# *Markov chain Monte Carlo I*
# *(Shorter) Introduction*

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# *Notation*

- Let $\theta$ denote unobservable vector quantities or population parameters of interest (such as the per-contact probability of transmission from an infected person to a susceptible person)
- Let $y$ denote the observed data (such as the number of infecteds and uninfecteds who were exposed)
- Let $\tilde{y}$ or $y_{n+1}$ denote unknown, but potentially observable quantities, such as the infection outcome of the next contact between an infected person and a susceptible person.

# *Bayesian Inference*

- Bayesian statistical conclusions about a parameter $\theta$, or unobserved data $\tilde{y}$, are made in terms of probability statements.
- These probability statements are conditional on the observed value of $y$.
- They can be written as $p(\theta|y)$ or $p(\tilde{y}|y)$
- We also implicitly condition on known values of any covariates.

# *Bayes' rule*

- To make probability statements about $\theta$ given $y$, we start with a model providing the joint probability distribution for $\theta$ and $y$.
- The joint probability mass or density function can be written as a product of two densities that are often referred to as the prior distribution $p(\theta)$ and the sampling distribution (or data distribution) $p(y|\theta)$

$$p(\theta, y) = p(\theta)p(y|\theta)$$

- Simply conditioning on the known value of the data $y$, using the basic property of conditional probability known as Bayes' rule, yields the posterior density

$$p(\theta|y) = \frac{p(\theta, y)}{p(y)} = \frac{p(\theta)p(y|\theta)}{p(y)}$$

# *Bayes' rule, cont'd*

- Simply conditioning on the known value of the data $y$, using the basic property of conditional probability known as Bayes' rule, yields the posterior density

$$p(\theta|y) = \frac{p(\theta, y)}{p(y)} = \frac{p(\theta)p(y|\theta)}{p(y)}$$

- where $p(y) = \sum_\theta p(\theta)p(y|\theta)$ and the sum is over all possible values of $\theta$
- or $p(y) = \int p(\theta)p(y|\theta)d\theta$ in the case of continuous $\theta$

# *Prior, likelihood, and posterior*

- Let
  - $y = (y_1, \ldots, y_n)$: observed data
  - $f(y|\theta)$: model for the observed data, usually a probability distribution
  - $\theta$: vector of unknown parameters, assumed a random quantity
  - $\pi(\theta)$: prior distribution of $\theta$
- The posterior distribution for inference concerning $\theta$ is

$$f(\theta|y) = \frac{f(y|\theta)\pi(\theta)}{\int f(y|u)\pi(u)du}.$$

# *Posterior and marginal density of y*

- The integral $\int f(y|u)\pi(u)du$, the marginal density of the data $y$, does not depend on $\theta$.
- When the data $y$ are fixed, then the integral can be regarded as a normalizing constant $C$.
- In high dimensional problems, the integral can be very difficult to evaluate.
- Evaluation of the complex integral $\int f(y|u)\pi(u)du$ was a focus of much Bayesian computation.

# *Advent of MCMC Methods*

- With the advent of the use of Markov chain Monte Carlo (MCMC) methods,
  $\longrightarrow$ one could avoid evaluating the integral, making use of the unnormalized posterior density.

$$f(\theta|y) \propto f(y|\theta)\pi(\theta).$$

- Equivalently, if we denote the likelihood function or sampling distribution by $L(\theta)$, then

$$\begin{aligned} f(\theta|y) &\propto L(\theta)\pi(\theta). \\ \text{posterior} &\propto \text{likelihood} \times \text{prior} \end{aligned}$$

- We will show how this works.

# *Other Uses of MCMC Methods*

- Can simplify otherwise difficult computations.
- Sometimes a likelihood would be easy to evaluate if some data had been observed that was not observed or is unobservable.
- Examples:
  - infection times,
  - time of clearing infection,
  - when someone is infectious,
  - chains of infection.
- MCMC methods can be used to augment the observed data to make estimation simpler.

# *Transmission probability*

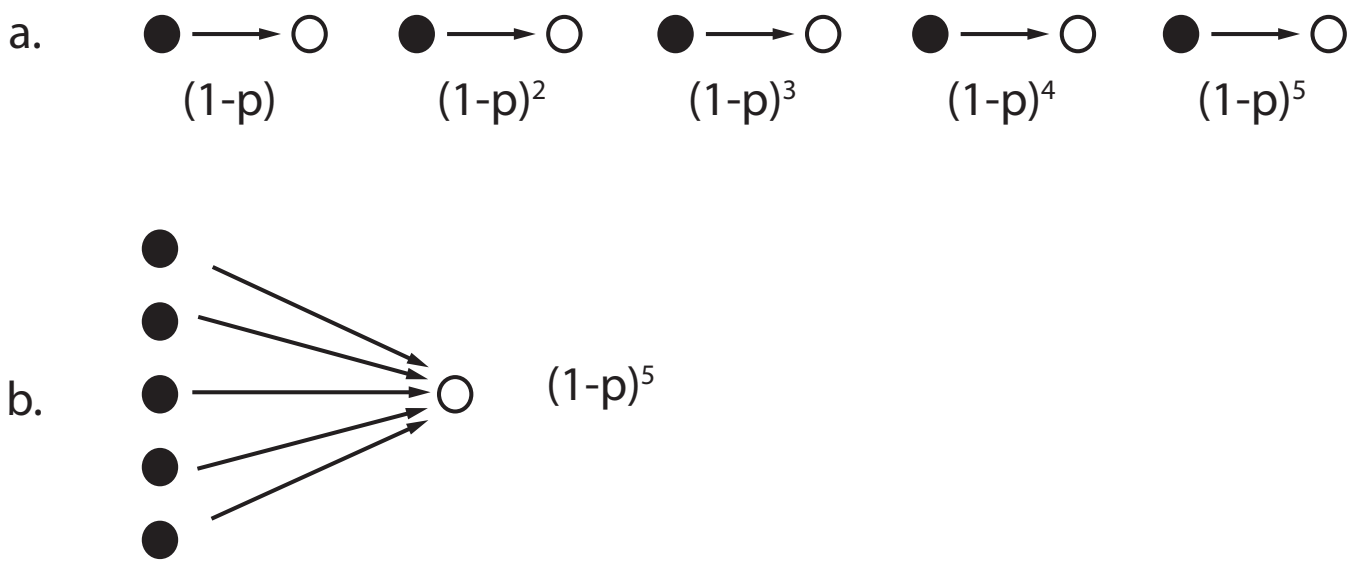
- $p$ is the probability an infective infects a susceptible: transmission probability
- $q = 1 - p$ is the probability a susceptible escapes infection when exposed to an infective: escape probability
- Transmission versus escape ? which is the "success" and which the "failure" ?
- Given there are $n$ exposures, and $y$ infections, what is the estimate of the transmission probability?
- Given there are $n$ exposures, and $n - y$ escapes, what is the estimate of the escape probability?

# *Chain-binomial model*

- Assume independent households
- One person in each household introduces the infection into the household (index case).
- Infections occur within households in generations of infection (discrete time).
- $p$ is the probability an infective infects a susceptible in a household in a generation
- $q = 1 - p$ is the probability a susceptible escapes infection when exposed to an infective in a household

# *Reed-Frost Chain Binomial Model*

*Figure :* Independent exposures = independent Bernoulli trials



# *Chain Binomial Model*

*Table :* Chain binomial probabilities in the Reed-Frost model in $N$ households of size 3 with 1 initial infective and 2 susceptibles, $S_0 = 2, I_0 = 1$

| Chain | Chain probability | Frequency | at p=0.4 | at p=0.7 | Final number infected |
|---|---|---|---|---|---|
| $1 \longrightarrow 0$ | $q^2$ | $n_1$ | 0.360 | 0.090 | 1 |
| $1 \longrightarrow 1 \longrightarrow 0$ | $2pq^2$ | $n_{11}$ | 0.288 | 0.126 | 2 |
| $1 \longrightarrow 1 \longrightarrow 1$ | $2p^2q$ | $n_{111}$ | 0.192 | 0.294 | 3 |
| $1 \longrightarrow 2$ | $p^2$ | $n_{12}$ | 0.160 | 0.490 | 3 |
| Total | 1 | $N$ | 1.00 | 1.00 | |

# *Chain binomial model*

- Data: The observations are based on outbreaks of measles in Rhode Island 1929–1934.
- The analysis is restricted to $N = 334$ families with three susceptible individuals at the outset of the epidemic.
- Assume there is a single index case that introduces infection into the family.
- The actual chains are not observed, just how many are infected at the end of the epidemic.
- So the frequency of chains $1 \longrightarrow 1 \longrightarrow 1$ and $1 \longrightarrow 2$ are not observed.
- MCMC can be used to augment the missing data, and estimate the transmission probability $p$.

# *Chain Binomial Model*

*Table :* Rhodes Island measles data: chain binomial probabilities in the Reed-Frost model in $N = 334$ households of size 3 with 1 initial infective and 2 susceptibles, $N_3 = n_{111} + n_{12} = 275$ is observed

| Chain | Chain probability | Frequency | Observed frequency | Final number infected |
|---|---|---|---|---|
| $1 \longrightarrow 0$ | $q^2$ | $n_1$ | 34 | 1 |
| $1 \longrightarrow 1 \longrightarrow 0$ | $2pq^2$ | $n_{11}$ | 25 | 2 |
| $1 \longrightarrow 1 \longrightarrow 1$ | $2p^2q$ | $n_{111}$ | not observed | 3 |
| $1 \longrightarrow 2$ | $p^2$ | $n_{12}$ | not observed | 3 |
| Total | 1 | $N$ | 334 | |

# *Conjugate prior distributions*

- Conjugacy: the property that the posterior distribution follows that same parametric form as the prior distribution.
- Beta prior distribution is conjugate family for binomial likelihood: posterior distribution is Beta
- Gamma prior distribution is conjugate family for Poisson likelihood: posterior distribution is Gamma

# *Conjugate prior distributions*

- Simply put, conjugate prior distributions in tandem with the appropriate sampling distribution for the data have the same distribution as the posterior distribution.
- Conjugate prior distributions have computational convenience.
- They can also be interpreted as additional data.
- They have the disadvantage of constraining the form of the prior distribution.

# *More on prior distributions*

- **Nonconjugate** prior distributions can be used when the shape of the prior knowledge or belief about the distribution of the parameters of interest does not correspond to the conjugate prior distribution.

- **Noninformative** prior distributions carry little population information and are generally supposed to play a minimal role in the posterior distribution.
  $\longrightarrow$They are also called diffuse, vague, or flat priors.

- Computationally nonconjugate distributions can be more demanding.

# *Data and Sampling Distribution*

- Goal: Inference on the posterior distribution of the transmission probability

- Suppose that $n$ people are exposed once to infection
  - $y$ become infected ("successes")
  - $n - y$ escape infection ("failures")

- Let
  - $p =$ transmission probability
  - $1 - p = q =$ escape probability
- Binomial sampling distribution

$$L(y|p) = \text{Bin}(y|n, p) = \binom{n}{y} p^y (1-p)^{n-y} = \binom{n}{y} p^y q^{n-y}$$

# *Specify the Prior Distribution of p*

- To perform Bayesian inference, we must specify a prior distribution for $p$.
- We specify a Beta prior distribution:

$$p \sim \text{Beta}(\alpha, \beta)$$

$$\text{Beta}(p|\alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha-1}(1-p)^{\beta-1}, \alpha > 0, \beta > 0.$$

- Mean: $E(p|\alpha, \beta) = \frac{\alpha}{\alpha+\beta}$
- Variance: $\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)} = \frac{E(p|\alpha,\beta)[1-E(p|\alpha,\beta)]}{\alpha+\beta+1}$

# *Specify the Prior Distribution of p*

- We specify a Beta prior distribution:

$$\begin{aligned} p &\sim \text{Beta}(\alpha, \beta) \\ \pi(p) &= \text{Beta}(p|\alpha, \beta) \\ \text{Beta} &\propto p^{\alpha-1}(1-p)^{\beta-1}. \end{aligned}$$

- Looks similar to binomial distribution
- $\alpha > 0$, $\beta > 0$, "prior sample sizes"

# *Posterior distribution of p*

- The posterior distribution of the transmission probability $p$, $f(p|y)$:

$$
\begin{array}{rcl}
f(p|y) & \propto & p^y(1-p)^{n-y}p^{\alpha-1}(1-p)^{\beta-1} \\
\text{posterior} & & \text{likelihood} \times \textit{prior} \\
& = & p^{y+\alpha-1}(1-p)^{n-y+\beta-1} \\
& \propto & \text{Beta}(p|\alpha+y, \beta+n-y)
\end{array}
$$

- The role of $\alpha$ and $\beta$ as prior sample sizes is clear.

# *Posterior mean of $\theta$*

- Posterior mean of $p$
  $\longrightarrow$ posterior probability of success (transmission) for a future draw from the population:

$$E(p|y) = \frac{\alpha + y}{\alpha + \beta + n}$$

- posterior mean always lies between the prior mean $\alpha/(\alpha + \beta)$ and the sample mean $y/n$.

# *Uniform prior distribution*

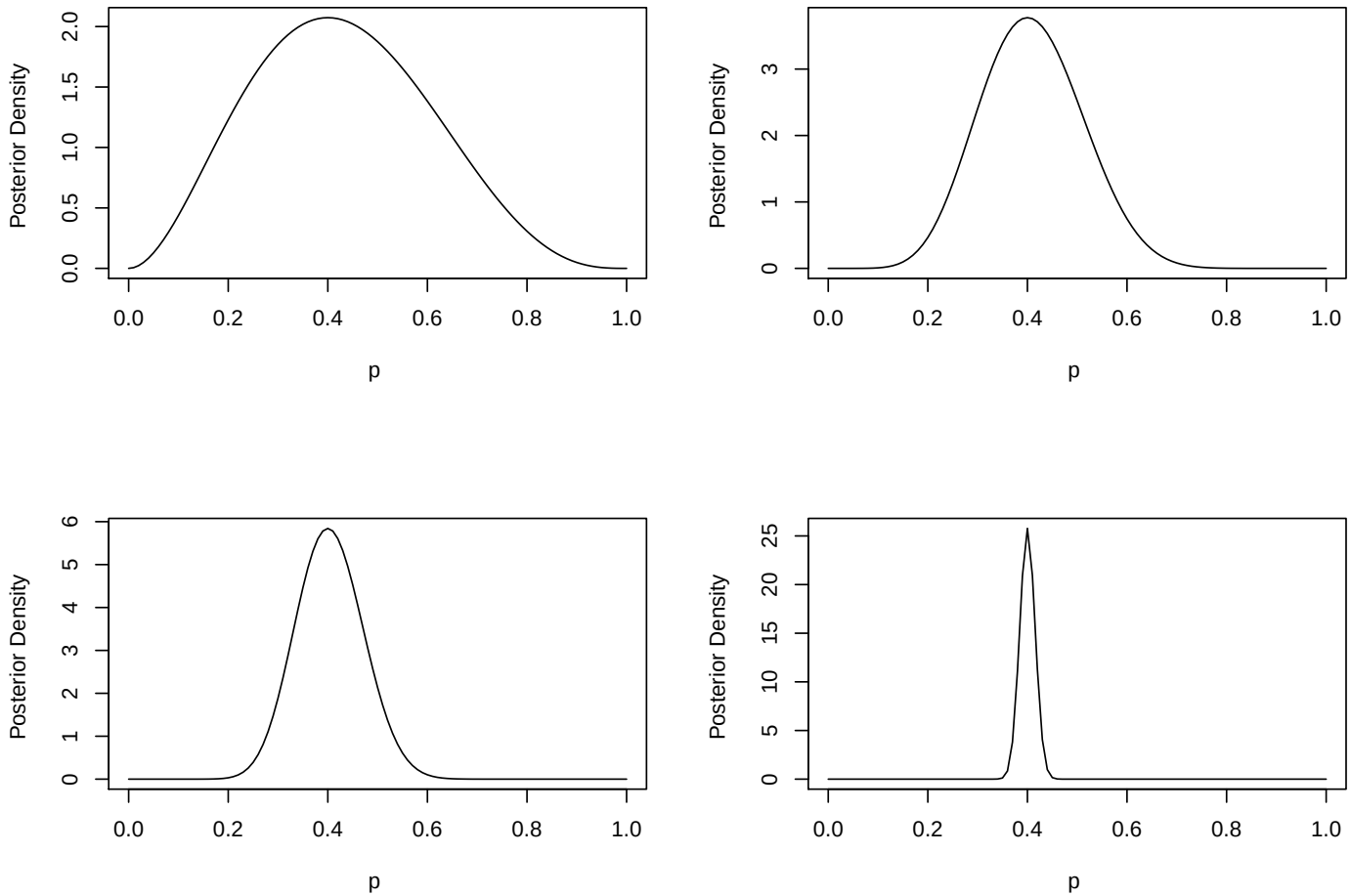
- The uniform prior distribution on [0,1] corresponds to $\alpha = 1$, $\beta = 1$. Essentially no prior information on $p$.

$$f(p|y) = \text{Beta}(p|y+1, n-y+1)$$

- Let's see how the posterior distribution of the transmission probability depends on the amount of data given a uniform prior distribution (Sample mean $y/n = 0.40$).

| $n$, number exposed | $y$, number infected |
|---|---|
| 5 | 2 |
| 20 | 8 |
| 50 | 20 |
| 1000 | 400 |

*Figure :* R program: Posterior distribution with differing amounts of data. Uniform Beta prior, Binomial sampling distribution.



# *References*


- Gelman, A, Carlin, JB, Stern, HS, Dunson, DB, Vehtari, A, Rubin, DB. *Bayesian Data Analysis*, Chapman and Hall/CRC, third edition, 2014.
- Carlin, BP and Louis, TA. *Bayesian Methods for Data Analysis*, CRC Press, third edition, 2008.

# *Introductory Practical in R*

- Do the exercises described in PracticalBayes12020.pdf.
- A video is available explaining Rstudio and the practical.
- The R code is available in bayesintro2020.R.
- This practical also has an exercise where you vary the amount of prior data keeping the amount of observed data constant to see how it affects the posterior distribution.
- If you already are familiar with R, this will be a simple exercise.

# *Chain Binomial Model*

*Table :* Rhodes Island measles data: chain binomial probabilities in the Reed-Frost model in $N = 334$ households of size 3 with 1 initial infective and 2 susceptibles, $N_3 = n_{111} + n_{12} = 275$ is observed

| Chain | Chain probability | Frequency | Observed frequency | Final number infected |
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# *Complete data likelihood for q*

- The multinomial complete data likelihood for $q$:

$$f(n_1, n_{11}, N_3, n_{111}|q)$$

$$= \binom{334}{n_1, n_{11}, n_{111}, N_3 - n_{111}} (q^2)^{n_1} (2q^2p)^{n_{11}} (2qp^2)^{n_{111}} (p^2)^{N_3 - n_{111}}$$

- The observed data are $(n_1, n_{11}, N_3)$, but we do not observe $n_{111}$.

- We could estimate $q$ using a marginal model, but won't.

# *Gibbs sampler for chain binomial model*

- The general idea of the Gibbs sampler is to sample the model unknowns from a sequence of full conditional distributions and to loop iteratively through the sequence.
- To sample one draw from each full conditional distribution at each iteration, it is assumed that all of the other model quantities are known at that iteration.
- In the theoretical lectures, it will be shown that the Gibbs sampler converges to the posterior distribution of the model unknowns.
- In the Rhode Island measles data, we are interested in augmenting the missing data $n_{111}$ and estimating the posterior distribution of $q$, the escape probability.

# *Gibbs sampler for chain binomial model*

- The joint distribution of the observations $(n_1, n_{11}, N_3)$ and the model unknowns $(n_{111}, q)$ is

$$f(n_1, n_{11}, N_3, n_{111}, q) = f(n_1, n_{11}, N_3, n_{111}|q) \times f(q)$$

complete data likelihood $\times$ prior

- We want to make inference about the joint posterior distribution of the model unknowns

$$f(n_{111}, q|n_1, n_{11}, N_3)$$

- This is possible by sampling from the full conditionals (Gibbs sampling): $f(q|n_1, n_{11}, N_3, n_{111})$ and $f(n_{111}|n_1, n_{11}, N_3, q)$

# *Algorithm for Gibbs sampler for chain binomial model*

1. Start with some initial values $(q^{(1)}, n_{111}^{(1)})$
2. For $t = 1$ to $M$ do
3. Sample $q^{(t+1)} \sim f(q|n_1, n_{11}, N_3, n_{111}^{(t)})$
4. Sample $n_{111}^{(t+1)} \sim f(n_{111}|n_1, n_{11}, N_3, q^{(t+1)})$
5. end for
6. How to get the two full conditionals in this model?

# *Full conditional of chain* $1 \longrightarrow 1 \longrightarrow 1$

- Assume $q$ is known
- Compute the conditional probability of chain $1 \to 1 \to 1$ when outbreak size is $N = 3$:

$$\Pr(1 \to 1 \to 1 | N = 3, q) = \frac{\Pr(N = 3, 1 \to 1 \to 1 | q)}{\Pr(N = 3 | q)}$$

$$= \frac{\Pr(N = 3 | 1 \to 1 \to 1, q) \Pr(1 \to 1 \to 1 | q)}{\Pr(N = 3 | 1 \to 1 \to 1, q) \Pr(1 \to 1 \to 1 | q) + \Pr(N = 3 | 1 \to 2, q) \Pr(1 \to 2 | q)}$$

$$= \frac{2p^2 q}{2p^2 q + p^2} = \frac{2q}{2q + 1}, \quad (0 \leq q < 1)$$

# *The full conditional of $n_{111}$*

- We have found that

$$\Pr(1 \to 1 \to 1 | N = 3, q) = \frac{2q}{2q+1}$$

- So the full conditional distribution of $n_{111}$ is

$$n_{111} | (n_1, n_{11}, N_3, q) \sim \text{Binomial}(275, 2q/(2q+1))$$

# *The full conditional of q*

- Assume that $n_{111}$ is known, that is, assume we know the complete data $(n_1, n_{11}, N_3, n_{111})$
- Assume a prior distribution for $q$: $q \sim \text{Beta}(\alpha, \beta)$,

$$f(q) \equiv f(q|\alpha, \beta) \propto q^{\alpha-1}(1-q)^{\beta-1}$$

- The full conditional distribution of $q$ :

$$f(q|n_1, n_{11}, N_3, n_{111}, \alpha, \beta) \propto f(n_1, n_{11}, N_3, n_{111}|q, \alpha, \beta) f(q|\alpha, \beta)$$

$$\propto \underbrace{q^{2n_1+2n_{11}+n_{111}} p^{n_{11}+2N_3}}_{\text{complete data likelihood}} \times \underbrace{q^{\alpha-1}(1-q)^{\beta-1}}_{\times \text{ prior}}$$

# *The full conditional of q*

- The full conditional distribution of $q$ is thus a Beta distribution

$$q|\text{complete data}, \alpha, \beta \sim \text{Beta}(2n_1 + 2n_{11} + n_{111} + \alpha, n_{11} + 2N_3 + \beta)$$

- A uniform prior on $q$ corresponds to $\alpha = 1$, $\beta = 1$.

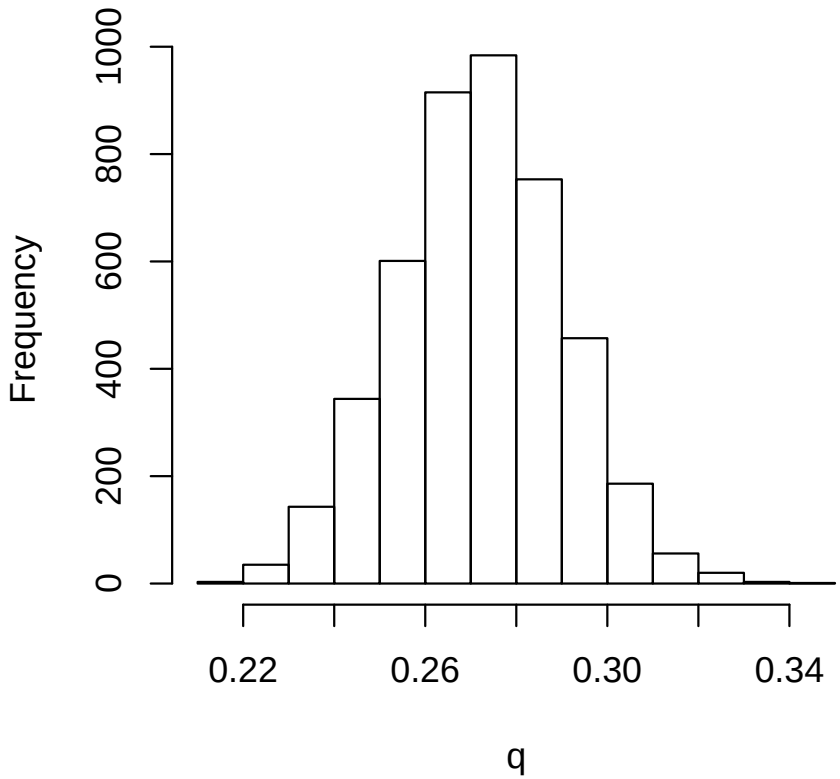
- With the complete data, a natural point estimate of the escape probability would be the mean of the Beta distribution, i.e., the proportion of "escapes" out of all exposures:

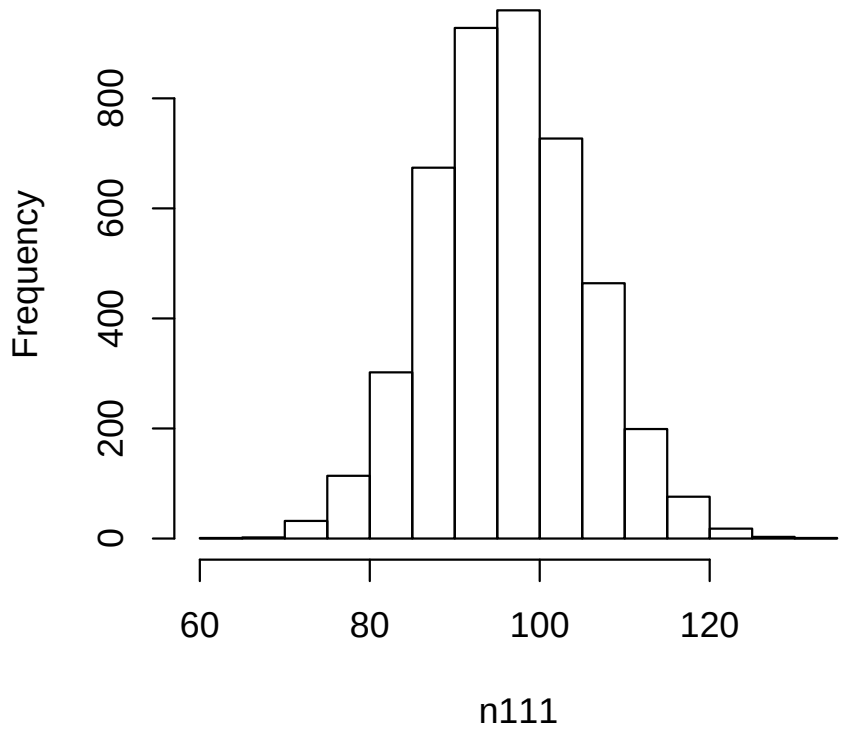
$$\frac{2n_1 + 2n_{11} + n_{111} + \alpha}{2n_1 + 3n_{11} + 3n_{111} + 2n_{12} + \alpha + \beta}$$

# *Algorithm for Gibbs sampler for chain binomial model*

1. Start with some initial values $(q^{(1)}, n_{111}^{(1)})$
2. For $t = 1$ to $M$ do
3. Sample $q^{(t+1)} \sim \text{Beta}(2n_1 + 2n_{11} + n_{111}^{(t)} + \alpha, n_{11} + 2N_3 + \beta)$
4. Sample $n_{111}^{(t+1)} \sim \text{Binomial}(275, 2q^{(t+1)}/(2q^{(t+1)} + 1))$
5. end for
6. Get summaries of the marginal posterior distributions.

# *Approx. posterior distributions of* $q$ *and* $n_{111}$



# *Lab: First Gibbs Sampler*

- Next will be the lab with first Gibbs sampler computational exercise.
- PracticalChain_binomial.pdf