

PREDICTIVE INFERENCE TOOLS FOR RESEARCHERS

by

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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

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

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

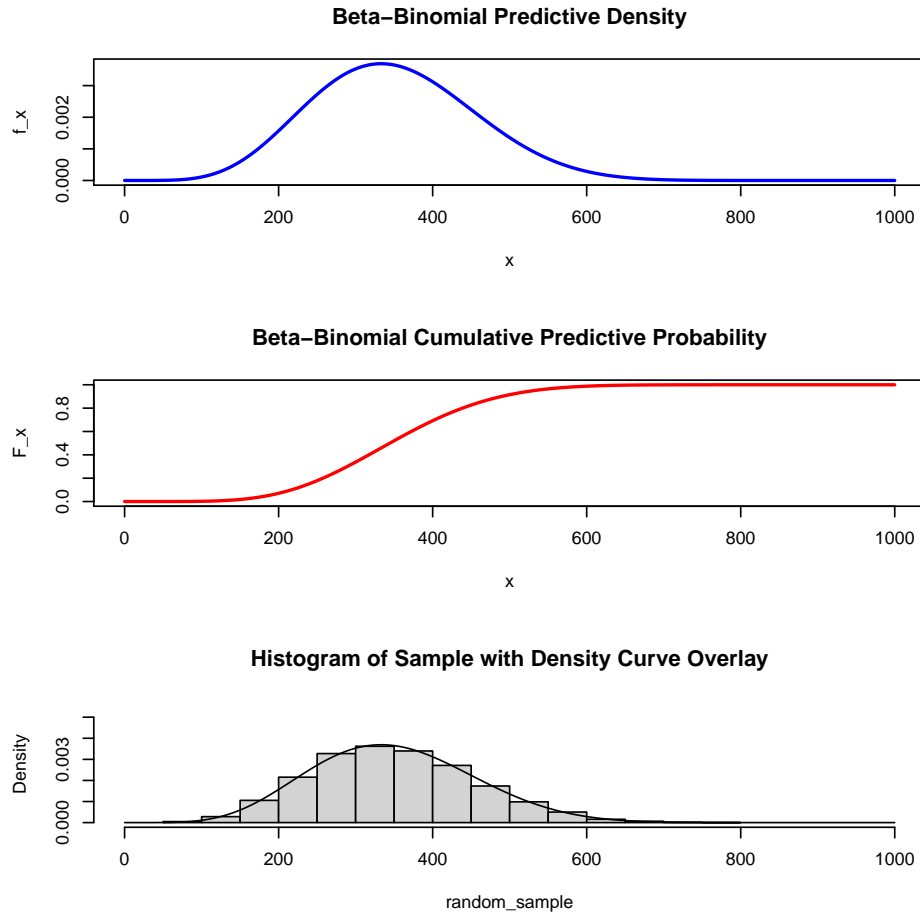
$$\begin{aligned} \Pr[R = r | t] &= \int \binom{M}{r} \theta^r (1 - \theta)^{M-r} p(\theta | X^{(N)}) d\theta \\ &= \binom{M}{r} \int \theta^r (1 - \theta)^{M-r} \frac{\Gamma(N + \alpha + \beta)}{\Gamma(t + \alpha) \Gamma(N - t + \beta)} \theta^{t+\alpha-1} (1 - \theta)^{N-t+\beta-1} d\theta \\ &= \frac{M!}{r!(M-r)!}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

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(δ, γ) prior for θ ,

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

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

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

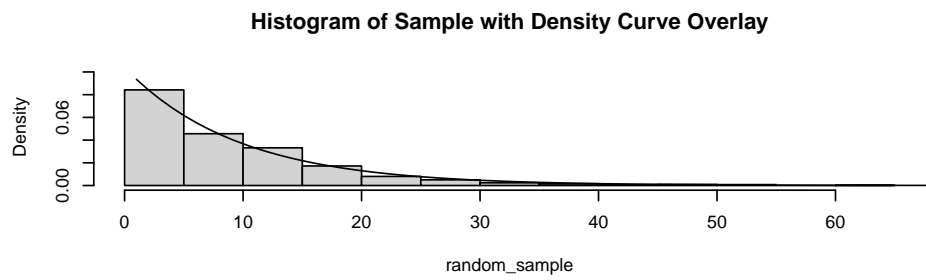
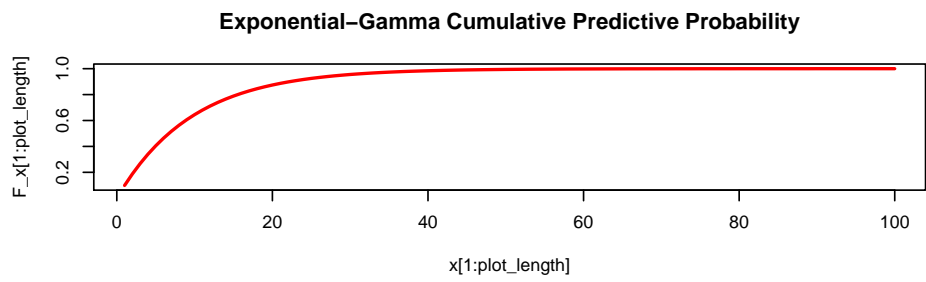
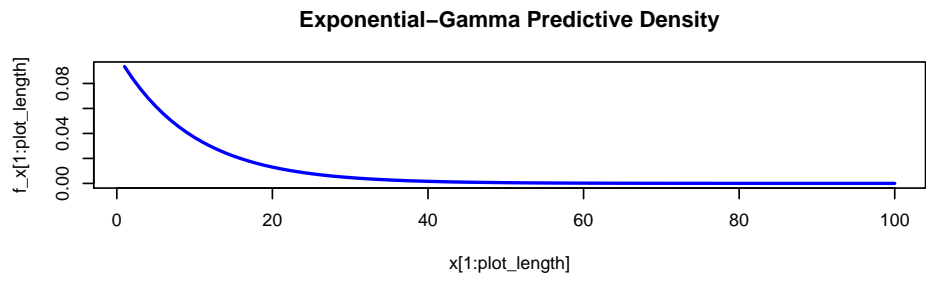
(simplifying by constructing a $\text{Gamma}(d + \delta + 1, \gamma + N\bar{x} + x)$ density in the final integrand.)

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: $\tilde{y} \sim NB(\alpha + \sum y_i, \beta + n)$, for which

$$\begin{aligned}
E[\tilde{Y}|y_1, \dots, y_n] &= \frac{a + \sum y_i}{b + n} = E[\theta|y_1, \dots, y_n]; \\
\text{Var}[\tilde{Y}|y_1, \dots, y_n] &= \frac{a + \sum y_i}{b + n} \frac{b + n + 1}{b + n} \\
&= \text{Var}[\theta|y_1, \dots, y_n] \times (b + n + 1) \\
&= E[\theta|y_1, \dots, y_n] \times \frac{b + n + 1}{b + n}
\end{aligned}$$

[Showing here that it is indeed a NB distribution]

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

so

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

[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

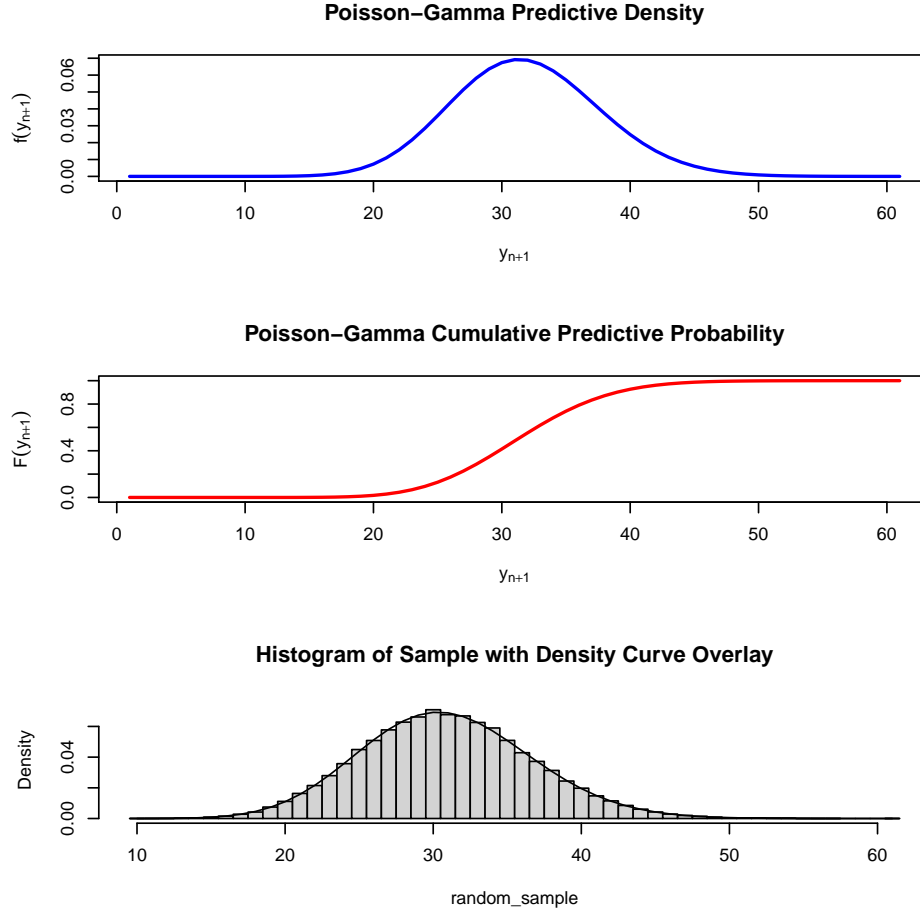
This result has been used to create standard format R functions `dpredPG()`, `ppredPG()`, and `rpredPG()` for the Poisson-Gamma distribution for density, cumulative probability, and random sampling, respectively (see appendix). These functions are exercised in the following example.

Developing the random sample function `rpredPG()`: I need to establish the support of the predictive distribution f_x from which to sample. the `uniroot()` function is not working because it keeps feeding non-integer values to `dnbinom()`. Strategy: a modified bisection method as follows:

1. set a desired tolerance ϵ .
2. Find the expected value E_x (closed formula, see above).
3. Step to the right of E_x by whole integers, in the sequence $E_x + \{1, 2, 4, \dots, 2^n\}$, stopping at $U = f_x(E_x + 2^n) < 0$. This is the upper bound for the bisection method.
4. Bisect the interval, rounding to the nearest integer. Call the resulting mid-interval number B .
5. If B is positive, test whether $0 \leq f_x(B) \leq \epsilon$. If so, DONE. If not:
6. Establish new interval, choosing endpoints from E_x , B , and U so that the interval straddles 0, and repeat the steps until the condition in step 5 is reached.

3.3.3 Example

Suppose we have 10 prior observations with counts 27, 79, 21, 100, 8, 4, 37, 15, 3, 97. Let $\alpha = 11$ and $\beta = 3$. For $\tilde{y} = 1 : 100$ possible future occurrences, the figures below show the predictive distribution from `dpredPG()`, the cumulative distribution from `ppredPG()`, and a histogram of random draws from `rpredPG()`.



3.4 Normal Observation with Normal-Inverse Gamma Prior

3.4.1 One sample

3.4.1.1 Derivation [Hoff p. 69ff]

Let $\{Y_1, \dots, Y_n | \theta, \sigma^2\} \stackrel{i.i.d.}{\sim} N(\theta, \sigma^2)$. Then the joint sampling density is

$$\begin{aligned}
 p(y_1, \dots, y_n | \theta, \sigma^2) &= \prod_{i=1}^n p(y_i | \theta, \sigma^2) \\
 &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{y_i - \theta}{\sigma}\right)^2} \\
 &= (2\pi\sigma^2)^{-n/2} e^{-\frac{1}{2}\sum_{i=1}^n \left(\frac{y_i - \theta}{\sigma}\right)^2}.
 \end{aligned}$$

It can be shown that $\{\sum y_i^2, \sum y_i\}$ and hence $\{\bar{y}, s^2\}$ are sufficient statistics, where $\bar{y} = \sum y_i / n$ and $s^2 = \sum (y_i - \bar{y})^2 / (n - 1)$.

⋮

Skipping ahead

⋮

posteriors given Jeffrey's Prior:

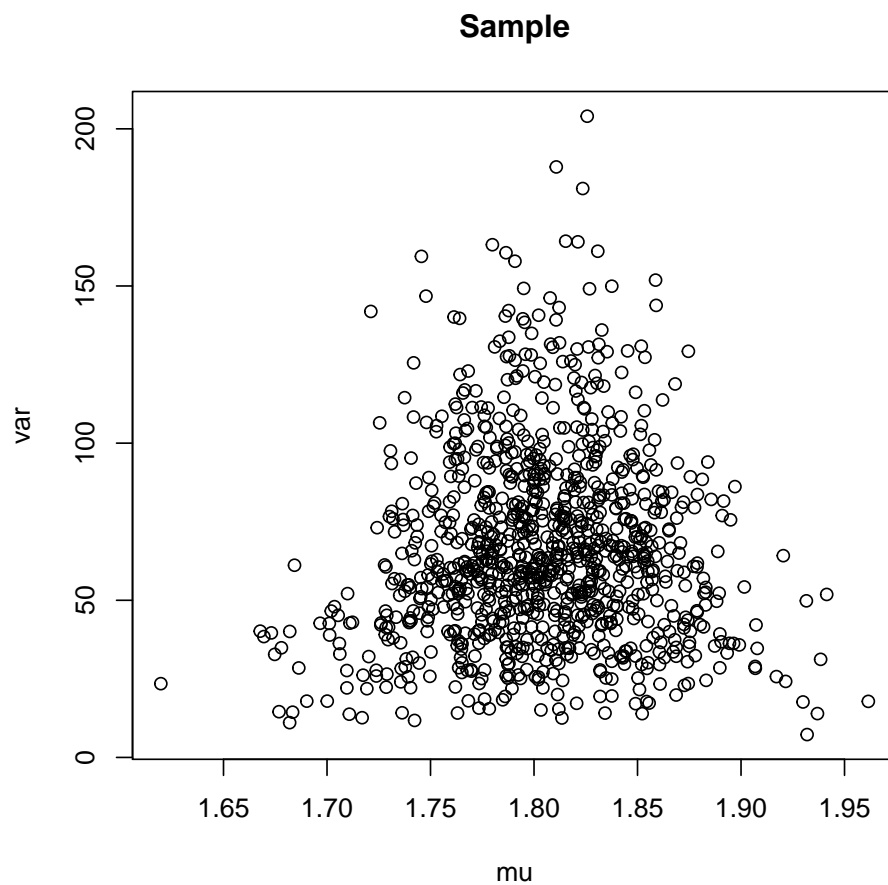
$$\{1/\sigma^2|y_1, \dots, y_n\} \sim \text{gamma}\left(\frac{n}{2}, \frac{1}{2n} \sum (y_i - \bar{y})^2\right)$$

same as

$$\{1/\sigma^2|y_1, \dots, y_n\} \sim \text{gamma}\left(\frac{n}{2}, \frac{1}{2} \sum (y_i - \bar{y})^2\right)$$

$$\{\theta|\sigma^2, y_1, \dots, y_n\} \sim \text{normal}\left(\bar{y}, \frac{\sigma^2}{n}\right)$$

dig into Bedrick notes and homework for Jeffrey's prior



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