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POSTERIOR MOMENTS COMPUTED BY MIXED INTEGRATION

H.K. VAN DIJK AND T. KLOEK

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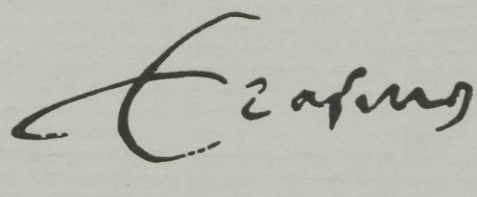

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POSTERIOR MOMENTS COMPUTED BY MIXED INTEGRATION

by H.K. van Dijk and T. Kloek

Abstract

A flexible numerical integration method is proposed for the computation of moments of a multivariate posterior density with different tail properties in different directions. The method (called mixed integration) amounts to a combination of classical numerical integration and Monte Carlo integration. Mixed integration is parsimonious in the sense that the method makes use of the same parameters as the more restrictive multivariate normal importance function.

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June 1983

1. INTRODUCTION

Our research is directed towards the efficient computation of posterior moments of measurable functions of parameters of econometric models in multivariate cases.

Given our prior assumptions these posterior moments cannot be evaluated using analytical integration methods without gross approximation errors or excessive computational costs. In earlier work [4, 8] we made use of Monte Carlo integration methods [2, 6]. As an example of an econometric model we took the well known simultaneous equation model, which is nonlinear in the sense that the expected values of the endogenous variables are usually nonlinear functions of the parameters of interest θ. As a Monte Carlo integration method we made use of importance sampling.

Our application of importance sampling may be described briefly as follows. Let $g(\theta)$ be a measurable function of the parameters of interest θ, where g may be a scalar, a vector or a matrix. Standard examples of g are elements of θ and $\theta\theta'$, but we are also interested in marginal posterior densities [4] and in nonlinear functions of θ such as short-run and long-run multipliers [8]. Our purpose is the efficient computation of

$$(1) \qquad E\, g(\theta) = \frac{\int g(\theta)w(\theta)I(\theta)d\theta}{\int w(\theta)I(\theta)d\theta}$$

The weight function $w(\theta)$ is defined as $p(\theta)/I(\theta)$, where $p(\theta)$ is a kernel of a multivariate posterior density function and the importance function $I(\theta)$ is a multivariate density function with properties to be discussed below. The region of integration in (1) is the set of all θ satisfying $I(\theta) > 0$. The importance function is supposed to be a good approximation of $p(\theta)$, so that $w(\theta)$ is roughly a constant, and the importance function is supposed to have convenient Monte Carlo properties, so that it is relatively easy to generate random drawings from it. As an importance function we made use of the truncated multivariate Student t density. For details we refer to [4, 8]. We shall use the term simple importance sampling for the approach used in [4, 8].

In several econometric applications we found that the surface of the posterior density of a nonlinear model may be ill behaved. An important reason for this phenomenon is small sample size. Then the question arises whether such a density can be approximated with a reasonable degree of accuracy by a multivariate Student t density. A limitation of the Student t is its symmetry,

while truncation of the density is helpful only in special cases. Since our experience with the Student t density was not always successful, we started to consider alternative approaches.

In the present paper we consider the case where the kernel of the posterior density $p(\theta)$ is unimodal but has different tail properties in different directions and we propose a flexible numerical integration method, which is intended to handle this situation. The method proposed transforms the s-dimensional parameter space of vectors θ into another s-dimensional parameter space of pairs (η, ρ), where η is an (s-1)-dimensional vector and ρ a scalar. For ρ we take $\pm$ d, where d is a measure of the distance between a point $\theta^{(i)}$, generated at random, and a point θ^0, a location estimate of θ. As a location estimate we take e.g. the posterior mode or a preliminary estimate of the posterior mean. The vector η is taken as the direction $(\theta^{(i)} - \theta^0)/\rho^{(i)}$ with one coordinate deleted to avoid degeneracy. After having performed the transformation, we generate a vector $\eta^{(i)}$ by means of Monte Carlo and apply classical numerical integration with respect to ρ given $\eta^{(i)}$. So the method amounts to a combination of classical numerical integration and Monte Carlo integration. We call it the mixed integration method. More details on the transformation are given in Section 2 and the Appendix. The mixed integration method is discussed in Section 3. Further comments are contained in Section 4, while our conclusions are given in Section 5.

2. A TRANSFORMATION

In this section we describe a particular transformation of a multivariate normal random variable. We start by defining a multivariate normal density function on the parameter space as

$$I(\theta) = (2\pi)^{-\frac{1}{2}s}|V|^{-\frac{1}{2}}\exp[-\tfrac{1}{2}(\theta - \theta^0)'V^{-1}(\theta - \theta^0)] \tag{2}$$

with $-\infty < \theta_j < \infty$, $j = 1, \ldots, s$. Here θ^0 is the posterior mode or a (possibly rough) first stage estimate of the posterior mean; V is minus the inverse of the Hessian of the log posterior evaluated at θ^0 or another preliminary estimate of the posterior covariance matrix. For more details on the choice of parameters for importance functions we refer to [8, Section 4; and 10].

Next, we partition $\theta - \theta^0$ and V^{-1} as

$$(3) \qquad \theta - \theta^0 = \begin{bmatrix} u \\ v \end{bmatrix} \qquad V^{-1} = \begin{bmatrix} P & q \\ q' & r \end{bmatrix}$$

where v and r are scalars.

We shall make use of

$$(4) \qquad d := (u'Pu + 2u'qv + rv^2)^{\frac{1}{2}}$$

$$(5) \qquad \bar{v} := E(v|u) = -\frac{u'q}{r}$$

Note that d measures the distance from θ to θ^0 according to a norm based on V^{-1} and that $\bar{v}$ is the mean value of the conditional normal distribution of v given u, which is called the regression function [1, p.29]. We partition the region of integration of θ as

$$(6) \qquad \begin{aligned} S_1 &= \{\theta \mid \theta \in \mathbb{R}^s \text{ and } v \geq \bar{v}\} \\ S_2 &= \{\theta \mid \theta \in \mathbb{R}^s \text{ and } v < \bar{v}\} \end{aligned}$$

The transformation that carries θ into (η, ρ) is given by the following transformation formulae,

$$(7) \qquad \begin{aligned} (\eta, \rho) = T_1(\theta) &= \left(\frac{u}{d}, d\right) \qquad \text{if } v \geq \bar{v} \\ (\eta, \rho) = T_2(\theta) &= \left(-\frac{u}{d}, -d\right) \quad \text{if } v < \bar{v} \end{aligned}$$

The regions of integration of (η, ρ) are given by

$$(8) \qquad \begin{aligned} S_1' &= \{(\eta, \rho) \mid \rho \in \mathbb{R}^+, \eta \in \Omega\} \\ S_2' &= \{(\eta, \rho) \mid \rho \in \mathbb{R}^-, \eta \in \Omega\} \end{aligned}$$

where $\mathbb{R}^+$ and $\mathbb{R}^-$ are the sets of positive and negative real numbers, respectively. The characterization of Ω will be discussed in the Appendix. Note that the sign of ρ determines the region of integration S_1' or S_2'.

The inverse transformation that carries (η, ρ) into θ is defined on S_1' and S_2' as the function

$$(9) \qquad (u,\ v) = T^{-1}(\eta,\ \rho) = \left(\rho\eta,\ -\frac{q'\eta}{r}\rho + \frac{\rho}{r}\sqrt{D(\eta)}\right)$$

with

$$(10) \qquad D(\eta) = (q'\eta)^2 + r(1 - \eta'P\eta)$$

where we make use of (4) and (7). Note that v can be rewritten as

$$(11) \qquad v = \bar{v} + \frac{\rho}{r}\sqrt{D(\eta)}$$

So the transformation $T_i(\theta)$ maps the elements of S_i onto S_i', i = 1, 2. The purpose of the inequality conditions in (7) is to make this transformation one-to-one. We shall give a geometric interpretation below.

The Jacobian determinant J, obtained by taking derivatives of u and v with respect to η and ρ, equals

$$(12) \qquad J = \rho^{s-1}J_2(\eta)$$

with

$$(13) \qquad J_2(\eta) = D^{-\frac{1}{2}}(\eta)$$

which can straightforwardly be verified. So the absolute value of the Jacobian determinant $|J|$ is the same in both regions of integrations.

The density function of (η, ρ) is given by

$$(14) \qquad \begin{aligned} I^*(\eta, \rho) &= I\left[T^{-1}(\eta, \rho)\right]|J| \\ &= (2\pi)^{-\frac{1}{2}s}|V|^{-\frac{1}{2}}\exp(-\tfrac{1}{2}\rho^2)|\rho|^{s-1}J_2(\eta) \end{aligned}$$

where we have deleted an index for the region of integration S_1' or S_2' [5, pp.156 and 157], because the density of (η, ρ) is invariant with respect to changing the region of integration. This result is due to the symmetry properties of the multivariate normal density.

A geometric interpretation of the transformation of the random variables θ is presented in Figure 1. At the top we have drawn a contour of a bivariate

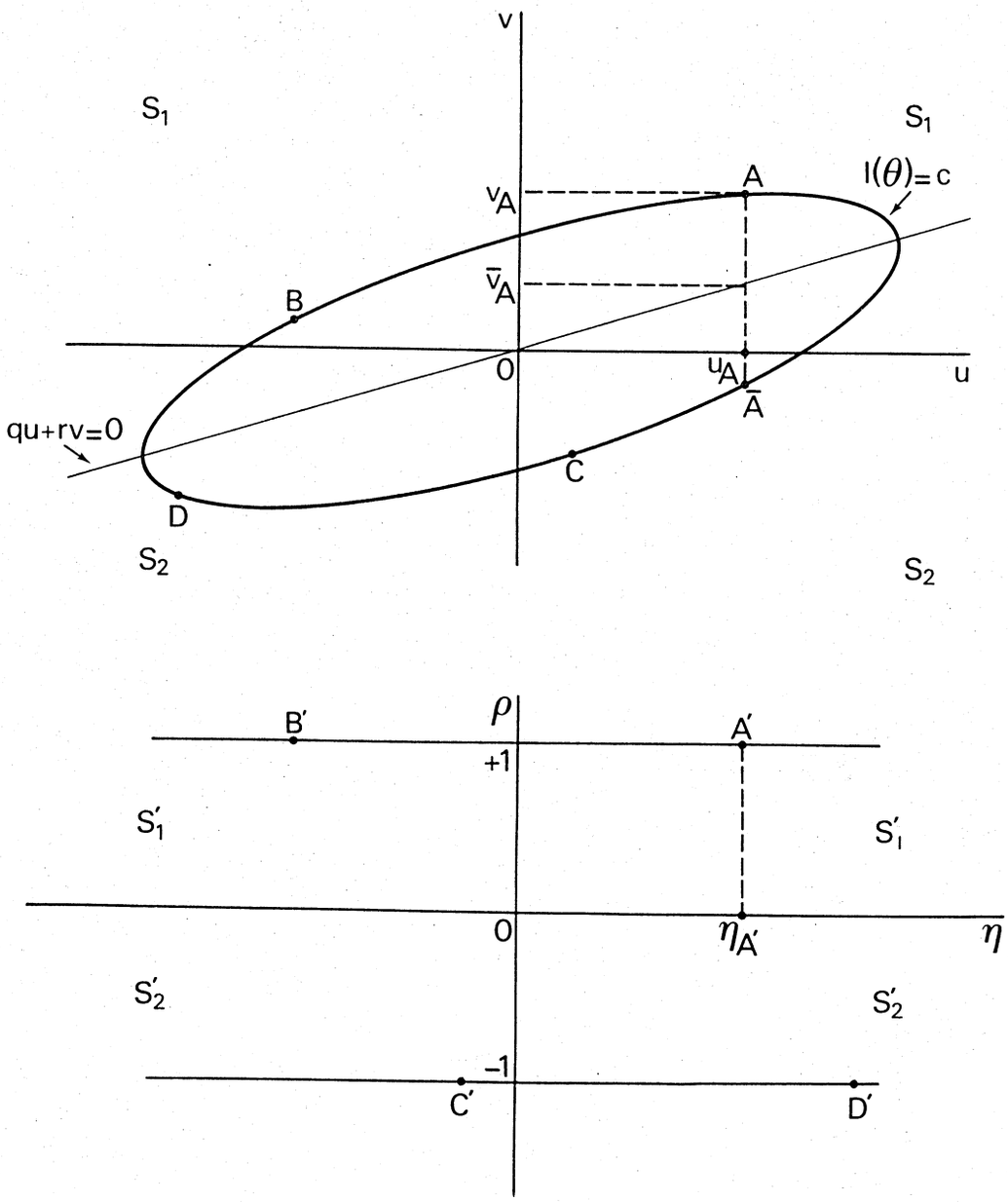

Fig.1 A transformation of the bivariate normal random variable $\theta=(u,v)$ into (η,ρ)

normal importance function $I(\theta) = c$ with $\theta^0 = 0$ and $d = 1$, for convenience only. The regression line $qu + rv = 0$ partitions the region of integration of θ-elements into S_1 and S_2 [compare (6)]. Consider the point A generated at random from $I(\theta)$. A is an element of S_1 because $v_A > \bar{v}_A$ [see (7)]. It follows that A is mapped into the point $A' \in S_1'$ at the bottom of Figure 1, where A' has the coordinates $\eta_{A'} = u_A$ and $\rho_{A'} = +1$. A similar analysis can be given for B. The points C and D are elements of S_2 for which $\rho = -1$ and $\eta = -u$. Note that C' and D' [in the (η, ρ) space] are reflected with respect to the vertical axis compared with C and D.

We conclude this section with a remark. If we do not use the inequality conditions of (7), the transformation of θ into (η, ρ) will be two-to-one in the following way. Let $\eta = u/\rho$ and $\rho = d$, instead of the transformation (7). Then the inverse transformation $\theta = T^{-1}(\eta, \rho)$ will give two solutions of v that are not symmetric around θ^0. This is illustrated in Figure 1. Consider the point $A' = (\eta_{A'}, +1)$ at the bottom. Given $u_A = \eta_{A'}$ [compare (9)], it is seen that there exist two solutions of θ: the points A and $\bar{A}$ on the contour $I(\theta) = c$. This is a disadvantage for practical applications. Another disadvantage of the two-to-one transformation is the asymmetric treatment of the elements of θ. In order to define the direction η one may delete any element of the s-vector $(\theta - \theta^0)$ instead of the last one. In such a case one obtains s+1 solutions of θ by inverting the transformation. Because of these disadvantages we have constructed the transformation described.

3. THE MIXED INTEGRATION METHOD

In this section we apply the transformation of Section 2 to the integrals of equation (1). We write the numerator as $A = A_1 + A_2$ where

$$A_i = \int_{S_i} g(\theta)w(\theta)I(\theta)d\theta \qquad (i = 1, 2) \tag{15}$$

The denominator is handled in the same way after substitution of $g(\theta) = 1$. By making use of the inverse transformation (9) we can write A_i in terms of η and ρ. Let

$$g(\theta) = g[T^{-1}(\eta, \rho)] =: g^*(\eta, \rho) \tag{16}$$

$$w(\theta) = \frac{p[T^{-1}(\eta, \rho)]}{I[T^{-1}(\eta, \rho)]} =: w^*(\eta, \rho)$$

Using (12), (14) and (16) we find

$$w^*(\eta, \rho)I^*(\eta, \rho) = \frac{p[T^{-1}(\eta, \rho)]}{I[T^{-1}(\eta, \rho)]} I[T^{-1}(\eta, \rho)]|J| \tag{17}$$

$$= p[T^{-1}(\eta, \rho)]|\rho|^{s-1}J_2(\eta)$$

Note that the importance function has been dropped from (17). We shall comment on this result in the next section. By making use of (14) and (16) we can write the first of the two integrals in (15) as

$$A_1 = \iint_{S_1'} g^*(\eta, \rho)w^*(\eta, \rho)I^*(\eta, \rho)d\eta d\rho \tag{18}$$

We assume that appropriate regularity conditions are satisfied and substitute (17) into (18). Then one obtains

$$A_1 = \int_{\Omega} \{\int_{\mathbb{R}^+} g^*(\eta, \rho)p[T^{-1}(\eta, \rho)]|\rho|^{s-1}d\rho\}J_2(\eta)d\eta \tag{19}$$

Similar results can be obtained for A_2, where the integration with respect to ρ is over $\mathbb{R}^-$. We recall from Section 2 that the importance function (14) is invariant with respect to the sign of ρ, but we emphasize that the expressions in (16)-(19) will usually not be invariant.

Now suppose we draw N vectors $\eta^{(i)}$ from a distribution with a density proportional to $J_2(\eta)$. Then we may estimate A_1 by means of

$$\bar{A}_1 \propto \frac{1}{N} \sum_{i=1}^{N} \{\int_{\mathbb{R}^+} g^*(\eta^{(i)}, \rho)p[T^{-1}(\eta^{(i)}, \rho)]|\rho|^{s-1}\}d\rho \tag{20}$$

The proportionality sign in (20) is necessary since we have not bothered about the question which part of the integration constant of (2) corresponds to η and which part to ρ. If we treat the numerator and the denominator of (1) in the same way the constants will cancel. The generation of the random drawings η is done by drawing θ from (2) and deriving η through (4) and (7). The one-dimensional integrals in (20) are calculated by means of classical numerical integration methods. There are two reasons for this choice. First, classical integration procedures are known to be quite efficient in handling one-dimensional integration problems. Second, in the type of nonlinear problems we

are interested in, it will be difficult to find a good importance function, since for certain values of η the expression $p[T^{-1}(\eta, \rho)]$ considered as a function of ρ will decrease faster than a normal density as $|\rho|$ tends to infinity, while for other values of η it may decrease slowly as a Student t density with a few degrees of freedom only. Anyway, this is our experience with the examples we studied in [9, 10, 11]. In fact, the integrals in (20) may not converge at all for a diffuse prior when ρ tends to infinity. In our own applications we have taken a prior which is positive on a bounded region only, but the approach of this section can be applied to integration over $\mathbb{R}^s$ provided the integrals exist.

For the practical application of the integration approach we shall discuss one further development. Suppose $\theta^{(i)}$ is a point generated at random from the normal importance function (2). Given $\theta^{(i)}$ we know which transformation formula, $T_1(\theta)$ or $T_2(\theta)$, we have to take from (7). Suppose we take T_1 which gives $(\eta^{(i)}, \rho^{(i)})$. Numerical integration is then performed on the half-line through the points θ^0 and $\theta^{(i)}$, consisting of all positive multiples of $(\theta^{(i)} - \theta^0)$. In case one has to take T_2 (instead of T_1) one performs numerical integration along the half line consisting of all negative multiples of $(\theta^{(i)} - \theta^0)$. One may generate another direction $\eta^{(i+1)}$ (through $\theta^{(i+1)}$) as a next step. We recommend however a modification in the practical application of the integration procedure. Clearly the points $\theta^{(i)} - \theta^0$ and $\theta^0 - (\theta^{(i)} - \theta^0)$ are symmetric around θ^0. Suppose as before that $\theta^{(i)}$ is a point generated at random. Let $\theta^0 - (\theta^{(i)} - \theta^0)$ be the next point to be considered. Then one can perform one-dimensional numerical integration along the line consisting of θ^0 plus all positive and negative multiples of $(\theta^{(i)} - \theta^0)$. This method of generating one point by Monte Carlo and the next one by a symmetry argument is well known in the literature as <u>antithetic</u> sampling [2, 6]. It implies that we replace (20) by

$$\hat{A} \propto \frac{1}{2N} \sum_{i=1}^{N} \left\{ \int_{-\infty}^{\infty} g^*(\eta^{(i)}, \rho) p[T^{-1}(\eta^{(i)}, \rho)] |\rho|^{s-1} d\rho \right\} \tag{21}$$

We divide by 2N since each point drawn is used twice. The posterior kernel is not defined at $\rho = 0$ but since this event has measure zero it is of no importance in the computation of the integrals.

In our integration approach the proportionality (21) is the basic formula for the estimation of the integral A. Since this approach amounts to a combination of classical numerical integration and Monte Carlo integration, we

call it the mixed integration method. In the next section we give some further comments.

4. FURTHER COMMENTS

First, it seems useful to compare the present approach with an alternative we tried before. In [10] we gave pictures of some very skew posterior densities. Student t densities necessarily yield bad approximations in such cases since they are essentially symmetric. Existing families of skew multivariate densities, such as Wishart and poly-t, might be considered but it is rather difficult to fit them to a given posterior. We also considered products of univariate skew densities fitted along the main axes, but the results were not encouraging. Compared with these alternatives the present approach has the advantage that it is both flexible and parsimonious. By flexible we mean that we perfectly follow the shape of the posterior when we integrate with respect to ρ. By parsimonious that we do not introduce additional parameters to describe the shape of the importance function, given preliminary posterior mode estimates or first-stage integration results on posterior mean and covariance matrix.

Second, one might observe that the reciprocal of the density function $I[T^{-1}(\eta, \rho)]$ does not appear in (19)-(21) in the same way it appears in (1) through $w(\theta)$. If we are interested in computing the integral

$$\int g(\theta)p(\theta)d\theta \tag{22}$$

and if $p(\theta)$ has no convenient Monte Carlo properties, we substitute $p(\theta)$ by $[p(\theta)/I(\theta)]I(\theta)$ in order to obtain an expression containing a density from which we can conveniently draw points $\theta^{(i)}$ at random. If we apply the transformation defined by (3)-(7), we can rewrite (22) as follows

$$\begin{aligned}&\iint g[T^{-1}(\eta, \rho)]p[T^{-1}(\theta, \rho)]|J|d\rho d\eta = \\ &\int\{\int g[T^{-1}(\eta, \rho)]p[T^{-1}(\eta, \rho)]|\rho|^{s-1}d\rho\}J_2(\eta)d\eta\end{aligned} \tag{23}$$

compare Section 2 and, in particular, (12). Since $J_2(\eta)$ is already proportional to a density with convenient Monte Carlo properties there is no reason to introduce an importance function in this stage. In fact, when defining the transformation we have already implicitly introduced our

importance function. Note that the posterior kernel of (η, ρ) is decomposed as a conditional density of ρ given η and a marginal density of η. We have incorporated the importance function $I(\theta)$ of (2) explicitly in our derivation since we want to emphasize the link between the kernel $J_2(\eta)$ and the normal density $I(\theta)$ that is used to generate the random directions $\eta^{(i)}$ $(i = 1, \ldots, N)$. We note that there exists a computational efficiency problem with respect to the generation of the random directions. This is illustrated in Figure 2a below [compare comment four].

Third, we mention that one can use the same integral with respect to ρ for different functions $g^*(\eta, \rho)$. For instance, when one is interested in the computation of the first order moments of the vector $\theta - \theta^0$ one takes for g the elements of u and v. But (given η) these are constant multiples of p [compare (9)]. As a consequence only one integral with respect to ρ has to be computed for all elements of θ in (21). So moments of linear functions of θ are easy to compute. This holds similarly for the zero order and second order moments of θ. Marginal posterior densities may be approximated by making use of the integration results for the case $g(\theta) = 1$ on some interval and zero elsewhere [4, Section 7]. Moments of complicated nonlinear functions of θ require additional numerical integrations.

Fourth, a geometric interpretation of some of the features of mixed integration is illustrated for $s = 2$ in Figures 2a and 2b. In Figure 2a we have drawn a contour of a posterior density $p(\theta) = c$ with the mode $\theta^0 = 0$, for convenience only. The point A, generated at random from a bivariate normal importance function with $\theta^0 = 0$, is located on the contour $I(\theta) = c$. Numerical integration can be performed on the line through the points -A and A by making use of antithetic sampling. Note that (-)A is mapped into (-)A' [compare also Figure 1]. Typical shapes of the function $p[T^{-1}(\eta_{A'}, \rho)]|\rho|$, considered as a function of ρ given $\eta_{A'}$, are shown in Figure 2b. The different shapes illustrate the flexibility of mixed integration. Furthermore, Figure 2a illustrates that it is less efficient to take a standard normal importance function ($V = I$) because one should generate more lines in the direction of the main diagonal than orthogonal to it.

Finally, we mention two cases in the literature where a transformation of the multivariate normal density is considered with a Jacobian factor that differs from (12) and (13) only with respect to the expression of $J_2(\eta)$. First, Anderson [1, pp. 175 and 176] and Kendall and Stuart [3, pp. 246 and 247] give the transformation of normal variables into polar coordinates.

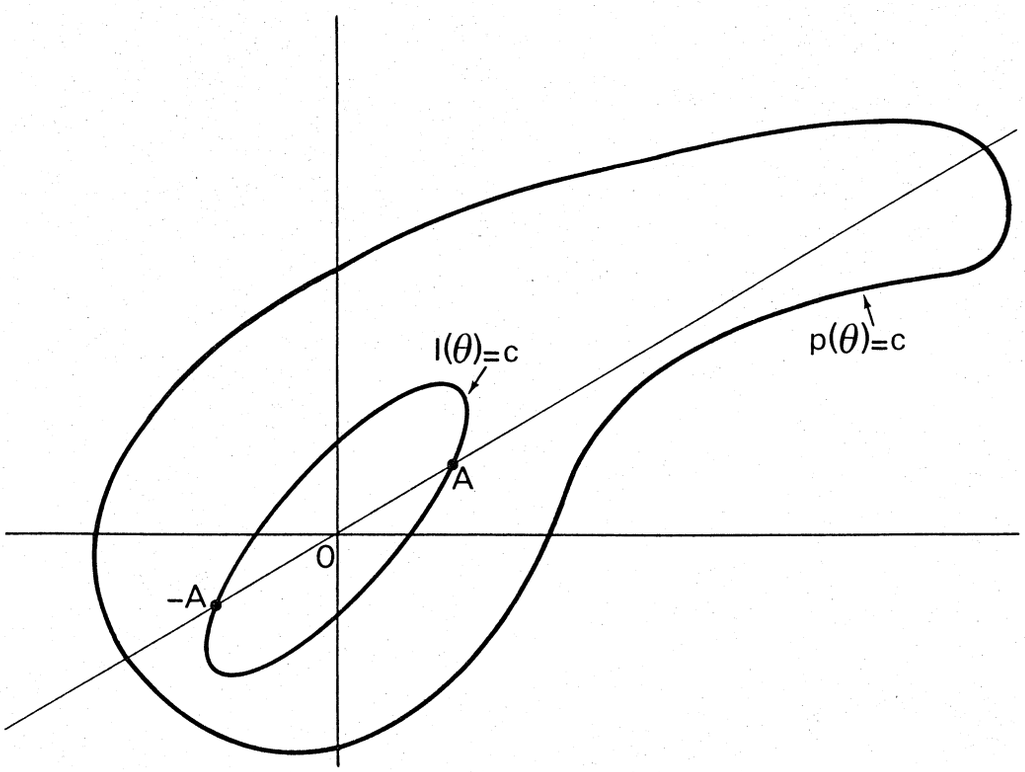

Fig. 2a Contours of the posterior density $p(\theta)=c$ and the normal importance function $I(\theta)=c$ with $\theta^{o}=0$

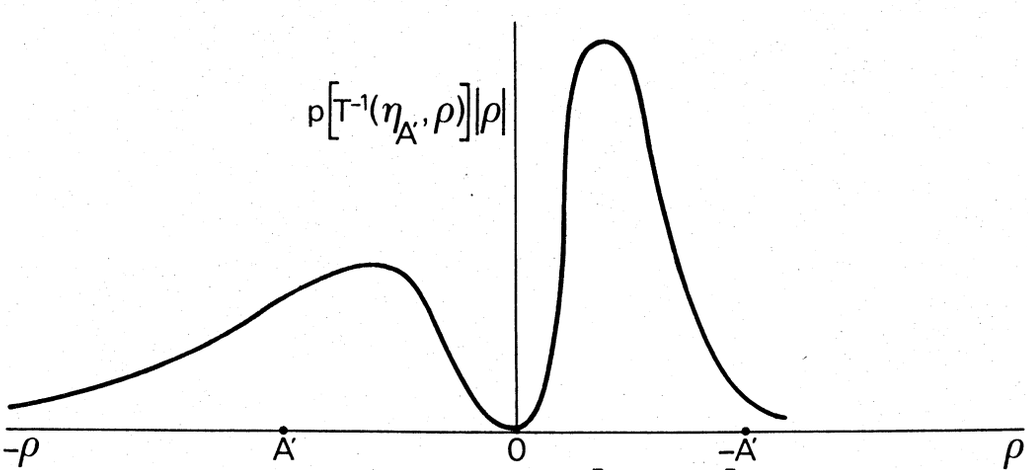

Fig. 2b Typical shapes of the function $p\left[T^{-1}(\eta_{A'},\rho)\right]|\rho|$ considered as a function of ρ given $\eta_{A'}$

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We have opted for (7) since it appears relatively easy for practical applications. Second, Trotter and Tukey [7] make use of a transformation of normal random variables in what is known as Conditional Monte Carlo. In this approach a possibly awkward parameter space is enlarged to a more suitably chosen space. Details are discussed in [2, Chapter 6]. By contrast, we have reduced the s-dimensional parameter space of θ-elements into an (s-1)-dimensional space of η-elements. Our approach has the advantage of being parsimonious with respect to the number of parameters of the importance function.

5. CONCLUSIONS

In this paper we have proposed a flexible numerical integration method that can be used for the computation of posterior moments in case the multivariate posterior density has different tail properties in different directions. The method is parsimonious because one makes only use of the parameters of the more restrictive multivariate normal importance function, which will approximate the tail behavior of the posterior mentioned above very poorly. Increased flexibility is, of course, not a free good. But the price of one-dimensional numerical integration along lines in the parameter space is not very restrictive on modern computers. Practical experience with several examples, for instance with the Klein-Goldberger model, which involves thirty-dimensional numerical integration [9], indicates the feasibility of the mixed integration approach in a case where simple importance sampling failed to converge. In [11] we compared mixed integration and simple importance sampling with an alternative Monte Carlo method where the importance function consists of a finite mixture of multivariate normal densities. The particular mixture used was tailor-made for the example studied. In other words, the finite mixture approach can probably not be applied to arbitrary models, without first studying the properties of their likelihood functions. The results of some experiments indicate that an importance function based on mixtures is rather efficient but that mixed integration appears robust and can be used in a rather mechanical way. Of course, more experience is needed in this area before any final conclusions can be given.

APPENDIX

The set Ω in equation (8) may be defined as

$$\Omega = \{\eta | \eta \in \mathbb{R}^{s-1} \text{ and } \eta' V_1 \eta \leq 1\} \tag{24}$$

where

$$V_1 := P - q \frac{1}{r} q' \tag{25}$$

The characterization of Ω is based on the following argument. We start with (2) and (3) and note that v is a real number. Next, given an (η, ρ) the corresponding value of v is obtained from the inverse transformation (9). Suppose the discriminant $D(\eta)$ in (9) is negative. Then there is no real solution for v. This is a contradiction. Therefore, using the definition of $D(\eta)$ in (10), we have

$$\eta' q q' \eta - r \eta' P \eta + r \geq 0 \tag{26}$$

This inequality can be rewritten, by making use of (25), as

$$\eta' V_1 \eta \leq 1 \tag{27}$$

So Ω is an ellipsoid provided V_1 is positive definite. It is straightforward to verify, using (2) and (3), that V_1 is the inverse of the covariance matrix of the vector u. The covariance matrix of the multivariate normal random variable θ in (2) is positive definite. Then the covariance matrix (and the inverse of the covariance matrix) of u is positive definite [1, p. 337].

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