SC7 Bayes Methods

Third problem sheet (Sections 7-9.3.1 of lecture notes).

Section A

1. Suppose $X = x$ is a draw from an Ising model distribution $X \sim \pi(\cdot|\theta)$ on an $m \times m$ lattice, so that for $i = 1, 2, ..., n$ with $n = m^2$, $x_i \in \{0, 1\}$ and $x = (x_1, ..., x_n)$ with $n = m^2$. Let N_i be the set of neighbors of pixel i on the square lattice. Let $\#x$ denote the number of disagreeing neighbors, that is

$$\#x = \frac{1}{2}\sum_{i=1}^{m^2}\sum_{j\in N_i}\mathbb{I}_{x_i\neq x_j}.$$

Under the Ising model, $\pi(x|\theta) = \exp(-\theta\#x)/Z(\theta)$ where $Z(\theta)$ is a normalising constant.

Suppose we don't observe X itself but instead observe $Y = y_{obs}$ with $y_{obs} = (y_{obs1}, ..., y_{obsn})$ and $Y_i|x_i \sim N(x_i, \sigma^2)$ iid for $i = 1, 2, ..., n$. Here $\sigma > 0$ is known and a prior $\theta \sim \mathrm{Exp}(2)$ is elicited for θ.

(a) Write down the posterior $\pi(\theta, x|y_{obs})$ in terms of the model elements and explain why it is doubly intractable when $m \gg 1$.

Solution:

$$\pi(\theta, x|y_{obs}) \propto \left[\prod_{i=1}^{n} N(y_{obsi}; x_i, \sigma^2)\right]\frac{e^{-\theta\#x}}{Z(\theta)}\mathrm{Exp}(\theta; 2)$$

is DI beacuse $Z(\theta) = \sum_{x\in\{0,1\}^n}\exp(-\theta\#x)$ is intractable.

(b) Consider the statistic for $y \in R^n$

$$S(y) = \frac{1}{2}\sum_{i=1}^{m^2}\sum_{j\in N_i}(y_i - y_j)^2$$

and distance measure $d(s - s') = |s - s'|$. Briefly motivate this choice of of the ABC statistic $S(y)$ [Hint: what happens when $\sigma \ll 1$.].

Solution: When the observation noise σ is small, $S(y) \simeq \#x$ which is sufficient for θ. In this case when $\delta \to 0$ conditioning on $d(s - s') < \delta$ approximates conditioning on the sufficient statistic $\#x$ so the ABC posterior should approximate the exact posterior well at small σ and δ.

(c) An MCMC algorithm for $X \sim \pi(x|\theta)$ is available. Give an ABC algorithm targeting $\pi(\theta|d(S(Y), S(y_{obs})) < \delta)$ using the MCMC algorithm to simulate $X \sim \pi(x|\theta)$.

Solution:

(1) Simulate $\theta \sim \pi(\theta)$, $x \sim \pi(x|\theta)$ (using the MCMC algorithm) and $y \sim N(y; x, \sigma^2 I_n)$.

(2) If $d(S(y), S(y_{obs})) < \delta$ return θ and stop, otherwise goto (1).

2. Consider a linear regression $y_i = x_i^T \beta + \epsilon_i$ with covariates $x_i \in R^p$ and $\epsilon_i \sim N(0, \sigma^2)$, $i = 1, \dots, n$. There are p parameters $\beta \in R^p$ with prior $\pi(\beta) = \prod_j \pi(\beta_j)$. For $j = 1, \dots, p$ let $z_j \in \{0, 1\}$ be indicator variables. The component priors are

$$\pi(\beta_j|z_j) = (1 - z_j) N(\beta_j; 0, \sigma_1^2) + z_j N(\beta_j; 0, \sigma_2^2)$$

where $0 < \sigma_1 \ll \sigma_2$ are prior hyperparameters which we suppose are fixed. The prior for $z = (z_1, \dots, z_p)$ is $\pi_Z(z) = \prod_j \pi_Z(z_j)$ where $\pi_Z(z_j) = \Pr(Z_j = 0) = w$ for some $w \in (0, 1)$.

(a) By considering the limit $\sigma_1 \to 0$, explain the relation between this prior and the spike and slab prior (end Section 8.2.1 in lecture notes). Recall that the regression parameters in that setup are $\tilde{\theta}_j = z_j \theta_j$ and $y_i = \sum_i x_i^T \tilde{\theta} + \epsilon_i$ and suppose the prior for θ is $N(0, \sigma_2^2 I_p)$ and the prior for z is the same as above.

Solution: The marginal of the spike and slab prior for $\tilde{\theta}_j = z_j \theta_j$ averaged over z_j is

$$\tilde{\pi}(\tilde{\theta}_j) = w \delta_0(\tilde{\theta}_j) + (1 - w) N(\tilde{\theta}_j; 0, \sigma_2^2).$$

Let $A \subset R$ be any open set in R. The prior probability for $\tilde{\theta}_j \in A$ is

$$\tilde{\pi}(A) = w \mathbb{I}_{0 \in A} + (1 - w) \int_A N(\tilde{\theta}_j; 0, \sigma_2^2) d\tilde{\theta}_j.$$

The marginal for the prior above is

$$\pi(\beta_j) = w\, N(\beta_j; 0, \sigma_1^2) + (1 - w)\, N(\beta_j; 0, \sigma_2^2)$$

so when σ_1 approaches zero the prior probability for $\beta_j \in A$ converges to

$$\begin{aligned} \lim_{\sigma_1 \to 0} \pi(A) &= w \lim_{\sigma_1 \to 0} \int_A N(\beta_j; 0, \sigma_1^2) d\beta_j + (1 - w) \int_A N(\beta_j; 0, \sigma_2^2) d\beta_j \\ &= w \mathbb{I}_{0 \in A} + (1 - w) \int_A N(\beta_j; 0, \sigma_2^2) d\beta_j. \end{aligned}$$

Since $\Pr(\tilde{\theta}_j \in A) = \lim_{\sigma_1 \to 0} \Pr(\beta_j \in A)$ on all open sets in R^p, the priors are equal in the limit, so the posteriors will converge. We can think of the setup with β as a smoothed version of the spike and slab prior.

(b) What are the relative merits of the two priors? When is one prefered to the other?

Solution: A bit outside the course, but there are computational advantages in working with continuous variables (the β setup, summing out z). Many good MCMC schemes rely on taking derivatives, and most easily implemented variational Bayes methods use automatic differentiation of the log-posterior. From a modeling perspective, it is often the case that effects are never "truly" zero, even when the model is correct. There is a weak effect, possibly through correlation with unmeasured confounding variables. However, the true spike and slab is more parsimonious, and there are settings where an effect is truly absent.

Section B (Part C/OMMS to hand in solutions to Section B)

3. (ABC) We considered a version of ABC related to the rejection algorithm. Consider the following MCMC-ABC algorithm[1], targeting $\pi(\theta|y)$ (approximately) using the statistics $S(y)$, distance $d(S', S)$ and threshold δ. The observation model is $p(y|\theta)$ and the prior is $\pi(\theta)$. Suppose $X_t = \theta$.

   Step 1. Simulate $\theta' \sim q(\theta'|\theta)$ and $y' \sim p(y'|\theta')$.

   Step 2. If $d(S(y'), S(y)) < \delta$ then accept θ' (set $X_{t+1} = \theta'$) with probability

$$\alpha(\theta'|\theta) = \min\left\{1, \frac{\pi(\theta')q(\theta|\theta')}{\pi(\theta)q(\theta'|\theta)}\right\}$$

   and otherwise reject θ' (set $X_{t+1} = \theta$).

   (a) Show this algorithm targets $\pi(\theta|d(S(Y), S(y)) < \delta)$ (y is fixed here and $Y \sim p(\cdot|\theta)$).

   (b) Suppose we have $y_i \sim \text{Poisson}(\Lambda)$, $i = 1, 2, ..., n$ with $n = 5$. Prior $\lambda \sim \Gamma(\alpha = 1, \beta = 1)$. Give the ABC-MCMC algorithm targeting $\pi(\lambda|y)$ (approximately). Take $S(y) = \bar{y}$, $d(\bar{y}', \bar{y}) = |\bar{y}' - \bar{y}|$ and $\delta = 0.5$.

4. (Model averaging) Consider a normal linear model allowing for outliers. Let X be an $n \times p$ design matrix with rows $x_i = (x_{i,1}, ..., x_{i,p})$ and first column $X_{i,1} = 1, i = 1, ..., n$. Let β be a p-component parameter vector with β_1 the regression intercept. Let z be a latent

[1] Marjoram et al, "Markov chain Monte Carlo without likelihoods", PNAS (2003).

indicator variable with $z_i = 1$ if (y_i, x_i) is an outlier and $z_i = 0$ otherwise. The response $y_i \sim N(x_i\beta, \sigma^2)$ if $z_i = 0$ and $y_i \sim N(x_i\beta, \rho\sigma^2)$ if $z_i = 1$. Here ρ is a variance inflation factor defining outliers (and ρ is fixed, so for eg we take $\rho = 9$ in Q10 below). Let p be the probability that any single given data point is an outlier.

(a) The model parameters are β, σ, p and the n-component vector z. The choice of ρ defining outliers is fixed. Write down the likelihood $L(\beta, \sigma, z; y)$.

(b) Write down the posterior $p(\beta, \sigma, p, z|y)$ if the priors are $p \sim \text{Beta}(1, 9)$, $\beta_i/2.5 \sim t(1)$, iid for $i = 1, ..., p$ and $z_i \sim \text{Bern}(p)$, iid for $i = 1, ..., n$ and $\sigma \sim 1/\sigma$.

(c) The columns of $X_{2:p}$ are centred to mean zero. Show that, conditional on $z_i = 0, i = 1, ..., n$ (no outliers) and σ, β_1 is independent of $\beta_2, ..., \beta_p$ in the posterior. Why might this be desirable for MCMC analysis?

(d) An MCMC sampler targeting $\pi(\beta, \sigma, p, z|y)$ is given. Explain (a) how you would use the MCMC output to test if a given data point is an outlier, (b) how you would sample the model averaged posterior $\pi(\beta, \sigma, p|y)$ and (c) how you would form a point estimate $\hat{\beta}_i,\ i \in \{1, ..., p\}$ for β_i if your loss function is the square error $|\hat{\beta}_i - \beta_i|^2$.

5. (MCMC with a Jacobian) Consider an MCMC algorithm targeting $\pi(\theta) \propto \theta^{-1/2}/(1 + \theta^2)$ with $\theta > 0$ a scalar random variable. In the following ν is a fixed parameter of the MCMC and $t(\nu)$ denotes the student-t distribution with ν degrees of freedom.

(a) Calculate the acceptance probability for the MCMC proposal $u \sim t(\nu)$, $\theta' = \theta^u$.

(b) Comment briefly on how you would decide a value for ν.

6. If $\pi(\theta)$ is a prior for θ then an inference scheme is a rule $\psi(\theta; \pi, y)$ for updating belief for θ given data y. For example in Bayesian inference $\psi_{Bayes}(\theta; \pi, y) = \pi(\theta|y)$ but in ABC at fixed δ, $\psi_{\Delta,\delta}(\theta; \pi, y) = \pi(\theta|Y \in \Delta_y(\delta))$.

For $1 \le j < n$ let $y_{1:j} = (y_1, ..., y_j)$ and $y_{j+1:n} = (y_{j+1}, ..., y_n)$ so we split the data into two sets. Suppose the data are conditionally independent, so

$$p(y|\theta) = \prod_{i=1}^{n} p(y_i|\theta).$$

A belief update is *order-coherent* for conditionally independent data if

$$\psi(\theta; \pi, y) = \psi(\theta; \psi(\theta; \pi, y_{1:j}), y_{j+1:n})$$

for all $j \in \{1, 2, ..., n-1\}$ (the posterior from the first data set is the prior for the next).

(a) Show that Bayesian inference is order-coherent.

(b) Show that ABC with fixed δ is not in general order coherent. *Hint: take summary statistic $S(y) = y$ and Euclidean distance measure $d(y, y') = ||y - y'||$ and give a counter-example.*

(c) Let $C_y(\delta)$ be the rectangular prism $C_y(\delta) = \{y' \in R^n : |y_i - y'_i| < \delta \ \forall \ i = 1, ..., n\}$. Show that inference with $\psi_{C,\delta}(\theta; \pi, y) = \pi(\theta|Y \in C_y(\delta))$ is order-coherent.

Section C

7. (MCMC with a Jacobian) Let $\theta \in \Re^p$ be a p-component parameter vector with prior $\pi(\theta)$ and $y \in \Re^n$ an n-component data vector with observation model $y \sim p(y|\theta)$. the parameters are positive, and satisfy an order constraint, $0 < \theta_1 < \theta_2 < ... < \theta_p < \infty$.

(a) Consider the following MCMC proposal. Draw $u_1 \sim U(1/2, 2)$ and $u_2 \sim N(0, \sigma^2)$ where $\sigma > 0$ is a fixed parameter of the MCMC. Set $\theta' = u_1\theta + u_2$, that is $\theta'_i = u_1\theta_i + u_2, \ i = 1, 2, ..., p$. Calculate the acceptance probability $\alpha(\theta'|\theta)$ in as much detail as you can.

Solution: If

$$g(u) = U(u_1; [1/2, 2])N(u_2; 0, \sigma^2)$$

and

$$\psi(\theta, u) = (u_1\theta + u_2, u')$$

then u' satisfies $\psi(\theta', u') = (\theta, u)$. That means

$$u'_1(u_1\theta + u_2) + u'_2 = \theta$$

for every θ. This has the unique solution $u'_1 = 1/u_1, \ u'_2 = -u_2/u_1$. The acceptance probability is

$$\alpha(\theta'|\theta) = \min\left\{1, \ \frac{p(y|\theta')\pi(\theta')g(u')}{p(y|\theta)\pi(\theta)g(u)} \left|\frac{\partial(\theta', u')}{\partial(\theta, u)}\right|\right\}.$$

The Jacobian for

$$(\theta, (u_1, u_2)) \ \rightarrow \ (u_1\theta + u_2, (1/u_1, -u_2/u_1))$$

is

$$\begin{aligned} \left|\frac{\partial(\theta', u')}{\partial(\theta, u)}\right| &= \begin{pmatrix} u_1 I_p & 0_p & 0_p \\ \theta & -1/u_1^2 & u_2/u_1^2 \\ 1_p^T & 0 & -1/u_1 \end{pmatrix} \\ &= u_1^{p-3}. \end{aligned}$$

The acceptance probability is then

$$\alpha(\theta'|\theta) = \mathbb{I}_{\theta_1>0} \min\left\{1,\ \frac{p(y|\theta')\pi(\theta')N(-u_2/u_1;0,\sigma^2)}{p(y|\theta)\pi(\theta)N(u_2;0,\sigma^2)}u_1^{p-3}\right\}.$$

Notice we set the acceptance probability equal zero if we shift $\theta_1 \leq 0$.

(b) Explain qualitatively why the proposal scheme above is not irreducible (for example in the "computer measure"). A MCMC algorithm which has an update with a second distinct proposal mechanism alternates between the two updates. Outline briefly (in a sentence) a suitable "second update".

Solution: Shift-and-scale is not irreducible. For example the function $(\theta_p - \theta_i)/(\theta_p - \theta_1)$ is invariant under shift-and-scale, so something more is certainly needed.

Add a random walk update which picks a random component and applies a simple random walk proposal to that component. This is clearly irreducible on its own.

Remark (not required) If the target is heavy tailed the SRW update will mix very slowly. For example the mean $\bar{\theta}$ will hardly move at each update. The shift-and-scale update will move the parameter vector in and out of the tail efficiently. The mean moves to $u_1\bar{\theta} + u_2$, so we may almost double or halve it in a single update. Similarly the statistic $\min(\theta)$ *(ie, θ_1) may mix much more rapidly due to the global shift u_2.*

8. Continuing question 4 in Section B, the `hills` data are often used to illustrate outlier detection. The finishing time is transformed to make the response more normal, and the covariates for height climbed and distance covered are scaled and centred.

```
> data(hills); a=hills
> a$y=sqrt(a$time); a$climb=scale(a$climb); a$dist=scale(a$dist)
```

We would like to fit a normal linear model `y~climb+dist` to these data, allowing for possible outliers and carrying out model averaging over the outlier labels z. In the file ProblemSheet3-25.R is MCMC code for this problem. Run the MCMC, test for outliers and give an 95% HPD interval for the outlier probability p.

Solution: Relevant output from the MCMC in ProblemSheet3-25.R:

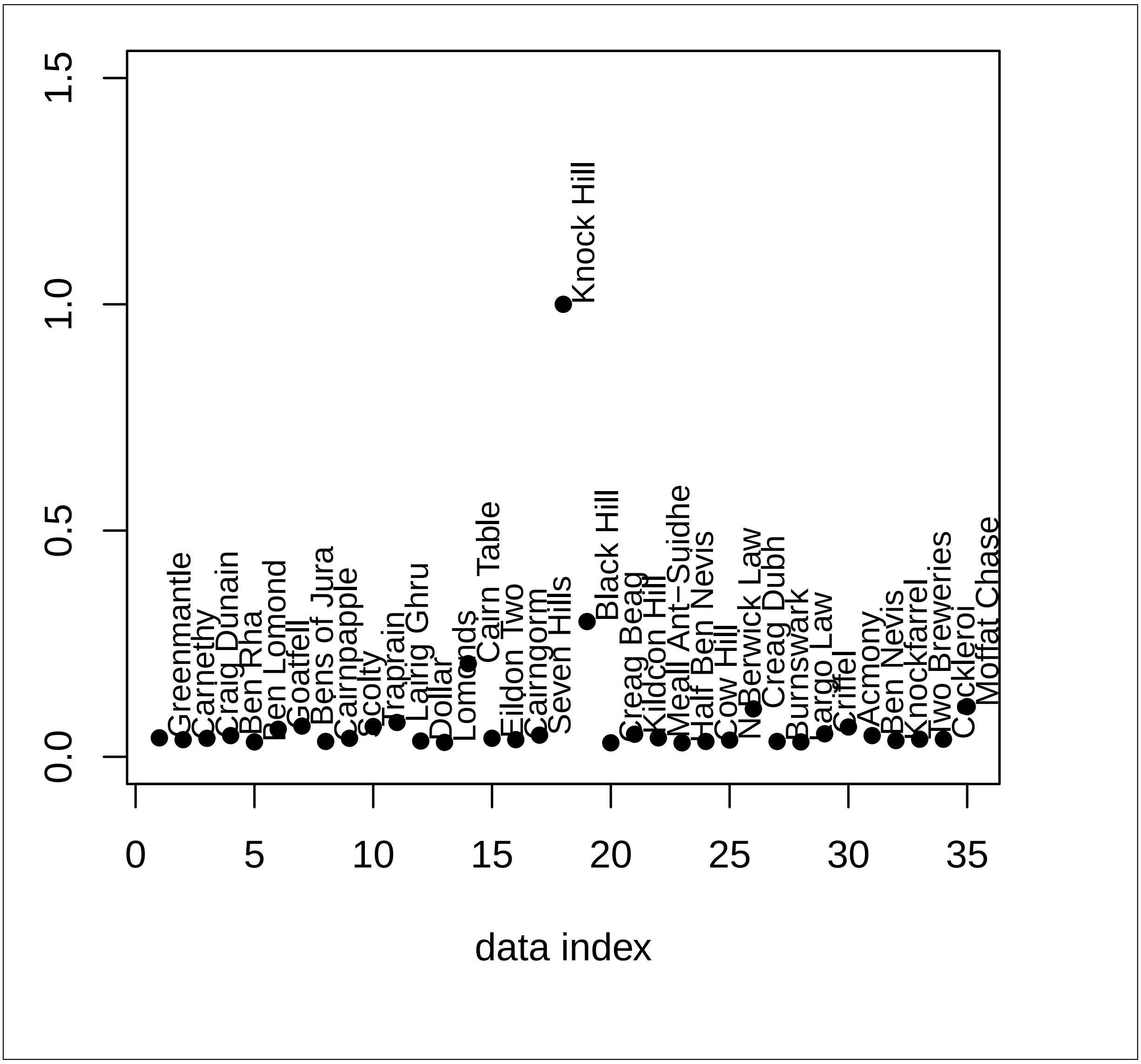
```
#MCMC T-steps code fitting outlier model,
#Z is T x n indicator for outlier,
#Theta is T x 5 columns (p, beta_1:3, sigma)

#outlier probabilities - posterior mean - see graph below
op=apply(Z,2,mean);
plot(1:n,op,pch=16,ylim=c(0,1.5),xlab=’data index’,
     ylab=’outlier probability’);
text(1:n,op,row.names(a),srt=90,pos=4,cex=0.8)

#parameter estimates means etc
summary(as.mcmc(Theta))

> HPDinterval(as.mcmc(Theta))
            lower      upper
p       0.002366977 0.20708522
beta1   0.886371617 0.92233162
beta2   0.108723124 0.17823598
beta3   0.215467656 0.28730858
sigma   0.049710874 0.08822158
attr(,"Probability")
[1] 0.95
```

Running this gives outlier posterior probabilities `op`$[1 : $`n`$]$ plotted below. The 95% HPD interval for the outlier probability p is $[0.00, 0.21]$, (`var1` in the MCMC output).



9. Continuing question 5 in Section B, implement the MCMC and check your answer!

Solution: An implementation can be found in ProblemSheet3-25.R.

10. (RJ targeting inhomogeneous Poisson point process) Let $[L, U]$ be an interval and $\lambda : [L, U] \to \mathbb{R}^+$. In an inhomogeneous Poisson point process (IPP) the probability for an event in a small interval δt is $\lambda(t)\delta t + o(\delta t)$. The sample space is $\Omega = \cup_{n=0}^{\infty}\Omega_n$ where $\Omega_0 = \{\emptyset\}$ and

$$\Omega_n = \{y \in [L, U]^n : L < y_1 < y_2 < \cdots < y_n < U\}.$$

The probability density to realise any particular point pattern $y \in \Omega,\ y = (y_1, \dots, y_n)$ is

$$p(y|\lambda) = \exp(-\Lambda) \prod_{i=1}^{n} \lambda(y_i)$$

where $\Lambda = \int_L^U \lambda(t)dt$. Denote by $|y|$ the number of points in the ordered set y.

(a) Let $Y \sim p(\cdot|\lambda)$ and let $N = |Y|$. Show that $N \sim \text{Poisson}(\Lambda)$.

Solution: $\Pr(N = n) = \Pr(Y \in \Omega_n)$ so

$$\begin{aligned}
\Pr(N = n) &= \int_{\Omega_n} dp(y|\lambda) \\
&= \exp(-\Lambda) \int_L^U \lambda(y_n) \int_L^{y_n} \lambda(y_{n-1}) \cdots \int_L^{y_2} \lambda(y_1)\, dy_1\, dy_2 \dots dy_n \\
&= \exp(-\Lambda) \int_L^U \lambda(y_n) \int_L^U \lambda(y_{n-1}) \cdots \int_L^U \lambda(y_1)\, dt_1\, dt_2 \dots dt_n \ \times \frac{1}{n!} \\
&= \exp(-\Lambda)\Lambda^n/n!
\end{aligned}$$

The integral over the unconstrained $t \in [L, U]^n$ can be written as a sum of integrals over the spaces constrained to respect one of the $n!$ different orders. All these integrals are equal so when we remove the constraint we just divide by $n!$.

(b) Give a reversible jump MCMC algorithm to sample $Y \sim p(\cdot|\lambda)$.

Solution: We only need two moves for irreducibility: add a point or delete a point. Suppose the current state is $Y_t = y$ and $|y| = n$. Choose one of the moves with probability ξ_{add} and $\xi_{del} = 1 - \xi_{add}$. Suppose we take $\xi_{add} = 1/2$.

add a point If we choose to add a point then take $t \sim U[L, U]$ and set $y' = \text{sort}(y_1, \dots, y_n, t)$. The acceptance probability is

$$\begin{aligned}
\alpha(y'|y) &= \min\left\{1,\ \frac{p(y'|\lambda)\xi_{del}(n+1)^{-1}}{p(y|\lambda)\xi_{add}(U-L)^{-1}}\right\} \\
&= \min\left\{1,\ \lambda(t)\frac{(U-L)}{(n+1)}\right\}
\end{aligned}$$

delete a point If we choose to delete a point then if $n = 0$ set $\alpha(y'|y) = 0$. Otherwise, choose a point $i \sim U\{1, \dots, n\}$ and set $y' = y_{-i}$ (ie, remove the point y_i from the points in y). The acceptance probability is

$$\begin{aligned}
\alpha(y'|y) &= \min\left\{1,\ \frac{p(y'|\lambda)\xi_{add}(U-L)^{-1}}{p(y|\lambda)\xi_{del}n^{-1}}\right\} \\
&= \min\left\{1,\ \lambda(y_i)^{-1}\frac{n}{(U-L)}\right\}.
\end{aligned}$$

do accept/reject step With probability $\alpha(y'|y)$ set $Y_{t+1} = y'$ and otherwise set $Y_{t+1} = y$.

(c) Implement this and check the samples you realise satisfy $|Y| \sim \text{Poisson}(\Lambda)$.

Solution: See the code in ProblemSheet3-25.R.

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