### STAT314/461 Bayesian Inference

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### Things to discuss

- lab this week
- office hours
- Week 6

#### What we will cover this term

not necessarily in exactly this order

- Bayesian computation from direct simulation to Markov Chain Monte Carlo methods.
  - rejection sampling
  - importance sampling
  - Metropolis-Hastings algorithm
  - Gibbs Sampler
- Hierarchical Models
- Problems of the "missing data type"

Computation will be in R

#### **Assignments**

- 20/09 due 1/10 max 10% for STAT314
- 4/10 due 15/10, max 10% for STAT314
- exact dates may change depending on how fast we go.

Best 4 of 5 assignments will count for your grade.

### Things we need to know about aside from Bayesian Inference

- logistic regression
- multivariate normal distribution (see dmvnorm() in the mvtnorm package)
- R programming:
  - For loops
  - While loops
  - functions using and writing?
- setting priors

### Recap on Bayesian Inference

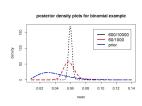
### Recap on Bayesian Inference: Some big Bayesian ideas

#### What is Bayesian modelling?

- An approach to statistical modelling which makes explicit use of probability models for
  - observables (data)
  - parameters of models
- Uses the data actually observed to update the prior distribution (pre-data) for the parameters to a posterior distribution (post-data);  $p(\theta|\text{data})$
- "Statistics is the study of uncertainty; Uncertainty should be measured by probability." (Denis Lindley, 2000)

#### Review some basics

The aim is always p(unknown|data)



- aka the posterior distribution think "post-data" distribution
- computation of the posterior requires:
  - a model for the data
  - a model for the parameters of the data model the "prior" or "prior model"
  - $(model \equiv statistical model (recognises uncertainty))$
- the prior (think "pre-data" or "pre current data) allows information about the problem that is not in the data to be brought to the analysis

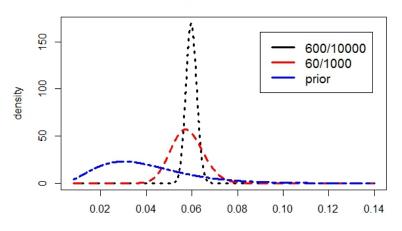
### Some features of Bayesian modelling and inference

- A full distribution is available for inference; not just point estimates, standard errors and intervals.
- So its easy to make inferences like  $Pr(\theta > c|\text{data}) = 0.1$ .
- Given a posterior distribution for model parameters, inferences for observables not yet seen follows straightforwardly from the rules of probability theory.

#### The idea of using a distribution for inference

Suppose we are interested in estimating a binomial proportion; e.g proportion unemployed:

#### posterior density plots for binomial example



#### Bayesian Inference: More formally

Suppose Y denotes some variable of interest, e.g. income  $Y_i$  - value of Y for  $i^{th}$  individual

**Y** collection of *Y* values,  $\mathbf{Y} = (Y_1, Y_2, ...)$ 

We model  ${f Y}$  as a random variable with distribution

$$p(\mathbf{Y}|\theta) = f_{\mathbf{Y}}(\mathbf{Y}|\theta) \tag{1}$$

Usually assume conditional independence so

$$p(\mathbf{Y}|\theta) = \prod_{i} p(Y_{i}|\theta) = \prod_{i} f_{Y}(Y_{i}|\theta)$$
 (2)

We observe  $\mathbf{Y}^{obs} = (Y_1, Y_2, \dots, Y_n)$ 

The first job for a Bayesian is to compute

$$p(\theta|\mathbf{Y}^{obs}) = \frac{p(\mathbf{Y}^{obs}|\theta)p(\theta)}{\int p(\mathbf{Y}^{obs}|\theta)p(\theta) \,\mathrm{d}\theta}$$
$$\propto p(\mathbf{Y}^{obs}|\theta)p(\theta)$$

(3)

#### Bayesian Inference: Likelihood and Prior

$$p(\theta|\mathbf{Y}^{obs}) \propto p(\mathbf{Y}^{obs}|\theta)p(\theta)$$
 (4)  
 Likelihood × Prior

**Likelihood** - probability density for observing the data actually seen, under the assumed model; a function of  $\theta$ . Compute it using the model  $p(\mathbf{Y}|\theta) = f_{\mathbf{Y}}(\mathbf{Y}|\theta)$ .

Under conditional independence  $p(\mathbf{Y}|\theta) = \prod_{i=1}^{i=n} f_{\mathbf{Y}}(Y_i|\theta)$ . e.g. suppose  $\mathbf{Y}^{obs} = (400, 1012, 961)$ ; assuming conditional independence (given  $\theta$ ), the likelihood function is

$$p(\mathbf{Y}^{obs}|\theta) = f_Y(400|\theta) \times f_Y(1012|\theta) \times f_Y(961|\theta)$$
 (5)

**Prior** - probability model for  $\theta$  which represents information about  $\theta$  that is not contained in the observed data.

#### Bayesian Inference for observables not yet seen

e.g. for

- future observations
- missing observations

Just use probability theory to compute

$$p(\mathbf{Y}^{new}|\mathbf{Y}^{obs}) = \int p(\mathbf{Y}^{new}|\mathbf{Y}^{obs},\theta)p(\theta|Y^{obs}) d\theta$$
 (6)

Can think of integration as Monte Carlo simulation

- draw  $\theta$  from  $p(\theta|\mathbf{Y}^{obs})$
- draw  $\mathbf{Y}^{new}$  from  $p(\mathbf{Y}^{new}|\mathbf{Y}^{obs},\theta)$ . Under conditional independence this amounts making independent draws from the data model  $p(Y|\theta) = f_Y(Y|\theta)$ .

#### Likelihood, prior and Bayesian computation

$$p(\theta|\mathbf{Y}^{obs}) = \frac{p(\mathbf{Y}^{obs}|\theta)p(\theta)}{\int p(\mathbf{Y}^{obs}|\theta)p(\theta) d\theta}$$
(7)

- But notice we have been emphasising the numerator of (7), sometimes called the unnormalised posterior  $q(\theta|\mathbf{Y}^{obs}) = p(\mathbf{Y}^{obs}|\theta)p(\theta)$ .
- The Monte Carlo methods we will study generally only need the unnormalised posterior.
- This is a good thing:
  - We specify the prior; we derive the likelihood from the model for the data that we specify. Hence the unnormalised posterior can always be written down and computed.
  - In realistic applications the integration in the denominator can be high-dimensional and difficult.

# Introduction to Monte Carlo methods for Bayesian Computation

# Some basic ideas in the use of Monte Carlo methods for posterior computation (1)

- Suppose we can simulate from  $p(\theta|\mathbf{Y}^{obs})$
- Let  $h(\theta)$  be some function of  $\theta$
- We can approximate  $E(h(\theta)|\mathbf{Y}^{obs}) = \int h(\theta)p(\theta|\mathbf{Y}^{obs}) d\theta$  using the following Monte Carlo (MC) algorithm
  - (i) for i in  $1: n_{\text{sim}}$  draw  $\theta_{(i)}$  from  $p(\theta|\mathbf{Y^{obs}})$  compute  $h_{(i)} = h(\theta_{(i)})$  store  $\theta_{(i)}, h_{(i)}$
  - (ii) set

$$\hat{E}(h(\theta)|\mathbf{Y}^{\mathbf{obs}}) = \frac{\sum_{i=1}^{n_{sim}} h_{(i)}}{n_{sim}}$$

### Basic ideas in Monte Carlo computation (2)

Many things we are interested in are integrals and can be written as expectations of  $h(\theta)$  for some choice of  $h(\theta)$ :

**Expectation**:  $h(\theta) = \theta$ 

$$E(\theta|\mathbf{Y}^{obs}) = \int \theta p(\theta|\mathbf{Y}^{obs}) \,\mathrm{d}\theta$$

**Variance**:  $h(\theta) = (\theta - E(\theta|\mathbf{Y}^{obs}))^2$ 

$$V(\theta)|\mathbf{Y}^{obs}) = \int (\theta - E(\theta|\mathbf{Y}^{obs}))^2 p(\theta|\mathbf{Y}^{obs}) d\theta$$

**Tail probability** e.g.  $h(\theta) = I_c(\theta)$ , where  $I_c(\theta) = 1$  if  $\theta \le c$ ;  $I_c(\theta) = 0$  if  $\theta > c$ .

$$Pr(\theta < c|\mathbf{Y}^{obs}) = \int_{\infty}^{c} p(\theta|\mathbf{Y}^{obs}) d\theta$$
$$= \int I_{c}(\theta) p(\theta|\mathbf{Y}^{obs}) d\theta$$

#### Basic ideas in Monte Carlo computation:(2b)

**Interval Probability**  $h(\theta) = I_{(a,b)}(\theta) = 1$  if  $a \le \theta \le b$ ;  $I_{(a,b)} = 0$ , otherwise.

$$\Pr(a \le \theta \le b | \mathbf{Y}^{obs}) = \int_{a}^{b} p(\theta | \mathbf{Y}^{obs}) \, \mathrm{d}\theta \tag{8}$$

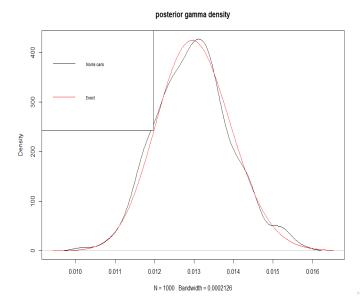
$$\int I_{(a,b)}(\theta) p(\theta|\mathbf{Y}^{obs}) d\theta \tag{9}$$

So, generate  $\theta=(\theta_1,\ldots,\theta_M)$  from the posterior, count up the number of theta values falling in (a,b) and divide by M. As  $b\to a$  this gets pretty close to density estimation. e.g.

plot(density(rgamma(n=1000, shape=alpha+sumY,
rate=beta+sumN))

General idea, in practice, is to draw values of  $\theta$  from  $p(\theta|\mathbf{Y}^{obs})$  and approximate features of the posterior by the corresponding features of the sample of  $\theta$  values.

### Compare Monte Carle density estimate with exact density



### Basic ideas in Monte Carlo computation (3)

Recall:

$$p(\theta|\mathbf{Y}^{obs}) = \frac{p(\mathbf{Y}^{obs}|\theta)p(\theta)}{\int p(\mathbf{Y}^{obs}|\theta)p(\theta) d\theta}$$
(10)

Setting  $h(\theta) = p(\mathbf{Y}^{obs}|\theta)$ , i.e the likelihood, we can see that the normalising constant (denominator) in the posterior also has the form of an expectation, but over the prior. So this is a bit different from the other examples where integration is over the posterior for  $\theta$ . In principle we could apply the standard MC algorithm to approximate  $K(\mathbf{Y}^{obs}) = \int p(\mathbf{Y}^{obs}|\theta)p(\theta)\,\mathrm{d}\theta$  by repeatedly sampling values from  $p(\theta)$ , computing  $p(\mathbf{Y}^{obs}|\theta) = \prod_{i=1}^n p(Y_i|\theta)$  for each generated theta, and taking the average.

But  $\prod_{i=1}^n p(Y_i|\theta)$  rapidly gets very small, which leads to numerical problems. We need to be a bit more clever to evaluate the normalizing constant (fortunately we, mostly, don't need to explicitly)

#### Aside: Laplace approximation to the normalising constant

$$p(\theta|\mathbf{Y}^{obs}) = \frac{p(\mathbf{Y}^{obs}|\theta)p(\theta)}{\int p(\mathbf{Y}^{obs}|\theta)p(\theta) d\theta} = \frac{q(\theta|\mathbf{Y}^{obs})}{\int q(\theta|\mathbf{Y}^{obs})}$$
(11)

Let  $u(\theta) = \log(q(\theta))$  and suppose  $u(\theta)$  is maximised at  $\theta = \hat{\theta}$ , so  $\hat{\theta}$  is the posterior mode. Let  $u''(\theta) = \frac{d^2}{du(\theta)^2}$  and Let r denote the dimension of  $\theta$ 

$$K(\mathbf{Y}^{\mathbf{obs}}) = \int (q(\theta|\mathbf{Y}^{obs})) \, \mathrm{d}\theta \approx q(\hat{\theta}|\mathbf{Y}^{obs}) (2\pi)^{r/2} |-u''(\hat{\theta})|^{-1/2} \quad (12)$$

In practice we would compute

$$\log(K(\mathbf{Y}^{\mathbf{obs}})) \approx u(\hat{\theta}|\mathbf{Y}^{\mathbf{obs}}) + (r/2)\log(2\pi) - 0.5\log|-u''(\hat{\theta})|$$
(13)

$$= \sum_{i=1}^{n} \log(p(Y_i|\hat{\theta})) + \log(p(\hat{\theta})) + (r/2) \log(2\pi) - 0.5 \log|-u''(\hat{\theta})|$$
(14)

can often then work with  $\log(p(\theta|\mathbf{Y}^{obs})) \approx \log(q(\theta|\mathbf{Y}^{obs})) - \log(\hat{K}(\mathbf{Y}^{obs}))$  where  $\log(\hat{K}(\mathbf{Y}^{obs}))$  is rhs of (14)

## Basic ideas of Monte Carlo computation (4): Work on the log-scale for intermediate calculations

- To avoid numerical problems we will usually work on the log<sub>e</sub> scale when evaluating likelihoods and posterior distributions; leaving exponentiating as late as possible.
- For example, in the Metropolis-Hastings algorithm, to be considered later, it is necessary to evaluate the a ratio of posterior densities computed at different values of  $\theta$ . Instead of working with  $r_{MH} = p(\theta_1|\mathbf{Y})/p(\theta_2|\mathbf{Y})$  directly we work with  $\log(r_{MH}) = \log(p(\theta_1|\mathbf{Y})) \log(p(\theta_2|\mathbf{Y}))$  e.g. Instead of determining  $(r_{MH}>1)$  we determine  $\log(r_{MH}>0)$

### Basic ideas in Monte Carlo computation (5): Monte Carlo error

- Yes, Monte Carlo methods provide approximations to posterior distributions.
- Monte Carlo error is under the control of the analyst reduce error by increasing the Monte Carlo sample size!
- We can get a sense of the Monte Carlo error.
- For simple Monte Carlo methods this is fairly straightforward, at least for the expected value (of  $\theta$  or  $h(\theta)$ ).
- if  $\theta_{n_{sim}}=(\theta_{(1)},\theta_{(2)},\dots\theta_{n_{sim}})$  are  $n_{sim}$  independent draws from the posterior and  $s(\theta_{n_{sim}})$  is the standard deviation of the draws, then  $s(\theta_{n_{sim}})/\sqrt{n_{sim}}$  is a reasonable approximation to the Monte Carlo error, for the expectation.

### Basic ideas in Monte Carlo computation (6): More on Monte Carlo error

- $s(\theta_{n_{sim}})$  is an approximation to the posterior standard deviation, so  $V(\theta_{n_{sim}}) = s(\theta_{n_{sim}})^2$  is an approximation to the posterior variance.
- So, in a loose sense, we can think of

$$V^{ ext{tot}}(\boldsymbol{\theta}_{n_{sim}}) = V(\boldsymbol{\theta}_{n_{sim}}) + \frac{V(\boldsymbol{\theta}_{n_{sim}})}{n_{sim}}$$
 (15)

$$=V(\theta_{n_{sim}})(1+\frac{1}{n_{sim}}) \tag{16}$$

as a measure of total uncertainty about heta

- For  $n_{sim}=100$ , total uncertainty is about 1% greater than posterior uncertainty; Total standard deviation is about  $\sqrt{1+1/100}\approx 0.5\%$  greater than posterior standard deviation.
- Monte Carlo error can be often be a small contributor to total uncertainty.

#### Basic ideas in Monte Carlo computation (7): Some caveats

- Caveat 1: approximating extreme posterior quantiles requires a bigger Monte Carlo sample size than approximating the posterior expectation,
- Caveat 2: The above arguments are based on the premise that we can draw n<sub>s</sub> im values independently from the posterior. The more complex Monte Carlo methods we will look at later generate correlated draws and approximation of the Monte Carlo standard error in this case is more difficult. For a given n<sub>sim</sub>, the Monte Carlo standard error will be greater for correlated draws than for independent draws.

### Applications of direct Monte carlo simulation

# Direct simulation of the posterior of a function of random variables $\operatorname{Ex}(1)$

Consider a simple two-group study: people randomly allocated to group  $\boldsymbol{A}$  or  $\boldsymbol{B}$ 

- Group A 10 people given drug A; 7 successes (respond to treatment)
- Group B 10 people given drug B; 3 successes

#### A model for these data:

Conditional Independence:

$$p(Y_A, Y_B | \theta_A, \theta_B, N_A, N_B) = p(Y_A | \theta_A, N_A) p(Y_B | \theta_B, N_B)$$

$$Y_A \sim \text{Binomial}(\theta_A, N_A)$$
  
 $Y_B \sim \text{Binomial}(\theta_B, N_B)$ 

Suppose  $p(\theta_A, \theta_B) = p(\theta_A)p(\theta_B)$  and  $\theta_A \sim \text{Beta}(1, 1)$ ,  $\theta_B \sim \text{Beta}(1, 1)$ Suppose further that we are interested in the relative risk,  $\text{rr} = \theta_A/\theta_B$ .

# Simulating the posterior of a function of random variables (2)

- Ultimately we want p(rr|data) where here data is  $(Y_A, Y_B)$  and we regard as  $N_A$ ,  $N_B$  as known constants, fixed by the investigator.
- first step is to obtain the posterior for the model parameters

$$\begin{split} \rho(\theta_A, \theta_B | \mathrm{data}) &\propto \rho(Y_A, Y_B | \theta_A, \theta_B, N_A, N_B) \rho(\theta_A) \rho(\theta_B) \\ &= [\rho(Y_A | \theta_A, N_A) \rho(\theta_A)] \times [\rho(Y_B | \theta_B, N_B) \rho(\theta_B)] \\ &= [\mathrm{Binomial}(Y_A | \theta_A, N_A)] [\mathrm{Beta}(\theta_A | 1, 1)] \\ &\times [\mathrm{Binomial}(Y_B | \theta_B, N_B)] [\mathrm{Beta}(\theta_B | 1, 1)] \\ &= [\mathrm{Beta}(\theta_A | Y_A + 1, N_A - Y_A + 1)] \times \\ &\times [\mathrm{Beta}(\theta_B | Y_B + 1, N_B - Y_B + 1)] \end{split}$$

# Simulating the posterior of a function of random variables (3)

$$p(\theta_A, \theta_B | \text{data}) = [\text{Beta}(\theta_A | Y_A + 1, N_A - Y_A + 1)] \times \times [\text{Beta}(\theta_B | Y_B + 1, N_B - Y_B + 1)]$$
(17)

It is easy to simulate the joint posterior for  $(\theta_A, \theta_B)$ . Just draw values independently from the appropriate  $\operatorname{Beta}$  distributions. Almost as easy to simulate the posterior of  $\operatorname{rr} = \theta_A/\theta_B$ :

```
for (i in 1:n_{sim}) { draw \theta_A^{(i)} from Beta(Y_A + 1, N_A - Y_A + 1) draw \theta_B^{(i)} from Beta(Y_B + 1, N_B - Y_B + 1) set rr^{(i)} = \theta_A^{(i)}/\theta_B^{(i)} store rr^{(i)} }
```

Summarise stored rr values (see R script posterior\_rr.r)

# Direct simulation of function of parameters: Ex. 2 Cancer rates by DHB

see R markdown file cancer\_example.pdf and /or  $cancer_example.rmd$ 

- If  $\lambda_i$  is the underlying rate of tongue cancer for the  $i^{th}$  DHB we can, using Monte Carlo simulation, compute quantites like  $\Pr(\lambda_i > \lambda_j, \forall j \neq i | \mathbf{Y})$  i.e the posterior probability that the  $i^{th}$  DHB has the largest underlying cancer rate among all DHBs. We can compute this probability for each DHB.
- We can also compute the posterior distribution for the rank-order of DHBs, wrt tongue cancer rates.
- These types of inferences are difficult to obtain analytically

Useful probability decompositions for Monte Carlo simulation (and Bayesian Inference in general)

#### Direct simulation for a vector of random variables

We can always write a joint distribution as a product of a marginal and conditional distribution, e.g.

$$p(Y_1, Y_2) = p(Y_1)p(Y_2|Y_1)$$

Extends automatically to vectors or arbitrary length:

$$p(Y_1, Y_2, \ldots, Y_k) = p(Y_1)p(Y_2|Y_1)p(Y_3|Y_2, Y_1), \ldots, p(Y_k|Y_{k-1}, \ldots, Y_1)$$

And, of course this holds for any vector of r.v's, not just observables, so we might sometimes model a parameter vector as

$$p(\theta_1, \theta_2, \dots, \theta_k) = p(\theta_1)p(\theta_2|\theta_1)p(\theta_3|\theta_2, \theta_1), \dots, p(\theta_k|\theta_{k-1}, \dots, \theta_1)$$

The point is we are breaking a multivariate distribution into a sequence of univariate (more generally, low-dimensional) distributions - often easier to model and simulate. If you are lucky you can take advantage of conditional independencies to simplify further.

# Sequence of conditionals approach also applies to a combination of parameters and observables; and holds conditionally

$$p(\theta, Y_{n+1}|Y_1, \dots, Y_n) = p(\theta|Y_1, \dots, Y_n)p(Y_{n+1}|\theta, Y_1, \dots, Y_n)$$
 (18)

If  $Y_1, \ldots, Y_n$  are the observed data we will of often write expressions such as (18) as

$$p(\theta, Y_{n+1}|\text{data}) = p(\theta|\text{data})p(Y_{n+1}|\theta, \text{data}).$$
(19)

If the Y's are modelled as conditionally independent given  $\theta$ :

$$p(Y_1, Y_2, \dots | \theta) = \prod_{i} p(Y_i | \theta)$$
 (20)

(19) simplifies to

$$p(\theta, Y_{n+1}|\text{data}) = p(\theta|\text{data})p(Y_{n+1}|\theta) \tag{21}$$