SFS 2023 Short Course – Bayesian Applications in Environmental and Ecological Studies with R and Stan

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Introduction

- Statistical inference mode hypothetical deduction implemented through three basic "problems" (Fisher 1921)
 - 1. Problem of formulation what is the distribution of the response variable
 - 2. Problem of estimation how to estimate parameters of the model (from problem 1)
 - 3. Problem of distribution how to evaluate the model once we have the data
- A mathematical summary of statistical inference
 - The probability distribution density function of the response variable y: $\pi(y,\theta)$
 - Observing data $y_1, y_2 \cdots, y_n$, we want to know the joint distribution of $\pi(y_1, y_2, \cdots, y_n, \theta)$. True for both classical and Bayesian inference.
 - Classical statistics $\pi(y_1, \dots, y_n, \theta) = \pi(y_1, \dots, y_n \mid \theta)\pi(\theta)$ The likelihood function: $L(\theta; y) = \pi(y_1, \dots, y_n \mid \theta)$ and MLE

 - Sampling distribution uncertainty
 - Bayesian statistics -

 - * $\pi(y_1, \dots, y_n, \theta) = \pi(y_1, \dots, y_n \mid \theta) \pi(\theta) = \pi(\theta \mid y_1, \dots, y_n) \pi(y_1, \dots, y_n)$ * Posterior distribution $\pi(\theta \mid y_1, \dots, y_n) = \frac{\pi(y_1, \dots, y_n \mid \theta) \pi(\theta)}{\pi(y_1, \dots, y_n)} \propto \pi(y_1, \dots, y_n \mid \theta) \pi(\theta)$
 - * Combining estimation and distribution
- Bayesian inference is a generalization of MLE-based classical inference: MLE is the mode of posterior distribution with uniform prior

From Mathematics to Computation

- Derivative (classical) versus integration (Bayesian)
 - MLE: find parameter values that maximize the likelihood function $\hat{\theta} = arg \ max_{\theta \in \Theta} L(\theta; y)$
 - Bayesian: $\pi(\theta \mid y_1, \dots, y_n) = \frac{\pi(y_1, \dots, y_n \mid \theta) \pi(\theta)}{\int_{\pi} \pi(y_1, \dots, y_n \mid \theta) \pi(\theta) d\theta}$
- Classical statistics: a collection of efficient numerical algorithms for quantifying MLEs from a number of classes of models
 - Historically, tabulated results
 - Now, implemented in software such as SAS, SPSS, and R
- Bayesian statistics: Using Monte Carlo simulation to avoid integration
 - Markov chain Monte Carlo simulation (MCMC) algorithm drawing random numbers of θ from its density function (or a function proportional to its density function)
 - Posterior distributions of model parameters evaluated using random samples from their posterior distributions
 - The Bayesian posterior is proportional to $L(\theta; y_1, \dots, y_n)\pi(\theta)$
 - If y_1, \dots, y_n i.i.d., $L(\theta; y_1, \dots, y_n) = \prod_{i=1}^n L(\theta; y_i)$ and

- The posterior

$$\log (\pi(\theta \mid y_1, \dots, y_n)) = \log (\pi(\theta)) + \sum_{i=1}^n \log (L(\theta; y_i))$$

- Stan via rstanin R:
 - A program implements MCMC when $\log (\pi(\theta))$ and $\log (L(\theta; y_i))$ are provided.

Example – Snake Fungal Disease

- Estimating the prevalence of fungal infection in a population of protected snake species in Michigan
 - qPCR test with false positive rate (probability) f_p and false negative rate f_n .
 - In a sample of n snakes, y tested positive
 - What is the prevalence of the disease in the population (θ)
- Response variable y modeled by the binomial distribution

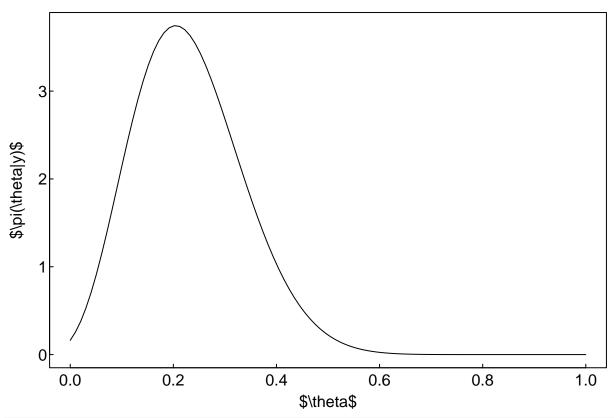
$$y \sim Bin(p, n)$$

where p is the probability of testing positive, and $p = \theta(1 - f_n) + (1 - \theta)f_p$

- The likelihood function $L = p^y(1-p)^{n-y}$
- Log likelihood: $\log(L) = y \log(p) + (n-y) \log(1-p)$
- Using a beta distribution prior for θ : $\pi(\theta) \propto \theta^{\alpha} (1-\theta)^{\beta}$
- The log posterior density $\pi(\theta \mid y, n) \propto \alpha \log(\theta) + \beta \log(1-\theta) + y \log(p) + (n-y) \log(1-p)$
- Computational options:
 - Classical statistics: $\hat{p} = y/n$, $\hat{\theta} = \frac{\hat{p} f_p}{1 (f_p + f_n)}$ (because MLE is transformation invariant). Uncertainty: variance of $\hat{p} \approx (1 \hat{p})\hat{p}/n$, variance of $\hat{\theta}$ is $(1/(1 f_p f_n))^2(1 \hat{p})\hat{p}/n$

```
n <- 20
y <- 5
fn <- 0.05
fp <- 0.07
p_hat <- y/n
p_hat_sd <- sqrt(p_hat*(1-p_hat)/n)
theta_hat <- (p_hat - fp)/(1-fp-fn)
theta_hat_sd <- p_hat_sd/(1-fp-fn)</pre>
```

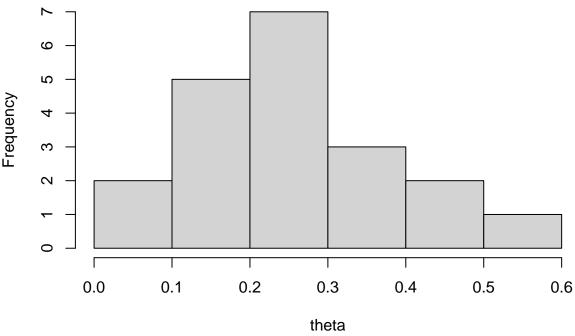
• Bayesian 1: brute force numerical integration Calculating the posterior density over a grid between 0 and 1 and normalize the results.



• Bayesian 2: Monte Carlo simulation Directly draw random numbers from the posterior distribution using the inverse-CDF method

```
## Using evenly spaced pdf from Chapter 1
post_impft_cdf <- function(x=5, n=20, fp=0.07, fn=0.05, k=100){
    theta <- seq(0, 1,, k)
    fpst <- theta*(1-fn) + (1-theta)*fp
    post <- x*log(fpst) + (n-x)*log(1-fpst)
    return(cumsum(exp(post)/sum(exp(post))))
}

post_cdf <- data.frame(theta=seq(0,1,,5000), cdf=post_impft_cdf(k=5000))
u <- runif(n)
tmp <- apply(post_cdf, 1, function(x, unf))</pre>
```



```
mean(theta)

## [1] 0.2572915

sd(theta)

## [1] 0.111202

median(theta)

## [1] 0.2474495

quantile(theta, prob=c(0.05,0.95))

## 5% 95%
```

• Bayesian 3: Using Metropolis-Hastings algorithm (See Section 2.4.1) An acceptance-rejection method (Section 2.3.2) with a candidate-generating distribution function and the acceptance probability probability is based on the ratio of posterior density function at two points. As a result, we only need to know the posterior density upto a proportional constant.

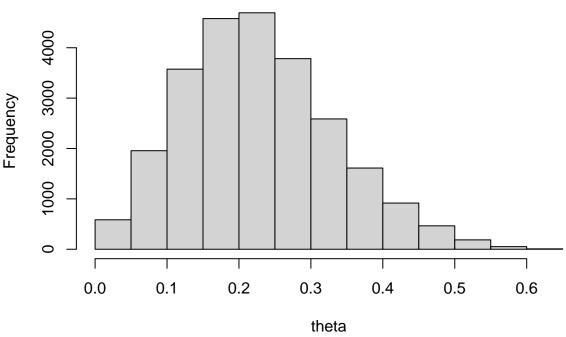
0.09684937 0.43089618

```
set.seed(10)
n_sims<-50000
theta <- numeric()
theta[1] <- runif(1) # initial value</pre>
```

```
n <- 20
x <- 5
log_lk <- function(theta, x=5, n=20, fp=0.07, fn=0.05){
    pp <- theta*(1-fn)+(1-theta)*fp
    llk <- x*log(pp)+(n-x)*log1p(-pp)
    return(llk)
}

for (j in 1:n_sims){
    y <- runif(1) ## unif(0,1) as the candidate-generating function
    alpha <- exp(log_lk(y)-log_lk(theta[j]))
    if (runif(1) < alpha) theta[j+1] <- y
    else theta[j+1] <- theta[j]
}

theta <- theta[round(1+n_sims/2):n_sims]
hist(theta)</pre>
```



```
mean(theta)

## [1] 0.2276803

sd(theta)

## [1] 0.104186

median(theta)
```

[1] 0.2176312

```
quantile(theta, prob=c(0.05,0.95))
## 5% 95%
## 0.07138723 0.41652067
```

Stan using rstan

• Bayesian 4: Using Stan The basic task of Bayesian computation is to derive the posterior distribution $\pi(\theta \mid y_1, \dots, y_n) \propto \pi(\theta) L(\theta; y_1, \dots, y_n)$

Using Stan, we draw random samples of the unknown parameters θ from their joint posterior distribution. As we know from the Metropolis-Hastings algorithm, we can draw random samples by knowing the posterior density upto a proportional constant. The rest can be automatic using a computer. In a Bayesian computing software, we need to provide three groups of information to formulate the MCMC algorithm. 1. Input data (e.g., y, n, f_p, f_n) 2. Parameters to be estimated 3. The likelihood function and prior distributions Stan puts the above three groups of information in three code blocks. For the snake fungal example, we have $x = 5, n = 20, f_p = 0.07$ and $f_n = 0.05$. The response variable (y) is assumed to follow a binomial distribution $y \sim Bin(p, n)$, with the probability of a positive result being $p = \theta(1 - f_n) + (1 - \theta)f_p$). Translating to Stan, we have

```
### Stan Code ###
snake_code1 <- "
  data{
    int<lower=1> n;
    int<lower=0> y;
    real<lower=0,upper=1> fn;
    real<lower=0,upper=1> fp;
}
parameters{
    real<lower=0,upper=1> theta;
}
model{
    theta ~ beta(1,1);
    y ~ binomial(n, theta*(1-fn) + (1-theta)*fp );
}
"
```

We can also specify log-likelihood function directly by changing the model block to:

or directly use the log-probability function come with Stan:

6

```
transformed parameters{
    real<lower=Omupper=1> p_pos;
    p_pos = theta*(1-fn)+(1-theta)*fp;
}
model{
    theta ~ beta(0,1);
    target += binomial_lpmf(y | n, p_pos);
}
```

Here we used beta(1,1) (the same as uniform between 0 and 1) as the non-informative prior of θ . Because its density is a constant, we can omit the line theta ~ beta(1,1);.

Before we can run the Stan (code snake_code1), we need to load the package rstan and set some options

```
packages(rv)
packages(rstan)
packages(car)
rstan_options(auto_write = TRUE)
options(mc.cores = min(c(parallel::detectCores(), 8)))

nchains <- min(c(parallel::detectCores(), 8))
niters <- 5000
nkeep <- 2500
nthin <- ceiling((niters/2)*nchains/nkeep)</pre>
```

After that, we typically follow the following steps.

fit1 <- stan_model(model_code = snake_code1)</pre>

1. Compile the model

##

##

```
## Trying to compile a simple C file
## Running /usr/lib/R/bin/R CMD SHLIB foo.c
## using C compiler: 'gcc (Ubuntu 11.3.0-1ubuntu1~22.04) 11.3.0'
## gcc -I"/usr/share/R/include" -DNDEBUG
                                          -I"/usr/lib/R/site-library/Rcpp/include/" -I"/usr/lib/R/sit
## In file included from /usr/lib/R/site-library/RcppEigen/include/Eigen/Core:88,
##
                    from /usr/lib/R/site-library/RcppEigen/include/Eigen/Dense:1,
                    from /usr/lib/R/site-library/StanHeaders/include/stan/math/prim/mat/fun/Eigen.hpp:1
##
##
                    from <command-line>:
## /usr/lib/R/site-library/RcppEigen/include/Eigen/src/Core/util/Macros.h:628:1: error: unknown type na
##
     628 | namespace Eigen {
         | ^~~~~~
##
  /usr/lib/R/site-library/RcppEigen/include/Eigen/src/Core/util/Macros.h:628:17: error: expected '=',
##
     628 | namespace Eigen {
##
```

/usr/lib/R/site-library/RcppEigen/include/Eigen/Core:96:10: fatal error: complex: No such file or di

2. Organizing input data, initial values, and parameters to monitor using a function

from <command-line>:

make: *** [/usr/lib/R/etc/Makeconf:191: foo.o] Error 1

96 | #include <complex>

compilation terminated.

In file included from /usr/lib/R/site-library/RcppEigen/include/Eigen/Dense:1,

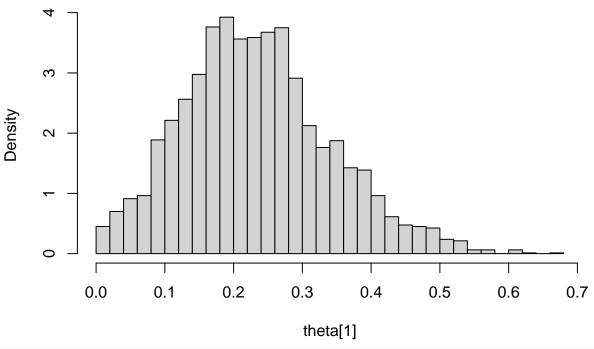
```
input_snake <- function(y=5, n=20, nchns=nchains){
  data <- list(y=y,n=n, fp=0.07,fn=0.05)
  inits <- list()
  for (i in 1:nchns)
    inits[[i]] <- list(theta=runif(1))
    pars=c("theta")
  return(list(data=data, inits=inits, pars=pars))
}</pre>
```

3. Run the model

```
input.to.stan <- input_snake()</pre>
fit2keep <- sampling(fit1, data = input.to.stan$data,</pre>
                     init=input.to.stan$inits,
                     pars = input.to.stan$pars,
                     iter=niters, thin=nthin,
                     chains=nchains)
print(fit2keep)
## Inference for Stan model: c835acd4430be9e9eca5cbd7565db810.
## 8 chains, each with iter=5000; warmup=2500; thin=8;
## post-warmup draws per chain=313, total post-warmup draws=2504.
##
##
                                                     75% 97.5% n_eff Rhat
           mean se_mean
                          sd
                               2.5%
                                       25%
                                              50%
                                     0.16
## theta
           0.23
                   0.00 0.11
                               0.05
                                             0.23
                                                    0.30
                                                          0.47 2526
## lp__ -13.60
                   0.02 0.89 -16.20 -13.77 -13.25 -13.05 -13.00 2183
                                                                          1
## Samples were drawn using NUTS(diag_e) at Fri May 12 13:45:39 2023.
## For each parameter, n_eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor on split chains (at
## convergence, Rhat=1).
```

4. Processing output

```
stan_out <- rstan::extract(fit2keep)
theta <- rvsims(stan_out$theta)
rvhist(theta)</pre>
```



quantile(stan_out\$theta, prob=c(0.05,0.95))

5% 95% ## 0.07248955 0.42349034

Why Bayesian?

With Stan, Bayesian inference can be readily applied to more complex problems that are impossible for classical MLE. More importantly, Bayesian inference using Stan can provide useful information on model formulation and identify potential problems. Bayesian inference is also the best approach for information accumulation.

Information accumulation

Suppose that we conducted a new survey of the snake fungal disease a year after the initial study to update the prevalence. Or, we may want to evaluate the temporal trend of the disease prevalence in the subsequent years.

All the methods we used resulted in a consistent estimate of the prevalence of about 22% with a wide range of between 0.07-0.4. The uncertainty reflects the small sample size. Suppose that we now have a new sample of $n_2 = 12$ and $y_2 = 4$. Using classical statistics, we either estimate the prevalence using only the second sample, assuming that the prevalence has changed or combine the data (i.e., n = 35 and y = 9), assuming the population stays the same.

With a Bayesian approach, we can summarize the posterior of θ from the first sample to form a prior of θ and update the prior using the new data. We typically use a beta distribution to summarize the distribution of a probability. Given the mean and standard deviation of 0.23 and 0.11 (from the Stan model), we propose a beta distribution with parameters $\alpha = 3.52$ and $\beta = 11.56$ (based on the method of moments). The prior can also be from similar studies elsewhere. All we need is an estimate of the mean and a likely range. We can treat the likely range as the usual 95% confidence interval (roughly 4 times standard deviation), from which derive a rough estimate of the standard deviation.

```
ybar <- mean(stan_out$theta)
s2 <- var(stan_out$theta)
alpha0 <- ybar*(ybar*(1-ybar)/s2 - 1)
beta0 <- alpha0*(1-ybar)/ybar
alpha0+beta0</pre>
```

[1] 14.58325

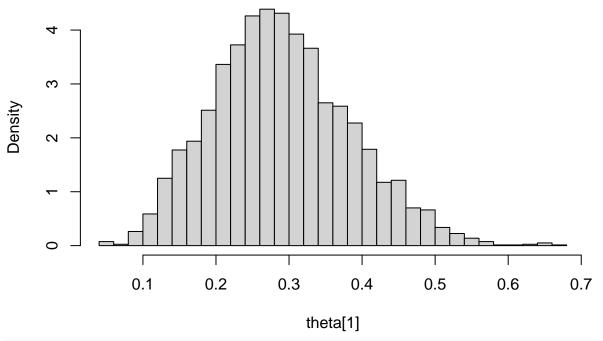
Once the initial estimates of α_0 and β_0 are available, we can further revise the estimate based on our assessment of the relevancy of the prior to our data at hand. For example, the relevancy of the prior may be measured by $\alpha + \beta$ if we interpret the sum as the sample size from which the prior was derived. For example, $\alpha_0 + \beta_0 = 15$, somewhat smaller than the sample size we used (20), perhaps, because of the imperfect detection of the qPCR method. If we want to weight the prior less than 15 data points, we can rescale the prior parameter by setting $\alpha_0 + \beta_0 = n_0$ while keeping $\alpha_0/(\alpha_0 + \beta_0)$ the same (equals to \bar{y}).

We now need additional data for the model:

```
### Stan Code ###
snake_code2 <- "</pre>
  data{
    int<lower=1> n;
    int<lower=0> y;
    real<lower=0,upper=1> fn;
    real<lower=0,upper=1> fp;
    real<lower=0> alpha0;
    real<lower=0> beta0;
  }
  parameters{
    real<lower=0,upper=1> theta;
  transformed parameters{
   real<lower=0,upper=1> p_pos;
   p_pos = theta*(1-fn)+(1-theta)*fp;
}
model{
   theta ~ beta(alpha0,beta0);
   target += binomial_lpmf(y | n, p_pos);
}
11
fit2 <- stan model(model code = snake code2)
## Trying to compile a simple C file
```

```
## Running /usr/lib/R/bin/R CMD SHLIB foo.c
## using C compiler: 'gcc (Ubuntu 11.3.0-1ubuntu1~22.04) 11.3.0'
## gcc -I"/usr/share/R/include" -DNDEBUG
                                          -I"/usr/lib/R/site-library/Rcpp/include/" -I"/usr/lib/R/sit
## In file included from /usr/lib/R/site-library/RcppEigen/include/Eigen/Core:88,
##
                    from /usr/lib/R/site-library/RcppEigen/include/Eigen/Dense:1,
##
                    from /usr/lib/R/site-library/StanHeaders/include/stan/math/prim/mat/fun/Eigen.hpp:1
##
                    from <command-line>:
##
  /usr/lib/R/site-library/RcppEigen/include/Eigen/src/Core/util/Macros.h:628:1: error: unknown type na
##
     628 | namespace Eigen {
         | ^~~~~~
##
## /usr/lib/R/site-library/RcppEigen/include/Eigen/src/Core/util/Macros.h:628:17: error: expected '=',
```

```
##
     628 | namespace Eigen {
##
## In file included from /usr/lib/R/site-library/RcppEigen/include/Eigen/Dense:1,
                    from /usr/lib/R/site-library/StanHeaders/include/stan/math/prim/mat/fun/Eigen.hpp:1
##
                    from <command-line>:
## /usr/lib/R/site-library/RcppEigen/include/Eigen/Core:96:10: fatal error: complex: No such file or di
      96 | #include <complex>
##
##
## compilation terminated.
## make: *** [/usr/lib/R/etc/Makeconf:191: foo.o] Error 1
input_snake2 <- function(n=12, y=5, alpha, beta, nchns=nchains){
  data <- list(y=y,n=n, fp=0.07,fn=0.05, alpha0=alpha, beta0=beta)
  inits <- list()</pre>
  for (i in 1:nchns)
    inits[[i]] <- list(theta=runif(1))</pre>
 pars=c("theta")
  return(list(data=data, inits=inits, pars=pars))
input.to.stan <- input_snake2(alpha=alpha0, beta=beta0)</pre>
fit2keep <- sampling(fit2, data = input.to.stan$data,</pre>
                     init=input.to.stan$inits,
                     pars = input.to.stan$pars,
                     iter=niters, thin=nthin,
                     chains=nchains)
print(fit2keep)
## Inference for Stan model: dbd499ca160d39389db648d57b572370.
## 8 chains, each with iter=5000; warmup=2500; thin=8;
## post-warmup draws per chain=313, total post-warmup draws=2504.
##
                          sd
                                2.5%
                                        25%
                                              50%
                                                    75% 97.5% n_eff Rhat
           mean se_mean
## theta
           0.29
                   0.00 0.09
                               0.13
                                     0.22 0.28 0.35 0.49 2453
                   0.02\ 0.74\ -12.30\ -10.45\ -9.99\ -9.80\ -9.75\ 2315
## lp__ -10.27
## Samples were drawn using NUTS(diag_e) at Fri May 12 13:46:03 2023.
## For each parameter, n_eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor on split chains (at
## convergence, Rhat=1).
stan_out <- rstan::extract(fit2keep)</pre>
theta <- rvsims(stan_out$theta)</pre>
rvhist(theta)
```



```
quantile(stan_out$theta, prob=c(0.05,0.95))
```

```
## 5% 95%
## 0.1432169 0.4541387
```

From here, we can evaluate whether the prevalence is increased by calculating the probability that the posterior is larger than the prior:

```
prior<-rvbeta(1, alpha0, beta0)
Pr(theta>prior)
```

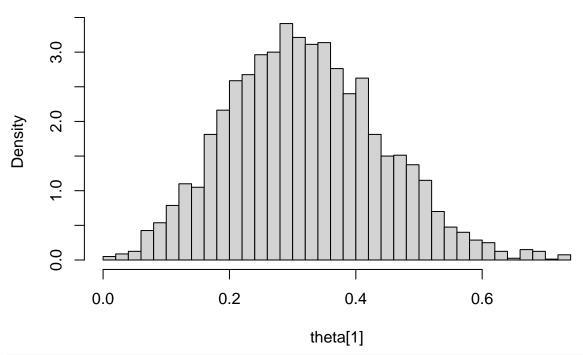
[1] 0.67475

If we down weight the prior by setting $\alpha_0 + \beta_0 = 6$, half of the data from the current year, the new prior data are n = 12, y = 5, we simply rerun the model by changing only the input data:

```
## Inference for Stan model: dbd499ca160d39389db648d57b572370.
## 8 chains, each with iter=5000; warmup=2500; thin=8;
## post-warmup draws per chain=313, total post-warmup draws=2504.
##
## mean se_mean sd 2.5% 25% 50% 75% 97.5% n_eff Rhat
```

```
## theta 0.32    0.00 0.12 0.10 0.24 0.31 0.40 0.56 2613    1
## lp__ -5.50    0.02 0.81 -7.94 -5.66 -5.19 -5.01 -4.96 2459    1
##
## Samples were drawn using NUTS(diag_e) at Fri May 12 13:46:06 2023.
## For each parameter, n_eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor on split chains (at
## convergence, Rhat=1).

stan_out <- rstan::extract(fit2keep)
theta <- rvsims(stan_out$theta)
rvhist(theta)</pre>
```



```
quantile(stan_out$theta, prob=c(0.05,0.95))
## 5% 95%
## 0.1273145 0.5224719
Pr(theta>prior)
```

[1] 0.7095

Realistic modeling

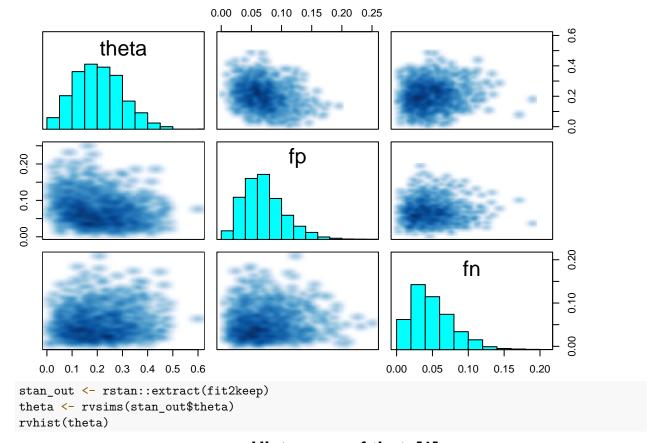
Most likely, we don't know exactly the values of f_p and f_n . But we may have prior knowledge on their likely values, from which we can derive prior distributions of f_p and f_n . For example, the values $f_p = 0.07$ and $f_n = 0.05$ are estimated from similar tests elsewhere based on over 50 tests. We can use the beta distribution to quantify the prior knowledge:

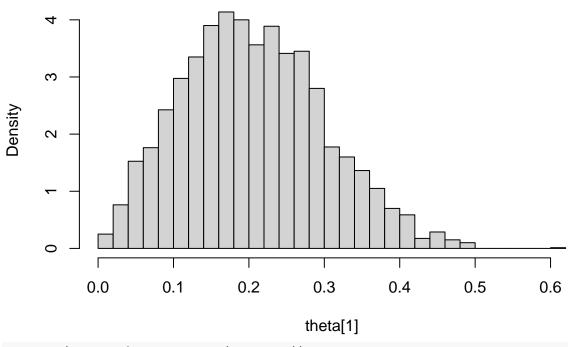
```
a_p < 0.07*50
b_p < 50-a_p
a_n < 0.05*50
b_n = 50-a_n
```

Now the only change needed is to include f_p and f_n as parameters and their the priors:

```
### Stan Code ###
snake code3 <- "
  data{
    int<lower=1> n;
    int<lower=0> y;
    real<lower=0> alpha0;
    real<lower=0> beta0;
    real<lower=0> a_p;
    real<lower=0> b_p;
    real<lower=0> a_n;
    real<lower=0> b_n;
  }
  parameters{
    real<lower=0,upper=1> theta;
    real<lower=0,upper=1> fn;
    real<lower=0,upper=1> fp;
  transformed parameters{
   real<lower=0,upper=1> p_pos;
   p_pos = theta*(1-fn)+(1-theta)*fp;
model{
   theta ~ beta(alpha0,beta0);
   fp ~ beta(a_p, b_p);
   fn ~ beta(a_n, b_n);
   target += binomial_lpmf(y | n, p_pos);
}
fit3 <- stan_model(model_code = snake_code3)</pre>
## Trying to compile a simple C file
## Running /usr/lib/R/bin/R CMD SHLIB foo.c
## using C compiler: 'gcc (Ubuntu 11.3.0-1ubuntu1~22.04) 11.3.0'
## gcc -I"/usr/share/R/include" -DNDEBUG
                                           -I"/usr/lib/R/site-library/Rcpp/include/"
                                                                                        -I"/usr/lib/R/sit
## In file included from /usr/lib/R/site-library/RcppEigen/include/Eigen/Core:88,
##
                    from /usr/lib/R/site-library/RcppEigen/include/Eigen/Dense:1,
##
                    from /usr/lib/R/site-library/StanHeaders/include/stan/math/prim/mat/fun/Eigen.hpp:1
                    from <command-line>:
##
## /usr/lib/R/site-library/RcppEigen/include/Eigen/src/Core/util/Macros.h:628:1: error: unknown type na
##
     628 | namespace Eigen {
         | ^~~~~~~
##
  /usr/lib/R/site-library/RcppEigen/include/Eigen/src/Core/util/Macros.h:628:17: error: expected '=',
##
##
     628 | namespace Eigen {
##
## In file included from /usr/lib/R/site-library/RcppEigen/include/Eigen/Dense:1,
##
                    from /usr/lib/R/site-library/StanHeaders/include/stan/math/prim/mat/fun/Eigen.hpp:1
##
                    from <command-line>:
  /usr/lib/R/site-library/RcppEigen/include/Eigen/Core:96:10: fatal error: complex: No such file or di
##
##
      96 | #include <complex>
                    ^~~~~~~
##
## compilation terminated.
```

```
## make: *** [/usr/lib/R/etc/Makeconf:191: foo.o] Error 1
input_snake3 <- function(n=20, y=5, alpha, beta, ap, bp, an, bn, nchns=nchains){
  data <- list(y=y,n=n, fp=0.07,fn=0.05, alpha0=alpha, beta0=beta, a_p=ap, b_p=bp, a_n=an, b_n=bn)
  inits <- list()</pre>
  for (i in 1:nchns)
    inits[[i]] <- list(theta=runif(1))</pre>
 pars=c("theta", "fp", "fn")
 return(list(data=data, inits=inits, pars=pars))
}
input.to.stan <- input_snake3(alpha=alpha0, beta=beta0, ap=a_p, an=a_n, bp=b_p, bn=b_n)
fit2keep <- sampling(fit3, data = input.to.stan$data,</pre>
                     init=input.to.stan$inits,
                     pars = input.to.stan$pars,
                     iter=niters, thin=nthin,
                     chains=nchains)
print(fit2keep)
## Inference for Stan model: 0475852eeb748112a6964ce34adbc0ce.
## 8 chains, each with iter=5000; warmup=2500; thin=8;
## post-warmup draws per chain=313, total post-warmup draws=2504.
##
##
           mean se mean
                          sd
                               2.5%
                                       25%
                                              50%
                                                      75% 97.5% n eff Rhat
## theta
           0.21
                   0.00 0.09
                               0.04
                                      0.14
                                             0.20
                                                     0.27
                                                            0.40 2477
                               0.02
                                      0.05
## fp
           0.07
                   0.00 0.03
                                             0.07
                                                     0.09
                                                            0.15 2476
                                                                          1
                   0.00 0.03
                               0.01
                                      0.03
                                             0.04
## fn
           0.05
                                                    0.07
                                                            0.12 2716
                                                                          1
                   0.02 1.26 -32.30 -29.64 -28.74 -28.13 -27.61 2666
## lp__ -29.05
## Samples were drawn using NUTS(diag_e) at Fri May 12 13:46:31 2023.
## For each parameter, n_eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor on split chains (at
## convergence, Rhat=1).
pairs(fit2keep, pars=c("theta", "fp", "fn"))
## Warning in par(usr): argument 1 does not name a graphical parameter
## Warning in par(usr): argument 1 does not name a graphical parameter
## Warning in par(usr): argument 1 does not name a graphical parameter
```





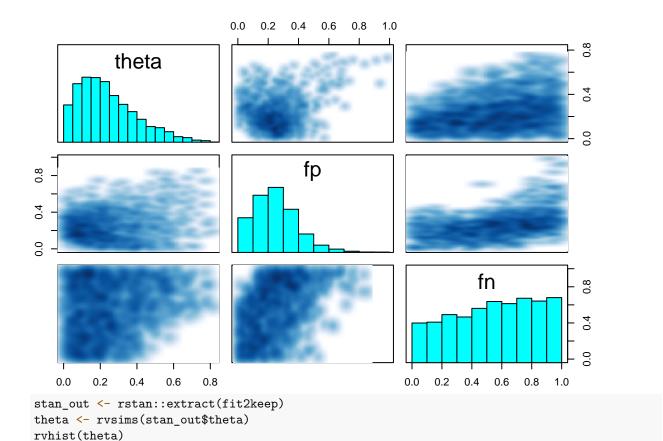
quantile(stan_out\$theta, prob=c(0.05,0.95))

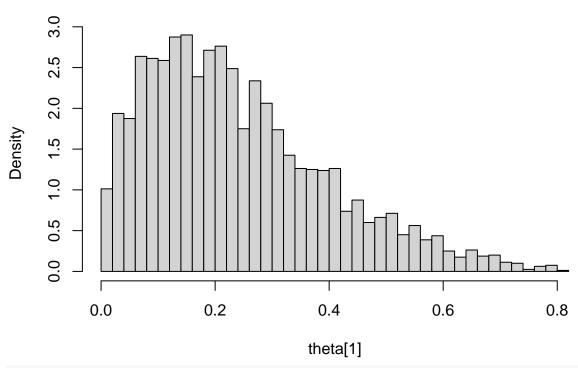
5% 95%

Identifiability

What happens if we have no prior information of f_p and f_n ? We could try to use non-informative prior beta(1,1) (uniform between 0 and 1). However, it is unlikely that we can simultaneously identify all three parameters. Mathematically, information in the data is represented in the likelihood function, consisting of products of θf_p and θf_n . In other words, the data have information of the two products. To definitely separate them, we need additional information. If we can try because we can, Stan will let us know that something is wrong.

```
input.to.stan <- input_snake3(alpha=alpha0, beta=beta0, ap=1, an=1, bp=1, bn=1)
fit2keep <- sampling(fit3, data = input.to.stan$data,
                     init=input.to.stan$inits,
                     pars = input.to.stan$pars,
                     iter=niters, thin=nthin,
                     chains=nchains)
print(fit2keep)
## Inference for Stan model: 0475852eeb748112a6964ce34adbc0ce.
## 8 chains, each with iter=5000; warmup=2500; thin=8;
## post-warmup draws per chain=313, total post-warmup draws=2504.
##
##
                              2.5%
                                      25%
                                             50%
                                                   75% 97.5% n_eff Rhat
          mean se_mean
                         sd
## theta
         0.24
                  0.00 0.16
                              0.02
                                     0.12
                                           0.21
                                                  0.33
                                                       0.61
                                                              2231
                  0.00 0.14
                              0.02
                                     0.14
                                           0.24
                                                  0.33
                                                       0.59
                                                              2542
## fp
          0.25
                                                                      1
## fn
          0.55
                  0.01 0.28
                              0.03
                                     0.32
                                           0.57
                                                 0.79 0.98
                                                              2172
                                                                      1
## lp__
         -9.72
                  0.03 1.39 -13.27 -10.34 -9.36 -8.71 -8.16
                                                              2412
                                                                      1
## Samples were drawn using NUTS(diag_e) at Fri May 12 13:46:35 2023.
## For each parameter, n eff is a crude measure of effective sample size,
## and Rhat is the potential scale reduction factor on split chains (at
## convergence, Rhat=1).
pairs(fit2keep, pars=c("theta", "fp", "fn"))
## Warning in par(usr): argument 1 does not name a graphical parameter
## Warning in par(usr): argument 1 does not name a graphical parameter
## Warning in par(usr): argument 1 does not name a graphical parameter
```





quantile(stan_out\$theta, prob=c(0.05,0.95))

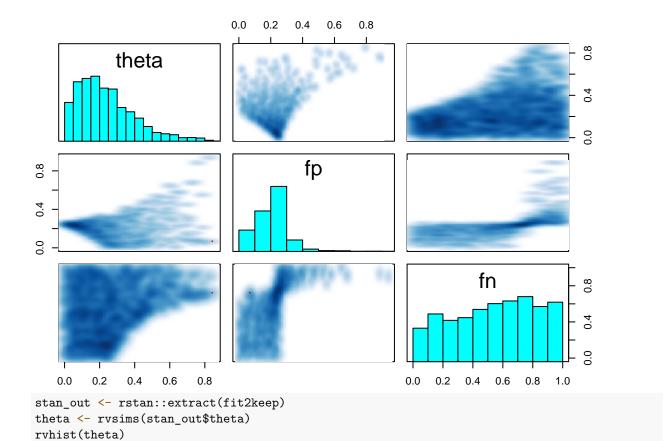
5% 95%

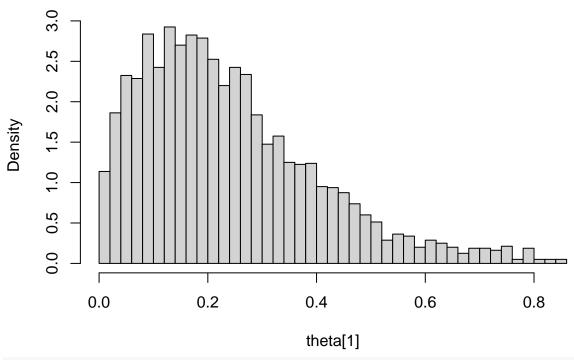
0.03663341 0.55183609 To show the non-identifiability clearly, we increase the sample size from n=20 to n=2000input.to.stan <- input_snake3(n=2000, y=500, alpha=alpha0, beta=beta0, ap=1, an=1, bp=1, bn=1) fit2keep <- sampling(fit3, data = input.to.stan\$data,</pre> init=input.to.stan\$inits, pars = input.to.stan\$pars, iter=niters, thin=nthin, chains=nchains) ## Warning: There were 1 divergent transitions after warmup. See ## https://mc-stan.org/misc/warnings.html#divergent-transitions-after-warmup ## to find out why this is a problem and how to eliminate them. ## Warning: Examine the pairs() plot to diagnose sampling problems ## Warning: Tail Effective Samples Size (ESS) is too low, indicating posterior variances and tail quant ## Running the chains for more iterations may help. See ## https://mc-stan.org/misc/warnings.html#tail-ess print(fit2keep) ## Inference for Stan model: 0475852eeb748112a6964ce34adbc0ce. ## 8 chains, each with iter=5000; warmup=2500; thin=8; ## post-warmup draws per chain=313, total post-warmup draws=2504. ## ## mean se_mean 2.5% 25% 50% 75% 97.5% n_eff Rhat sd 0.24 0.00 0.16 0.02 ## theta 0.12 0.21 0.33 0.65 1128 1.01 ## fp 0.21 0.00 0.10 0.03 0.15 0.22 0.26 0.41 1627 1.00 ## fn 0.54 0.01 0.28 0.04 0.31 0.56 0.78 0.98 2319 1.00 ## lp__ -12.15 0.04 1.42 -15.77 -12.78 -11.80 -11.13 -10.52 1416 1.00 ## ## Samples were drawn using NUTS(diag_e) at Fri May 12 13:46:39 2023. ## For each parameter, n eff is a crude measure of effective sample size, ## and Rhat is the potential scale reduction factor on split chains (at ## convergence, Rhat=1).

pairs(fit2keep, pars=c("theta", "fp", "fn"))

Warning in par(usr): argument 1 does not name a graphical parameter
Warning in par(usr): argument 1 does not name a graphical parameter

Warning in par(usr): argument 1 does not name a graphical parameter





quantile(stan_out\$theta, prob=c(0.05,0.95))

5% 95%

0.03559549 0.55986941

Examine the marginal distributions is not enough.

Summary

Using Stan in R is a natural way for implementing Bayesian modeling. Writing the Stan model requires us explicitly formulate a model, identify parameters of interest, and provide any prior information we have on the parameters. The strong diagnostic feature of Stan makes model evaluation simple. A typical Bayesian inference workflow starts with writing down the response variable model (what is the likely probability distribution model and how the mean parameter relates to predictors). From the likelihood function, we identify parameters of interest and relevant prior information. We then organize all available information into three basic blocks (data, parameters, and model) to construct the Stan model code. Because the MCMC algorithm in Stan is constructed through a function proportional to the log-posterior density, the log-likelihood function in a Stan model does not have to be based on a known distribution function (e.g., the normal distribution).