(N)}\right) d\theta$$

$$= \binom{M}{r} \int \theta^r (1-\theta)^{M-r} \frac{\Gamma(N+\alpha+\beta)}{\Gamma(t+\alpha)\Gamma(N-t+\beta)} \theta^{t+\alpha-1} (1-\theta)^{N-t+\beta-1} d\theta$$

$$= \frac{M!}{r!(M-r)!} \frac{\Gamma(N+\alpha+\beta)}{\Gamma(t+\alpha)\Gamma(N-t+\beta)} \int \theta^{r+t+\alpha-1} (1-\theta)^{M-r+N-t+\beta-1} d\theta$$

$$= \frac{\Gamma(M+1)\Gamma(N+\alpha+\beta)\Gamma(r+t+\alpha)\Gamma(M-r+N-t+\beta)}{\Gamma(r+1)\Gamma(M-r+1)\Gamma(t+\alpha)\Gamma(N-t+\beta)\Gamma(M+N+\alpha+\beta)}$$

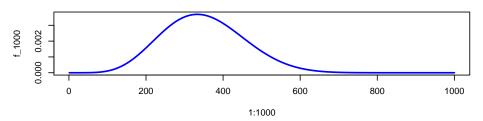
3.1.2 R Implementation

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

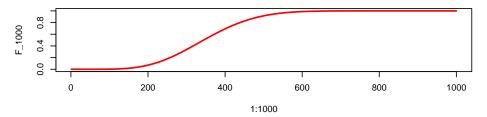
3.1.3 Example

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().

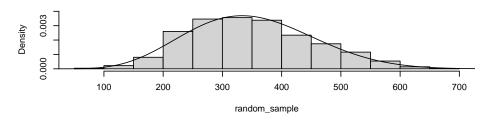
Beta-Binomial Predictive Density



Beta-Binomial Cumulative Predictive Probability



Histogram of Sample with Density Curve Overlay



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 $x_{d+1},...,x_N$, 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 $\Pr(x > \theta) = 1 - \Pr(x \le \theta) = 1 - F(x|\theta) = 1 - (1 - e^{-\theta x}) = e^{-\theta x}$. 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(δ, γ) prior for θ ,

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

we obtain the posterior

$$p(\theta|X^{(N)}) = \frac{p(x^{(N)}|\theta)p(\theta)}{\int p(X^{(N)}|\theta)p(\theta)d\theta}$$

$$= \frac{\theta^{d}e^{-\theta N\bar{x}} \cdot \frac{\gamma^{\delta}\theta^{\delta-1}e^{-\gamma\theta}}{\Gamma(\delta)}}{\int \left(\theta^{d}e^{-\theta N\bar{x}} \cdot \frac{\gamma^{\delta}\theta^{\delta-1}e^{-\gamma\theta}}{\Gamma(\delta)}\right)d\theta}$$

$$= \frac{\frac{\gamma^{\delta}}{V(\delta)} \left(\theta^{d+\delta-1}e^{-\theta(\gamma+N\bar{x})}\right)}{\frac{\gamma^{\delta}}{V(\delta)} \int \left(\theta^{d+\delta-1}e^{-\theta(\gamma+N\bar{x})}\right)d\theta}$$

$$= \frac{\frac{(\gamma+N\bar{x})^{d+\delta}}{\Gamma(d+\delta)} \left(\theta^{d+\delta-1}e^{-\theta(\gamma+N\bar{x})}\right)d\theta}{\frac{(\gamma+N\bar{x})^{d+\delta}}{\Gamma(d+\delta)} \int \left(\theta^{d+\delta-1}e^{-\theta(\gamma+N\bar{x})}\right)d\theta}$$

$$= \frac{(\gamma+N\bar{x})^{d+\delta}}{\Gamma(d+\delta)} \int \left(\theta^{d+\delta-1}e^{-\theta(\gamma+N\bar{x})}\right)d\theta$$

$$= \frac{(\gamma+N\bar{x})^{d+\delta}}{\Gamma(d+\delta)} \int \left(\theta^{d+\delta-1}e^{-\theta(\gamma+N\bar{x})}\right)d\theta$$

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

$$P(X = x | \theta, X^{(N)}) = \int p(\theta | X^{(N)}) p(x | \theta) d\theta$$

$$= \int \frac{(\gamma + N\bar{x})^{d+\delta} \theta^{d+\delta-1} e^{-\theta(\gamma + N\bar{x})}}{\Gamma(d+\delta)} \cdot \theta e^{-\theta x} d\theta$$

$$= (d+\delta)(\gamma + N\bar{x})^{d+\delta} \int \frac{\theta^{(d+\delta+1)-1} e^{-\theta(\gamma + N\bar{x} + x)}}{(d+\delta)\Gamma(d+\delta)} d\theta$$

$$= \frac{(d+\delta)(\gamma + N\bar{x})^{d+\delta}}{(\gamma + N\bar{x} + x)^{d+\delta+1}} \int \frac{(\gamma + N\bar{x} + x)^{d+\delta+1} \theta^{(d+\delta+1)-1} e^{-\theta(\gamma + N\bar{x} + x)}}{\Gamma(d+\delta + 1)} d\theta$$

$$= \frac{(d+\delta)(\gamma + N\bar{x})^{d+\delta}}{(\gamma + N\bar{x} + x)^{d+\delta+1}}$$

$$= \frac{(d+\delta)(\gamma + N\bar{x})^{d+\delta}}{(\gamma + N\bar{x} + x)^{d+\delta+1}}$$

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

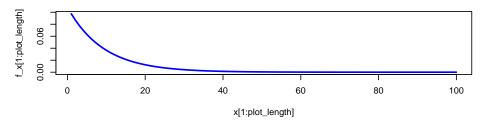
3.2.2 R Implementation

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.

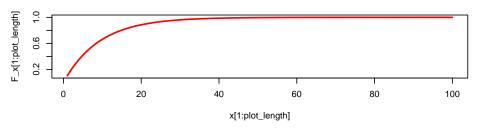
3.2.3 Example

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().

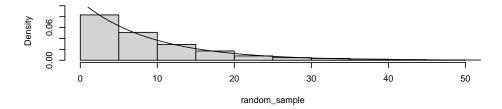
Exponential-Gamma Predictive Density



Exponential-Gamma Cumulative Predictive Probability



Histogram of Sample with Density Curve Overlay



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

$$P(Y_1 = y_1, ..., Y_n = y_n | \theta) = \prod_{i=1}^n p(y_i | \theta)$$

$$= \prod_{i=1}^n \frac{1}{y!} \theta^{y_i} e^{-\theta}$$

$$= \left(\prod_{i=1}^n \frac{1}{y!}\right) \theta^{\sum y_i} e^{-n\theta}$$

$$= c(y_1, ..., y_n) \theta^{\sum y_i} e^{-n\theta}$$

and

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

Then we have posterior distribution

$$p(\theta|y_1, ..., y_n) = \frac{p(y_1, ..., y_n|\theta) p(\theta)}{\int_{\theta} p(y_1, ..., y_n|\theta) p(\theta)}$$

$$= \frac{p(y_1, ..., y_n|\theta) p(\theta)}{p(y_1, ..., y_n)}$$

$$= \frac{1}{p(y_1, ..., y_n)} \theta^{\sum y_i} e^{-n\theta} \frac{\beta^{\alpha}}{\Gamma(\alpha)} \theta^{\alpha-1} e^{-\beta\theta}$$

$$= C(y_1, ..., y_n, \alpha, \beta) \theta^{\alpha+\sum y_i - 1} e^{-(\beta+n)\theta}$$

$$\sim \text{Gamma} \left(\alpha + \sum y_i, \beta + n\right).$$

Here

$$C(y_{1},...,y_{n},\alpha,\beta) = \frac{1}{p(y_{1},...,y_{n})} \cdot \frac{\beta^{\alpha}}{\Gamma(\alpha)}$$

$$= \frac{1}{\int_{\theta} p(y_{1},...,y_{n}|\theta) p(\theta)} \cdot \frac{\beta^{\alpha}}{\Gamma(\alpha)}$$

$$= \frac{1}{\int_{\theta} \left(\prod \frac{1}{y_{i}!}\right) \theta^{\sum y_{i}} e^{-n\theta} \left(\frac{\beta^{\alpha}}{\Gamma(\alpha)}\right) \theta^{\alpha-1} e^{-\beta\theta}} \cdot \left(\frac{\beta^{\alpha}}{\Gamma(\alpha)}\right)$$

$$= \frac{1}{\left(\prod \frac{1}{y_{i}!}\right) \frac{\Gamma(\alpha+\sum y_{i})}{(\beta+n)^{\alpha+\sum y_{i}}} \int_{\theta} \frac{(\beta+n)^{\alpha+\sum y_{i}}}{\Gamma(\alpha+\sum y_{i})} \theta^{\sum y_{i}+\alpha-1} e^{-(\beta+n)\theta}}$$

$$= \frac{\prod_{i=1}^{n} y_{i}! (\beta+n)^{\alpha+\sum y_{i}}}{\Gamma(\alpha+\sum y_{i})}$$

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

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

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

$$p(\tilde{y}|y_{1},...,y_{n}) = \frac{p(y_{1},...,y_{n},\tilde{y})}{p(y_{1},...,y_{n})} = \frac{p(y_{1},...,y_{n+1})}{p(y_{1},...,y_{n})} = \frac{\frac{1}{C_{n+1}}\frac{\beta^{\alpha}}{p(\alpha)}}{\frac{1}{C_{n}}\frac{\beta^{\alpha}}{p(\alpha)}} = \frac{C_{n}}{C_{n+1}}$$

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

$$= \frac{\Gamma\left(\alpha+\sum_{i=1}^{n+1}y_{i}\right)(\beta+n)^{\alpha+\sum_{i=1}^{n}y_{i}}}{(y_{n+1}!)\Gamma\left(\alpha+\sum_{i=1}^{n}y_{i}\right)(\beta+n+1)^{\alpha+\sum_{i=1}^{n+1}y_{i}}}$$

$$= \frac{\Gamma\left(\alpha+\sum_{i=1}^{n}y_{i}+\tilde{y}\right)(\beta+n)^{\alpha+\sum_{i=1}^{n}y_{i}}}{(\tilde{y}!)\Gamma\left(\alpha+\sum_{i=1}^{n}y_{i}\right)(\beta+n+1)^{\alpha+\sum_{i=1}^{n}y_{i}+\tilde{y}}}$$

$$= \frac{\Gamma\left(\alpha+\sum_{i=1}^{n}y_{i}+\tilde{y}\right)(\beta+n+1)^{\alpha+\sum_{i=1}^{n}y_{i}+\tilde{y}}}{\Gamma(\tilde{y}+1)\Gamma(\alpha+\sum_{i=1}^{n}y_{i})\cdot\left(\frac{\beta+n}{\beta+n+1}\right)^{\alpha+\sum_{i=1}^{n}y_{i}+\tilde{y}}} \cdot \left(\frac{1}{\beta+n+1}\right)^{\tilde{y}}$$

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

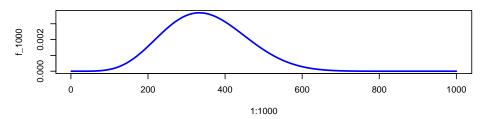
$$\theta \sim NB(\alpha, \beta) \Rightarrow p(\theta) = \begin{pmatrix} \theta + \alpha - 1 \\ \alpha - 1 \end{pmatrix} \left(\frac{\beta}{\beta + 1} \right)^{\alpha} \left(\frac{1}{\beta + 1} \right)^{\theta}$$

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

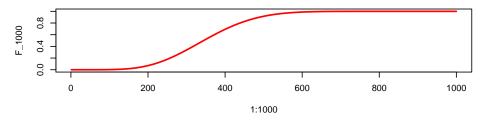
[This is the result in Hoff. The straightforward derivation below is off by a constant multiple. Need to figure out what went awry.]

$$\begin{split} p\left(\tilde{y}|y_{1},...,y_{n}\right) &= \int_{0}^{\infty} p\left(\tilde{y}|\theta,y_{1},...,y_{n}\right) p\left(\theta|y_{1},...,y_{n}\right) d\theta \\ &= \int p\left(\tilde{y}|\theta\right) p\left(\theta|y_{1},...,y_{n}\right) d\theta \\ &= C \int \left(\frac{1}{\tilde{y}!} \theta^{\tilde{y}} e^{-\theta}\right) \theta^{\alpha + \sum y_{i} - 1} e^{-(\beta + n)\theta} d\theta \\ &= \frac{C}{\tilde{y}!} \int \theta^{\tilde{y} + \alpha + \sum y_{i} - 1} e^{-(\beta + n + 1)\theta} d\theta \\ &= \frac{C\Gamma\left(\tilde{y} + \alpha + \sum y_{i}\right)}{\Gamma\left(\tilde{y} + 1\right)\left(\beta + n + 1\right)^{\tilde{y} + \alpha + \sum y_{i}}} \int \frac{(\beta + n + 1)^{\tilde{y} + \alpha + \sum y_{i}}}{\Gamma\left(\tilde{y} + \alpha + \sum y_{i}\right)} \theta^{\tilde{y} + \alpha + \sum y_{i-1}} e^{-(\beta + n + 1)\theta} d\theta \\ &= C \cdot \frac{\Gamma\left(\tilde{y} + \alpha + \sum y_{i}\right)}{\Gamma\left(\tilde{y} + 1\right)\left(\beta + n + 1\right)^{\tilde{y} + \alpha + \sum y_{i}}} \\ &= \frac{\prod_{i=1}^{n} y_{i}!(\beta + n)^{\alpha + \sum y_{i}}}{\Gamma(\alpha + \sum y_{i})} \cdot \frac{\Gamma\left(\tilde{y} + \alpha + \sum y_{i}\right)}{\Gamma\left(\tilde{y} + 1\right)\left(\beta + n + 1\right)^{\tilde{y} + \alpha + \sum y_{i}}} \\ &= \prod_{i=1}^{n} y_{i}! \cdot \frac{\Gamma\left(\tilde{y} + \alpha + \sum y_{i}\right)}{\Gamma\left(\tilde{y} + 1\right)\Gamma\left(\alpha + \sum y_{i}\right)} \cdot \left(\frac{\beta + n}{\beta + n + 1}\right)^{\alpha + \sum y_{i}} \cdot \left(\frac{1}{\beta + n + 1}\right)^{\tilde{y}} \end{split}$$

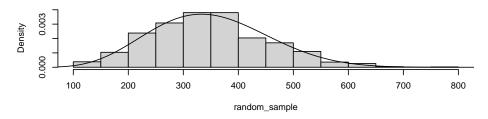
Beta-Binomial Predictive Density



Beta-Binomial Cumulative Predictive Probability



Histogram of Sample with Density Curve Overlay



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