International Journal of Statistical Sciences *ISSN 1683–5603*
Vol. 9(Special Issue), 2009, pp 33-57

On a Directionally Adjusted Metropolis-Hastings Algorithm

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[Received December 1, 2008; Accepted February 17, 2009]

Abstract

We propose a new Metropolis-Hastings algorithm for sampling from smooth, unimodal distributions; a restriction to the method is that the target be optimizable. The method can be viewed as a mixture of two types of MCMC algorithm; specifically, we seek to combine the versatility of the random walk Metropolis and the efficiency of the independence sampler as found with various types of target distribution. This is achieved through a directional argument that allows us to adjust the thickness of the tails of the proposal density from one iteration to another. We discuss the relationship between the acceptance rate of the algorithm and its efficiency. We finally apply the method to a regression example concerning the cost of construction of nuclear power plants, and compare its performance to the random walk Metropolis algorithm with Gaussian proposal.

Keywords and Phrases: Independence Sampler, Random Walk Metropolis Algorithm, Student Distribution, Hessian Matrix, Markov Chain Monte Carlo.

AMS Classification: 62E17; 62E20.

1 Introduction

Metropolis-Hastings algorithms have countless applications in science. They aim to provide a sample from a distribution of interest, the target distribution, often too complex or high-dimensional to allow for direct sampling. These efficient sampling methods are particularly popular in Bayesian statistics, where the distribution of interest in often intractable. In statistics however, their application is far from limited to the Bayesian framework, and they can be useful in the classical (or frequentist) approach. In hypothesis testing for instance, it may be of interest to determine an exact p-value; this may be the case when examining new or existing methods for computing p-values, or simply when performing a study about their accuracy (see Bédard et al. 2007).

Common to all Metropolis-Hastings algorithms is the need for selecting a proposal density q, which is used to propose values to be potentially included in the sample. The characteristics of the chosen q define the type of algorithm that is used. The most popular class of Metropolis-Hastings algorithms is undoubtedly that of the random walk Metropolis (RWM) algorithms. The proposal density of these algorithms is centered around the current value of the Markov chain (or, in other words, the current value of the sample); standard choices for the proposal distribution are the normal and the uniform distributions. The proposal density of a RWM algorithm thus evolves over time, and this results in an algorithm that is versatile and extremely easy to apply. In fact, practitioners need to make very few adjustments before using this algorithm; they only need to tune the variance of the proposal distribution in the case of a normal proposal, or its range in the case of a uniform proposal. There already exist guidelines in the literature to facilitate this step (Roberts et al. 1997; Roberts and Rosenthal 2001; Bédard 2006 and 2007). As a drawback to the wide applicability of RWM algorithms, we notice however that their convergence may be lengthy. This should not come as a surprise when taking into account the versatility of the sampling method, which may be applied to sample from virtually any target distribution.

A second class of Metropolis-Hastings algorithms contains the independence samplers. For this class of algorithm, the proposal density q is independent of the previous values in the Markov chain. From one iteration to another, the proposal density thus remains the same. When applying MCMC methods, the selection of the proposal distribution always involves a compromise: the closer it is to the target distribution, the more difficult it is to generate moves from the proposal distribution but the more efficient is the sampling method. Under this scheme, we have the opportunity to select a proposal distribution which is close to the target distribution in a certain sense. Hence, the independence sampler has the potential of enjoying better convergence properties than the RWM algorithm, but it necessitates a better understanding of the target distribution. Generally, independence samplers are more problem-specific than RWM algorithms, but they also require more work in order to come up with a well-suited proposal density.

In this paper, we introduce a new sampling algorithm that could be classified between RWM algorithms and independence samplers. In other words, we attempt to combine the versatility of the RWM algorithm and the performance of the independence sampler to obtain samples from smooth and unimodal target densities. As is the case for the independence sampler, the location of the new proposal distribution is fixed over time; the tails of the proposal distribution however are fine tuned by what we call a directional adjustment. This feature ensures that the tails of the target distribution are not neglected; this is an important detail, particularly when the estimation of tail probabilities is of interest as was the case in Bédard et al. (2007).

The paper is arranged as follows. In Section 2, we introduce some notation and describe the type of target distribution for which the new algorithm is designed. In Section 3, we develop the theory behind the directionally adjusted argument, and in Section 4 we summarize the necessary steps for implementing the algorithm. To illustrate its application and its performance, we consider 3- and 8-parameter regression examples in Sections 5 and 6, and compare the new method to both the independence sampler and the RWM algorithm. We conclude the paper with a discussion in Section 7.

Compared to the RWM algorithm, the resulting algorithm reduces significantly the variances of estimates; it also produces a high acceptance rate. The acceptance rate of an algorithm is defined as the proportion of proposed moves that are accepted as suitable values for the sample. In the case of RWM algorithms, a high acceptance rate is by no mean an indicator of efficiency for the algorithm; on the contrary it generally is a sign that the algorithm is exploring the state space too slowly and thus performing sub-efficiently. In the case of an independence sampler, we are not aware of any theoretical result stating that efficiency is implied by, or somehow related to a high acceptance rate. For instance, an independence sampler with a high acceptance rate might indicate that we sample too much from regions with high target density, and consequently that the proposal distribution is poorly suited to the problem at hand. Intuitively however, we can deduce that a high acceptance rate is a favorable attribute in our case. Indeed, if we are positive that we are not undersampling the tails of the target density, then a high acceptance rate indicates that we are not wasting energy in proposing too great a number of unsuitable values for the target; in other words, the proposal is a good fit!

2 Some Notation

Consider an n-dimensional target density $\pi(\mathbf{x})$, $\mathbf{x} = (x_1, \ldots, x_n)$. Suppose that we are interested in obtaining a sample from this density of interest, but that unfortunately there is no simple way to achieve this directly. We might then use the very general Metropolis-Hastings algorithm (Metropolis et al. 1953; Hastings 1970), which is implemented through the following procedure.

Given that the current sample value is $\mathbf{x}_j$, we propose a new value for the sample by generating a value $\mathbf{y}_{j+1}$ from a preferred proposal distribution with density $q(\mathbf{y}_{j+1} | \mathbf{x}_j)$. Then, we accept this proposed value as the new sample value (i.e. we set $\mathbf{x}_{j+1} = \mathbf{y}_{j+1}$) with probability $\alpha(\mathbf{x}_j, \mathbf{y}_{j+1})$, where

$$\alpha(\mathbf{x}_j, \mathbf{y}_{j+1}) = 1 \wedge \frac{\pi(\mathbf{y}_{j+1})\, q(\mathbf{x}_j | \mathbf{y}_{j+1})}{\pi(\mathbf{x}_j)\, q(\mathbf{y}_{j+1} | \mathbf{x}_j)}; \tag{2.1}$$

otherwise, we repeat the current value in the sample and set $\mathbf{x}_{j+1} = \mathbf{x}_j$. If we then repeat this $N-1$ times from an initial $\mathbf{x}_0$ we will obtain a nominal sample of size N.

This sampling method is very general and might exhibit peformances that are dramatically different depending on which type of proposal density is selected. As mentioned previously, one approach is to use the extremely popular RWM algorithm. Usually, the RWM algorithm employs a proposal density with independent components:

$$q\left(\mathbf{y}_{j+1}\left|\mathbf{x}_j\right.\right) = \prod_{i=1}^{n} q_i\left(y_{j+1,i}\left|\mathbf{x}_j\right.\right),$$

where $q_i\left(y_{j+1,i}\left|\mathbf{x}_j\right.\right)$ is the density for the ith component of $\mathbf{y}_{j+1}$. For instance, one might set $\mathbf{Y}_{j+1} \sim N\left(\mathbf{x}_j, \sigma^2 I_n\right)$ for some $\sigma > 0$, with I_n the n-dimensional identity matrix. The center of the proposal distribution is thus spanning the state space over time. This is a convenient practice, but as soon as we are dealing with a multi-dimensional target distribution which does not possess independent components, as is usually the case, this independence assumption between the proposal components becomes suboptimal.

Nonetheless, applying the method does not require a very thorough study of the target density, and may not be much hassle to implement. If we are lucky, we might even benefit from a reasonable convergence rate to the stationary distribution. However in particular situations, where the density of interest is heavy-tailed for instance, the RWM algorithm may take more time to explore the space and may exhibit a slower convergence to stationarity, which may be frequent in the asymptotic context (as $n \to \infty$).

Now in the case where the target density π is smooth and unimodal and if we are able to maximize the density function, then we may be able to take advantage of this extra information to come up with a refined proposal distribution. In fact, the initial idea would be to design a proposal density that mimics the target density at its maximum. In other words, we would like our proposal density not only to have the same mode as the target density, but also similar curvature properties at the maximum.

For this, let $\hat{\mathbf{x}} = \arg\sup_{\mathbf{x}} \pi\left(\mathbf{x}\right)$ be the point at which the target density attains its maximum (the mode), and let $\pi\left(\hat{\mathbf{x}}\right)$ be the value of the density at that maximum. Recall that the Hessian matrix of the target density is defined as

$$\begin{bmatrix} \frac{\partial^2\pi}{\partial x_1^2} & \frac{\partial^2\pi}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2\pi}{\partial x_1 \partial x_n} \\ \frac{\partial^2\pi}{\partial x_2 \partial x_1} & \frac{\partial^2\pi}{\partial x_2^2} & \cdots & \frac{\partial^2\pi}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2\pi}{\partial x_n \partial x_1} & \frac{\partial^2\pi}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2\pi}{\partial x_n^2} \end{bmatrix}, \tag{2.2}$$

and will typically be negative definite when evaluated at the mode $\hat{\mathbf{x}}$; accordingly we take $\hat{H} = -\partial^2 \log \pi\left(\mathbf{x}\right) / \partial\mathbf{x}\partial\mathbf{x}^T \left.\right|_{\mathbf{x}=\hat{\mathbf{x}}}$ to be the negative Hessian of the log-density at the maximum $\hat{\mathbf{x}}$.

A natural choice for a proposal distribution would then be to select a normal density, whose location and scaling are adjusted to match $\hat{\mathbf{x}}$ and $\hat{H}^{-1}$ respectively. This, however, illustrates well the problem at hand: the resulting proposal distribution is one that is static, i.e. whose location does not vary through time, but whose maximum does mimic that of the target distribution. Using a proposal distribution whose location is static calls for a certain level of caution, mainly to ensure that we are not undersampling from certain areas of the state space. Indeed, it is well-known that the normal density has short tails. It is therefore reasonable to wonder what would happen if we aimed at sampling from a target distribution with long tails? Since the normal distribution seldom proposes moves located far out in the tails, we might expect to either neglect the tails of the target distribution, or have to run the algorithm for a very long time before it converges to the stationary distribution. In order to design an efficient proposal distribution whose location is fixed through time, it is thus necessary to ensure that it has tails that are heavy enough to match those of the target distribution.

How does the acceptance rate of an algorithm relate to the efficiency of the proposed method? For the case of RWM algorithms, it is commonly acknowledged that a high proportion of accepted moves is usually far from guaranteeing any level of perfomance in the algorithm. In the case of a Gaussian proposal distribution for instance, a high acceptance rate might reveal that very small steps are taken at every iteration, and consequently that the algorithm explores its state space inefficiently. In fact, theoretical results prove that for high-dimensional target distributions, the proportion of accepted moves that yields the fastest convergence to the stationary distribution is smaller or equal to 25% (Roberts et al. 1997; Bédard 2006, 2007).

In the case of a proposal distribution whose location is fixed, the acceptance rate must be interpreted differently. Indeed, because the location of the proposal distribution does not span the state space but rather remains fixed, it is important that it does not neglect any region where the target density is positive. In the cases we consider, where the location of both the target and proposal densities are identical, excessively high or low acceptance rates could be indicators of two different concerns. A high acceptance rate could indicate that the proposal distribution is concentrated in regions where the target possesses a high density only, thus ignoring other regions with lower, but positive density; such a proposal distribution could then wrongly lead us to oversample from some regions. At some opposite, the tails of the proposal distribution could be considerably heavier than those of the target distribution and too great a number of improbable values for the target would be proposed; this would translate into a reduced acceptance rate, and would consequently alter the speed of convergence of the algorithm.

As long as we are totally sure that the proposal distribution selected does not neglect any region of the state space, a high acceptance rate is then an indicator that the proposal is a good fit for the target considered. Although this is quite intuitive, we are not aware of any general theoretical result confirming this as yet. This might be related to the fact that for a general form of the target density, it is not straight-forward to design a well-suited proposal distribution with a fixed location that would allow to observe such an implication. In the following section, we introduce a directionally adjusted proposal distribution that attempts to resolve this issue.

3 A Directionally Adjusted Proposal Distribution

3.1 Centering and Scaling the Student Distribution

We aim at sampling efficiently from a smooth and unimodal n-dimensional target density π. Under this setting, the regions most likely to be neglected using a proposal density that is centered around $\hat{\mathbf{x}}$ and scaled according to $\hat{H}^{-1}$ are the tails of the target density. As mentioned in the previous section, a normal proposal would not be a wise choice due to its short tails. To overcome this problem, we consider a distribution with heavier tails, the n-dimensional Student density with f degrees of freedom; in its canonical form, designated $\text{Student}_f\,(0, I_n)$, this density satisfies

$$\begin{aligned} q_f\,(\mathbf{t}) &= \frac{\Gamma\left(\frac{f+n}{2}\right)}{\pi^{n/2}\Gamma\left(\frac{f}{2}\right)}\left(1+t_1^2+\ldots+t_n^2\right)^{-\frac{f+n}{2}} \\ &= \frac{\Gamma\left(\frac{f+n}{2}\right)}{\pi^{n/2}\Gamma\left(\frac{f}{2}\right)}\left(1+\mathbf{t}'\mathbf{t}\right)^{-\frac{f+n}{2}}, \end{aligned} \tag{3.1}$$

where $\mathbf{t}' = (t_1, \ldots, t_n)$. Samples from this distribution are easily generated from any statistical package. Indeed, an observation from an n-dimensional canonical Student distribution with f degrees of freedom can be obtained as

$$\mathbf{t}' = \left(\frac{z_1}{\chi_f}, \ldots, \frac{z_n}{\chi_f}\right), \tag{3.2}$$

where $z_1, \ldots, z_n$ are independent observations from a standard normal distribution and χ_f^2 is an observation from a chi-square distribution with f degrees of freedom.

The negative Hessian of the log density at $\mathbf{t} = \mathbf{0}$ for the n-dimensional canonical Student (3.1) is equal to $(f+n)\,I_n$. Adjusting the location and scaling to match the location and Hessian of the target density at its mode, the proposal then becomes a $\text{Student}_f\left(\hat{\mathbf{x}}, (f+n)\,\hat{H}^{-1}\right)$. For this we then relocate and rescale the generated $\mathbf{t}$'s to obtain

$$\mathbf{y} = \hat{\mathbf{x}} + (f+n)^{1/2}\,\hat{H}^{-1/2}\mathbf{t}, \tag{3.3}$$

where $\hat{H}^{1/2}$ is a right square root matrix of $\hat{H} = (\hat{H}^{1/2})'(\hat{H}^{1/2})$, or alternatively we might use the relation

$$\mathbf{y} = \hat{\mathbf{x}} + \mathbf{w}/\chi_f,$$

where $\mathbf{w}$ designates an observation from a multivariate normal $MN\left(\mathbf{0}, (f+n)\,\hat{H}^{-1}\right)$.

The general form of the relocated and rescaled proposal density is given as

$$q_f(\mathbf{y}) = \frac{\Gamma\left(\frac{f+n}{2}\right)}{\pi^{n/2}\Gamma\left(\frac{f}{2}\right)} \left(1 + \frac{(\mathbf{y}-\hat{\mathbf{x}})' \hat{H} (\mathbf{y}-\hat{\mathbf{x}})}{f+n}\right)^{-\frac{f+n}{2}} \frac{\left|\hat{H}^{1/2}\right|}{(f+n)^{n/2}}. \tag{3.4}$$

Now all that is left is choosing the degrees of freedom f of the distribution. What value of f would produce the optimal speed of convergence for the algorithm? On the one hand, the parameter f has to be small enough to yield tails that are at least as heavy as those of the target density; on the other hand, a too-small value for f could yield unnecessarily heavy tails that would slow down the convergence of the algorithm. Furthermore, we have not yet considered the fact that the picture might vary as we study different directions with the target density; indeed, the target densities considered are often far from spherically symmetrical and the behavior of the tails can vary widely over the state space.

Because of the generality of the target densities studied, a natural decision for the degrees of freedom f of the proposal distribution would be to allow it to vary over time as opposed to choosing a value fixed for the duration of the algorithm. We find this approach to be more efficient, particularly for target densities departing from the spherical assumption.

3.2 Expressing Sample Values in Terms of Direction and Departure

The choice of f will then be redetermined at each iteration of the algorithm. For this, we favor an approach that allows us to match as closely as possible the target and proposal distributions, while ensuring that the tails of the target are not neglected. The idea we propose for selecting the degrees of freedom f in any given iteration is based on the following decomposition, and is outlined in Section 3.3.

The discussion is easier if $\hat{\mathbf{x}} = \mathbf{0}$, the Hessian $\hat{H} = I_n$ is the identity, and thus the root $\hat{H}^{1/2} = I_n$; accordingly we assume this here and address the more general case later. Looking from the maximum of the target density, we examine the target π in the direction of the current state. Suppose that the current state of the algorithm is $\mathbf{x}_j$; we refer to $\mathbf{u}_j = \mathbf{x}_j / |\mathbf{x}_j|$ as the direction of $\mathbf{x}_j$, where $|\mathbf{x}| = \sqrt{x_1^2 + \ldots + x_n^2}$ is the norm of the vector $\mathbf{x}$. The directional argument $\mathbf{u}_j$ is approximately uniformly distributed on a unit sphere in $\mathbb{R}^n$; its density, $\tilde{\pi}(\mathbf{u}_j)$, can then be approximated by $\tilde{\pi}(\mathbf{u}) \approx 1/A_n$, where $A_n = 2\pi^{n/2}/\Gamma(n/2)$ is the surface area of the sphere. Furthermore a random uniform value $\mathbf{u}$ can easily be generated by taking $z_1, \ldots, z_n$ from a unit normal and then standardizing

$$\mathbf{u}' = \frac{(z_1, \ldots, z_n)}{|\mathbf{z}|}. \tag{3.5}$$

According to this method, every sample point can then be expressed as $\mathbf{x}_j = \mathbf{u}_j \cdot s_j$; $\mathbf{u}_j$ is itself an n-dimensional vector indicating the direction of the current sample point $\mathbf{x}_j$ from the mode of the target density, while $s_j = |\mathbf{x}_j|$ gives the radial departure of this sample point from the mode. Analogously, the target density can be reexpressed in terms of the directional and departure variables as $\tilde{\pi}(\mathbf{u}_j, s_j) = \tilde{\pi}(s_j \,|\mathbf{u}_j)\, \tilde{\pi}(\mathbf{u}_j)$.

Using this information and continuing with the assumption that $\hat{\mathbf{x}} = \mathbf{0}$ and $\hat{H} = I_n$, we would like to sample from some proposal density q that is as similar as possible to π; although we chose a Student proposal, we momentarily generalize this choice in the following way. A proposed $\mathbf{y}_{j+1}$ can be decomposed in a similar manner into its own directional and departure arguments: $\mathbf{y}_{j+1} = \mathbf{u}_{j+1}^{prop} \cdot s_{j+1}^{prop}$. We can then reexpress the proposal density $q\left(\mathbf{y}_{j+1}\right)$ accordingly as

$$\tilde{q}\left(\mathbf{u}_{j+1}^{prop}, s_{j+1}^{prop}\right) = \tilde{q}\left(s_{j+1}^{prop} \middle| \mathbf{u}_{j+1}^{prop}\right) \tilde{q}\left(\mathbf{u}_{j+1}^{prop}\right).$$

Here we now take the marginal uniform density approximation of $\tilde{\pi}\left(\mathbf{u}\right)$ as an appropriate sampling process for the proposed direction, $\mathbf{u}_{j+1}^{prop}$. In other words, it suffices to generate the proposed direction from (3.5). To have maximum agreement between the target and proposal densities, we then choose $\tilde{q}\left(s_{j+1}^{prop} \middle| \mathbf{u}_{j+1}^{prop}\right)$ as being an accessible approximation to the conditional target $\tilde{\pi}\left(s_j \left| \mathbf{u}_j \right.\right)$.

In our case, we are restricting the proposal distribution to be a Student distribution with f degrees of freedom. The standardized Student$_f$ density function, designated Student$_f(0, (f + n)I_n)$, is given by

$$q_f\left(\mathbf{T}\right) = \frac{\Gamma\left(\frac{f+n}{2}\right)}{\pi^{n/2}\Gamma\left(\frac{f}{2}\right)} \left(1 + \frac{\mathbf{T}'\mathbf{T}}{f+n}\right)^{-\frac{f+n}{2}} (f+n)^{-n/2}; \tag{3.6}$$

it is such that $\hat{\mathbf{T}} = \mathbf{0}$ and $\hat{H} = I_n$. Furthermore, $\mathbf{T} = (f+n)^{1/2}\, \mathbf{t}$ can be generated by using $\mathbf{t}$ as in (3.2).

For a given $\mathbf{u}_{j+1}^{prop}$, we then choose $\tilde{q}\left(s_{j+1}^{prop} \middle| \mathbf{u}_{j+1}^{prop}\right) = q_f\left(s_{j+1}^{prop} \middle| \mathbf{u}_{j+1}^{prop}\right)$, where $f = f\left(\mathbf{u}_{j+1}^{prop}\right)$ is chosen to make $q_f\left(s_{j+1}^{prop} \middle| \mathbf{u}_{j+1}^{prop}\right)$ close to $\tilde{\pi}\left(s_{j+1}^{prop} \middle| \mathbf{u}_{j+1}^{prop}\right)$. The resulting proposal is thus a Student distribution whose degrees of freedom depend on the proposed direction $\mathbf{u}_{j+1}^{prop}$. For generating s_{j+1}^{prop} from the standardized Student$_f$ (3.6) but given the direction $\mathbf{u}_{j+1}^{prop}$, we can use the $(z_1, \ldots, z_n)$ that gave us the direction $\mathbf{u}_{j+1}^{prop}$ and then obtain the departure as $s_{j+1}^{prop} = (f+n)^{1/2}|\mathbf{z}|/\chi_f$; this gives the sample value $\mathbf{u}_{j+1}^{prop} \cdot s_{j+1}^{prop}$. This is easily implemented due to the rotational symmetry of the standardized Student$_f$ distribution and we are thus in fact sampling from the conditional Student given the direction and having the degrees of freedom determined by the direction.

3.3 Selecting the Degrees of Freedom

We have already argued that a Student density would be a sensible choice for the proposal distribution in the case of a smooth, unimodal target density centered at the origin with Hessian $\hat{H} = I_n$. In this special context, how do we choose an appropriate degrees of freedom for a given iteration? By first generating $\mathbf{u}_{j+1}^{prop}$, we determine in which direction we are going to propose a new value for the algorithm. We then choose a fixed departure, say s^*, which yields a point that is appropriately out in the tail of the target density. The degrees of freedom of the proposal density, f_{j+1}^{prop}, is then chosen so that the target and proposal densities have the same drop-off from the value at the origin to the value at the point $\mathbf{u}_{j+1}^{prop} \cdot s^*$; this reasonably results in good agreement for the tails of the two densities in the direction $\mathbf{u}_{j+1}^{prop}$.

After having determined the degrees of freedom f for a given iteration, we then generate a proposed departure s_{j+1}^{prop} by first generating a χ_f to use in (3.2) together with the $(z_1, \ldots, z_n)$ that generated the $\mathbf{u}_{j+1}^{prop}$, as mentioned in the previous section. In effect we are using a conditional Student distribution special to the direction in order to mimic the target in that direction as much as possible. The proposed value is thus $\mathbf{u}_{j+1}^{prop} \cdot s_{j+1}^{prop}$, which is then accepted or rejected according to the usual acceptance function for the Metropolis-Hastings algorithm.

This procedure results in a proposal density that reproduces the behavior of the target at the maximum and accomodates the form of the tails. At each iteration, the proposal is chosen to match the tail in that generated direction of interest. The choice of f_{j+1}^{prop} for the simplistic case of a one-dimensional target density is illustrated in Figure 1. The target density represented in this figure (solid curve) possesses a relatively heavy tail on the right hand side, and a light tail on the left hand side. When sampling in a direction pointing to the right for such a target density, we propose the Student distribution (dashed curve) with a heavier tail (i.e., smaller degrees of freedom) than if we were sampling in the opposite direction. From the graph, we also notice the point at which the proposal and target densities intersect; for this the target has been rescaled vertically so the drop-off is from a common maximum.

Finding the degrees of freedom f_{j+1}^{prop} for a given iteration involves solving the equation

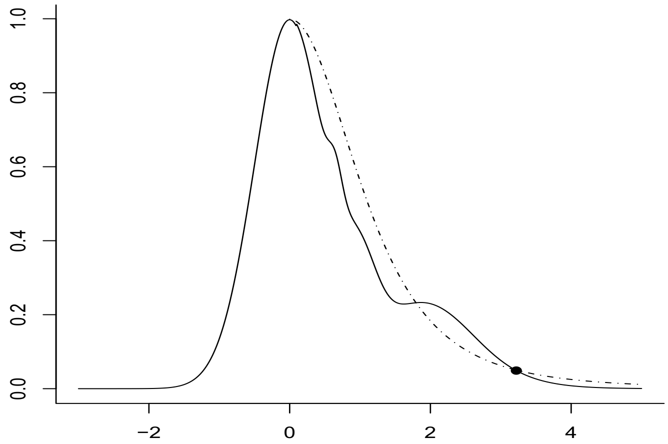
$$\begin{aligned} \frac{\pi\left(\mathbf{u}_{j+1}^{prop} \cdot s^*\right)}{\pi\left(\mathbf{0}\right)} &= \frac{q_{f_{j+1}^{prop}}\left(\mathbf{u}_{j+1}^{prop} \cdot s^*\right)}{q_{f_{j+1}^{prop}}\left(\mathbf{0}\right)} \\ &= \left(1 + \frac{\left(\mathbf{u}_{j+1}^{prop} \cdot s^*\right)'\left(\mathbf{u}_{j+1}^{prop} \cdot s^*\right)}{f_{j+1}^{prop} + n}\right)^{-\frac{f_{j+1}^{prop}+n}{2}}, \end{aligned} \tag{3.7}$$

where $\mathbf{u}_{j+1}^{prop}$ is the generated direction for a new value, and s^* is the distance from the mode to the point where we want the proposal and target densities to intersect in the direction $\mathbf{u}_{j+1}^{prop}$.

There does not exist a closed-form solution for f_{j+1}^{prop} in the previous equation. In practice, it is not necessary to solve for the exact value of f_{j+1}^{prop} in (3.7); for pragmatic reasons, we restrict f_{j+1}^{prop} to be an integer value between 1 (Cauchy distribution) and 50 (near normal distribution). If we let $r^2 = 2\log\left\{\pi\left(\mathbf{0}\right)/\pi\left(\mathbf{u}_{j+1}^{prop} \cdot s^*\right)\right\}$ be the target likelihood ratio quantity and let $Q^2 = \left(\mathbf{u}_{j+1}^{prop} \cdot s^*\right)'\left(\mathbf{u}_{j+1}^{prop} \cdot s^*\right)$ be the quadratic departure for the standardized Student, we can solve for $f_{j+1}^{prop} + n = \overline{f}$ using

$$\overline{f}\log\left(1 + \frac{Q^2}{\overline{f}}\right) = r^2. \tag{3.8}$$

Figure 1: Graph of the target (solid) and proposal (dashed) densities when proposing a value in the direction pointing to the right of the graph. The intersection point is $\mathbf{u}_{j+1}^{prop} \cdot s^*$.



This can be achieved by scanning the values for f_{j+1}^{prop} in $\{1, 2, \ldots, 50\}$ and choosing the closest fit.

3.4 Choosing s^*

There remains one issue to be discussed before being ready to implement the outlined method. We mentioned that we choose the degrees of freedom of the proposal distribution at every iteration so that both the target and proposal densities intersect at an appropriate point in the tail in the given direction. How do we choose s^*, the departure from the mode at which we would like to force an agreement between the target and proposal densities?

To address this issue we once again focus on the standardized version of the target density where we have $\hat{\mathbf{x}} = 0$ and $\hat{H} = I_n$; it should be emphasized that this adjustment does not limit the proposed method as we shall see in Section 4. If the target happened to correspond to the case where the coordinates are independent and approximately normal, then we would have $\mathbf{Y} \sim N(\mathbf{0}, I_n)$ and the distribution of $(s_{j+1}^{prop})^2 = |\mathbf{y}_{j+1}|^2$ given $\mathbf{u}_{j+1}^{prop} = \mathbf{y}_{j+1}/|\mathbf{y}_{j+1}|$ would be a chi square with n degrees of freedom. Consequently, the conditional distribution for departure of the proposed value given its direction, $s_{j+1}^{prop}|\mathbf{u}_{j+1}^{prop}$, would simply be chi in distribution with n degrees of freedom; an approximate mean value for this is $\sqrt{n}$. We thus suggest forcing the target and proposal densities to intersect at a departure of $s^* = \lambda\sqrt{n}$ from the mode, where λ is a tuning parameter. From our experience, λ can be chosen to be 2 or 3 for instance; when chosen in this range, the exact value of the tuning parameter usually has an insignificant impact on the performance of the algorithm.

Accordingly we examine the target distribution drop off at such a distance in the chosen direction and use a degrees of freedom f that boosts the tails of the proposal distribution to match those of the target. We thus choose f to give $\tilde{\pi}\left(s^*|\mathbf{u}_{j+1}^{prop}\right)/q_f\left(s^*|\mathbf{u}_{j+1}^{prop}\right)$ to the degree possible with f in a sensible range of $1, \ldots, 50$.

The resulting proposal density is thus one that has the same location and the same curvature at the maximum as the target density but that also replicates the tail thickness in the direction of the proposed sample value. The Metropolis-Hastings algorithm can then be carried through as usual, by proposing a value from a multivariate Student with the designated degrees of freedom, and then accepting or rejecting this proposed value according to the usual acceptance probability. Overall this results in an algorithm whose proposal has central form that stays fixed throughout time, but whose tails becomes thicker or lighter from one iteration to another depending on the direction from the center of the distribution.

We do note a small technical point concerning the overall effective proposal density. We have spoken of having a particular curvature and Hessian at the maximum. By varying the degrees of freedom with direction we will have differing heights coming to the maximum from differing directions and indeed have a discontinuity at the maximum; this is of no practical significance.

4 The Algorithm

The sampling algorithm introduced herein is valid for general target densities π. To implement the method, it is however convenient to work with a standardized version of the target density. Specifically, we consider $\mathbf{x}^* = \hat{H}^{1/2}(\mathbf{x} - \hat{\mathbf{x}})$, where $\hat{H}^{1/2}$ is a right square root matrix of $\hat{H}$ such that $\hat{H} = (\hat{H}^{1/2})'\left(\hat{H}^{1/2}\right)$. This can easily be obtained with the functions `pdMat` and `pdFactor`, located in the package `nlme` of the statistical freeware **R**. This adjustment implies that $\hat{x}^* = 0$ and $\hat{H}^* = I_n$. The standardized target density satisfies

$$\pi^*(\mathbf{x}^*) = \pi\left(\hat{\mathbf{x}} + \hat{H}^{-1/2}\mathbf{x}^*\right)\left|\hat{H}^{-1/2}\right| \propto \pi\left(\hat{\mathbf{x}} + \hat{H}^{-1/2}\mathbf{x}^*\right) = \pi(\mathbf{x}),$$

where $\hat{H}^{-1/2}$ is the inverse of $\hat{H}^{1/2}$ and $\left|\hat{H}^{-1/2}\right|$ is the determinant of the former; we can thus access standardized density at $\mathbf{x}^*$ by using the original π with the $\mathbf{x}$ value obtained from the mapping $\mathbf{x} = \hat{\mathbf{x}} + \hat{H}^{-1/2}\mathbf{x}^*$.

We also assume that determinations of $\hat{\mathbf{x}}$ and $\hat{H}$ are available; in the statistical freeware **R** for instance, $\hat{\mathbf{x}}$ can usually be obtained with the function `nlm`. The Hessian can either be computed directly using the second derivatives of the density, or obtained numerically with the function `fdHess`. For the algorithm we assume that this standardization has been applied and is used for the following.

Given that $\mathbf{x}_j$ is the time-j state of the algorithm, we perform the following two preliminary steps if not available from preceding calculations:

a. Determine the direction of the standardized current sample value $\mathbf{x}_j^* = \hat{H}^{1/2}(\mathbf{x}_j - \hat{\mathbf{x}})$: $\mathbf{u}_j = \mathbf{x}_j^* / \left|\mathbf{x}_j^*\right|$.

b. Choose the integer value among $\{1, 2, \ldots, 50\}$ which is closest to the solution to (3.8) for $\mathbf{u}_j$; call it f_j.

Once these steps are executed, we are ready to iterate:

1. Generate $\mathbf{u}_{j+1}^{prop}$, an n-dimensional proposed direction, by using the relation in (3.5) (also record the magnitude $|\mathbf{z}_{j+1}|$, as it shall be used in Step 3).

2. Choose the integer value among $\{1, 2, \ldots, 50\}$ which is closest to the solution to (3.8) for $\mathbf{u}_{j+1}^{prop}$; call it f_{j+1}^{prop}.

3. Obtain a proposed departure s_{j+1}^{prop} by generating a value $\chi_{f_{j+1}^{prop}}$ from a chi distribution with f_{j+1}^{prop} degrees of freedom and letting $s_{j+1}^{prop} = (f_{j+1}^{prop} + n)^{1/2} \left|\mathbf{z}_{j+1}\right| / \chi_{f_{j+1}^{prop}}$ (where $|\mathbf{z}_{j+1}|$ has been obtained in Step 1).

4. Obtain the standardized proposed value through the relation

$$\mathbf{y}_{j+1}^* = \left(\mathbf{u}_{j+1}^{prop} \cdot s_{j+1}^{prop}\right).$$

5. Compute the acceptance probability of the proposed sample value

$$\alpha\left(\mathbf{x}_j^*, \mathbf{y}_{j+1}^*\right) = 1 \wedge \frac{\pi\left(\hat{\mathbf{x}} + \hat{H}^{-1/2}\mathbf{y}_{j+1}^*\right) q_{f_j}\left(\mathbf{x}_j^*\right)}{\pi\left(\hat{\mathbf{x}} + \hat{H}^{-1/2}\mathbf{x}_j^*\right) q_{f_{j+1}^{prop}}\left(\mathbf{y}_{j+1}^*\right)}, \tag{4.1}$$

   where $q_f\left(\mathbf{x}\right)$ is as in (3.6).

6. Generate a value r_{j+1} from a uniform distribution on $(0, 1)$.

7. If $r_{j+1} \leq \alpha\left(\mathbf{x}_j^*, \mathbf{y}_{j+1}^*\right)$, then accept the proposed move and set $\mathbf{x}_{j+1}^* = \mathbf{y}_{j+1}^*$, $f_{j+1} = f_{j+1}^{prop}$; otherwise, reject the move and let $\mathbf{x}_{j+1}^* = \mathbf{x}_j^*$, $f_{j+1} = f_j$.

8. Obtain $\mathbf{x}_{j+1} = \hat{\mathbf{x}} + \hat{H}^{-1/2}\mathbf{x}_{j+1}^*$.

9. Replace j by $j + 1$ and repeat these steps for N iterations.

As can be noticed, the preliminary steps (a) and (b) have to be carried out only at the very beginning of the algorithm, for the initial state $\mathbf{x}_0$. After that, they are naturally available from the preceding steps of the algorithm.

When performing Metropolis-Hastings algorithms, the normalization constants for the target and proposal densities are usually superfluous. Indeed, these densities only appear in ratio form in the acceptance probability. In the present case, since the choice for the degrees of freedom of the proposal density depends upon the direction in which the move is proposed, the normalization constants of the proposal density do not in general cancel, and they must then be explicitly included in the acceptance ratio; see (4.1).

Before introducing some examples in which we make use of the directionally adjusted algorithm, we verify that the reversibility condition is satisfied for this new method. This condition ensures that Metropolis-Hastings algorithms converge to the right distribution (i.e., the target distribution), and here can be expressed as

$$\begin{aligned}
&\pi^*\left(\mathbf{x}_j^*\right) q\left(\mathbf{y}_{j+1}^* \left| \mathbf{x}_j^*\right.\right) \alpha\left(\mathbf{x}_j^*, \mathbf{y}_{j+1}^*\right) d\mathbf{x}_j^* \, d\mathbf{y}_{j+1}^* \\
&\qquad\qquad = \pi^*\left(\mathbf{y}_{j+1}^*\right) q\left(\mathbf{x}_j^* \left| \mathbf{y}_{j+1}^*\right.\right) \alpha\left(\mathbf{y}_{j+1}^*, \mathbf{x}_j^*\right) d\mathbf{y}_{j+1}^* \, d\mathbf{x}_j^*.
\end{aligned}$$

In our particular case, the proposal density satisfies

$$q\left(\mathbf{y}_{j+1}^* \left| \mathbf{x}_j^*\right.\right) \equiv q\left(\mathbf{y}_{j+1}^*\right) = q_{f_{j+1}^{prop}}\left(\mathbf{y}_{j+1}^* \left| \mathbf{u}_{j+1}^{prop}\right.\right) \tilde{q}\left(\mathbf{u}_{j+1}^{prop}\right),$$

where $\tilde{q}$ is the uniform density on a sphere in $\mathbb{R}^n$. Since $\tilde{q}$ is in fact constant, we can reexpress the acceptance probability in Step 5 as

$$\alpha\left(\mathbf{x}_j^*, \mathbf{y}_{j+1}^*\right) = 1 \wedge \frac{\pi^*\left(\mathbf{y}_{j+1}^*\right) q_{f_j}\left(\mathbf{x}_j^* \left| \mathbf{u}_j\right.\right) \tilde{q}\left(\mathbf{u}_j\right)}{\pi^*\left(\mathbf{x}_j^*\right) q_{f_{j+1}^{prop}}\left(\mathbf{y}_{j+1}^* \left| \mathbf{u}_{j+1}^{prop}\right.\right) \tilde{q}\left(\mathbf{u}_{j+1}^{prop}\right)}.$$

Consequently, the left hand side of the reversibility condition becomes

$$\begin{aligned}
&\pi^*\left(\mathbf{x}_j^*\right) q_{f_{j+1}^{prop}}\left(\mathbf{y}_{j+1}^* \left| \mathbf{u}_{j+1}^{prop}\right.\right) \tilde{q}\left(\mathbf{u}_{j+1}^{prop}\right) \left(1 \wedge \frac{\pi^*\left(\mathbf{y}_{j+1}^*\right) q_{f_j}\left(\mathbf{x}_j^* \left| \mathbf{u}_j\right.\right) \tilde{q}\left(\mathbf{u}_j\right)}{\pi^*\left(\mathbf{x}_j^*\right) q_{f_{j+1}^{prop}}\left(\mathbf{y}_{j+1}^* \left| \mathbf{u}_{j+1}^{prop}\right.\right) \tilde{q}\left(\mathbf{u}_{j+1}^{prop}\right)}\right) \\
&= \pi^*\left(\mathbf{x}_j^*\right) q_{f_{j+1}^{prop}}\left(\mathbf{y}_{j+1}^* \left| \mathbf{u}_{j+1}^{prop}\right.\right) \tilde{q}\left(\mathbf{u}_{j+1}^{prop}\right) \wedge \pi^*\left(\mathbf{y}_{j+1}^*\right) q_{f_j}\left(\mathbf{x}_j^* \left| \mathbf{u}_j\right.\right) \tilde{q}\left(\mathbf{u}_j\right) \\
&= \pi^*\left(\mathbf{y}_{j+1}^*\right) q_{f_j}\left(\mathbf{x}_j^* \left| \mathbf{u}_j\right.\right) \tilde{q}\left(\mathbf{u}_j\right) \left(1 \wedge \frac{\pi^*\left(\mathbf{x}_j^*\right) q_{f_{j+1}^{prop}}\left(\mathbf{y}_{j+1}^* \left| \mathbf{u}_{j+1}^{prop}\right.\right) \tilde{q}\left(\mathbf{u}_{j+1}^{prop}\right)}{\pi^*\left(\mathbf{y}_{j+1}^*\right) q_{f_j}\left(\mathbf{x}_j^* \left| \mathbf{u}_j\right.\right) \tilde{q}\left(\mathbf{u}_j\right)}\right),
\end{aligned}$$

and the last equality is equivalent to the right hand side of the reversibility condition.

In the next two sections, we apply the sampling method described to obtain p- and s-values in two different regression studies.

5 Toy Example

5.1 Background

As a first example of the applicability and efficiency of the method, we shall focus on the regression example discussed in Bédard et al. (2007). Specifically we consider the following data, which has been generated from the null linear regression model $y_i = \alpha + \beta x_i + \sigma z_i$ with $\alpha = 0, \beta = 1$, $\sigma = 1$, and $k = 7$:

x_i	-3	-2	-1	0	1	2	3
y_i	-2.68	-4.02	-2.91	0.22	0.38	-0.28	0.03

The response variability is the Student density with 7 degrees of freedom (no connection with $k = 7$) and thus the density of the response can be expressed as

$$f(\mathbf{y}; \alpha, \beta, \sigma)\, d\mathbf{y} = \sigma^{-7} \prod_{i=1}^{7} h\left(\frac{y_i - \alpha - x_i\beta}{\sigma}\right) dy_i,$$

where $h(z)$ is the Student density with 7 degrees of freedom.

Let us suppose that we are interested in testing the hypothesis $\beta = 1$. This can be achieved from the Bayesian and the classical perspectives, by respectively computing the posterior survivor value (s-value) and the p-value. We shall examine the performance of the directionally adjusted algorithm under both approaches. This type of example is particularly appealing in the present context; indeed, it is interesting to see how the method performs for the evaluation of tail probabilities.

In the Bayesian setting, we select the default prior $d\alpha\ d\beta\ d\log\sigma$ to perform the analysis; this choice of prior distribution yields s- and p-values that are equivalent under both frameworks, as discussed in Bédard et al. (2007). The default prior selected points towards a more natural choice for the parameter of interest; we shall then use $(\alpha, \beta, \log\sigma)$ rather than (α, β, σ), a convenient parameterization which also has the advantage of avoiding boundary problems. The posterior distribution of $(\alpha, \beta, \log\sigma)$ is then

$$\pi_1\left(\alpha, \beta, \tau \left|\mathbf{y}^0\right.\right) d\alpha\, d\beta\, d\tau = c\, e^{-7\tau} \prod_{i=1}^{7} \left\{1 + \frac{(y_i^0 - \alpha - \beta x_i)^2}{7e^{2\tau}}\right\}^{-4} d\alpha\, d\beta\, d\tau. \tag{5.1}$$

To obtain the exact s-value for testing the hypothesis that β is equal to 1, it suffices to obtain a sample from this posterior density and to record the number of values of β located to the right of the value of interest:

$$s(\beta) = \frac{1}{N} \sum_{j=1}^{N} I\left(\beta_j \geq \beta\right) = \frac{1}{N} \sum_{j=1}^{N} I\left(\beta_j \geq 1\right), \tag{5.2}$$

where N is the size of the sample generated.

The approach for obtaining the exact p-value under the classical approach is discussed in details in Section 6, which considers a similar model. For now, we shall just mention that a sample needs to be obtained from a reparameterized density of interest

$$\pi_2\left(a,b,g\,\middle|\,\mathbf{d}^0\right)da\,db\,dg = c\,e^{5g}\prod_{i=1}^{7}\left(1+\frac{(a+bx_i+e^g d_i^0)^2}{7}\right)^{-4} da\,db\,dg, \tag{5.3}$$

where $d_i^0 = (y_i^0 - x_i b_0)/e^{g_0}$ and b_0, g_0 are the least-squares estimates from the data. The p-value can then be computed by using

$$p(\beta) = \frac{1}{N}\sum_{j=1}^{N} I\left(\frac{b_j}{e^{g_j}} < \frac{b_0-\beta}{e^{g_0}}\right) = \frac{1}{N}\sum_{j=1}^{N} I\left(\frac{b_j}{e^{g_j}} < \frac{b_0-1}{e^{g_0}}\right). \tag{5.4}$$

5.2 Simulations

We compare s- and p-values obtained when applying three different types of Metropolis-Hastings algorithms. In particular, we sample from the target densities π_1 in (5.1) and π_2 in (5.3) by using a random walk Metropolis algorithm with a normal proposal, an independence sampler with a Student$_7(\hat{\mathbf{x}}, (f+n)\hat{H}^{-1})$ proposal distribution, and the directionally adjusted algorithm described previously. We choose a proposal variance of 0.16 for the RWM algorithm; this parameter, just like the parameters of the independence proposal, have been selected so as to yield a reasonable speed of convergence for the algorithms.

In order to estimate the accuracy of the values obtained through each of the methods considered, we use the following approach. For each combination of algorithm and target density, we obtain a sample of size $N = 4,000,000$. We split this vector into 4,000 batches that each contains 1,000 consecutive sample values. In each batch, we drop the first 50 sample values and thus keep the remaining 950 sample values only. We can then compute the s- or p-values obtained from each batch using (5.2) or (5.4) respectively; this yields a vector containing 4,000 s- or p-values that are approximately independent from each other. The exact s- or p-value is estimated by recording the sample average of the 4,000 s- or p-values from the vector. The simulation standard deviation can then be obtained by computing the sample standard deviation of the vector and dividing this number by $\sqrt{4,000}$; for more details, we refer the reader to the appendix in Bédard et al. (2007). The numbers obtained under both the Bayesian and classical frameworks appear in Table 1. We also recorded the acceptance rate of each of the algorithms, as well as the average value of the proposed degrees of freedom ($\sum_{j=1}^{N} f_{j+1}^{prop}/N$) for the directionally adjusted algorithm.

The s- and p-values obtained are very similar for each of the three methods studied. It is interesting to note a significant decrease in the simulation standard deviation of the DA algorithm when compared to the RWM algorithm; in the Bayesian framework, the simulation standard deviation of the DA algorithm is reduced by a factor of about 1.8 compared to that of the RWM algorithm while in the classical framework, this factor is close to 2.2. We also

Table 1: Bayesian s-values and frequentist p-values for testing the hypothesis $\beta = 1$ using three different Metropolis-Hastings algorithms with 4.10^6 iterations.

Test procedure	p-value	s-value
RWM - Normal$(\mathbf{x}_j, 0.16)$	.10821	.10778
(Simulation SD)	$(.0^3 400)$	$(.0^3 475)$
{Acceptance rate}	{32.8%}	{36.7%}
Independence sampler - Student$_7(\hat{\mathbf{x}}, (f+n)\hat{H}^{-1})$	.10821	.10761
(Simulation SD)	$(.0^3 195)$	$(.0^3 355)$
{Acceptance rate}	{76.0%}	{62.7%}
DAMcMC	.10773	.10781
(Simulation SD)	$(.0^3 184)$	$(.0^3 268)$
{Acceptance rate}	{89.3%}	{66.5%}
[Mean f^{prop}]	[37.88]	[28.57]

observe that the Bayesian target density π_1 possesses longer tails than the frequentist target density π_2. This can be witnessed by checking the mean value of the proposed degrees of freedom recorded in Table 1.

The DA algorithm also shows some improvement over the independence sampler in terms of the simulation standard deviation although, as expected, the difference in efficiency is not as flagrant. Nonetheless, it is generally difficult to be certain of the appropriateness of the proposal distribution selected for an independence sampler, especially when working in large dimensions. When applying the DA algorithm, a suitable degrees of freedom is selected automatically at every iteration; since one needs not fix a conservative degrees of freedom to ensure a rapid convergence as is the case for the independence sampler, this results in a gain in efficiency.

It is not appropriate to compare the acceptance rate of the RWM algorithm with the acceptance rates of the independence sampler and DA algorithm. Indeed, the acceptance rate of the RWM algorithm might be tuned through the variance of the normal proposal; here, we used existing theory on the subject to select a proposal variance that should roughly yield a chain converging as fast as possible to its stationary distribution. We can however compare the acceptance rates obtained with the independence sampler and the DA algorithm. We notice that the acceptance rate of the DA algorithm is consistently and significantly higher than that obtained with the independence sampler; this intuitively tells us that the proposal density of the DA algorithm consists in a better fit for both our Bayesian and frequentist target densities. In particular, the acceptance rate of the DA algorithm for computing the p-value recorded in

Table 1 is surprisingly high, which means that the proposal density is even better suited for the target density (5.3) in the classical framework than for (5.1) in the Bayesian framework. In general, a large discrepancy between the acceptance rates of the independence sampler and DA algorithm might reveal an important variation in the tails behavior in different directions; it might also mean that the independence proposal is much too conservative.

Although longer to run than its competitors, we finally mention that the relative efficiency gained by using the DA algorithm makes it worth programming. For instance, running the DA algorithm for this toy example is no longer than about twice the running time of the RWM algorithm, and this factor decreases as the dimension of the target density increases. The difference between the running times of the independence sampler considered here and the DA algorithm are even less important; added to the extra advantages of the DA algorithm discussed earlier, it is preferable to use the latter.

6 Example

6.1 Background

We consider a dataset concerning the cost of construction of nuclear power plants (Example G; Cox and Snell, 1981). Specifically, we have information about 32 light water reactor (LWR) power plants constructed in the USA. The dataset includes 10 explanatory variables, in addition to a constant; it can be found in the Appendix, along with the description of the various explanatory variables.

The chosen response is the natural logarithm of the capital cost ($\log C$), and all the other quantitative variables have also been taken in log form ($\log S$, $\log T_1$, $\log T_2$, and $\log N$). According to the analysis in Cox and Snell (1981) and in Brazzale et al. (2007), a linear regression model seems suitable for this example. There are 4 explanatory variables that are dismissed as non significant ($\log T_1$, $\log T_2$, PR, and BW); see the ANOVA table on page 86 of Cox and Snell (1981). The indicated model thus uses the remaining 7 variables, these being the constant plus D, $\log S$, NE, CT, $\log N$, and PT. Of particular interest is how the capital cost C depends on N, the cumulative number of power plants constructed by each architect-engineer.

Brazzale et al. (2007) first investigated the suitability of a Student distribution with 4 degrees of freedom as the error distribution. The corresponding model is then

$$\mathbf{y} = X\beta + \sigma\mathbf{z},$$

where the design matrix X is the 32 x 7 matrix containing the chosen explanatory variables, and z is distributed according to a Student distribution with 4 degrees of freedom. The density of the response is then

$$f(\mathbf{y};\beta,\sigma)\,d\mathbf{y} = \sigma^{-n}\prod_{i=1}^{n} h\left(\frac{y_i - X_i\beta}{\sigma}\right)dy_i,$$

where $h(z)$ is the Student density with 4 degrees of freedom and X_i is the ith row of the design matrix.

The observed standardized residuals can be recorded as $\mathbf{d}^0 = \left(\mathbf{y}^0 - Xb^0\right)/s^0$ where for convenience we use the least squares regression coefficients b and the related error standard deviation s satisfying $s^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2/(n-r)$ with $n = 32$ and $r = 7$. The observed likelihood function is then

$$\begin{aligned} L^0(\beta, \sigma) &= \sigma^{-n} \prod_{i=1}^n h\left(\frac{y_i^0 - X_i\beta}{\sigma}\right) \\ &= \sigma^{-n} \prod_{i=1}^n h\left(\frac{s^0 d_i^0 - X_i\left(\beta - b^0\right)}{\sigma}\right). \end{aligned}$$

The residuals $\mathbf{d}^0$ have an effect on the precision of the estimates of β and σ when there is error structure other than the usual normal. This is partly reflected in the observed likelihood function $L^0(\beta, \sigma)$ and would then be available for default Bayesian analysis using the familiar default prior $\sigma^{-1}\ d\beta\ d\sigma$. By contrast with a full model $f(\mathbf{y}; \beta, \sigma)$ analysis the available precision is not taken account of. Accordingly we use the conditional model $f\left(\mathbf{y}\left|\mathbf{d}^0\right.; \beta, \sigma\right)$ obtained by conditioning on the identified standardized residuals $\mathbf{d}^0$:

$$f\left(b, s\left|\mathbf{d}^0\right.; \beta, \sigma\right) db\ ds \;=\; c\sigma^{-n} \prod_{i=1}^n h\left(\frac{sd_i^0 - X_i(\beta - b)}{\sigma}\right) s^{n-r-1} db\ ds,$$

where $n = 32$ and $n - r - 1 = 24$.

Now suppose we are interested in the kth regression coefficient; here $k = 6$ corresponding to the explanatory variable $\log N$. The corresponding standardized departure is $t_k = (b_k - \beta_k)/c_{kk}^{1/2}s$ where c_{kk} is the (k,k) element of the matrix $C = (X'X)^{-1}$; it has observed value $t_k^0(\beta_k) = (b_k^0 - \beta_k)/c_{kk}^{1/2}s^0$ and does of course depend on the value β_k being assessed. Due to invariance properties of the model it suffices to compare t_k^0 with the distribution of $t_k = b_k/c_{kk}^{1/2}s$ from the null model with $\beta = 0$ and $\sigma = 1$

$$f\left(b, s\left|\mathbf{d}^0\right.\right) db\ ds = c \prod_{i=1}^n h\left(sd_i^0 + X_i b\right) s^{n-r-1} db\ ds$$

on the $r+1$ dimensional space $\{b, s\}$, or with the distribution of $t_k = b_k/c_{kk}^{1/2}e^a$ from

$$f\left(b, a\left|\mathbf{d}^0\right.\right) db\ da = c \prod_{i=1}^n h\left(e^a d_i^0 + X_i b\right) e^{a(n-r)} db\ da \tag{6.1}$$

on $\mathbb{R}^{r+1}$; the latter can avoid boundary problems.

We thus wish to sample from the target (6.1) and evaluate the p-value function $p(\beta_k)$ that gives the percentage position of the observed data relative to the value β_k for the particular explanatory variable:

$$p\left(\beta_k\right) = \frac{\#\, t_k\left(b, s\right) < t_k^0\left(\beta_k\right)}{N}; \tag{6.2}$$

here N is the size of the simulation and the numerator gives the number of instances (b, s) yielding a value less than the observed $t_k^0(\beta_k)$.

6.2 Simulations

We compare p-values for testing $\beta_6 = -0.1$, $\beta_6 = -0.01$, and $\beta_6 = 0.02$; for each of these hypotheses, the p-values are obtained by applying the three Metropolis-Hastings algorithms considered in Section 5.2. To obtain an efficient speed of convergence for the RWM algorithm, we however select a proposal variance of 0.0001 (i.e. a proposal standard deviation of 0.01). The approach chosen for carrying the MCMC simulations and obtaining the desired p-values is the same as that described in that section. Specifically, we generate a sample of size 4,000,000 that we split into 4,000 batches, each containing 1,000 sample values. We then drop the first 50 values in each of the batches and compute the p-values from (6.2) by using the last 950 values of each batch only. From the resulting vector of 4,000 p-values, we obtain the sample mean and the simulation standard deviation (sample SD/$\sqrt{4,000}$; see Bédard et al. 2007) for each of the three sampling methods selected for comparison. Once again, we record the average acceptance rate of each algorithm, and the average value of the proposed degrees of freedom for the DA algorithm. The results of the simulations are recorded in Table 2; for each hypothesis, we also included the frequentist third order p-value. The general relationship between hypotheses and their corresponding p-value for different sampling methods is depicted in Figure 2.

Contrarily to the toy example of Section 5, the p-values obtained with the three sampling methods selected are not all very close for a given hypothesis. In this higher-dimensional setting, the RWM algorithm does not perform well for the task at hand, i.e. the computation of tail probabilities. In fact, the results obtained under this sampling scheme are very unstable; this can be witnessed by examining Figure 2, which shows two different runs of the RWM algorithm (the dashed curves). Although these two runs embrace the p-values obtained by applying the third order approximation and the DA algorithm, these results are far from agreeing with the latter. We do not however address this instability here; this issue shall be perused separately. The independence sampler and the DA algorithm both yield much more accurate and consistent results. The solid curve depicting the behavior of the DA algorithm agrees very closely with the plotted symbols representing the third order p-values. For clarity purposes, we did not include in the graph a curve for the independence sampler; we however precise that if such a curve were added, it would be impossible to dissociate from the DA curve.

Compared to the example of Section 5, the differences among the simulation standard deviations of the algorithms considered are greatly amplified; in particular, the simulation SD

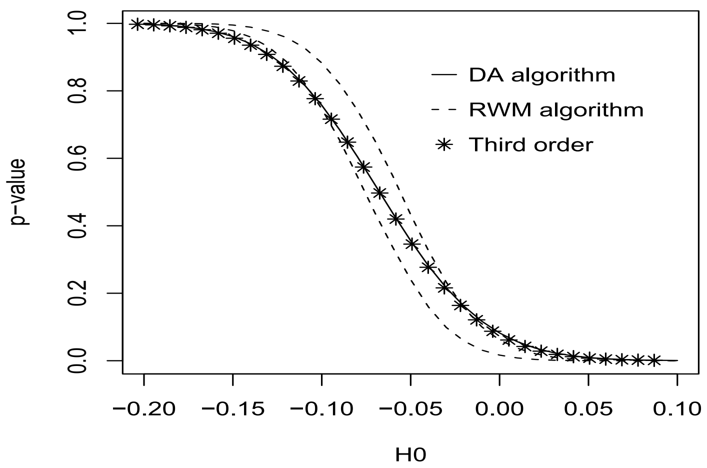
Table 2: Frequentist p-values for testing the hypotheses $\beta_6 = -0.1, -0.01, 0.02$ using three different Metropolis-Hastings algorithms with 4.10^6 iterations. The frequentist third order p-values are also included for comparison.

Test procedure	$\beta_6 = -0.1$	$\beta_6 = -0.01$	$\beta_6 = 0.02$
Thrid order	.75283	.10936	.03646
RWM - Normal$(\mathbf{x}_j, 0.0001)$	.88263	.09019	.01354
(Simulation SD)	$(.0^2399)$	$(.0^2388)$	$(.0^2135)$
$\{$Acceptance rate$\}$	$\{$34.5%$\}$	$\{$34.6%$\}$	$\{$34.5%$\}$
Independence sampler - Student$_7(\hat{\mathbf{x}}, (f + r + 1)\hat{H}^{-1})$	.75675	.11679	.03766
(Simulation SD)	$(.0^3482)$	$(.0^3341)$	$(.0^3185)$
$\{$Acceptance rate$\}$	$\{$36.9%$\}$	$\{$36.9%$\}$	$\{$36.9%$\}$
DAMcMC	.75712	.11695	.03746
(Simulation SD)	$(.0^3328)$	$(.0^3232)$	$(.0^3140)$
$\{$Acceptance rate$\}$	$\{$71.6%$\}$	$\{$71.6%$\}$	$\{$71.6%$\}$
[Mean f^{prop}]	[48.24]	[48.24]	[48.24]

of the DA algorithm is more than 16 times smaller than that of the RWM algorithm when testing $\beta_6 = -0.01$. Combining this with the fact that the discrepancies between the running times of the different sampling methods become less important as the dimension of the target density increases, this makes the DA algorithm a clear winner. An interesting detail to notice in this particular situation is the average proposed degrees of freedom recorded for the DA algorithm, which is close to 50, the maximum value allowed by this algorithm. This is a clear indication that overall, the tails of the target density are almost as short as those of a normal density. Even in such a case, where the target density is short-tailed and seems to behave nicely, the DA algorithm outdoes the RWM algorithm.

The acceptance rate of the DA algorithm is quite high compared to that of the independence sampler; in fact, the independence proposal used here (a Student$_7$ distribution) seems quite conservative compared to the average proposed degrees of freedom obtained from the DA algorithm and recorded in Table 2 (≈ 48). Hence, we can presume that the DA algorithm results in a Markov chain that is mixing more efficiently, by proposing moves that are more appropriate (and thus accepted more often) than those proposed by the independence sampler. This might also explain the fact that the simulation SDs obtained with the DA algorithm are significantly smaller than those obtained with the independence sampler.

Figure 2: Graph of p-values versus hypotheses H_0 obtained by using the DA (solid) and RWM (dashed) algorithms, as well as the third order approximation (symbols).



7 Discussion

We have introduced a new type of Metropolis-Hastings algorithm for sampling from smooth and unimodal target densities, the directionally adjusted (DA) algorithm. The idea behind this method can be divided in two steps: we first use the location and Hessian of the target density to build a proposal density that reproduces the target behavior at its maximum; we then let the tail thickness of the proposal be adjusted at every iteration, by an automatic procedure that attempts to match the tails of the target as closely and efficiently as possible.

We tested this sampling method on two different regression examples; the first example used simulated data, and the second one real data. Specifically, we evaluated the performance of the new algorithm by comparing it with the results produced by a RWM algorithm and an independence sampler. Performance was based on the accuracy of the estimates (p- and s-values along with their simulation standard deviations), the running times of the algorithms, as well as the acceptance rate produced by the methods.

In brief we have found that the DA algorithm consistently outperforms its competitors when looking at the accuracy of the estimates produced. The superiority of the DA algorithm is even more shocking when working in relatively high-dimensional settings, as the discrepancies between the running times of the RWM algorithm, independence sampler, and DA algorithm tend to vanish as the dimension of the target density increases. The results from Section 6 are particularly surprising, as they revealed that traditional sampling methods can go badly wrong when working in higher dimensions. The comparison of the acceptance rates obtained also allowed us to conclude that the DA algorithm yields Markov chains that are mixing more efficiently than those produced by the independence sampler.

8 Appendix

The dataset used in the example of Section 6 appears in Table 3; the description of the explanatory variables can be found in Table 4.

Table 3: Data on 32 LWR power plants in the USA

C	D	T_1	T_2	S	PR	NE	CT	BW	N	PT
460.05	68.58	14	46	687	0	1	0	0	14	0
452.99	67.33	10	73	1065	0	0	1	0	1	0
443.22	67.33	10	85	1065	1	0	1	0	1	0
652.32	68.00	11	67	1065	0	1	1	0	12	0
642.23	68.00	11	78	1065	1	1	1	0	12	0
345.39	67.92	13	51	514	0	1	1	0	3	0
272.37	68.17	12	50	822	0	0	0	0	5	0
317.21	68.42	14	59	457	0	0	0	0	1	0
457.12	68.42	15	55	822	1	0	0	0	5	0
690.19	68.33	12	71	792	0	1	1	1	2	0
350.63	68.58	12	64	560	0	0	0	0	3	0
402.59	68.75	13	47	790	0	1	0	0	6	0
412.18	68.42	15	62	530	0	0	1	0	2	0
495.58	68.92	17	52	1050	0	0	0	0	7	0
394.36	68.92	13	65	850	0	0	0	1	16	0
423.32	68.42	11	67	778	0	0	0	0	3	0
712.27	69.50	18	60	845	0	1	0	0	17	0
289.66	68.42	15	76	530	1	0	1	0	2	0
881.24	69.17	15	67	1090	0	0	0	0	1	0
490.88	68.92	16	59	1050	1	0	0	0	8	0
567.79	68.75	11	70	913	0	0	1	1	15	0
665.99	70.92	22	57	828	1	1	0	0	20	0
621.45	69.67	16	59	786	0	0	1	0	18	0
608.80	70.08	19	58	821	1	0	0	0	3	0
473.64	70.42	19	44	538	0	0	1	0	19	0
697.14	71.08	20	57	1130	0	0	1	0	21	0
207.51	67.25	13	63	745	0	0	0	0	8	1
288.48	67.17	9	48	821	0	0	1	0	7	1
284.88	67.83	12	63	886	0	0	0	1	11	1
280.36	67.83	12	71	886	1	0	0	1	11	1
217.38	67.25	13	72	745	1	0	0	0	8	1
270.71	67.83	7	80	886	1	0	0	1	11	1

Table 4: Notation for data in Table 3

C	Cost in dollars $\times 10^{-6}$, adjusted to 1976 base
D	Date construction permit issued
T_1	Time between application for and issue of permit
T_2	Time between issue of operating licence and construction permit
S	Power plant net capacity (MWe)
PR	Prior existence of an LWR on same site $(= 1)$
NE	Plant constructed in north-east region of USA $(= 1)$
CT	Use of cooling tower $(= 1)$
BW	Nuclear steam supply system manufactured by Babcock-Wilcox $(= 1)$
N	Cumulative number of power plants constructed by each architect-engineer
PT	Partial turnkey plant $(= 1)$

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