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# Simulation of multivariate normal rectangle probabilities and their derivatives Theoretical and computational results

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#### Abstract

An extensive literature in econometrics and in numerical analysis has considered the problem of evaluating the multiple integral  $P(\mathbf{B}; \mu, \Omega) = \int_a^b n(v - \mu, \Omega) \, \mathrm{d}v \equiv \mathbf{E}_V \mathbf{1}(V \in \mathbf{B})$ , where V is a m-dimensional normal vector with mean  $\mu$ , covariance matrix  $\Omega$ , and density  $n(v - \mu, \Omega)$ , and  $\mathbf{1}(V \in \mathbf{B})$  is an indicator for the event  $\mathbf{B} = \{V | a < V < b\}$ . A leading case of such an integral is the negative orthant probability, where  $\mathbf{B} = \{V | V < 0\}$ . The problem is computationally difficult except in very special cases. The multinomial probit (MNP) model used in econometrics and biometrics has cell probabilities that are negative orthant probabilities, with  $\mu$  and  $\Omega$  depending on unknown parameters (and, in general, on covariates). Estimation of this model requires, for each trial parameter vector and each observation in a sample, evaluation of  $P(\mathbf{B}; \mu, \Omega)$  and of its derivatives with respect to  $\mu$  and  $\Omega$ . This paper surveys Monte Carlo techniques that have been developed for approximations of  $P(\mathbf{B}; \mu, \Omega)$  and its linear and logarithmic derivatives, that limit computation while possessing properties that facilitate their use in iterative calculations for statistical inference: the Crude Frequency Simulator (CFS), Normal Importance Sampling (NIS), a Kernel-Smoothed Frequency Simulator (KFS), Stern's Decomposition

This paper collects and extends results obtained by the authors in Hajivassiliou and McFadden (1990), McFadden (1989), McFadden and Ruud (1990), and Ruud (1986, 1991).

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Simulator (SDS), the Geweke-Hajivassiliou-Keane Simulator (GHK), a Parabolic Cylinder Function Simulator (PCF), Deák's Chi-squared Simulator (DCS), an Acceptance/Rejection Simulator (ARS), the Gibbs Sampler Simulator (GSS), a Sequentially Unbiased Simulator (SUS), and an Approximately Unbiased Simulator (AUS). We also discuss Gauss and FORTRAN implementations of these algorithms and present our computational experience with them. We find that GHK is overall the most reliable method.

Key words: Simulation estimation; Monte Carlo integration; Discrete choice models; Multinomial probit models; Importance sampling; Acceptance/rejection; Gibbs resampling

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#### 1. Introduction

An extensive literature in econometrics and in numerical analysis<sup>1</sup> has considered the problem of evaluating the multiple integral

$$P \equiv P(\mathbf{B}; \mu, \Omega) = \int_{a}^{b} n(v - \mu, \Omega) \, dv \equiv \mathbf{E}_{V} \mathbf{1}(V \in \mathbf{B}), \tag{1}$$

where V is a m-dimensional normal random vector with mean  $\mu$ , covariance matrix  $\Omega$ , and density  $n(v - \mu, \Omega)$ , and  $\mathbf{1}(V \in \mathbf{B})$  is an indicator for the event  $\mathbf{B} = \{V \mid a < V < b\}$ . A leading case of such an integral is the negative orthant probability, where  $\mathbf{B} = \{V \mid V < 0\}$ . The problem is computationally difficult unless the dimension of the integral is less than four or the covariance matrix  $\Omega$  has a special structure, such as a factorial structure with a small number of factors.

The multinomial probit (MNP) model used in econometrics and biometrics has cell probabilities that are negative orthant probabilities, with  $\mu$  and  $\Omega$  depending on unknown parameters and, in general, on covariates.<sup>3</sup> Estimation of this

<sup>&</sup>lt;sup>1</sup> See Clark (1961), Daganzo (1980), Davis and Rabinowitz (1984), Dutt (1973, 1976), Fishman (1973), Hammersley and Handscomb (1964), Horowitz, Sparmonn, and Daganzo (1981), Moran (1984), Owen (1956), Rubinstein (1981), Stroud (1971), and Thisted (1988).

<sup>&</sup>lt;sup>2</sup> Where convenient, we write  $P(\mathbf{B}; \mu, \Omega)$  as  $P(a, b; \mu, \Omega)$ , or when  $a = -\infty$ , as  $P(b; \mu, \Omega)$ . Note that  $P(b; \mu, \Omega) \equiv P(0; \mu - b, \Omega)$  is the cumulative multivariate normal distribution, also denoted  $+(b; \mu, \Omega)$ . This setup covers all cases of interest, since components  $V_i$  for which both limits are infinite can be margined out analytically, and components  $V_i$  with  $a_i$  finite and  $b_i = +\infty$  can be converted to the previous case by a reversal of sign.

<sup>&</sup>lt;sup>3</sup> For example, see McFadden (1984).

model requires, for each trial parameter vector and each observation in a sample, evaluation of (1) and of its linear and logarithmic derivatives with respect to  $\mu$  and  $\Omega$ . This paper surveys Monte Carlo techniques that have been developed for approximation of (1) and its derivatives that limit computation while possessing properties that facilitate their use in iterative calculations for statistical inference. Section 2 presents the simulation methods we consider. An Appendix discusses GAUSS and FORTRAN algorithms implementing these methods. Section 3 describes the test problems we used to investigate the operational properties of the methods and summarizes our computational experience with them. Section 4 concludes the paper.

#### 2. Simulation methods

We begin by deriving the linear and logarithmic derivatives of choice probabilities, and then we discuss the simulation approaches we consider in this paper. After introducing some notation in Section 2.3, we explain the general principles of sequential sampling and acceptance/rejection techniques in Section 2.4, of unbiased and asymptotically unbiased simulation in Section 2.5, and of importance sampling in Section 2.6. We then discuss two variance-reduction methods (antithetic variates in Section 2.7 and control variates in Section 2.8). Sections 2.9 through 2.19 describe the eleven simulation techniques that we analyze in this paper. Table 1 summarizes the methods and the mnemonics we will adopt. We begin with the most direct method, the crude frequency simulator

Table 1						
Simulators for	P, V	P.	$\nabla_{\alpha}P$	$\nabla \log P$	and	$\nabla_{\alpha} \log P$

			Unbiased for		
Section	Name of simulator	Mnemonic	P	$\nabla P$	$V \log P$
2.9	Crude Frequency Simulator	CFS	У	n	n
2.10	Normal Importance Sampling Simulator	NIS	y	n	n
2.11	Kernel-Smoothed Frequency Simulator	KFS	ya	n	n
2.12	Stern Decomposition Simulator	SDS	y	n	n
2.13	Geweke Hajivassiliou-Keane Simulator	GHK	y	n	n
2.14	Parabolic Cylinder Function Simulator	PCF	у	n	n
2.15	Deák Chi-square Simulator	DCS	y	n	n
2.16	Acceptance/Rejection Simulator	ARS	_	-	у
2.17	Gibbs Sampler Simulator	GSS			y <sup>b</sup>
2.18	Sequentially Unbiased Simulator	SUS	n	n	n
2.19	Approximately Unbiased Simulator	AUS	n	n	n

<sup>&</sup>lt;sup>a</sup> Window parameter must approach 0.

<sup>&</sup>lt;sup>b</sup> Number of Gibbs resamplings must approach ∞.

(CFS), which computes the sample frequency of simulated draws from a binomial distribution with probability P. Next we describe a generalization of the CFS which employs the technique of importance sampling, thereby converting the sample frequency to a weighted sample frequency that can have a smaller sampling variance. We call this the normal importance sampling (NIS) simulator. The kernel-smoothed frequency simulator (KFS) generalizes the CFS by replacing the discrete zero-one outcome of the binomial experiment by a continuous outcome on the [0,1] interval. This simulator overcomes the discontinuities in the CFS with respect to the parameters of the underlying normal distribution, but is biased. The fourth through seventh simulators, the Stern decomposition simulator (SDS), the Geweke-Kajivassiliou-Keane simulator (GHK), the parabolic cylinder function (PCF) simulator, and the Deák chisquare simulator (DCS), are also applications of importance sampling like the NIS and are both smooth and unbiased. These simulators differ according to the importance sampling distribution that they use. All of the simulators, from CFS through DCS, are simulators of P and its derivatives.

A second group of simulators apply specifically to the logarithmic derivatives of P, because these simulators address the additional difficulties posed by the problem of sampling from a truncated normal distribution. The acceptance/rejection simulator (ARS) is another importance sampling technique which additionally filters out draws that fall outside an acceptance region determined by the truncation. The Gibbs sampler simulator (GSS) is an alternative method for sampling from the truncated multivariate normal distribution. The GSS is smooth in the distribution parameters, but the ARS is not. A third approach is taken in the sequentially unbiased simulators (SUS) which construct unbiased simulators of 1/P. The last method, approximately unbiased simulators (AUS), comprises a family of simulators that are approximately unbiased for 1/P. The members of this family can be constructed from most of the simulators of P in the first group.

#### 2.1. Derivatives of rectangle probabilities

The derivatives of (1) with respect to  $\mu$  and  $\Omega$  can be written:<sup>4</sup>

$$V_{\mu}P(\mathbf{B};\mu,\Omega) = \Omega^{-1} \int_{-\infty}^{+\infty} \mathbf{1}(v \in \mathbf{B})(v-\mu)n(v-\mu,\Omega) \,\mathrm{d}v$$

$$\equiv \Omega^{-1}\mathbf{E}_{\mathbf{V}}\mathbf{1}(V \in \mathbf{B})(V-\mu). \tag{2}$$

<sup>&</sup>lt;sup>4</sup> Eq. (3) is derived without imposing symmetry on the elements of  $\Omega$ , and is then simplified by using the symmetry of  $\Omega$  at the evaluation point. These formulas are due to Ruud (1986), and they can be demonstrated using the matrix derivatives  $\partial \log |A|/\partial A = A^{-1}$  and  $\partial A^{-1}/\partial A = -A^{-1} \otimes A^{-1}$ . If Γ is a lower triangular Choleski factor of  $\Omega$ , so that  $\Omega = \Gamma \Gamma'$ , then  $\nabla_r P = 2(\nabla_{\Omega} P)\Gamma$ .

(4)

$$\nabla_{\Omega} P(\mathbf{B}; \mu, \Omega) = \frac{1}{2} \Omega^{-1} \int_{-\infty}^{+\infty} \mathbf{1}(v \in \mathbf{B}) \left[ (v - \mu)(v - \mu)' - \Omega \right]$$

$$\times n(v - \mu, \Omega) \, \mathrm{d}v \cdot \Omega^{-1}$$

$$\equiv \frac{1}{2} \Omega^{-1} \mathbf{E}_{V} \mathbf{1}(V \in \mathbf{B}) \left[ (V - \mu)(V - \mu)' - \Omega \right] \cdot \Omega^{-1}. \tag{3}$$

These formulas imply

$$\nabla_{\mu} \log P(\mathbf{B}; \mu, \Omega) \equiv \nabla_{\mu} P(\mathbf{B}; \mu, \Omega) / P(\mathbf{B}; \mu, \Omega) = \Omega^{-1} \mathbf{E}_{V \mathbf{B}} (V - \mu),$$

$$\nabla_{\Omega} \log P(\mathbf{B}; \mu, \Omega) \equiv \nabla_{\mu} P(\mathbf{B}; \mu, \Omega) / P(\mathbf{B}; \mu, \Omega)$$

$$= \frac{1}{2} \Omega^{-1} \mathbf{E}_{VB} \left[ (V - \mu)(V - \mu)' - \Omega \right] \cdot \Omega^{-1}, \tag{5}$$

where  $\mathbf{E}_{V|\mathbf{B}}$  denotes expectation with respect to the conditional density  $n(v-\mu,\Omega,\mathbf{B}) \equiv \mathbf{1}(v \in \mathbf{B})n(v-\mu,\Omega)/P(\mathbf{B};\mu,\Omega)$ . Note that (2) and (3) are partial moments of the density, and (4) and (5) are conditional moments. It is useful for statistical applications to develop techniques for approximating (4)–(5) as well as (1)–(3).

Eqs. (1)–(3) can be written

$$H \equiv H(\mathbf{B}; \mu, \Omega) = \int_{-\infty}^{+\infty} \mathbf{1}(v \in \mathbf{B}) h(v) n(v - \mu, \Omega) \, \mathrm{d}v \equiv \mathbf{E}_{\mathbf{V}} \mathbf{1}(V \in \mathbf{B}) h(V), \quad (6)$$

and Eqs. (4) and (5) can be written

$$H_C = \mathbf{E}_{V|\mathbf{R}} h(V) \equiv H/P(\mathbf{B}; \mu, \Omega), \tag{7}$$

where h(v) is the polynomial array

$$h(v) = \begin{bmatrix} 1 & (v - \mu)'\Omega^{-1} \\ \Omega^{-1}(v - \mu) & \frac{1}{2} [\Omega^{-1}(v - \mu)(v - \mu)'\Omega^{-1} - \Omega^{-1}] \end{bmatrix}.$$
 (8)

Then the northwest element of H gives (1), the remainder of the first row gives (2), and the southeast subarray gives (3); the analogous elements of  $H_C$  give 1, (4), and (5).

#### 2.2. Simulation procedures

For statistical inference, it is often unnecessary to achieve high numerical accuracy in evaluation of (1)–(5). For example, simulating P by the frequency of the event  $\mathbf{I}(v \in \mathbf{B})$  in a number of Monte Carlo draws comparable to sample size will tend to produce statistics in which the variance introduced by simulation is at worst of the same magnitude as the variance due to the observed data. Further, when probabilities appear linearly across observations in an estimation criterion, independent unbiased simulation errors are averaged out. Then, a small, fixed number of draws per probability to be evaluated will be sufficient with increasing sample size to reduce simulation noise at the same rate as noise

from the observed data.<sup>5</sup> This makes it computationally feasible to treat statistical problems that require repeated evaluation of high-dimensional normal rectangle probabilities. McFadden (1989), Pakes and Pollard (1989), and McFadden and Ruud (1990) analyze the statistical properties of such estimators, and Hajivassiliou (1993a) surveys simulation estimation methods for limited dependent variable models.

The first seven methods we will discuss in this paper, CFS through DCS, simulate H. Methods ARS and GSS simulate  $H_C$  by drawing from the conditional distribution of V given  $V \in \mathbf{B}$ . Method SUS approximates  $H_C = H/P$  using independent unbiased simulators of H and 1/P. Method AUS is similar, but uses a biased simulator of 1/P to speed computation. Some versions of AUS require a positive simulator of P. This is guaranteed by NIS, SDS, GHK, PCF, DCS, and by KFS if a positive kernel is used. The number of draws required in ARS is random. The remaining methods will in general use a fixed number of repetitions, which may in statistical applications increase with sample size.

To understand what is perhaps the most intuitive simulation method, write the random vector V as

$$V = \mu + \Gamma \eta, \tag{9}$$

where  $\eta$  is an independent standard normal vector of dimension m and  $\Gamma$  is a lower triangular Choleski factor of  $\Omega$ , so  $\Omega = \Gamma \Gamma'$ . A simple approach to approximating (6) is to make repeated Monte Carlo draws for  $\eta$ , use (9) to calculate V for each parameter vector, and then form an empirical analogue of the expectation in (6). Below we call this the *crude frequency simulator* (CFS) of  $P(\mathbf{B}; \mu, \Omega)$  and its derivatives. Similarly, a crude frequency simulator for  $H_C$  can

$$0 = N^{1/2} \mathbf{E}_N s(\hat{\theta}, \eta),$$

where s is an approximation (involving Monte Carlo elements  $\eta$ ) to a function  $\sigma(\theta)$  of P and its derivatives that has expectation zero at the true parameter  $\theta^{o}$ , and  $\mathbf{E}_{N}$  denotes empirical expectation over an independent sample of size N. Then, one can write

$$\begin{split} 0 &= N^{1/2} \mathbf{E}_N s(\hat{\theta}, \eta) \\ &\equiv N^{1/2} \mathbf{E}_N \sigma(\theta^o) + N^{1/2} \mathbf{E}_N \big[ s(\theta^o, \eta) - \sigma(\theta^o) \big] + N^{1/2} \mathbf{E}_N \big[ \sigma(\hat{\theta}) - \sigma(\theta^o) \big] \\ &+ N^{1/2} \mathbf{E}_N \big[ s(\hat{\theta}, \eta) - \sigma(\hat{\theta}) - s(\theta^o, \eta) + \sigma(\theta^o) \big]. \end{split}$$

Under standard regularity conditions, the first term is asymptotically normal, reflecting the noise in the observations, and the third term is proportional to  $\sqrt{N}(\hat{\theta}-\theta^a)$ . The last term will be of order  $o_p(1)$  for simulators that satisfy a stochastic equicontinuity condition. When s is a smooth function of crude frequency simulators of P,  $\nabla_\mu P$ , etc., obtained using R Monte Carlo draws, the second term will behave like  $\sqrt{N/R}$  times an expression that is asymptotically normal, so that it will be comparable in magnitude to the first term when R and N are proportional. If, in addition, there is any averaging out of simulation noise across observations, the second term may be of order  $o_p(1)$  when R and N are proportional, or comparable in magnitude to the first term for fixed R.

<sup>&</sup>lt;sup>5</sup> In outline, suppose  $\hat{\theta}$  is an M-estimator that solves

be formed by rejecting draws of V that do not satisfy the conditioning event  $V \in \mathbf{B}$ , and then forming an empirical analogue of the conditional expectation in (7) using the accepted draws. The advantages and disadvantages of the frequency simulators are discussed in Section 2.9 below.

## 2.3. General notation

Before discussing the simulation techniques, it is useful to introduce the following notation. For a vector of indices  $(1, \ldots, n)$ , we use the notation '< j' to denote the subvector  $(1, \ldots, j-1)$ , and '-j' to denote the subvector that excludes component j. Thus, for a matrix  $\Gamma, \Gamma_{j, < j}$  denotes a vector containing the first j-1 elements of row j, and  $\Gamma_{-j, -j}$  denotes the subarray excluding row j and column j. For a vector  $\eta, \eta_{< j}$  is the subvector of the first j-1 components, and  $\eta_{-j}$  is the subvector excluding component j.

## 2.4. Sequential sampling and acceptance/rejection methods

Some simulation techniques, such as the crude frequency simulators for  $H_C$  that reject draws not in **B**, require sequential sampling. Others, such as the crude frequency simulator for P, may employ sequential sampling for some purposes such as approximating 1/P. Sequential sampling may involve excessive computation if the yield of accepted points is low, so there is a payoff to techniques that increase yields. Sequential schemes also introduce the possibility of occasional lengthy computations. For computer implementation it is desirable to bound computation by building censoring rules into the sampling algorithms and taking account of the effects of this censoring on the statistical properties of the simulators.

Acceptance/rejection methods provide a mechanism for drawing from a conditional density when practical exact transformations from uniform or standard normal variates are not available. The following result is standard:

Lemma 1. Suppose f(x) is a m-dimensional density, and one wishes to sample from the conditional density  $f(\cdot | \mathbf{A})$  given the event  $x \in \mathbf{A}$ . Suppose g(x) is a density from which it is practical to sample, with the property that

$$\sup_{A} f(x)/g(x) \leqslant \alpha < +\infty.$$

Assume that either the support of g is A, or that it is practical to test if  $x \in A$ ; that it is practical to calculate f(x) and g(x); and that it is practical to calculate a bound  $\alpha$ .

<sup>&</sup>lt;sup>6</sup> See Devroye (1986) or Rubinstein (1981).

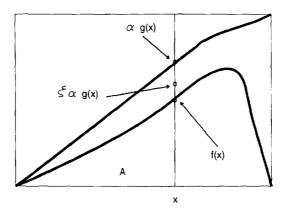


Fig. 1. Acceptance/rejection.

Draw x from g and  $\zeta$  from a uniform density on [0,1], repeat this process until a pair satisfying  $x \in \mathbf{A}$  and  $f(x) \ge \zeta \alpha g(x)$  is observed, and accept the associated x. Then, the accepted points have density  $f(x|\mathbf{A}) \equiv f(x)/f(\mathbf{A})$ .

*Proof.* Fig. 1 shows schematically that this method yields accepted points with the density  $f(x)/f(\mathbf{A})$ : One draws points uniformly from the area under  $\alpha g$ , and rejects them if they are above f, leaving a uniform distribution of points from the area f: Prob $(x\&accept) = g(x) \cdot [f(x)/g(x)\alpha]$ , implying Prob $(x|accept) = f(x)/f(\mathbf{A})$ , as desired.  $\square$ 

Suppose now that acceptance/rejection is used with a *censoring rule* that if the first r trials do not yield an acceptance, then the last draw from g(x) is accepted unconditionally. This method will be biased, but the bias is bounded at a geometric rate in r:

Lemma 2. Suppose the assumptions of Lemma 1 hold, with **A** the support of g. Suppose an acceptance/rejection sampling rule, with censoring after r trials. Let  $f^{(r)}(x|A)$  denote the density of x obtained by the censored A/R rule. Then, for any measurable function h(x) such that the expectation  $\int h(x)g(x) dx$  exists,

$$|\int h(x)f(x|A) dx - \int h(x)f^{(r)}(x|A) dx|$$

$$\leq |\int h(x)[g(x) - f(x)/f(\mathbf{A})] dx| \cdot [1 - f(\mathbf{A})/\alpha]^r. \tag{10}$$

*Proof.* The probability of acceptance on a trial, given x is drawn, is  $f(x)/\alpha g(x)$ , so that the unconditional probability of acceptance is

$$\int g(x) [f(x)/\alpha g(x)] dx = f(\mathbf{A})/\alpha.$$

Then, the probability of a rejection on the first r trials is  $[1 - f(\mathbf{A})/\alpha]^r$ , and the probability of x and acceptance on trial i is

$$\lceil 1 - f(\mathbf{A})/\alpha \rceil^{i-1} \lceil f(x)/\alpha g(x) \rceil g(x).$$

Then, the probability of x is

$$f^{(r)}(x|\mathbf{A}) = \sum_{i=1}^{r} \left[ 1 - f(\mathbf{A})/\alpha \right]^{i-1} f(x)/\alpha + \left[ 1 - f(\mathbf{A})/\alpha \right]^{r} g(x)$$
$$= \frac{1 - \left[ 1 - f(\mathbf{A})/\alpha \right]^{r}}{1 - \left[ 1 - f(\mathbf{A})/\alpha \right]} \cdot f(x)/\alpha + g(x) \left[ 1 - f(\mathbf{A})/\alpha \right]^{r}$$
$$= f(x|\mathbf{A}) + \left[ g(x) - f(x)/f(\mathbf{A}) \right] \cdot \left[ 1 - f(\mathbf{A})/\alpha \right]^{r}.$$

Since  $\alpha g(x)/f(\mathbf{A})$  dominates  $f(x)/f(\mathbf{A})$ ,  $\int h(x)f(x|\mathbf{A}) dx$  exists. Then forming the expectation using the formula above gives the result.

# 2.5. Unbiased and asymptotically unbiased simulators

The crude frequency simulators of H and  $H_C$  are all unbiased with finite variance, desirable properties that guarantee that when these expressions appear linearly in a condition defining a statistical estimator and the draws are independent across observations, a central limit theorem will operate to attenuate the effect of simulation noise on the estimator. For H, there are unbiased simulators that are smooth in parameters; we have not found smooth unbiased simulators for  $H_C$ . It may be advantageous for computation to work with smooth biased simulators, and increase the number of draws in statistical applications as iterative search proceeds or as sample size increases, to eliminate bias in the limit.

An important case where bias is an issue is simulation of 1/P in the expression  $(\nabla_{\mu}P)/P$  and  $(\nabla_{\Omega}P)/P$  for the logarithmic derivatives. Obviously, an unbiased simulator of P such as the crude frequency simulator for (1) does not yield an unbiased simulator of 1/P. One technique for achieving an unbiased simulator is based on the observation that 1/P is the expectation of the geometric distribution of the number of independent draws R from (9) required to yield  $V \in \mathbf{B}$ ; this can be simulated by drawing sequentially from (9) until  $V \in \mathbf{B}$  is observed. For P small, this method can require a large number of simulations. The following result, due to Ruud, refines the method first by using an upper bound on P, and second by reducing the variance in the simulation of the run length.

Lemma 3. Assume there is an event A such that:

- (i)  $\mathbf{E}_{\mathbf{V}}\mathbf{1}(V \in \mathbf{A})$  can be computed exactly.
- (ii)  $\mathbf{B} \subseteq \mathbf{A}$ .
- (iii) It is convenient to draw from  $n(v \mu, \Omega)$  conditioned on the event **A**.

Draw sequentially from the conditional distribution of V given  $\mathbf{A}$  until  $V \in \mathbf{B}$  is observed, and let R denote the number of draws required. Then,  $R/\mathbf{E}_V \mathbf{1}(V \in \mathbf{A})$  is an unbiased simulator of 1/P. The variance in the simulator is reduced by defining

$$R = 1 + O_1(1 + O_2(1 + O_3(1 + \cdots))), \tag{11}$$

where each  $Q_i$  is an independent unbiased simulator of  $\mathbf{E}_{V|\mathbf{A}}\mathbf{1}(V \notin \mathbf{B})$ , initially the  $Q_i$  are smooth simulators, and eventually  $Q_i = \mathbf{1}(V_i \notin \mathbf{B})$ , where the  $V_i$  are draws of V given  $\mathbf{A}$ .

*Proof.* 
$$\mathbf{E}R = \Pr(\mathbf{A})/\Pr(\mathbf{B}) = 1/\mathbf{E}_{V|\mathbf{A}}\mathbf{1}(V \in \mathbf{B});$$
 then  $ER/\mathbf{E}_{\mathbf{V}}\mathbf{1}(V \in \mathbf{A}) = 1/P.$  The alternative form for  $R$  has  $\mathbf{E}R = 1 + (\mathbf{E}Q_1)(1 + (\mathbf{E}Q_2))(1 + \cdots)) = \sum_{i=0}^{K} (1-P)^i = \Pr(\mathbf{A})/\Pr(\mathbf{B}),$  as required.  $\square$ 

If **A** can be chosen so that  $Pr(\mathbf{A})/Pr(\mathbf{B})$  is not too large, then the expected number of draws required in (11) is not impractically large, even for small P. For example, the event **A** that  $a_i < V_i < b_i$ , with i a specific component of V, has the properties:

- (i)  $\mathbf{E}_{\mathbf{V}}\mathbf{1}(V \in \mathbf{A}) = \Phi((b_i \mu_i)/\Omega_{ii}^{1/2}) \Phi((a_i \mu_i)/\Omega_{ii}^{1/2}).$
- (ii)  $\mathbf{A} \subseteq \mathbf{B}$ .
- (iii) It is easy to draw V conditioned on A by first drawing

$$V_i = \Phi^{-1}(\zeta \Phi((h_i - \mu_i)/\Omega_{ii}^{1/2}) + (1 - \zeta)\Phi((a_i - \mu_i)/\Omega_{ii}^{1/2})), \tag{12}$$

where  $\zeta$  is uniform on [0,1], and then drawing

$$V_{-i} = \mu_{-i} + \Omega_{-i,i} \Omega_{ii}^{-1} (V_i - \mu_i) + L \eta_{-i}, \tag{13}$$

where L is a Choleski factor of  $\Omega_{-i,-i} - \Omega_{-i,i}\Omega_{ii}^{-1}\Omega_{i,-i}$ . Choosing the i that minimizes  $\mathbf{E}_{\mathbf{v}}\mathbf{1}(V \in \mathbf{A})$  then provides a practical bound.

A continuous-in-parameters simulator of 1/P can be constructed, at the cost of some bias, using a variant of Lemma 3 suggested by Ruud:

Lemma 4. Make the assumptions of Lemma 3, except take

$$R = 1 + \sum_{i=1}^{r-1} \prod_{j=1}^{i} Q_j, \tag{14}$$

with the  $Q_i$  smooth independent unbiased simulators of  $\mathbf{E}_{V|\mathbf{A}}\mathbf{1}(V \notin \mathbf{B})$ . Then

$$1/P - (ER)/\mathbf{E}_{\mathbf{V}}\mathbf{1}(V \in \mathbf{A}) = (1 - \mathbf{E}_{V \mid A}\mathbf{1}(V \in \mathbf{B}))^{r}/P.$$
(15)

*Proof.* From the proof of Lemma 3,

$$\mathbf{E}R - 1/\mathbf{E}_{V|\mathbf{A}}\mathbf{1}(V \in \mathbf{B}) = \sum_{i=r}^{r} \prod_{j=1}^{i} \mathbf{E}Q_{j} = [\mathbf{E}_{V|\mathbf{A}}\mathbf{1}(V \notin \mathbf{B})]^{r}/\mathbf{E}_{V|\mathbf{A}}\mathbf{1}(V \in \mathbf{B}). \quad \Box$$

Suppose one simulates 1/P by a ratio  $N/r\mathbf{E}_V\mathbf{1}(V \in \mathbf{A})$ , where N is the random number of sequential draws necessary to obtain r occurrences of the event  $V \in \mathbf{B}$  given  $V \in \mathbf{A}$ , where the notation is as in Lemma 2. The following result due to McFadden, applied with  $U_i = 1/\mathbf{E}_V\mathbf{1}(V \in \mathbf{A})$  and  $W_i = \mathbf{1}(V \in \mathbf{B})$ , with V drawn from the density  $f(v|\mathbf{A})$ , bounds the bias in this simulator:

Lemma 5. Suppose  $(U_i, W_i)$  are independently identically distributed with  $U_i \ge 0, 1 \ge W_i$ ,  $\mathbf{E}W_i = \beta > 0$ , and  $\mathbf{E}U_i = \alpha > 0$ . Let r > 1 denote a positive constant. Suppose N is an integer-valued random variable defined as the first n such that  $\sum_{i=1}^{n} W_i \ge r$ . Then

$$\left| \mathbf{E} \sum_{i=1}^{N} U_i / \sum_{i=1}^{N} W_i - \alpha/\beta \right| \leqslant r^{-1} \alpha/\beta. \tag{16}$$

*Proof.* A lemma of Stein's (Siegmund, 1985, Prop. (2.19)) establishes  $P(N > n) < C\rho^n$ , for constants C > 0 and  $0 < \rho < 1$ , implying  $EN < +\infty$ . Then, Wald's identity (Siegmund, 1985, Prop. (2.20)) establishes  $E\sum_{i=1}^{N} U_i = \alpha EN$  and  $E\sum_{i=1}^{N} W_i = \beta EN$ . Then,  $r \le \beta EN < r + 1$ , implying

$$\mathbf{E} \sum_{i=1}^{n} U_i / \sum_{i=1}^{n} W_i \leq \alpha \mathbf{E} Nr < (\alpha/\beta)(1 + 1/r)$$

and

$$\mathbb{E} \sum_{i=1}^{n} U_{i} / \sum_{i=1}^{n} W_{i} \ge \alpha \mathbb{E} N / (m+1) \ge (\alpha/\beta) (1 - 1/(r+1)) > (\alpha/\beta) (1 - 1/r). \quad \Box$$

This result can also be applied when correlated draws are used in the numerator and denominator of expressions like  $(\nabla_u P)/P$ .

## 2.6. Importance sampling

Importance sampling is a general method for reducing the sampling variance of integrals computed by Monte Carlo integration. The CFS involves sampling V from the  $n(v - \mu, \Omega)$  p.d.f. and evaluating the indicator  $\mathbf{1}(V \in \mathbf{B})$ . A simple generalization of this procedure rewrites the rectangle probability  $P(\mathbf{B}; \mu, \Omega)$  in terms of another sampling distribution:

$$P(\mathbf{B}; \mu, \Omega) = \int \mathbf{1}(v \in \mathbf{B}) n(v - \mu, \Omega) \, \mathrm{d}v$$
$$= \int \left[ \mathbf{1}(v' \in \mathbf{B}) \frac{n(v' - \mu, \Omega)}{f(v'; \mu, \Omega)} \right] f(v'; \mu, \Omega) \, \mathrm{d}v'.$$

By sampling V' from the importance p.d.f. f and evaluating the weighted indicator function  $\mathbf{1}(V' \in \mathbf{B})n(V' - \mu, \Omega)/f(V'; \mu, \Omega)$ , one obtains an alternative

unbiased simulation of P. The first advantage that importance sampling offers is the ability to substitute sampling from f for sampling from n. It may be possible to sample f more quickly, or, in a more general setting, sampling from n may be infeasible. In addition, if f also has an analytical integral over a truncated sampling region C such that  $B \subseteq C$ , then this analytical integral can be exploited as an approximation to P:

$$P(\mathbf{B};\mu,\Omega) = \Pr\{V' \in \mathbf{C}\} \int_{\mathbf{C}} \left[\mathbf{1}(v' \in \mathbf{B}) \frac{n(v'-\mu,\Omega)}{f(v';\mu,\Omega)}\right] \frac{f(v';\mu,\Omega)}{\Pr\{V' \in \mathbf{C}\}} \, \mathrm{d}v'.$$

By drawing from the truncated p.d.f.  $f/\Pr\{C\}$ , fewer simulations are 'wasted' on outcomes of zero and, in effect,

$$\Pr\{V' \in \mathbb{C}\} \frac{n(v' - \mu, \Omega)}{f(v'; \mu, \Omega)}$$
 approximates  $P(\mathbf{B}; \mu, \Omega)$ .

When f is a good approximation to n, so that the ratio of densities n/f is relatively constant, the sampling variance of the importance-sampling simulator is small. The sampling variance of the CFS is P(1-P) and the sampling variance of the importance sampler is

$$\operatorname{var}(P_{\mathbf{C}} \cdot \mathbf{1}\{V' \in \mathbf{B}\} w(V')) = P_{\mathbf{C}}^2 \cdot P_{\mathbf{B}} \cdot [V(w(V')|V' \in \mathbf{B}) + (1 - P_{\mathbf{B}}) \cdot \mathbb{E}(w(V')|V' \in \mathbf{B})^2],$$

where  $P_{\mathbf{C}} \equiv \Pr\{V' \in \mathbf{C}\}\$ and  $P_{\mathbf{B}} \equiv \Pr\{V' \in \mathbf{B}\}\$ . In the extreme case f = n and  $\mathbf{C} = B$ , the latter is zero; clearly good approximations to n afford improvements over the CFS.

#### 2.7. Antithetic variates

The accuracy of simulators may be improved, for a given number of Monte Carlo draws, by use of antithetic variates. The principle of antithetic variates, which is to introduce negative correlation between successive Monte Carlo draws to reduce the variance of simulation sample averages, generalizes in the multivariate case to selection of a regular grid of points whose location is random. This technique can be employed in simulators of H and  $H_C$  when the method has sufficient symmetry.

In Monte Carlo simulation requiring draws of m-dimensional standard normal vectors, for example the crude frequency simulator, an approach due to Deák (1980a, b) has good antithetic properties: Draw m independent standard normal vectors, and save their lengths  $\rho_1, \ldots, \rho_m$ . Apply a Gram Schmidt orthonormalization to these vectors to create a random basis for m-space. Let  $v_1, \ldots, v_m$  denote the unit vectors in this basis. Each pair of unit vectors  $v_i$  and  $v_j$  with  $i \neq j$  define a great circle on the unit hypersphere. Generate 2m equally

spaced points on each great circle,

$$v_{ijk} = v_i \cos(\pi k/m) + v_j \sin(\pi k/m), \qquad k = 0, \dots, 2m - 1.$$

This gives a random antithetic grid on the unit hypersphere that is particularly useful for simulations based on spherical transformations. Scale each unit vector  $v_{ijk}$  by the lengths  $\rho_1, \ldots, \rho_m$  to give an array of normal vectors in m-space. A further antithetic refinement uses the fact that the squared lengths of standard normal vectors in m-space have a chi-squared distribution with m degrees of freedom. Taking  $\rho_j^2 = invchi((\zeta + j)q, m), j = 0, \ldots, q - 1$ , where  $\zeta$  is a uniform [0,1] random number and  $invchi(\cdot, m)$  is the inverse of the chi-squared distribution, gives q antithetic lengths that are images of a random grid from the uniform distribution.

#### 2.8. Control variates

Control variates are random variables with analytic expectations that are positively correlated with the random variable whose expectation is to be simulated. Then, simulation variance can be reduced by simulating only the difference between the expectations of the variate of interest and the control variate. A possible control variate for  $\mathbf{1}(V \in \mathbf{B})h(V)$  is  $\mathbf{1}(V \in A)h(V)$ , where  $\mathbf{A}$  is the event  $a_i < V_i < b_i$ , with i a specific component of V. Then, for any  $\alpha$ ,

$$H = \alpha \mathbf{E}_{\mathbf{V}} \mathbf{1}(V \in \mathbf{A}) h(V) + \mathbf{E}_{\mathbf{V}} [\mathbf{1}(V \in \mathbf{B}) - \alpha \mathbf{1}(V \in \mathbf{A})] h(V). \tag{17}$$

The first expectation on the right-hand side of (17) has a closed form, given below. The second expectation requires simulation. This control variate is not guaranteed to reduce simulation noise, but generally simulations based on (17) will be more accurate than simulations based on (6) if  $\alpha$  is a moderately good preliminary estimate of  $[\mathbf{E}_{\mathbf{V}}\mathbf{1}(V \in \mathbf{A})h(V)]^{-1}\mathbf{E}_{\mathbf{V}}\mathbf{1}(V \in \mathbf{B})h(V)$ .

To obtain the analytic expression for  $E_V 1(V \in A)h(V)$ , first define the univariate standard normal partial moment

$$\Phi(t,k,\kappa) = \int_{-\infty}^{t} (v-\kappa)^k \phi(v) \, \mathrm{d}v.$$
 (18)

Integration by parts yields the recursion formulas

$$\Phi(t,0,\kappa) = \Phi(t),$$

$$\Phi(t,1,\kappa) = -\kappa \Phi(t) - \phi(t),$$

$$\Phi(t,k,\kappa) = (k-1)\Phi(t,k-2,\kappa) - \kappa \Phi(t,k-1,\kappa) - (t-\kappa)^{k-1}\phi(t),$$
(19)

for k > 1.

Now consider a multivariate normal density  $n(v - \mu, \Omega)$  of dimension m, written as the product of a univariate marginal density  $n(y - \mu_y, \Omega_{yy})$ 

and a dimension m-1 conditional density  $n(z - \mu_z - \Omega_{zz}^{-1}\Omega_{zy}(v_y - \mu_y), \Omega_{zz} - \Omega_{zy}\Omega_{yy}^{-1}\Omega_{yz})$ . Consider the array of partial moments

$$\begin{split} \Psi(t,k,\mu,\Omega) &= \int_{-\tau}^{+\tau} \mathbf{1}(y < t) y^{k} \\ &\times \begin{bmatrix} 1 & z - \mu_{z} & y - \mu_{y} \\ (z - \mu_{z})' & (z - \mu_{z})'(z - \mu_{z}) - \Omega_{zz} & (z - \mu_{z})'(y - \mu_{y}) - \Omega_{zy} \\ y - \mu_{y} & (y - \mu_{y})(z - \mu_{z}) - \Omega_{yz} & (y - \mu_{y})^{2} - \Omega_{yy} \end{bmatrix} \\ &\times n(z - \mu_{z} - (y - \mu_{y})\Omega_{yy}^{-1}\Omega_{yz}, \Omega_{zz} - \Omega_{zy}\Omega_{yy}^{-1}\Omega_{yz})n(y - \mu_{y}, \Omega_{yy}) dz dy \\ &= \begin{bmatrix} \Psi_{1} & \Psi_{z} & \Psi_{y} \\ \Psi'_{z} & \Psi_{zz} & \Psi_{y} \\ \Psi_{y} & \Psi_{yz} & \Psi_{yy} \end{bmatrix}. \end{split}$$

Then, letting 
$$\Phi_{j} = \Omega_{yy}^{1/2} \Phi((t - \mu_{y})/\sqrt{\Omega_{yy}}, j, -\mu_{y}/\sqrt{\Omega_{yy}}),$$

$$\Psi_{1} = \Phi_{k},$$

$$\Psi_{y} = \Phi_{k+1} - \mu_{y} \Phi_{k},$$

$$\Psi_{yy} = \Phi_{k+2} - 2\mu_{y} \Phi_{k+1} + (\mu_{y}^{2} - \Omega_{yy}) \Phi_{k},$$

$$\Psi_{z} = \Psi_{y} \Omega_{yy}^{-1} \Omega_{yz},$$

$$\Psi_{yz} = \Psi_{yy} \Omega_{yy}^{-1} \Omega_{yz},$$

$$\Psi_{zz} = \Omega_{zy} \Omega_{yy}^{-1} \Psi_{yy} \Omega_{yy}^{-1} \Omega_{yz}.$$
(21)

Then,  $\Psi(b,0,\mu,\Omega) = \Psi(a,0,\mu,\Omega)$ , with y corresponding to component i of V, gives  $\mathbf{E}_{\mathbf{v}}\mathbf{1}(V \in \mathbf{A})h(V)$ .

#### 2.9. Crude frequency simulator (CFS)

Recall Eq. (9), which states that the random vector V can be written as  $V = \mu + \Gamma \eta$ , where  $\eta$  is an independent standard normal vector of dimension m and  $\Gamma$  is a lower triangular Choleski factor of  $\Omega$ , so  $\Omega = \Gamma \Gamma'$ . The Crude Frequency Simulator (CFS) of  $P(\mathbf{B}; \mu, \Omega)$  and its derivatives is to make repeated Monte Carlo draws for  $\eta$ , use (9) to calculate V for each parameter vector, and then form an empirical analogue of the expectation in (6). A crude frequency

<sup>&</sup>lt;sup>7</sup> Frequency simulation of probabilities is a traditional method in numerical analysis; Lerman and Manski (1981) introduced this approach to estimation of multinomial probit models.

simulator for  $H_C$  can be formed by rejecting draws of V that do not satisfy the conditioning event  $V \in \mathbf{B}$ , and then forming an empirical analogue of the conditional expectation in (7) using the accepted draws. The CFS are quick to compute and ideal for parallel processing. However, they are *not* continuous in parameters, exhibiting jumps at parameter values yielding draws of V on the boundary of  $\mathbf{B}$ . These discontinuities, however, can slow iterative parameter search. The accuracy of the CFS can be improved by use of antithetic and control variates introduced earlier.

# 2.10. Normal importance sampling (NIS)

Suppose the integrand  $h(v)n(v - \mu, \Omega)$  in H can, with multiplication and division by a factor if necessary, be written as the product of a density  $\gamma(v)$ , whose support coincides with or contains **B**, from which it is easy to sample, and the remainder. Then, H can be written

$$H = \int \{\mathbf{1}(v \in \mathbf{B})h(v)n(v - \mu, \Omega)/\gamma(v)\}\gamma(v) dv$$
  

$$\equiv \mathbf{E}_{z}\mathbf{1}(v \in \mathbf{B})h(v)n(v - \mu, \Omega)/\gamma(v).$$
(22)

An empirical expectation using draws from  $\gamma(v)$  gives an unbiased simulator that is smooth in parameters, provided  $h(v)n(v-\mu,\Omega)/\gamma(v)$  is dominated by a function whose expectation with respect to the density  $\gamma$  exists. We term this Normal Importance Sampling (NIS). Importance sampling works well when  $h(v)n(v-\mu,\Omega)/\gamma(v)$  is fairly flat, and  $\gamma(v)$  concentrates probability in the same region as  $n(v-\mu,\Omega)$ .

For fast computation, choose  $\gamma$  so that the components are independent, or are obtained as simple transformations of independent variates. A possible choice of  $\gamma$  when the rectangle [a,b] is finite is the uniform distribution on this rectangle. Independent exponential densities,

$$\gamma(v) = \prod_{i=1}^{m} \exp((v_i - b_i)/c_i)/c_i, \tag{23}$$

where  $c_i$  are parameters that can be set as part of the simulation, are feasible; draws from this density are easily computed using  $v_i = b_i + c_i \cdot \log \zeta_i$ , where  $\zeta_i$  is

<sup>&</sup>lt;sup>8</sup> These discontinuities do not prevent use of these simulators for statistical inference. If  $\eta$  is not redrawn when parameters change so that 'chatter' is avoided, then these simulators are piecewise constant in parameters, and the manifolds on which discontinuities occur are linear. These properties imply a stochastic equicontinuity property that is sufficient to make the simulators well-behaved in statistical inference; see McFadden (1989).

<sup>&</sup>lt;sup>9</sup> See Quandt (1984) for a discussion of iterative parameter search algorithms.

a uniform [0,1] variate. This particular choice of  $\gamma(v)$  defines the NISE simulator. On alternative that is more likely to concentrate probability for  $\gamma$  in the same region as the multivariate normal is the product of truncated normals,

$$\gamma(v) = \prod_{i=1}^{m} \phi((v_i - \alpha_i)/c_i)/[\Phi((b_i - \alpha_i)/c_i) - \Phi((a_i - \alpha_i)/c_i)], \quad v \in \mathbf{B},$$
 (24)

with  $\alpha_i = \mu_i$  and  $c_i = \sqrt{\Omega_{ii}}$ . One can sample from this distribution using

$$v_i = \alpha_i + c_i \Phi^{-1}(\zeta_i \Phi((b_i - \alpha_i)/c_i) + (1 - \zeta_i) \Phi((a_i - \alpha_i)/c_i)), \tag{25}$$

with  $\zeta_i$  a uniform [0,1] variate. Using  $\gamma(v)$  given in (24) defines the NIST simulator.<sup>11</sup> Reduction in simulation variance is in principle achievable using antithetic variates, with the  $\zeta_i$  in dimension i drawn in repeated trials from a random grid on the unit interval. A variation on (24) for finite rectangles [a,b] is

$$\alpha_i = \mu_i + \Omega_{i, -i} \Omega_{-i, -i}^{-1} (b_{-i} + a_{-i})/2, \tag{26}$$

$$c_i^2 = \Omega_{ii} - \Omega_{i,-i} \Omega_{-i,-i}^{-1} \Omega_{-i,i}. \tag{27}$$

This takes some account of the shift in location of probability mass in the multivariate normal density induced by correlation and restriction to  $\bf B$ .

## 2.11. Kernel-smoothed frequency simulator (KFS)

The Kernel-smoothed Frequency Simulator, suggested by McFadden (1989), replaced the indicator function  $\mathbf{1}(v \in \mathbf{B})$  in the crude frequency simulator with the function

$$\mathcal{K}_{\mathbf{B},\omega}(v) \equiv \mathcal{K}((v-b)/\omega) - \mathcal{K}((v-a)/\omega),\tag{28}$$

where  $\mathscr{K}(v)$  is a smooth kernel function from  $\mathbf{R}^m$  onto [0,1] with  $\mathscr{K}(-\infty)=1$  and  $\mathscr{K}(+\infty)=0$ , and  $\omega$  is a window width parameter. The function  $\mathscr{K}_{\mathbf{B},\omega}(v)$  approaches  $\mathbf{I}(v\in\mathbf{B})$  as  $\omega\to 0$ . Then, the simulator is an average of  $\mathscr{K}_{\mathbf{B},\omega}(v)h(v)$ , with  $v=\mu+\Gamma\eta$ , over r Monte Carlo draws of an independent standard normal vector  $\eta$ . This simulator is smooth in parameters, a useful feature when the simulator is used within an iterative optimization. The simulator is a biased estimate of H for positive  $\omega$ , but in statistical applications one can shrink  $\omega$  as sample size increases:

<sup>10 &#</sup>x27;E' for exponential.

<sup>11&#</sup>x27;T' for truncated normals.

Lemma 6. Define  $C_{\lambda} = \{w \in \mathbb{R}^m | |w_i| \ge \lambda \text{ for all } i\}$ . Suppose there exist  $\lambda_0$ , K, and q > 0 such that for  $\lambda \ge \lambda_0$ ,

$$\sup_{w \in C_{+}} |\mathbf{1}(w < 0) - \mathscr{K}(w)| \leqslant K\lambda^{-q}. \tag{29}$$

Then there exists a constant K' > 0 such that for small  $\omega$ ,

$$|\int [\mathcal{K}_{\mathbf{B},\omega}(v) - \mathbf{1}(v \in \mathbf{B})]h(v)n(v - \mu, \Omega) \,\mathrm{d}v| < K'\omega^{q/(1+q)}. \tag{30}$$

*Proof.* The conditional expectation of h(V) with respect to the distribution of  $V_{-i}$  given  $V_i = v_i$  is bounded by a function  $K_1 + K_2(v_i - \mu_i)^2$  for some constants  $K_1, K_2$ . Then the integral of  $[\mathcal{K}((v-b)/\omega) - \mathbf{1}(v < b)]h(v)n(v - \mu, \Omega)$  over the region  $(v-b)/\omega \in \mathbf{C}_{\lambda}$  is bounded by  $K\lambda^{-q}$  tr  $(\Omega)$ , and over the region  $(v-b)/\omega \notin \mathbf{C}_{\lambda}$  is bounded by

$$\sum_{i=1}^{m} \int_{|v_{i}-b_{i}| < \lambda \omega} n(v_{i} - \mu_{i}, \Omega_{ii}) [K_{1} + K_{2}(v_{i} - \mu_{i})^{2}] dv_{i}$$

$$\leq \sum_{i=1}^{m} 2\lambda \omega \Omega_{ii}^{-1} [K_{1} + K_{2}((b_{i} - \mu_{i})^{2} + (\lambda \omega)^{2})].$$

Take  $\lambda = \omega^{-1/(1+q)}$  and combine the regions to conclude that the integral is bounded by  $\omega^{q/(1+q)}K'/2$  for some constant K'. Repeat the argument, replacing b by a, to obtain the bound (30).

Ruud has suggested starting iterative parameter search with a large  $\omega$ , and shrinking it as the search approaches convergence. This avoids many of the problems of handling discontinuities in search.

A variety of kernel functions  $\mathscr{K}$  can be employed such as a logistic function  $\mathscr{K}(v) = 1/(1 + e^{v_1} + \cdots + e^{v_m})$ , a normal kernel  $\mathscr{K}(v) = \prod_{i=1}^m \Phi(-v_i)$ , or a polynomial kernel  $\mathscr{K}(v) = \prod_{i=1}^m G(v_i)$ , where

$$G(y) = \begin{cases} 1 & \text{for } y \le -1, \\ (1 - y(2 + y))/2 & \text{for } -1 < y \le 0, \\ (1 - y(2 - y))/2 & \text{for } 0 < y < 1, \\ 0 & \text{for } y \ge 1. \end{cases}$$
(31)

The polynomial kernel is particularly quick to compute, and will generally be the method of choice. As in the case of the crude frequency simulator, antithetic draws can be used for  $\eta$  in (9). It is also possible in the case of the polynomial kernel to use a smoothed version  $[G((v_i - b)/\omega) - G((v_i - a)/\omega)]h(v)$  of the control variable  $\mathbf{1}(a_i < v_i < b_i)h(v)$ . Let y denote  $v_i$ , and z denote  $v_{-i}$ . Then,  $\Upsilon(\omega, b, \mu, \Omega) - \Upsilon(\omega, a, \mu, \Omega)$  is the expectation of the smoothed control variate,

where

$$\Upsilon(\omega, t, \mu, \Omega) = \int_{-\infty}^{+\infty} G((y - t)/\omega) \\
\times \begin{bmatrix}
1 & z - \mu_z & y - \mu_y \\
(z - \mu_z)' & (z - \mu_z)'(z - \mu_z) - \Omega_{zz} & (z - \mu_z)' & (y - \mu_y) - \Omega_{zy} \\
y - \mu_y & (y - \mu_y)(z - \mu_z) - \Omega_{yz} & (y - \mu_y)^2 - \Omega_{yy}
\end{bmatrix} \\
\times n(z - \mu_z - (y - \mu_y)\Omega_{yy}^{-1}\Omega_{yz}, \Omega_{zz} - \Omega_{zy}\Omega_{yy}^{-1}\Omega_{yz}) \\
\times n(y - \mu_y, \Omega_{yy}) dz dy.$$

Breaking up the domain of integration, one has, from (20),

$$\begin{split} \Upsilon(\omega, t, \mu, \Omega) &= \left[ (t - \omega)^2 \Psi(t - \omega, 0, \mu, \Omega) - 2t^2 \Psi(t, 0, \mu, \Omega) \right. \\ &+ (t + \omega)^2 \Psi(t + \omega, 0, \mu, \Omega) \right] / 2\omega^2 \\ &- \left[ (t - \omega) \Psi(t - \omega, 1, \mu, \Omega) - 2t \Psi(t, 1, \mu, \Omega) \right. \\ &+ (t + \omega) \Psi(t + \omega, 1, \mu, \Omega) \right] / \omega^2 \\ &+ \left[ \Psi(t - \omega, 2, \mu, \Omega) - 2\Psi(t, 2, \mu, \Omega) \right. \\ &+ \Psi(t + \omega, 2, \mu, \Omega) \right] / 2\omega^2. \end{split}$$

# 2.12. Stern decomposition simulator (SDS)

The Stern Decomposition, suggested by Stern (1992), writes  $V \sim V(\cdot; \mu, \Omega)$  as a sum V = Y + W, with  $Y \sim V(\cdot; \mu, \lambda^2 I)$  with  $W \sim V(\cdot; 0, \Omega - \lambda^2 I)$ . That is, V equals the sum of a 'small' independently distributed normal vector and a second normal vector that carries the information on the covariance matrix of V. Then, by the law of iterated expectations,

$$H = \int_{w} \left\{ \int_{y=a}^{b} h(y) \left[ \prod_{i=1}^{m} \phi((y_i - w_i - \mu_i)/\lambda)/\lambda \right] dy \right\} n(w, \Omega - \lambda^2 I) dw.$$
 (33)

The term in braces can be integrated analytically; then the SDS averages this interior integral over r Monte Carlo draws  $w = [\Omega - \lambda^2 I]^{1/2} \eta$ , where  $\eta$  is a standard normal vector and  $[\Omega - \lambda^2 I]^{1/2}$  is a Choleski factor of  $\Omega - \lambda^2 I$ . The array H can also be written, by multiplying and dividing by the density  $n(v, \Omega - \lambda^2 I)$ , as

$$H = C \cdot \int_{v} \{ \mathbf{1}(v \in \mathbf{B}) \exp\{-\lambda^{2} v'(\Omega - \lambda^{2} I)^{-1} \Omega^{-1} v/2 + \mu' \Omega^{-1} v \} \} n(v, \Omega - \lambda^{2} I) dv,$$
(34)

where  $C = \exp(-\mu'\Omega^{-1}\mu/2) [\det(\Omega - \lambda^2 I)/\det(\Omega)]^{1/2}$ . There are two possible interpretations of this simulator. First, (33) can be viewed as a kernel-smoothed variant of the integrand in (34). Second, (34) can be interpreted as a form of importance sampling, with  $n(\cdot, \Omega - \lambda^2 I)$  the convenient density from which Monte Carlo draws are made.

To obtain the analytic form for the term in braces in (33), define

$$q_{ik} = \lambda^k \left[ \Phi\left(\frac{b_i - \mu_i - w_i}{\lambda}, k, -\frac{2w_i}{\lambda}\right) - \Phi\left(\frac{a_i - \mu_i - w_i}{\lambda}, k, -\frac{2w_i}{\lambda}\right) \right], \quad (35)$$

where  $\Phi(t, k, \kappa)$  is the partial moment function (19). Define

$$Q = \prod_{i=1}^{m} q_{i0},\tag{36}$$

$$s = (q_{11}/q_{10}, \dots, q_{m1}/q_{m0})', \tag{37}$$

$$D = \text{diag}\{q_{i2}/q_{i0}\}. \tag{38}$$

Then, (33) becomes

$$H = \int_{w} Q \cdot \begin{bmatrix} 1 & s'\Omega^{-1} \\ \Omega^{-1}s & \frac{1}{2}\Omega^{-1}[D+s \cdot s' - \Omega]\Omega^{-1} \end{bmatrix} n(w, \Omega - \lambda^{2}I) dw.$$
 (39)

The SDS provides an unbiased smooth simulator. Again, accuracy can be enhanced using antithetics when drawing  $\eta$  to construct the simulated values  $w = (\Omega - \lambda^2 I)^{1/2} \eta$ . This simulator is fast to compute, but it can be computationally burdensome to determine  $\lambda$  such that  $\Omega - \lambda^2 I$  is positive definite, and accuracy falls when m is large and the eigenvalues of  $\Omega$  are uneven. The extension of the Stern simulator to derivatives is due to McFadden.

# 2.13. Geweke-Hajivassiliou-Keane simulator (GHK)

This simulator is based on sampling from recursive truncated normals after a Choleski transformation. The approach was suggested by Geweke (1989), and has been developed by Hajivassiliou, who proposed the weighting used here. Keane (1994) independently developed a weighting scheme of essentially the same form for a problem of estimating transition probabilities.

Consider the triangularizing transformation  $V = \mu + \Gamma \eta$ , where  $\Gamma$  is the Choleski factor of  $\Omega$ . The indicator  $\mathbf{1}(v \in \mathbf{B})$  is then transformed to  $\mathbf{1}(\mu + \Gamma \eta \in \mathbf{B})$ , which can be written recursively as the product of indicators of the events

$$\mathbf{B}_{j}(\eta_{< j}) = \{ \eta_{j} | (a_{j} - \mu_{j} - \Gamma_{j, < j} \eta_{< j}) / \Gamma_{jj} < \eta_{j} < (b_{j} - \mu_{j} - \Gamma_{j, < j} \eta_{< j}) / \Gamma_{jj} \},$$
(40)

for j = 1, ..., m. Define  $\phi(\eta_j | \mathbf{B}_j(\eta_{< j})) = \phi(\eta_j) \mathbf{1}(\eta_j \in \mathbf{B}_j(\eta_{< j})) / \Phi(\mathbf{B}_j(\eta_{< j}))$ , the conditional distribution of  $\eta_i$  given the event  $\mathbf{B}_i(\eta_{< i})$ . Define a weight

$$\omega(\eta) = \prod_{j=1}^{m} \Phi(\mathbf{B}_{j}(\eta_{< j})). \tag{41}$$

Then

$$H = \int h(\mu + \Gamma \eta) \omega(\eta) \prod_{i=1}^{m} \phi(\eta_i | \mathbf{B}_j(\eta_{< j})) \, \mathrm{d}\eta. \tag{42}$$

The following result gives the GHK simulator:

Lemma 7. An unbiased simulator of H is an average of  $h(\mu + \Gamma \eta)\omega(\eta)$ , where  $\omega(\eta)$  is the weighting function (41), over draws constructed recursively from the one-dimensional conditional densities  $\phi(\eta_i | \mathbf{B}_i(\eta_{\le i}))$  by taking

$$\eta_{j} = \Phi^{-1}(\zeta_{j}\Phi((a_{j} - \mu_{j} - \Gamma_{j, < j}\eta_{< j})/\Gamma_{jj}) 
+ (1 - \zeta_{j})\Phi((b_{j} - \mu_{i} - \Gamma_{j, < j}\eta_{< j})/\Gamma_{jj}),$$
(43)

where the  $\zeta_j$  are draws from the uniform [0,1] density. When **B** is a finite rectangle, there is a constant c > 0 such that for each  $\varepsilon$ ,  $0 < \varepsilon < 1$ ,

$$\operatorname{Prob}\left(\frac{\sum_{i=1}^{r}h(\mu+\Gamma\eta_{i})\omega(\eta_{i})}{\sum_{i=1}^{r}\omega(\eta_{i})}-H_{C}>\varepsilon\right)<\exp(-rc\varepsilon^{2}).$$
(44)

*Proof.* It is immediate from (42) that the GHK simulator of H is unbiased. Now consider the simulator of  $H_C$  in (44). Write  $\mathbf{A} = \{\eta | \mu + \Gamma \eta \in \mathbf{B}\}$  and let  $\tilde{\eta}$  denote a random vector in  $\mathbf{A}$  drawn recursively using (43). Then,

$$\begin{split} \mathbf{E}_{V|V\in\mathbf{B}}h(V) &= \mathbf{E}_{\eta|\eta\in A}h(\mu + \Gamma\eta) \\ &= \frac{\int\limits_{\eta\in A}h(\mu + \Gamma\eta)\prod\limits_{k=1}^{m}\phi(\eta_k)\,\mathrm{d}\eta_k}{\prod\limits_{k=1}^{m}\phi(\eta_k)\,\mathrm{d}\eta_k} \\ &= \frac{\int\limits_{\eta\in A}h(\mu + \Gamma\eta)\omega(\eta)\prod\limits_{k=1}^{m}\left[\phi(\eta_k)/\Phi(\mathbf{B}_k(\eta_{< k}))\right]\,\mathrm{d}\eta_k}{\int\limits_{\eta\in A}\omega(\eta)\prod\limits_{k=1}^{m}\left[\phi(\eta_k)/\Phi(\mathbf{B}_k(\eta_{< k}))\right]\,\mathrm{d}\eta_k} \\ &= \left[\mathbf{E}_{\tilde{\eta}}h(\mu + \Gamma\tilde{\eta})\right]/\mathbf{E}_{\tilde{\eta}}\omega(\tilde{\eta}). \end{split}$$

To obtain the bound (44) when **B** is finite, note that in this case there is a bound  $c_1$  on every component of the array  $h(\mu + \Gamma \eta)\omega(\eta)$ . Then, by Hoeffding's inequality,

$$\operatorname{Prob}\left(\frac{1}{r_{i}}\sum_{i=1}^{r}h(\mu+\Gamma\eta_{i})\omega(\eta_{i})-H>\varepsilon_{1}\right)<\exp\left[-r\varepsilon_{1}^{2}/2c_{1}^{2}\right].\tag{45}$$

Choose  $\varepsilon_1 = \varepsilon P^2/(2 + c_1)$ . Suppose the event in (45) does not occur. Then,

$$\frac{\sum\limits_{i=1}^{r}h(\mu+\Gamma\eta_{i})\omega(\eta_{i})}{\sum\limits_{i=1}^{r}\omega(\eta_{i})}-H_{C}\leqslant\frac{\frac{1}{r}\sum\limits_{i=1}^{r}h(\mu+\Gamma\eta_{i})\omega(\eta_{i})-H}{\frac{1}{r}\sum\limits_{i=1}^{r}\omega(\eta_{i})}+|H_{C}|\cdot\frac{\frac{1}{r}\sum\limits_{i=1}^{r}\omega(\eta_{i})-P}{\frac{1}{r}\sum\limits_{i=1}^{r}\omega(\eta_{i})}$$

$$\leq \varepsilon_1/(P-\varepsilon_1) + c_1\varepsilon_1/P(P-\varepsilon_1) \leq \varepsilon$$

so that the event in (44) does not occur. Therefore, letting  $c = P^4/2c_1^2(2 + c_1)^2$ , the probability of the event in (44) is at most  $\exp(-rc\varepsilon^2)$ .

The GHK simulator can be interpreted as importance sampling using the recursive truncated standard normal densities. It has proven fast, with low noise, even when probabilities are small. Börsch-Supan and Hajivassiliou (1993) use this simulator<sup>12</sup> to define the method of smoothly simulated maximum likelihood and show that this method exhibits excellent properties for limited dependent variable models that are otherwise difficult to estimate. In principle, it is possible to use antithetic variates in (43), starting from a random grid of size q drawn from the uniform distribution in each step of the recursion. In practice, this produces  $q^m$  points, which is impractically large in many problems.<sup>13</sup>

# 2.14. Parabolic cylinder function simulator (PCF)

Consider a spherical transformation  $V=b+\rho\cdot v$  about the upper limit b of **B**, where v is in the unit sphere and  $\rho$  is a nonnegative scalar. The Jacobean of the transformation from V to  $(v_1,\ldots,v_{m-1},\rho)$  is  $\rho^{m-1}/v_m$ , where  $v_m=\left[1-v_1^2-\cdots-v_{m-1}^2\right]^{1/2}$ . Then, the multivariate normal density  $n(V-\mu,\Omega)$  expressed in terms of the transformed variables is

$$f(\rho|v)q(v|\mu - b, \Omega) = (2\pi)^{-m/2} |\Omega|^{-1/2} \exp[-(\rho v - (\mu - b))^{\alpha}] \times \Omega^{-1}(\rho v - (\mu - b))/2] \rho^{m-1}/v_m.$$

<sup>12</sup> Which they term the 'Smooth, Recursive Conditioning' simulator.

<sup>&</sup>lt;sup>13</sup>Some of the desirable features of antithetic variates can be obtained by sampling without replacement from a large random grid.

In this expression, the conditional density of  $\rho$  given v is

$$f(\rho|v) = \rho^{m-1} \exp[-(\rho - (\mu - b)'\Omega^{-1}v/v'\Omega^{-1}v)^2(v'\Omega^{-1}v)/2]/K(v), \quad (46)$$

with

$$K(v) = \int_{0}^{x} \rho^{m-1} \exp\left[-(\rho - (\mu - b)'\Omega^{-1}v/v'\Omega^{-1}v)^{2}(v'\Omega^{-1}v)/2\right] d\rho,$$

and the marginal distribution of v is

$$q(v|\mu - b, \Omega) = K(v)(2\pi)^{-m/2}|\Omega|^{-1/2}\exp[-(\mu - b)'\Omega^{-1}(\mu - b)/2 + (v'\Omega^{-1}(\mu - b))^2/2v'\Omega^{-1}v]/v_m.$$

When  $\mu - b = 0$  and  $\Omega = I$ , so that the distribution of v on the unit sphere is uniform,  $q(v|0,I) = (2\pi)^{-m/2} \int_0^\infty \rho^{m-1} \exp[-\rho^2/2] \, \mathrm{d}\rho/v_m = \pi^{-m/2} \Gamma(m/2)/2v_m$ . Define an importance sampling weight

$$\begin{split} s(v) &\equiv q(v|\mu - b, \Omega)/q(v|0, I)K(v) \\ &= \exp[-(\mu - b)'\Omega^{-1}(\mu - b)/2 \\ &+ (v'\Omega^{-1}(\mu - b))^2/2v'\Omega^{-1}v]/\Gamma(m/2)2^{m/2-1}|\Omega|^{1/2}. \end{split}$$

Define

$$\bar{\rho}(v) = \min_{i} n(a_i - b_j)/v_j, \tag{48}$$

and note that it is positive for v < 0. Then,

$$H = \int_{v \le 0} \left( \int_{\rho=0}^{\rho(v)} h(b + \rho v) f(\rho|v) \, \mathrm{d}\rho \right) K(v) s(v) q(v|0, I) \, \mathrm{d}v. \tag{49}$$

Define

$$C(i, \alpha, \beta, \gamma) = \int_{0}^{\gamma} \rho^{i} \exp\left[-\alpha(\rho - \beta/\alpha)^{2}/2\right] d\rho.$$
 (50)

This function satisfies

$$C(0,\alpha,\beta,\gamma) = (2\pi/\alpha)^{1/2} \left[ \Phi((\alpha\gamma - \beta)/\sqrt{\alpha}) - \Phi(-\beta/\sqrt{\alpha}) \right], \tag{51}$$

$$C(1, \alpha, \beta, \gamma) = (\exp[-\beta^2/2\alpha] - \exp[-\alpha(\gamma - \beta/\alpha)^2/2])/\alpha + C(0, \alpha, \beta, \gamma)\beta/\alpha.$$
(52)

$$C(i, \alpha, \beta, \gamma) = C(i - 1, \alpha, \beta, \gamma)\beta/\alpha + C(i - 2, \alpha, \beta, \gamma)(i - 1)/\alpha$$
$$- \gamma^{i-1} \exp[-\alpha(\gamma - \beta/\alpha)^2/2]/\alpha, \tag{53}$$

with (53) obtained by integration by parts for i > 1. Then, C can be computed by recursion in i. We term C a parabolic cylinder function, as it is closely related to a standard class of mathematical functions with this name. When  $\beta = 0$ , this function is proportional to a chi-square cumulative distribution function,

$$C(i, \alpha, 0, \gamma) = 2^{(i-1)/2} \cdot \Gamma((i+1)/2) \cdot \alpha^{-(i+1)/2} \cdot \gamma_{i+1}^2(\alpha \gamma^2).$$

The function K(v) in (46) satisfies  $K(v) = C(m-1, v'\Omega^{-1}v, (\mu-b)'\Omega^{-1}v, \infty)$ . Define

$$C_{i}(v) \equiv K(v) \int_{\rho=0}^{\rho(v)} \rho^{i} f(\rho | v) d\rho$$

$$= C(i + m - 1, v'\Omega^{-1}v, (\mu - b)'\Omega^{-1}v, \bar{\rho}(v)). \tag{54}$$

Then

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}$$

satisfies

$$H_{11} = \mathbf{E}_{v} C_{0}(v) s(v),$$

$$H_{21} = H'_{12}, = \Omega^{-1} \mathbf{E}_{v} [C_{1}(v)v + (b - \mu)C_{0}(v)] s(v),$$

$$H_{22} = \frac{1}{2} \Omega^{-1} \mathbf{E}_{v} [C_{2}(v)vv' - C_{1}(v) \{v(\mu - b)' + (\mu - b)v'\}$$

$$+ C_{0}(v) \{(\mu - b)(\mu - b)' - \Omega\} ] s(v) \Omega^{-1},$$

$$(55)$$

where the expectation is with respect to the uniform density on the unit sphere. The PCF simulator is obtained by averaging the array (55) over a sample of draws of v from the uniform distribution on the unit sphere intersecting the negative orthant, and can be interpreted as importance sampling with this comparison distribution. The draws can be made by first drawing a standard normal vector  $\eta$ , reversing the signs of positive components so that it is negative, and then defining  $v = \eta/\sqrt{\eta'\eta}$ . This has the effect of drawing from q(v|0,I) conditioned on v < 0. To remove this conditioning, the simulation average must be divided by  $2^m$ , the number of orthants. This simulator was suggested by McFadden (1989).

<sup>&</sup>lt;sup>14</sup> See Abramowitz and Stegun (1964, p. 685) and Spanier and Oldham (1987).

# 2.15. Deák chi-square simulator (DCS)

A spherical transformation about the mean of the multivariate distribution is  $V = \mu + \rho \cdot v$ , where again  $\rho$  is a scalar and v is a point in the unit sphere. We use the notation of the previous section, with  $\mu$  replacing b, so that  $s(v) = 1/2^{m/2-1} \Gamma(m/2) |\Omega|^{1/2}$  and, analogously to  $C_i(v)$ ,

$$D_i(v) \equiv K(v) \int \mathbf{1}(\mu + \rho v \in \mathbf{B}) \rho^i f(\rho | v) \, \mathrm{d}\rho.$$
 (56)

This expression can be evaluated analytically using (46)–(53), yielding

$$D_i(v) = C(i+m-1, v'\Omega^{-1}v, 0, \rho'(v)) - C(i+m-1, v'\Omega^{-1}v, 0, \rho''(v)),$$

where  $\rho'(v)$  and  $\rho''(v)$  are the largest and smallest values of  $\rho$  satisfying the inequalities  $a - \mu < \rho v < b - \mu$ . Then,  $0 \le \rho''(v) \le \rho'(v)$ ,

$$\rho'(v) = \min \left\{ \min_{v_j \ge 0} (b_j - \mu_j) / v_j, \min_{v_j \le 0} (a_j - \mu_j) / v_j \right\},$$

$$\rho''(v) = \max \left\{ 0, \max_{v_j \ge 0} (a_j - \mu_j) / v_j, \max_{v_j \le 0} (b_j - \mu_j) / v_j \right\},$$
(57)

where by convention 0/0 = 0, and  $0 = \rho''(v) = \rho'(v)$  whenever (57) fails to yield a nondegenerate interval in the positive half-line. Taking the expectation of  $D_i(v)s(v)$  with respect to the uniform distribution on the unit sphere,

$$\mathbf{E}_{V}D_{i}(v)s(v) = K'(v'\Omega^{-1}v)^{-(m+i)/2} \times \left[\chi_{i+m}^{2}(v'\Omega^{-1}v\rho'(v)^{2}) - \chi_{i+m}^{2}(v'\Omega^{-1}v\rho''(v)^{2})\right], \tag{58}$$

with  $K' = 2^{i/2} \Gamma((m+i)/2) / \Gamma(m/2) |\Omega|^{1/2}$ . Then

$$H = \begin{bmatrix} \mathbf{E}_{v} D_{0}(v) s(v) & \mathbf{E}_{v} D_{1}(v) v' s(v) \Omega^{-1} \\ \Omega^{-1} \mathbf{E}_{v} D_{1}(v) v s(v) & \frac{1}{2} \Omega^{-1} \mathbf{E}_{v} [D_{2}(v) v v' - D_{0}(v) \Omega] s(v) \Omega^{-1} \end{bmatrix},$$
(59)

with (58) used to evaluate the terms. The DCS simulator is obtained by drawing an antithetic random grid of points r on the unit sphere, as described in Section 2.7, and forming the empirical expectation corresponding to the array in (59). It is unbiased for H and smooth in parameters. This simulator for P is due to Deák (1980a, b); the extension to obtain the derivatives of P was suggested by Chunrong Ai.

#### 2.16. Acceptance/rejection simulator (ARS)

An Acceptance/Rejection Simulator calculates an empirical analogue of the expectation  $H_C = \mathbf{E}_{V|V \in \mathbf{B}} h(V)$  by constructing draws from the conditional distribution of V given  $\mathbf{B}$ . The crudest form of ARS is to sample from the unconditional distribution of V using (9), reject points not in  $\mathbf{B}$  until r accepted

points are found, and form an average of h(V) over the accepted points. More generally, the procedure in Lemma 1 permits improvement in the yield of the method by sampling from a comparison distribution that puts little or no weight outside **B** and has the property that the ratio of the comparison density to the target density is uniformly bounded above by a small number. Nevertheless, yields tend to be low, making computation heavy, for small P.

A point  $V = \mu + \Gamma \eta$  may, for given  $\eta$ , move from the rejection to the acceptance region with small changes in the parameters, introducing discontinuities in the ARS. Using an approach suggested by Ruud, Hajivassiliou, and McFadden (1990) show that the ARS nevertheless has a stochastic equicontinuity property that enables its use in statistical applications.

Possible comparison distributions for A/R sampling are independent exponential or truncated normal distributions in V-space, but greater yields can be obtained using the recursive truncated normal distribution (43) employed in the GHK simulator. The following lemmas give protocols for use of independent exponential or recursive truncated normal comparison distributions. Lemma 8 is due to McFadden (1989), Lemma 9 to Hajivassiliou and McFadden (1990).

Lemma 8. Draw  $v_i = b_i + (\log \zeta_i)\lambda_i$ , i = 1, ..., m, where the  $\lambda_i$  are positive constants chosen for the simulation and the  $\zeta_i$  are uniform [0, 1], and accept v if

$$\log \zeta_0 \leqslant -(v-\mu)'\Omega^{-1}(v-\mu)/2 - \lambda'(v-\mu) - \lambda'\Omega\lambda/2.$$

Then, the accepted V are distributed  $n(v - \mu, \Omega)$  conditioned on  $V \in \mathbf{B}$ , and the average of (8) over the accepted points is an unbiased simulator of  $H_C$ .

*Proof.* Apply Lemma 1 to the density  $\prod_{i=1}^{m} \lambda_i \exp[\lambda_i(v_i - b_i)]$  on  $v \leq b$ .

A suitable choice for  $\lambda$  might be  $\lambda_i = \sqrt{\Omega_{ii}}$ .

Lemma 9. Draw n sequentially using

$$\eta_{j} = \Phi^{-1}(\zeta_{j}\Phi((a_{j} - \mu_{j} - \Gamma_{j, < j}\eta_{< j})/\Gamma_{jj}) + (1 - \zeta_{j})\Phi((b_{j} - \mu_{j} - \Gamma_{j, < j}\eta_{< j})/\Gamma_{jj})),$$

and accept  $v = \mu + \Gamma \eta$  if  $\zeta_0 \leq \prod_{i=2}^m [\Phi(\mathbf{B}_i(\eta_{< i})/\alpha_i]$ , where the  $\zeta_i$  are uniform [0,1] random variates,  $\alpha_i = \Phi((b_i - a_i)/2\Gamma_{ii}) - \Phi(-(b_i - a_i)/2\Gamma_{ii}) \leq 1$ , and

$$\mathbf{B}_{i}(\eta_{< i}) = \left\{ \eta_{i} | a_{i} - \mu_{i} - \Gamma_{i, \leq i} \eta_{< i} \right\} / \Gamma_{ii} < \eta_{i} < (b_{i} - \mu_{i} - \Gamma_{i, \leq i} \eta_{< i}) / \Gamma_{ii} \right\}.$$

Then, the accepted V are distributed  $n(v - \mu, \Omega)$  conditioned on  $V \in \mathbf{B}$ , and the average of (8) over the accepted points is an unbiased simulator of  $H_C$ .

*Proof.* The protocol samples sequentially from the recursive truncated normal density  $g(\eta) = \prod_{i=1}^{m} \phi(\eta_i)/\Phi(\mathbf{B}_i(\eta_{< i}))$ , with  $\eta_i \in \mathbf{B}_i(\eta_{< i})$ . For this density,

$$f(\eta)/g(\eta) = \prod_{i=1}^{m} \Phi(\mathbf{B}_{i}(\eta_{< i})),$$

implying

$$1 \geqslant \alpha \geqslant \sup_{\eta \in \mathbf{B}} \prod_{i=1}^{m} \Phi(\mathbf{B}_{i}(\eta_{< i})) \geqslant \int \prod_{i=1}^{m} \Phi(\mathbf{B}_{i}(\eta_{< i})) \cdot g(\eta) \, \mathrm{d}\eta \equiv P. \tag{60}$$

In particular,

$$\Phi(\mathbf{B}_1) = \Phi((b_1 - \mu_1)/\Gamma_{11}) - \Phi((a_1 - \mu_1)/\Gamma_{11}) \equiv \alpha_1 \tag{61}$$

and

$$\sup_{\eta_i \in \mathbf{B}_i(\eta_{< i})} \Phi(\mathbf{B}_i(\eta_{< i})) \leqslant \sup_{z} \left[ \Phi((b_i - \mu_i - z)/\Gamma_{ii} - \Phi((a_i - \mu_i - z)/\Gamma_{ii})) \right], \tag{62}$$

$$\Phi((b_i - a_i)/2\Gamma_{ii}) - \Phi(-(b_i - a_i)/2\Gamma_{ii}) \equiv \alpha_i$$

and one can take  $\alpha = \prod_{i=1}^{m} \alpha_i \leq 1$ . The result then follows from Lemma 1.  $\square$ 

We term the acceptance/rejection variant that is defined by Lemma 8 the ARSE simulator, while we use ARSR to refer to the method of recursively sampling from truncated normal densities, as described in Lemma 9.15

#### 2.17. Gibbs sampler simulator (GSS)

The Gibbs Sampler Simulator of  $H_C$  is based on a Markov chain that utilizes computable univariate truncated normal densities to construct transitions, and has the desired truncated multivariate normal as its limiting distribution. The simulator was developed by Hajivassiliou, starting from stochastic relaxation methods studied by Geman and Geman (1984). The following result establishes the theoretical properties of the simulator:

Lemma 10. Suppose **B** is finite. Start from any  $v^{(0)} \in \mathbf{B}$ . Define a recursive procedure with steps i = 1, ..., m in rounds j = 1, ..., r. Suppose at step i in round j,  $v^{(j-1)}$  and  $v^{(j)}$  have been determined. Define

$$v_i^{(j)} = \kappa_{ij} + \sigma_i \Phi^{-1}(\zeta_{ij} \Phi((b_i - \kappa_{ij})/\sigma_i) + (1 - \zeta_{ij}) \Phi((a_i - \kappa_{ij})/\sigma_i)),$$
 (63)

<sup>&</sup>lt;sup>15</sup> It may be possible to increase the acceptance level in Lemma 9 in special cases by considering the structure of **B** in more detail. For example, when the below-diagonal terms of  $\Gamma$  are all nonnegative, the supremum in (62) can be defined recursively, using the previous bounds on  $\eta_{< i}$ .

where the  $\zeta_{ij}$  are independent uniform [0, 1] variates,

$$\kappa_{ij} = \mu_i + \Omega_{i,-i} \Omega_{-i,-i}^{-1} \begin{bmatrix} v_{< i}^{(j)} - \mu_{< i}^{(j)} \\ v_{> i}^{(j-1)} - \mu_{> i}^{(j-1)} \end{bmatrix}, \tag{64}$$

and

$$\sigma_i = [\Omega_{ii} - \Omega_{i,-i}\Omega_{-i,-i}^{-1}\Omega_{-i,i}]^{1/2}.$$
(65)

Note that  $v \in \mathbf{B}$ . Let  $\mathbf{E}_{(r)}$  denote expectation with respect to the distribution of the vector V obtained after r rounds of (63). Then, there exists  $\rho \in (0,1)$  and  $\mathbf{K} > 0$  such that

$$|\mathbf{E}_{(r)}h(V) - H_C| < K\rho^r. \tag{66}$$

Proof. See Hajivassiliou and McFadden (1990).

# 2.18. Sequentially unbiased simulator (SUS)

A family of unbiased simulators of  $H_C = H/P$  can be formed from independent unbiased simulators of H and of 1/P. Lemma 3 describes an unbiased simulator for 1/P: Let A denote the event  $a_i < V_i < b_i$ , where i is a specified component of V. For  $r \ge 0$  initial steps, independent unbiased simulators  $Q_j$  of  $1 - \Pr(\mathbf{B})/\Pr(\mathbf{A})$  are constructed, using the analytic expression for  $\Pr(\mathbf{A})$  and any of the smooth unbiased simulators of  $\Pr(\mathbf{B})$  provided by NIS, SDS, GHK, PCF, or DCS. After the initial r steps,  $V_i$  are drawn, conditional on  $\mathbf{A}$ , as detailed in (12) and (13). This sampling proceeds sequentially, setting  $Q_j = 1$ , until the event  $V_i \in \mathbf{B}$  is observed. Then (11) provides an unbiased simulator of 1/P. The purpose of the smooth simulators in the first r steps is to reduce the variance in the simulation of 1/P. For numerical purposes, this method coincides with the following simulator when an extremely large censoring point r, the predetermined limit for the number of steps, is used.

#### 2.19. Approximately unbiased simulator (AUS)

Assume **B** compact. The Gibbs Sampler Simulator for  $H_C$  is only approximately unbiased, although convergence is at a geometric rate. The GHK simulator (42) for  $H_C$  was also shown to have geometric convergence. Using the method, Lemma 4 for simulating 1/P, it is also possible to use the NIS, SDS, PCF, or DCS simulators to get smooth, approximately unbiased simulators of  $H_C$  with the property that the bias converges to zero at a geometric rate in the number of repetitions r. The KFS with a positive kernel, such as the normal or logistic, satisfies Lemma 6 for all q > 0. Taking  $\omega$  proportional to  $e^{-\alpha r}$  for some  $\alpha > 0$  then implies that Lemma 4 can be used for this simulator, with the bias introduced by kernel-smoothing contributing an additional bias term of order

 $e^{-\alpha rq/(1-q)}$  to the geometric bias coming from the truncation at r in Lemma 4. Again, a geometric rate is achieved overall.

In principle, the method in Lemma 5 could also be used to construct approximately unbiased simulators of  $H_C$ . This method might be better than the method in Lemma 4 for small r and some simulators, but for large r the geometric rate achieved in Lemma 4 will dominate the 1/r rate achieved in Lemma 5.

# 3. Test problems and computational results

The Appendix describes a series of GAUSS and FORTRAN procedures for simulation of multivariate normal rectangle probabilities and the derivatives of these probabilities with respect to the mean and covariances of the normal distribution. <sup>16</sup> In this section, we describe the test problems we used to evaluate the operational characteristics of these algorithms and then discuss the findings from our computational experiments.

# 3.1. Description of the test problems

A case that yields multivariate normal rectangle probabilities that are easily calculated analytically or by quadrature is the one-factor model,

$$V = \mu + S\eta + \Lambda\varepsilon, \tag{67}$$

where S is an  $m \times m$  diagonal matrix with diagonal elements  $s_i$ ,  $\Lambda$  is an  $m \times 1$  array of factor loadings,  $\mu$  is an  $m \times 1$  vector of means,  $\eta$  is an  $m \times 1$  vector of independent standard normal variates, and  $\varepsilon$  is an independent  $m \times 1$  standard normal vector. Given  $\varepsilon$ , the constraints require

$$S^{-1}(a - \mu - \Lambda \varepsilon) < \eta < S^{-1}(b - \mu - \Lambda \varepsilon). \tag{68}$$

Define

$$Q_i = \Phi((b_i - \mu_i - \lambda_i \varepsilon)/s_i) - \Phi((a_i - \mu_i - \lambda_i \varepsilon)/s_i)$$
(69)

and

$$q_i = \phi((b_i - \mu_i - \lambda_i \varepsilon)/s_i) - \phi((a_i - \mu_i - \lambda_i \varepsilon)/s_i). \tag{70}$$

Then.

$$P = \int_{-\infty}^{+\infty} \left( \prod_{i=1}^{m} Q_{i} \right) \phi(\varepsilon) \, \mathrm{d}\varepsilon, \tag{71}$$

$$\partial P/\partial \mu_m = (-1/s_m) \int_{-\infty}^{+\infty} \left( \prod_{i=1}^{m-1} Q_i \right) q_m \phi(\varepsilon) \, \mathrm{d}\varepsilon, \tag{72}$$

<sup>&</sup>lt;sup>16</sup> Both versions of the programs are available from the authors upon request.

and

$$\partial P/\partial \lambda_m = (-1/s_m) \int_{-\infty}^{+\infty} \left( \prod_{i=1}^{m+1} Q_i \right) q_m \varepsilon \phi(\varepsilon) \, \mathrm{d}\varepsilon. \tag{73}$$

These expressions can be evaluated by one-dimensional Gaussian quadrature, and in a few cases evaluated analytically, which will provide benchmarks to gauge the accuracy of the 13 simulation algorithms in the experiments below. One analytic case occurs when the factor is loaded only on the last alternative, so that it is equivalent to a change in the scale of  $V_m$ : transform  $s_m$  to  $(s_m^2 + \lambda_m^2)^{1/2}$  and  $\lambda_m$  to zero, so that the terms  $Q_i$  and  $q_m$  are independent of  $\varepsilon$ , and  $Q_m$  and  $q_m$  are evaluated at the transformed values, <sup>17</sup> obtaining

$$P = \left(\prod_{i=1}^{m} Q_{i}\right),$$

$$\partial P/\partial \mu_{m} = -\left(\prod_{i=1}^{m-1} Q_{i}\right) q_{m} \cdot (s_{m}^{2} + \lambda_{m}^{2})^{-1/2},$$

$$\partial P/\partial \lambda_{m} = -\left(\prod_{i=1}^{m-1} Q_{i}\right) q_{m} \left\{(b_{m} - \mu_{m}) - (a_{m} - \mu_{m})\right\} \lambda_{m} \cdot (s_{m}^{2} + \lambda_{m}^{2})^{-3/2}.$$

$$(74)$$

A second analytic case occurs when  $a=-\infty$ , b=0,  $\mu=0$ , S is the identity matrix, and  $\Lambda$  is a vector of ones. Then,

$$P = \int_{-\infty}^{+\infty} \Phi(-\varepsilon)^m \phi(-\varepsilon) d\varepsilon = 1/(m+1),$$

$$\partial P/\partial \mu_m = \int_{-\infty}^{+\infty} \Phi(-\varepsilon)^{m-1} \phi(-\varepsilon)^2 d\varepsilon,$$

$$\partial P/\partial \lambda_m = \int_{-\infty}^{+\infty} \Phi(-\varepsilon)^{m-1} \phi(-\varepsilon)^2 \varepsilon d\varepsilon.$$
(75)

Finally, we analyzed the case of a random effect combined with an autoregressive structure of order one, for which no analytic solution exists. This model is given by

$$V_{ni} = \varepsilon_n + \eta_{ni}, \quad \eta_{ni} = \rho \eta_{n,i-1} + v_{ni}, \quad i = 1, \dots, m,$$
 (76)

<sup>&</sup>lt;sup>17</sup> The convolution  $\Pr(V_m < v_m) = \int_{-\infty}^{+\infty} \Phi((v_m - \mu_m - \lambda_m v)/s_m)\phi(v) dv = \Phi((v_m - \mu_m)/(\sqrt{s_m^2 + \lambda_m^2}))$  is used to obtain the analytic form.

where  $\varepsilon$  and v are mutually independent, the random effect  $\varepsilon_n$  is i.i.d. over n, and the AR(1) innovation  $v_{ni}$  is i.i.d. over both n and i. Since the evaluation of the probability, linear derivative, and logarithmic derivative expressions in this case requires numerical integration of the order of the dimension m, it was not tractable computationally to use numerical quadrature as a benchmark. Instead we chose in this case to obtain benchmark results by averaging a very large number of simulations (20,000) of the GHK method, which as it will become clear below, seems overall to be the most reliable procedure throughout the cases studied.

## 3.2. Comparative performance

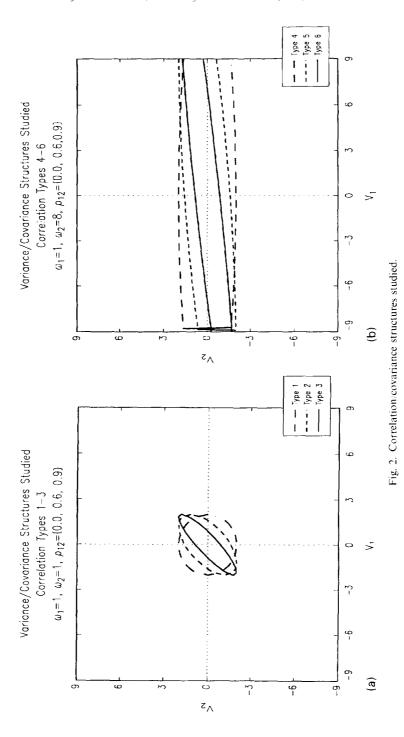
For each computational experiment we used 500 Monte Carlo repetitions of all 13 simulation algorithms. The number of simulations in calculating empirical expectations of the *H* matrix function was chosen endogenously by our programs, so as to require approximately the same time for each simulation method. The specific results reported in this section were obtained through the GAUSS implementation of the routines on 386/16MHz personal computers.

Figs. 2-6 describe the first series of experiments, in which truncated normal vectors V of dimension m=2 were generated, having the factor structure (67). Fig. 2 gives the six types of correlation/covariance structure<sup>18</sup> we studied, with  $\omega_1 = 1$ ,  $\omega_2 = \{1 \text{ or } 8\}$ , and  $\rho_{12} = \{0, 0.6, \text{ or } 0.9\}$ , where  $\text{var}V_i \equiv \omega_i$  and  $\text{cov}(V_1, V_2) \equiv \rho_{12} \cdot \omega_1 \cdot \omega_2$ . Fig. 3 describes the 14 different rectangles/restrictions<sup>19</sup> we investigated. These rectangles were chosen so as to analyze the effect of symmetry around either or both axes, as well as the location of them either close to the center of the distribution or far out in the tails. Hence, the results summarized in Figs. 4-6 refer to the 84 cases,  $\{A1, A2, \dots, N5, N6\}$ , that are obtained by combining these six correlation structures with the 14 sets of restrictions. Table 2a summarizes the characteristics of these 84 experiments in terms of the exact probability and the condition number and determinant of the variance-covariance matrix  $\Omega$  in each case. In Table 2b we give the explicit loadings in terms of the factor structure (67) for the six variance-covariance structures used in the experiments, i.e.,

$$S \equiv \begin{pmatrix} s_1 & 0 \\ 0 & s_2 \end{pmatrix}$$
 and  $\Lambda \equiv \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix}$ .

<sup>&</sup>lt;sup>18</sup> Indexed by a number from 1 to 6.

<sup>&</sup>lt;sup>19</sup> Indexed by a letter from A to N.



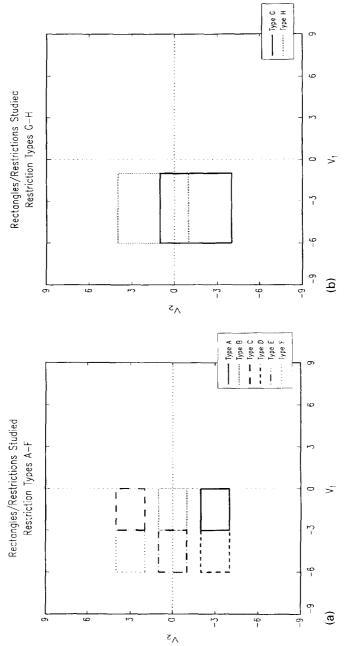
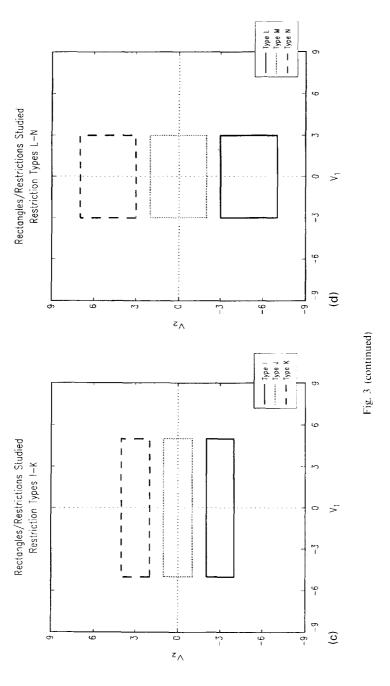
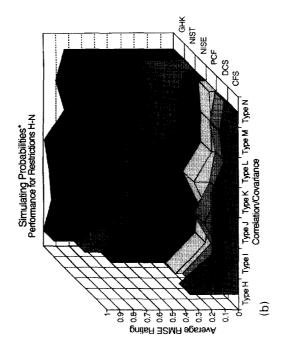


Fig. 3. Rectangles/restrictions studied.





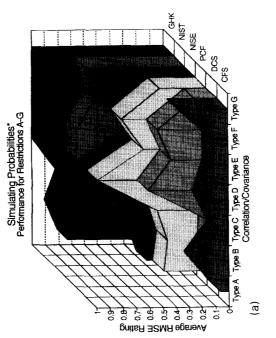


Fig. 4

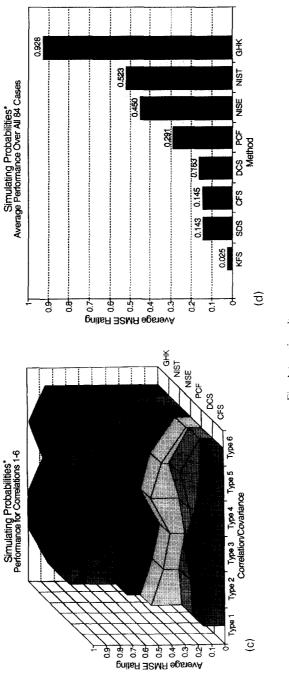
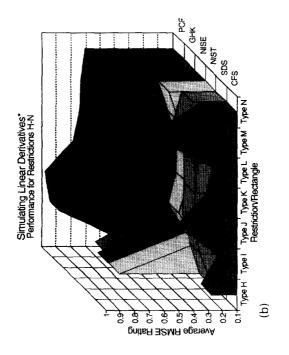


Fig. 4 (continued)



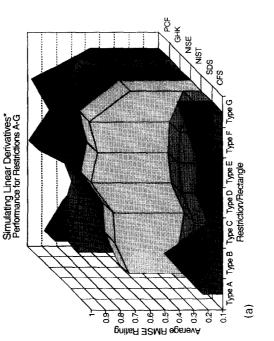
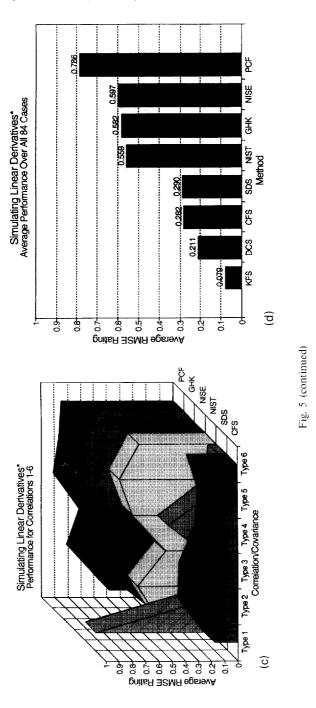
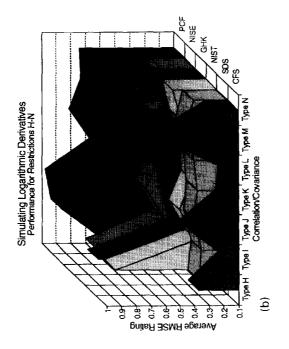
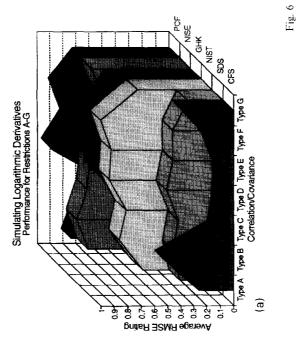


Fig. 5







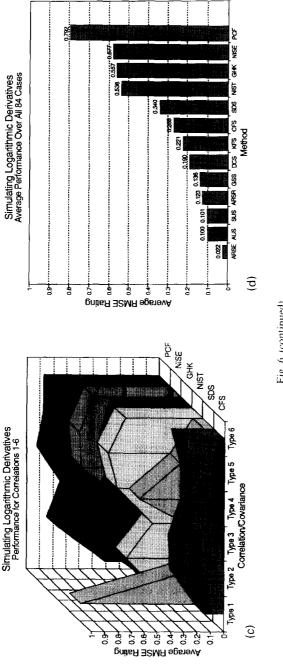


Fig. 6 (continued)

Table 2a Characteristics of 84 experiments, restrictions  $\{A-N\} \times \text{variance covariances } \{1-6\}$ , exact probability of each case

Restrictions	Variance-covariances							
	1	2	3	4	5	6		
A (3 × 2)	0.01133	0.02113	0.02143	0.04625	0.05656	0.07206		
$B(3\times2)$	0.34042	0.34112	0.34135	0.04960	0.04973	0.04974		
C (3×2)	0.01133	0.00095	8.601e-08	0.04625	0.03617	0.02069		
D $(3 \times 2)$	4.101e-05	0.00081	0.00174	0.00017	3.674e-05	9.799e-11		
$E(3 \times 2)$	0.00092	0.00023	2.662e-08	0.00013	1.366e-05	1.118e-11		
$F(3 \times 2)$	4.101e-05	1.036e-09	1.123e-13	0.00017	4.088e-06	1.633e-12		
$G(5 \times 5)$	0.12977	0.15259	0.15422	0.03720	0.03134	0.00792		
$H(5 \times 5)$	0.12977	0.08309	0.04057	0.03720	0.01960	0.00129		
$I = (10 \times 2)$	0.02272	0.02272	0.02272	0.09276	0.09276	0.09276		
$J = (10 \times 2)$	0.68269	0.68269	0.68269	0.09948	0.09948	0.09948		
$K(10 \times 2)$	0.02272	0.02272	0.02272	0.09276	0.09276	0.09276		
L (6 × 4)	0.00135	0.00121	0.00074	0.16260	0.16295	0.16304		
$M(6 \times 4)$	0.95192	0.95311	0.95444	0.19688	0.19738	0.19741		
$N(6 \times 4)$	0.00135	0.00121	0.00074	0.16260	0.16295	0.16304		
Cond. num. $(\Omega)$	1.000	3.999	18.999	63.999	101.139	345.446		
Det. $(\Omega)$	1.000	0.640	0.190	64.000	40.960	12.160		

After the name of each restriction type, the dimensions of the rectangle appear in parentheses.

Table 2b Characteristics of 84 experiments, factor structures of variance–covariances [1-6]

	$\Omega(1)$	$\Omega(2)$	$\Omega(3)$	$\Omega(4)$	$\Omega(5)$	$\Omega(6)$
S <sub>1</sub>	0.0	0.0	0.0	0.0	0.0	0.0
i <sub>2</sub>	1.0	0.8	0.43589	8.0	6.4	3.48712
·1	1.0	1.0	1.0	1.0	1.0	1.0
-2	0.0	0.6	0.9	0.0	4.8	7.2
$\frac{2}{1}$	1.0	1.0	1.0	1.0	1.0	1.0
$\sigma_2^2 = s_2^2 + \lambda_2^2$	1.0	1.0	1.0	64.0	64.0	64.0
$ alpha_{1,2} = \lambda_{\ell} \omega_2 $	0.0	0.6	0.9	0.0	0.6	0.9

For each one of the 84 cases studied, we rated the methods in terms of root-mean-squared-error relative to the best method for that case, e.g., a RMSE rating of 0.5 means that the method in question exhibited double the RMSE of the method with the lowest RMSE for that case. Analytically, 20

<sup>&</sup>lt;sup>20</sup> Interested readers may request from the authors considerably more detailed tables that report bias, variance, mean-squared-error, quantiles, robust statistics, and timing results for all cases studied.

Probabilities		Linear derivati	ves	Logarithmic derivatives		
GHK	0.928	PCF 0.786		PCF	0.792	
NIST	0.523	NISE 0.597		NISE	0.577	
NISE	0.450	GHK 0.582		GHK	0.557	
PCF	0.291	NIST 0.559		NIST	0.536	
DCS	0.163	SDS 0.290		SDS	0.340	
CFS	0.145	CFS 0.282		CFS	0.268	
SDS	0.143	DCS 0.211		KFS	0.221	
KFS	0.025	KFS 0.079		DCS	0.190	
AUS	n/a	AUS n/a		GSS	0.136	
ARSE	n/a	ARSE n/a		ARSR	0.123	
ARSR	n/a	ARSR n/a		SUS	0.101	
GSS	n/a	GSS n/a		AUS	0.100	
SUS	n/a	SUS n/a		ARSE	0.022	

Table 3
Average RMSE ratings across 84 cases

Average RMSE rating of method  $j \equiv \frac{1}{84} \sum_{k=1}^{84} \text{RMSE}$  (best method in case k)/RMSE (method j for case k).

n/a = not applicable.

Average RMSE rating of method i

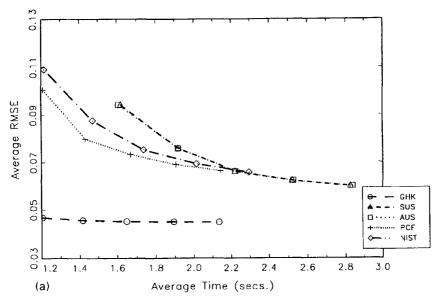
$$\equiv \frac{1}{84} \sum_{k=1}^{84} \text{RMSE (best method for case } k) / \text{RMSE (method } j \text{ in case } k).$$

In each figure the results are presented in four subfigures, (a) to (d). The first two report performance ratings for each of the 14 restriction types, averaging across all six correlation structures, with subfigures (a) and (b) giving cases A–G and H–N respectively. Subfigure (c) reports performance for each of the six types of correlation, averaging across the 14 restriction types. Finally, in subfigure (d) we report overall performance, averaging across all 84 correlation/restriction cases. The results of simulating probabilities appear in Fig. 4, those for simulating linear derivatives in Fig. 5, and those for logarithmic derivatives in Fig. 6. Overall the 84 cases studied, the average ratings of the various methods are also summarized in Table 3.

Our results support the following conclusions: GHK can be recommended as unambiguously the most reliable method for simulating normal rectangle probabilities, achieving an overall rating of 93%, compared to only 52% for the next best method, NIST.<sup>21</sup> For simulating derivative expressions, the PCF method exhibited the highest overall rating, 79% for linear and 79% for logarithmic, while NISE was second and GHK third for both types of derivatives. It is

<sup>&</sup>lt;sup>21</sup> Indeed, GHK achieved a first-place rating in over 70 of the 84 cases studied.





Simulating Linear Derivatives
Performance of Best Five Methods over Six typical cases

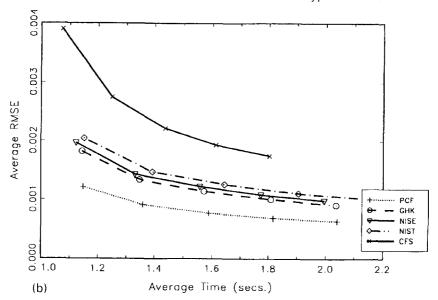
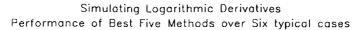


Fig. 7. Changing number of simulations:  $\times 1$ ,  $\times 2$ ,  $\times 3$ ,  $\times 4$ ,  $\times 5$ .



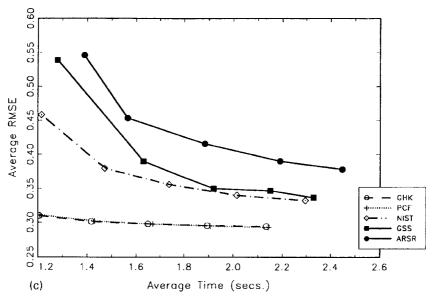
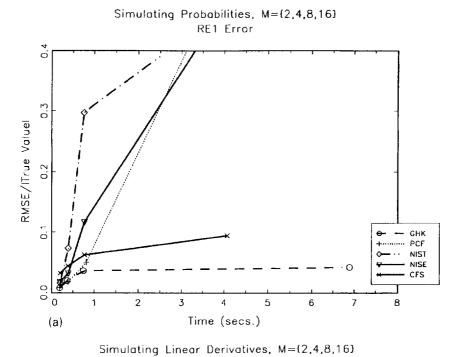


Fig. 7 (continued)

interesting to note that the normal importance sampling methods, NISE and NIST, seem to perform fairly well, bettered only by GHK in the case of probabilities, and by one (PCF) or two (PCF and GHK) methods in the case of derivatives. What Figs. 4–6 illustrate more clearly than the overall ratings table above is that GHK appears more robust than all other methods, in that it performs at or near the top in each one of the 84 cases studied. In particular, it performs even more impressively relative to the other algorithms in the most difficult cases of either high correlation among the elements of V and/or very low probability mass in the restriction region.

In the next set of computational experiments we investigated the consequences for the performance of the simulation methods of increasing the number of simulations used. We selected six cases out of the 84 possible ones discussed above<sup>22</sup> in such a way as to provide a wide range for the performance of the preferred method, GHK. The results are summarized in Fig. 7, where the actual RMSE of each of the five best methods, averaged over these six cases, is plotted against the time required to perform  $1 \times, 2 \times, 3 \times, 4 \times,$  and  $5 \times$  the original

<sup>&</sup>lt;sup>22</sup> A5, G6, K1, K2, L3, and L4.



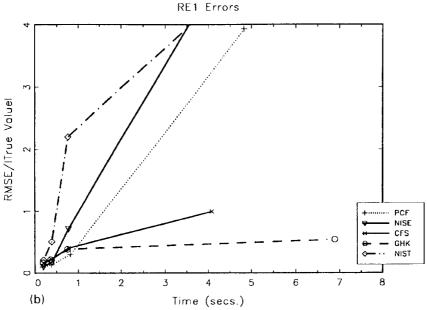
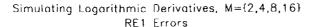


Fig. 8. Increasing dimension, RE1 errors:  $M = \{2, 4, 8, 16\}$ .



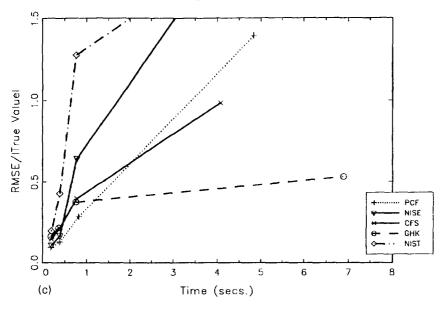


Fig. 8 (continued)

number of simulations used. The results again highlight the superior performance of GHK, especially for simulating probabilities. For linear derivatives, PCF has a slight edge over GHK, while for logarithmic derivatives, there is virtually a tie between GHK and PCF.

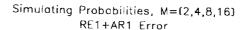
In the final set of experiments, we analyzed the impact on RMSE of increasing the dimension m of the problem. Figs. 8–9 report results for the five best methods for  $m = \{2, 4, 8, \text{ or } 16\}$ . In Fig. 8, the  $m \times 1$  multivariate normal vector V has the *one-factor* structure (RE1)

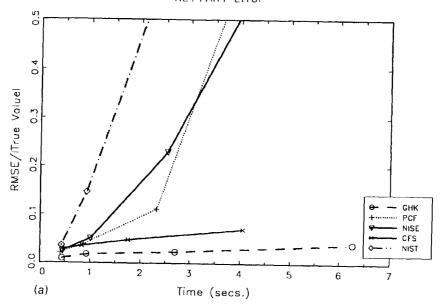
$$V_{ni} = \varepsilon_n + v_{ni}, \tag{75'}$$

with  $\sigma_v = 1$  and  $\sigma_\varepsilon = 1$ . In Fig. 9, the *one-factor plus AR(1)* structure (RE1AR1) was used

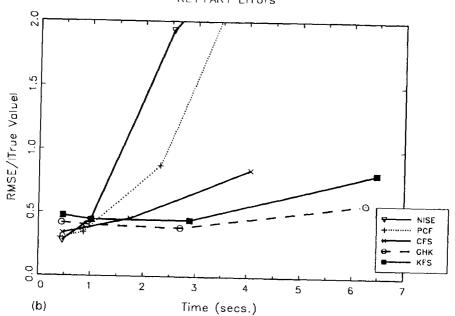
$$V_{ni} = \varepsilon_n + \eta_{ni}, \quad \eta_{ni} = \rho \eta_{n,i-1} + v_{ni}, \quad i = 1, \dots, m,$$
 (76')

with  $\sigma_v = 0.6$ ,  $\sigma_t = 1$ , and  $\rho = 0.8$ . The parameters were chosen so as to generate cases for which GHK is not the dominating method. In particular, the restriction region in these experiments was the all-negative orthant, which with the addition of a very high degree of serial correlation implies that the probability of





Simulating Linear Derivatives, M={2,4,8,16} RE1+AR1 Errors



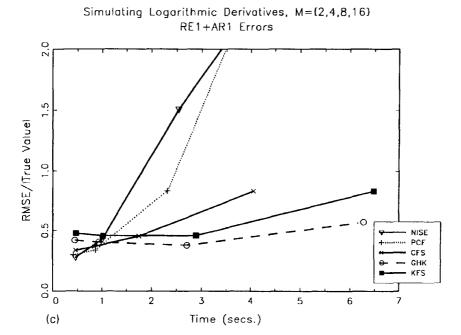


Fig. 9 (continued)

being in the restricted region is not very small.<sup>23</sup> Fig. 8 shows that GHK remains the only reliable method when the dimension is increased: the performance of GHK is uniformly superior, whether one simulates probabilities, linear derivatives, or logarithmic derivatives. The other methods perform especially poorly as m rises. Finally, Fig. 9 shows the effects of increasing the serial correlation through the addition of the AR(1) structure. The methods least affected by increasing m are GHK and CFS, with GHK once again exhibiting the most satisfactory performance.<sup>24</sup>

It should be noted that the results presented here discriminate against methods, like GSS, that are *not vectorizable*, since GAUSS is particularly efficient for vector operations. In preliminary timings using our FORTRAN code, we confirmed that methods that are difficult to vectorize then gain in relative speed. The impact of vectorization techniques on the performance of the

<sup>&</sup>lt;sup>23</sup> The true probability was 0.3333 for m = 2, 0.2001 for m = 4, 0.1095 for m = 8, and 0.0565 for m = 16 in the RE1 case, and 0.3974, 0.2855, 0.1753, and 0.0939 respectively for the RE1AR1 case.

<sup>&</sup>lt;sup>24</sup> In view of the relatively high probabilities in this last set of experiments, it is not surprising that CFS performs well in them.

simulation algorithms we studied is potentially a very important issue that merits further investigation, a task undertaken in Hajivassiliou (1993b). We plan future work on this topic.

## 4. Conclusions

The problem of evaluating multivariate normal probabilities and their derivatives is an important one in econometrics and biometrics because such expressions appear in leading econometric models, such as the *multinomial probit* (MNP) and other limited dependent variable models based on normality. Estimation of these models requires, for each trial parameter vector and each observation in a sample, evaluation of such probability expressions and their derivatives. The problem is computationally difficult unless the dimension of the integral is less than four or the covariance matrix  $\Omega$  has a special structure, such as a factorial structure with a low number of factors.

This paper surveyed Monte Carlo techniques that have been developed for approximating normal orthant probabilities and their derivatives that limit computation while possessing properties that facilitate their use in iterative calculations for statistical inference. We considered the following methods: the Crude Frequency Simulator (CFS), two variants of Normal Importance Sampling (NISE and NIST), a Kernel-smoothed Frequency Simulator (KFS), Stern's Decomposition Simulator (SDS), the Geweke-Hajivassiliou-Keane Simulator (GHK), a Parabolic Cylinder Function Simulator (PCF), Deák's Chi-squared Simulator (DCS), two variants of Acceptance/Rejection Simulation (ARSE and ARST), the Gibbs Sampler Simulator (GSS), a Sequentially Unbiased Simulator (SUS), and an Approximately Unbiased Simulator (AUS). In an Appendix we described GAUSS and FORTRAN algorithms implementing these methods. We presented test problems we used to investigate the operational properties of the methods, focussing on RMSE rankings, and summarized our computational experience with them. We also examined the impact of increasing the number of simulations R and the dimension of the probability integral m. We concluded that the GHK simulator appears overall the most reliable method, especially for simulating orthant probabilities.

## **Appendix**

Description of GAUSS and FORTRAN procedures

The simulation methods presented in this paper have been coded in GAUSS and in FORTRAN. Both versions of the programs are available via anonymous FTP from the Internet site ftp.econ.yale.edu, subdirectory pub/vassilis/simulation. Each simulator procedure requires the following standard inputs; the

interpretation of some inputs may vary from routine to routine, and not all are used in all routines:

M = dimension of the multivariate normal.

VMU = mean of multivariate normal, an  $M \times 1$  vector,

 $W = \text{covariance matrix of multivariate normal, an } M \times M \text{ array,}$ 

WI = inverse of W,

C = lower triangular Choleski factor of W, an  $M \times M$  array,

A = lower bound of rectangles, an  $M \times 1$  vector {when the lower

bound is  $-\infty$ , set A = (-1.0E10)\*ONES(M, 1),

B = upper bound of rectangle, an  $M \times 1$  vector {when the upper

bound is  $\infty$ , set B = (1.0E10)\*ONES(M, 1),

NR = number of repetitions,

 $U = \text{random variates, an } M \times R \text{ array,}$ 

*PARM* = parameters and constants for the simulation.

The simulators all return  $\{P, HU, HC\}$ , where P is the scalar rectangle probability, HU is the  $(M+1)\times(M+1)$  array of unconditional partial moments (6), and HC is the  $(M+1)\times(M+1)$  array of conditional moments (7). Parts of the output not provided by a simulator are set to -999.

In the FORTRAN implementation, two additional inputs are required, MMAX and NRMAX, specifying the maximum values of M and R allocated at compilation time.

The programs include code for all statistical functions, spherical transformations, and antithetics routines that are required by the simulation algorithms, and hence are self-contained.<sup>25</sup>

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<sup>&</sup>lt;sup>25</sup> In the Monte Carlo experiments reported in this paper, the number 1753227 was used as the starting seed for generating the random variates.

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