# PREDICTIVE INFERENCE TOOLS FOR RESEARCHERS

by

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# 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

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

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

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

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

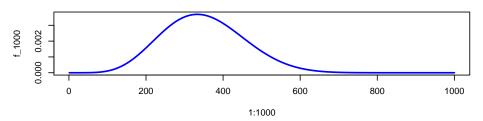
#### 3.1.2 R Implementation

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.

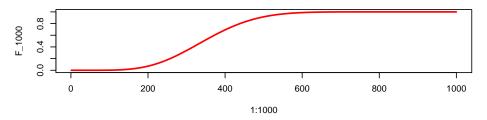
#### **3.1.3** Example

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().

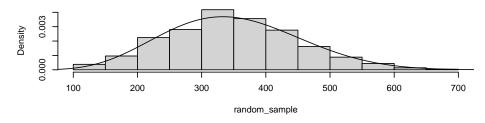
#### **Beta-Binomial Predictive Density**



#### **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( $\delta, \gamma$ ) prior for  $\theta$ ,

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

we obtain the posterior

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

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

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

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

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

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

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.)

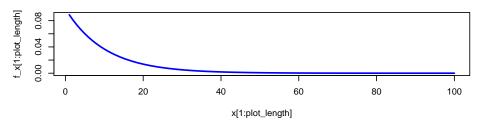
## 3.2.2 R Implementation

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.

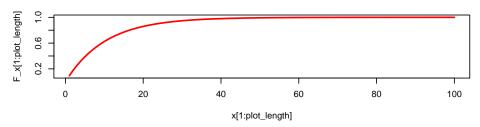
#### **3.2.3** Example

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().

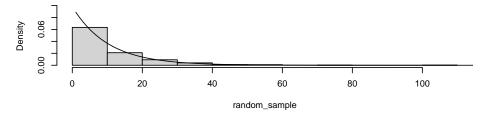
## **Exponential-Gamma Predictive Density**



## **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

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

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

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

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

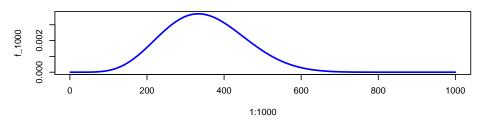
$$= \frac{\Gamma(\alpha+\sum_{i=1}^{n}y_{i})(\beta+n+1)^{\alpha+\sum_{i=1}^{n}y_{i}+\tilde{y}}}{\Gamma(\tilde{y}+1)\Gamma(\alpha+\sum_{i=1}^{n}y_{i})} \cdot \left(\frac{\beta+n}{\beta+n+1}\right)^{\alpha+\sum_{i=1}^{n}y_{i}+\tilde{y}}} \cdot \left(\frac{1}{\beta+n+1}\right)^{\tilde{y}}$$

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

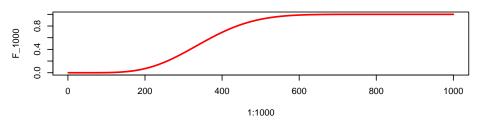
[This is the result in Hoff. The straightforward derivation below is off by a constant multiple. Need to figure out what went awry.]

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

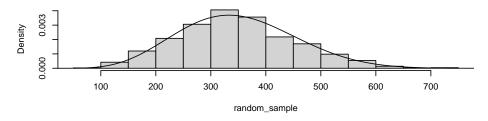
#### **Beta-Binomial Predictive Density**



#### **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