## MATS442 Stochastic simulation

The problems marked with $\mathbf{C}$ have a part which needs to be implemented in a computer programming language. Please return a single code file with the answers to these exercises by email to 〈santeri.j.karppinen(•at•)jyu.fi〉.

1. Suppose that $p$ and $q$ are probability densities on $\mathbb{R}$, satisfying $q(x)=0 \Longrightarrow p(x)=0$ and you have implemented self-normalised importance sampling, that is,

$$
X_{1}, \ldots, X_{n} \sim q(\cdot), \quad W_{k}^{(n)}=\frac{w_{u}\left(X_{k}\right)}{\sum_{j=1}^{n} w_{u}\left(X_{j}\right)}, \quad w_{u}(x)=c_{w} \frac{p(x)}{q(x)}
$$

(a) How can you estimate $\operatorname{Var}_{p}(X)$ using $\left(X_{1}, \ldots, X_{n}\right)$ and $\left(W_{1}^{(n)}, \ldots, W_{n}^{(n)}\right)$ ?
(Hint: Express $\operatorname{Var}_{p}(X)$ in terms of expectations.)
(b) Show that your estimator is consistent.
(c) How about quantiles, that is, for a given $\beta \in(0,1)$, how can you estimate the number $x_{\beta} \in \mathbb{R}$ such that $\mathbb{P}\left(X \leq x_{\beta}\right)=\beta$ where $X \sim p$ ?
(Hint: Think first what might be an estimator of $F(x)=\mathbb{P}(X \leq x)$.)
(d) $\left(^{*}\right)$ Can you show that the quantile estimator is consistent if $F$ is strictly increasing?
2. Consider Algorithm 6.13 (Metropolis-Hastings).
(a) Observe that $\left(X_{k}, Y_{k+1}\right)_{k \geq 1}$ is a Markov chain.
(b) Show that $\left(X_{k}, Y_{k+1}\right)_{k \geq 1}$ admits $\tilde{p}(x, y)=p(x) q(x, y)$ as invariant distribution.
(Hint: Use first the fact that $X_{k-1} \sim p \Longrightarrow X_{k} \sim p$, and then think about a conditional distribution of $Y_{k+1} \ldots$ )
(c) Where does the following average converge to:

$$
I_{p, q, \mathrm{WR}-\mathrm{MH}}^{(n)}(f):=\frac{1}{n} \sum_{k=1}^{n}\left[\alpha\left(X_{k}, Y_{k+1}\right) f\left(Y_{k+1}\right)+\left(1-\alpha\left(X_{k}, Y_{k+1}\right)\right) f\left(X_{k}\right) ?\right.
$$

(d) $\left(^{*}\right)$ Can you relate the $k:$ th term in the sum above to the conditional expectation of $f\left(X_{k+1}\right)$ given $X_{k}$ and $Y_{k+1}$ ? What does this mean regarding the variance of the $k$ :th term? What about the variance of the whole 'waste recycling' estimator $I_{p, q, \mathrm{WR}-\mathrm{MH}}^{(n)}(f)$ compared to $I_{p, q, \mathrm{MH}}^{(n)}(f)$ ?
3.C \& 4.C (worth 2 points). Consider a Metropolis-Hastings algorithm targetting the following unnormalised distribution in $\mathbb{R}^{2}$ :

$$
p_{u}([x, y])=\exp \left(-\frac{1}{2}\left(x^{2}+y^{2}\right)\right)+\exp \left(-\frac{1}{2}\left((x-7)^{2}+y^{2}\right)\right)
$$

You may use the following Julia function to calculate values of $\log p_{u}([x, y])$ :

```
function log_p_u(x, m1=[0.0,0.0], m2=[7.0,0.0])
    q1 = -.5(x-m1)'*(x-m1); q2 = -. 5(x-m2)'*(x-m2)
    q0 = max(q1, q2) # Avoid underflow of both exp's below
    return(q0 + log(exp(q1-q0) + exp(q2-q0)))
end
```

Use the proposal distribution $q(x, y)=\tilde{q}(y-x)$, where $\tilde{q}$ corresponds to $N\left(0,4 I_{2}\right)$, normal distribution in $\mathbb{R}^{2}$ with diagonal variance 4 .
(a) Implement this Metropolis-Hastings algorithm.
(b) Run the algorithm for 100000 iterations and with suitable burn-in, and calculate estimators for

$$
\mathbb{E}_{p}\left[f_{i}(X)\right] \quad \text { and } \quad \operatorname{Var}_{p}\left(f_{i}(X)\right),
$$

where $f_{i}(x):=x^{(i)}$, that is, $f_{1}(x, y):=x$ and $f_{2}(x, y):=y$.
(c) Calculate and inspect sample autocorrelations for $f_{i}\left(X_{1}\right), \ldots, f_{i}\left(X_{100000}\right)$ (using function autocor of StatsBase package).
(d) Calculate effective sample size by summing autocorrelations up to some truncation.
(e) Use the functions estimateBM and estimateSV of the code provided, which give estimates of $\sigma_{M H}^{2}$. Calculate the corresponding effective sample sizes, and compare to your result.
(f) Build up $95 \%$ confidence intervals to your estimators, using the estimated variance $\operatorname{Var}_{p}\left(f_{i}(X)\right)$ and effective sample sizes.
(g) (* optional) Repeat your experiments 1000 times, and check how many of your confidence intervals for $\mathbb{E}_{p}\left[f_{i}(X)\right]$ covered the true value (what are the true values?).
5. Let $p_{a}$ stand for the uniform distribution on the set

$$
C_{0} \cup C_{a}, \quad \text { where } \quad C_{t}:=\left\{(x, y) \in \mathbb{R}^{2}: x \in[t, t+1], y \in[t, t+1]\right\} .
$$

(a) Draw a picture of the set with $a=1 / 2$ and $a=1$.
(b) Describe a Gibbs sampler for $p_{a}$ with $a \in[0,1]$.
(c) Is the Gibbs sampler irreducible with $a=1$ ? How about $a \in(0,1)$ ?
(Precise proof is not necessary here, but explain your reasoning...)
6. Suppose $p_{u}$ is an unnormalised p.m.f. on $\mathbb{X}$ and $q(x, \cdot)$ a 'proposal' p.m.f.. Further assume that $h(x, \cdot)$ is a p.m.f. on non-negative integers $\mathbb{N}_{0}:=\{0,1, \ldots\}$ defined for each $x \in \mathbb{X}$, with the property

$$
\sum_{z \in \mathbb{N}} z h(x, z)=p_{u}(x) \quad \text { for each } x \in \mathbb{X}
$$

Consider a Markov chain ( $X_{k}, Z_{k}$ ) defined as follows: Start from $X_{0} \in \mathbb{X}, Z_{0}=1$ and for $k=1,2, \ldots$

- Draw $X_{k}^{*} \sim q\left(X_{k-1}, \cdot\right)$ and then $Z_{k}^{*} \sim h\left(X_{k}^{*}, \cdot\right)$.
- Draw $U_{k} \sim U(0,1)$ and set

$$
\left(X_{k}, Z_{k}\right)= \begin{cases}\left(X_{k}^{*}, Z_{k}^{*}\right), & \text { if } U_{k} \leq \frac{Z_{k}^{*}}{Z_{k-1}} \frac{q\left(X_{k}^{*}, X_{k-1}\right)}{q\left(X_{k-1}, X_{k}^{*}\right)}, \\ \left(X_{k-1}, Z_{k-1}\right), & \text { otherwise }\end{cases}
$$

(a) Write down the transition probability

$$
K\left((x, z),\left(x^{\prime}, z^{\prime}\right)\right)=\mathbb{P}\left(\left(X_{n}, Z_{n}\right)=\left(x^{\prime}, z^{\prime}\right) \mid\left(X_{n-1}, Z_{n-1}\right)=(x, z)\right)
$$

of this Markov chain.
(Hint: Write down first the 'compound proposal' $\tilde{q}\left((x, z),\left(x^{*}, z^{*}\right)\right)=\mathbb{P}\left(X_{k}^{*}=\right.$ $\left.x^{*}, Z_{k}^{*}=z^{*} \mid X_{k-1}=x, Z_{k}=z\right)$.)
(b) Observe that $h(x, z) z$ is an unnormalised distribution on $\mathbb{X} \times \mathbb{N}_{0}$ (why?), and show that $K$ is reversible with respect to $\pi(x, z) \propto h(x, z) z$.
(c) Suppose you know that the Markov chain $\left(X_{k}, Z_{k}\right)_{k \geq 1}$ is irreducible. What can you say about

$$
\lim _{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^{n} f\left(X_{k}\right) ?
$$

