## Part A Simulation and Statistical Programming HT19 Problem Sheet 4 - due Monday 5pm Week 1 of TT19

Please hand in the solutions at 24-29 St Giles, and email the R code, in a single well-commented R-script, to sinan.shi@stats.ox.ac.uk

1. (a) Give a Metropolis-Hastings algorithm with a stationary Gamma probability density function,

$$
\pi(x) \propto x^{\alpha-1} \exp (-\beta x), \quad x>0
$$

with parameters $\alpha, \beta>0$. Use the proposal distribution $Y \sim \operatorname{Exp}(\beta)$.
(b) Write an R function implementing your MCMC algorithm. Your function should take as input values for $\alpha$ and $\beta$ and a number $n$ of steps and return as output a realization $X_{1}, X_{2}, \ldots, X_{n}$ of a Markov chain targeting $\pi$. State briefly how you checked your code.
2. MCMC for Bayesian inference (first two parts were an exam Q in 2009)
(a) Let $X \sim \operatorname{Binomial}(n, r)$ be a binomial random variable with $n$ trials and success probability $r$. Let $\pi(x ; n, r)$ be the pmf of $X$. Give a Metropolis-Hastings Markov chain Monte Carlo algorithm with stationary pmf $\pi(x ; n, r)$.
(b) Suppose the success probability for $X$ is random, with $\operatorname{Pr}(R=r)=p(r)$ given by

$$
p(r)= \begin{cases}r & \text { for } r \in\{1 / 2,1 / 4,1 / 8, \ldots\}, \text { and } \\ 0 & \text { otherwise }\end{cases}
$$

An observed value $X=x$ of the Binomial variable in part (a) is generated by simulating $R \sim p$ to get $R=r^{*}$ say, and then $X \sim \operatorname{Binomial}\left(n, r^{*}\right)$ as before. Specify a Metropolis-Hastings Markov chain Monte Carlo algorithm simulating a Markov chain, $\left(R_{t}\right)_{t=0,1,2, \ldots}$ with equilibrium probability mass function $R_{t} \xrightarrow{d} p(r \mid x)$ where

$$
p(r \mid x) \propto \pi(x ; n, r) p(r)
$$

is called the posterior distribution for $r$ given data $x$.
(c) Write an R function implementing your MH MCMC algorithm with target distribution $p(r \mid x)$. Suppose $n=10$ and we observe $x=0$. Run your MCMC algorithm and estimate the mode of $p(r \mid x)$ over values of $r$.
3. Let $X$ be an $n \times p$ matrix of fixed covariates with $n>p$, and suppose that $X$ has full column rank $p$.
(a) Explain why the $p \times p$ matrix $X^{T} X$ is invertible.

Consider the linear model given by

$$
Y_{i}=\beta_{1} x_{i 1}+\beta_{2} x_{i 2}+\cdots+\beta_{p} x_{i p}+\varepsilon_{i}
$$

where $\varepsilon_{i} \sim N\left(0, \sigma^{2}\right)$.
(b) Write down the distribution of $Y_{i}$, and use it to write out the log-likelihood for $\beta=\left(\beta_{1}, \ldots, \beta_{p}\right)$.
(c) Show that the MLE is equivalent to minimising the sum of squares:

$$
R(\beta)=\sum_{i=1}^{n}\left(Y_{i}-\beta_{1} x_{i 1}-\cdots-\beta_{p} x_{i p}\right)^{2} .
$$

(d) By differentiating and writing the problem as a system of linear equations, show that the MLE is $\hat{\boldsymbol{\beta}}=\left(X^{T} X\right)^{-1} X^{T} Y$.
4. Consider the linear model $Y=X \beta+\epsilon$ where $Y$ is a vector of $n$ observations, $X$ is an $n \times p$ matrix with each column containing a different explanatory variable and $\epsilon$ is a vector of $n$ independent normal random errors with mean zero and unknown variance $\sigma^{2}$. The maximum likelihood estimator for $\beta$ is

$$
\hat{\beta}=\left(X^{T} X\right)^{-1} X^{T} Y .
$$

The sample variance is

$$
s^{2}=\frac{1}{n-p}\|X \hat{\beta}-Y\|^{2}
$$

where $p$ is the length of $\beta$. The standard error for $\beta$ is

$$
\operatorname{se}\left(\hat{\beta}_{i}\right)=s \sqrt{\left[\left(X^{T} X\right)^{-1}\right]_{i i}}
$$

(a) The trees data give Girth, Height and Volume measurements for 31 trees. Fit the model

$$
Y_{i}=\beta_{1}+x_{i}^{\text {height }} \beta_{2}+x_{i}^{\text {girth }} \beta_{3}+\epsilon_{i}
$$

using the R commands
> data(trees)
> summary(lm(Volume ~ Girth + Height, data=trees))
and briefly interpret the output.
(b) Write a function of your own (using solve() or your solution to question 3 , not $\operatorname{lm}()$ ) to fit a linear model. Your function should take the length 31 vector trees $\$$ Volume and the $31 \times 3$ matrix $\mathrm{X}=\mathrm{cbind}(1$, trees $\$$ Girth, trees $\$$ Height) as input and return estimates of $\beta$, the residual standard error $s$, and the standard errors of each $\beta_{i}$. Check your output against the corresponding results from the summary (lm()) output in (a).
5. Here is an algorithm to compute the QR factorisation of an $n \times p$ matrix $A$ with $p \leq n$. That is, it returns an $n \times p$ orthogonal matrix $Q$ and a $p \times p$ upper triangular matrix $R$ sich that $A=Q R$.
Let $|v|$ denote the Euclidean norm of a vector $v$. Let $A_{[, a: b]}$ denote the matrix formed from the columns $a, a+1, \ldots, b$ of $A$.

1. Create $n \times p$ matrix $Q$ and $p \times p$ matrix $R$.
2. Set $Q_{[, 1]}=A_{[, 1]} /\left|A_{[, 1]}\right|$ and $R_{11}=\left|A_{[, 1]}\right|$.
3. If $p=1$ then we are done; return $Q$ and $R$.
4. Otherwise (i.e. if $p>1$ ), set $R_{[1,2: p]}=Q_{[, 1]}^{T} A_{[, 2: p]}$ and $R_{[2: p, 1]}=\mathbf{0}$.
5. Set $A^{\prime}=A_{[, 2: p]}-Q_{[, 1]} R_{[1,2: p]}$. [Notice that $Q_{[, 1]} R_{[1,2: p]}$ is an outer product of an $n$ component column vector and $a$ ( $p-1$ ) component row vector, so $A^{\prime}$ is a new $n \times(p-1)$ matrix. Either make use of the outer() command or, if you use [ be careful to use the drop argument when forming these sub-matrices.]
6. Compute the QR factorisation of $A^{\prime}$ (so $A^{\prime}=Q^{\prime} R^{\prime}$ say).
7. Set $Q_{[, 2: p]}=Q^{\prime}$ and $R_{[2: p, 2: p]}=R^{\prime}$ and return $Q$ and $R$.
(a) Implement this algorithm as a recursive function in R . Your function should take as input an $n \times p$ matrix $A$ and return two matrices $Q$ and $R$ as a list. State briefly how you checked your function was correct.
(b) Using your QR function, and the R command backsolve(), give a least squares solution to the over-determined system

$$
X \beta=Y
$$

where $X$ and $Y$ take their values from the trees data in question 4.

