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USING MATHEMATICAL PROGRAMMING TO COMPUTE SINGULAR MULTIVARIATE NORMAL PROBABILITIES

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This paper describes two new, mathematical programming-based approaches for evaluating general, one- and two-sided, p-variate normal probabilities where the variance-covariance matrix (of arbitrary structure) is singular with rank $r (r < p)$, and r and p can be of unlimited dimensions. In both cases, principal components are used to transform the original, ill-defined, p-dimensional integral into a well-defined, r-dimensional integral over a convex polyhedron. The first algorithm that is presented uses linear programming coupled with a Gauss-Legendre quadrature scheme to compute this integral, while the second algorithm uses multi-parametric programming techniques in order to significantly reduce the number of optimization problems that need to be solved. The application of the algorithms is demonstrated and aspects of computational performance are discussed through a number of examples, ranging from a practical problem that arises in chemical engineering to larger, numerical examples.

Keywords: Singular multivariate normal distribution; Principal components; Linear programming; Parametric programming

1. INTRODUCTION

The multivariate normal distribution (MVN) plays an important rôle in a wide range of science, economic and engineering applications.

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As an example of this, consider a typical system that arises in chemical engineering – a heat exchanger network (Fig. 1). In this system, there are two hot process streams, $H1$ and $H2$, which must exchange heat with two cold streams, $C1$ and $C2$. The heat-capacities of all four streams and the outlet temperatures are given, but the inlet temperatures, denoted as T_1, T_2, T_3 and T_4, are uncertain and are described by normal probability density functions (*p.d.f.*s). The engineer's objective is to determine the probability that the system can be operated feasibly in the presence of these uncertainties.

Consider the case where $T_1 \sim N(620, 19.39)$, $T_2 \sim N(388, 19.39)$, $T_3 \sim N(583, 19.39)$ and $T_4 \sim N(313, 19.39)$. Using the analysis of Pistikopoulos and Mazzuchi (1990), it can be shown that the probability of feasible operation (or "stochastic flexibility") can be expressed as a one-sided probability:

$$\text{Prob} = P(\mathbf{X} \leq \mathbf{0}), \tag{1}$$

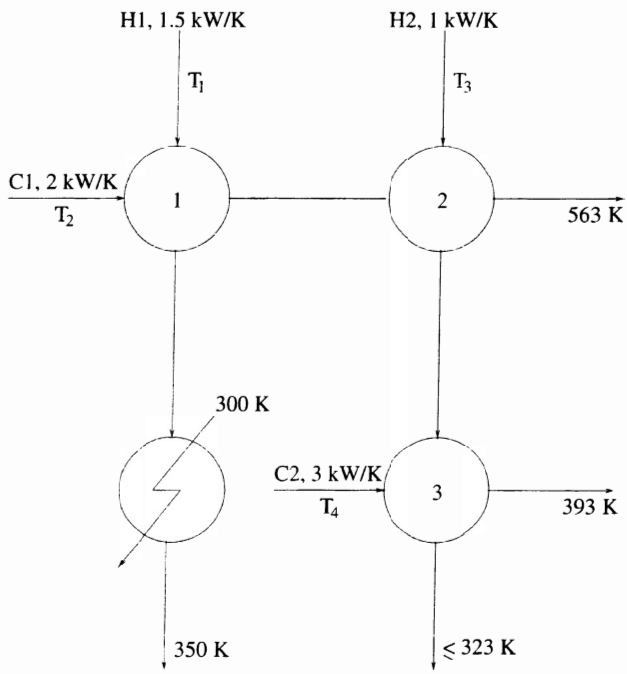

FIGURE 1 Motivating example: a heat exchanger network.

where $\mathbf{X} \sim N_3(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, and the vector of means, $\boldsymbol{\mu}$, and the variance-covariance matrix, $\boldsymbol{\Sigma}$, are given by:

$$\boldsymbol{\mu} = [-14, -10, -5]^T,$$

and

$$\boldsymbol{\Sigma} = \begin{bmatrix} 36.35625 & -24.2375 & -9.695 \\ -24.2375 & 48.475 & 14.5425 \\ -9.695 & 14.5425 & 4.8475 \end{bmatrix}.$$

Numerous methods exist in the literature for evaluating such MVN probabilities (see, for example, David, 1953; Plackett, 1954; Gupta, 1963; Milton, 1972; Drezner, 1992; Schervish, 1984, 1985; Genz and Kahaner, 1986; Evans and Swartz, 1988; Genz, 1992; Bunch *et al.*, 1993; Lohr, 1993; Joe, 1995 and Wang, 1997), while software is also commercially-available such as the G01HBF NAG sub-routine (NAG, 1998). Using the latter gives Prob = 0.9144 for (1).

Now consider the case where $T_1 \sim N(620, 69.39)$, $T_2 \sim N(388, 69.39)$, $T_3 \sim N(583, 69.39)$ and $T_4 \sim N(313, 69.39)$, as studied by Pistikopoulos and Mazzuchi (1990). This gives:

$$\text{Prob} = P(\mathbf{X} \leq \mathbf{0}), \tag{2}$$

where $\mathbf{X} \sim N_4(\boldsymbol{\mu}, \boldsymbol{\Sigma})$,

$$\boldsymbol{\mu} = [-19, -14, -10, -5]^T,$$

and

$$\boldsymbol{\Sigma} = \begin{bmatrix} 112.75875 & 78.06375 & 34.695 & 0 \\ 78.06375 & 130.10625 & -86.7375 & -34.695 \\ 34.695 & -86.7375 & 173.475 & 52.0425 \\ 0 & -34.695 & 52.0425 & 17.3475 \end{bmatrix}.$$

The difficulty with evaluating the probability in this instance is that $\boldsymbol{\Sigma}$ is a singular matrix. Thus, $|\boldsymbol{\Sigma}| = 0$, the inverse $\boldsymbol{\Sigma}^{-1}$ does not exist, and the *p.d.f.*, $f(\mathbf{x})$, which for a p-dimensional random vector $\mathbf{X}$ is given by

(Johnson and Wichern, 1988):

$$f(x) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right], \tag{3}$$

is ill-defined.

The fact that the calculation of probabilities involving such singular multivariate normal (SMVN) distributions is considerably more complicated than for the non-singular case, is reflected in the dearth of papers on the subject. Methods have been developed for the calculation of one- and two-sided percentage points (Bland and Owen, 1966; Nelson, 1991; Kwong, 1995; Kwong and Iglewicz, 1996; Soong and Hsu, 1997 and Kwong, 1998), but only for special forms of $\boldsymbol{\Sigma}$ (equicorrelated and product correlation structures). Pistikopoulos and Mazzuchi (1990) proposed lower and upper bounds on the value of a one-sided SMVN probability with arbitrary variance-covariance matrix using simple probability laws. While this procedure often results in tight bounds (for (2) it gives $0.6632 \leq \text{Prob} \leq 0.6654$), it involves the evaluation of a large number of non-singular MVN probabilities $\left(\sum_{i=1}^{p-1} {}^{p}C_i\right)$.

Kshirsagar (1972) described the use of principal components for evaluating SMVN probabilities and demonstrated the technique for an equicorrelated variance-covariance matrix. Rudolfer and Watson (1993) built on this idea to present methods for computing orthant probabilities, but limited to singular bivariate ($p=2$) and trivariate ($p=3$) distributions. The aim of this paper is to show how mathematical programming can be used to extend this latter approach to the evaluation of general, two-sided probabilities:

$$\begin{aligned}\text{Prob} = P[&(\alpha_1 \leq X_1 \leq \beta_1) \cap (\alpha_2 \leq X_2 \leq \beta_2) \\ &\cap \cdots \cap (\alpha_p \leq X_p \leq \beta_p)],\end{aligned} \tag{4}$$

for MVN distributions of *unrestricted* dimension p with singular variance-covariance matrices of arbitrary structure and *unrestricted* rank r ($r < p$).

The paper is structured as follows. In the next section, principal components theory is reviewed and it is shown how (4) can be transformed to an r-dimensional integral over a convex polyhedron. In Section 3, an algorithm is described for computing this integral which

uses linear programming coupled with a Gauss-Legendre quadrature scheme. Its application is illustrated with four examples, including a re-visitation of the heat exchanger network problem presented above. Finally, a second, alternative algorithm is described which uses multi-parametric linear programming techniques. Its potential for giving significant computational benefits is demonstrated with the heat exchanger network problem. The extension of this algorithm for efficiently determining percentage points is also discussed.

2. TRANSFORMATION USING PRINCIPAL COMPONENTS

Consider $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, where the vector of means and the variance-covariance matrix of rank r $(r < p)$ are given by

$$\boldsymbol{\mu} = [\mu_1, \mu_2, \ldots, \mu_p]^T, \tag{5}$$

and

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \sigma_1\sigma_2\rho_{12} & \cdots & \sigma_1\sigma_p\rho_{1p} \\ \sigma_1\sigma_2\rho_{12} & \sigma_2^2 & \cdots & \sigma_2\sigma_p\rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_1\sigma_p\rho_{1p} & \sigma_2\sigma_p\rho_{2p} & \cdots & \sigma_p^2 \end{bmatrix}, \tag{6}$$

respectively. Note that here, σ_i is the standard deviation of X_i, and ρ_{ij} is the correlation coefficient of X_i and X_j. The correlation matrix $\mathbf{C}$ is defined as:

$$\mathbf{C} = \begin{bmatrix} 1 & \rho_{12} & \cdots & \rho_{1p} \\ \rho_{12} & 1 & \cdots & \rho_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{1p} & \rho_{2p} & \cdots & 1 \end{bmatrix}, \tag{7}$$

and rank $(\mathbf{C}) = \text{rank}\,(\boldsymbol{\Sigma}) = r$. In order to utilise principal components for the problem at hand, the following transformation is first used (Rudolfer and Watson, 1993):

$$\mathbf{W} = \text{diag}\left(\sigma_1^{-1}, \sigma_2^{-1}, \ldots, \sigma_p^{-1}\right)\mathbf{X}. \tag{8}$$

This means that $\mathbf{W} \sim N_p(\boldsymbol{\mu}_w, \boldsymbol{\Sigma}_w)$, where

$$\boldsymbol{\mu}_w = [\mu_1/\sigma_1, \mu_2/\sigma_2, \ldots, \mu_p/\sigma_p]^T, \tag{9}$$

$$\boldsymbol{\Sigma}_w = \mathbf{C}, \tag{10}$$

and thus rank $(\boldsymbol{\Sigma}_w) = r$. Note that since $\boldsymbol{\Sigma}_w$ is a symmetric matrix, all its eigenvalues, λ_i, $i = 1, \ldots, p$, are real, and its rank is equal to the number of non-zero eigenvalues (Mardia *et al.*, 1979, pp. 465, 468). Hence, the eigenvalues can be written as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > 0$, and $\lambda_{r+1} = \lambda_{r+2} = \cdots = \lambda_p = 0$. Note also that (4) can now be written as:

$$\text{Prob} = P\left[\left(\frac{\alpha_1}{\sigma_1} \leq W_1 \leq \frac{\beta_1}{\sigma_1}\right) \cap \left(\frac{\alpha_2}{\sigma_2} \leq W_2 \leq \frac{\beta_2}{\sigma_2}\right) \cap \cdots \cap \left(\frac{\alpha_p}{\sigma_p} \leq W_p \leq \frac{\beta_p}{\sigma_p}\right)\right], \tag{11}$$

$$= P(\boldsymbol{\eta}_1 \leq \mathbf{W} \leq \boldsymbol{\eta}_2), \tag{12}$$

$$= \int_{\{\mathbf{W}: \boldsymbol{\eta}_1 \leq \mathbf{W} \leq \boldsymbol{\eta}_2\}} f(\mathbf{W})\, d\mathbf{W}, \tag{13}$$

where $f(\mathbf{W})$ is the (ill-defined) *p.d.f.* of $\mathbf{W}$,

$$\boldsymbol{\eta}_1 = [\alpha_1/\sigma_1, \alpha_2/\sigma_2, \ldots, \alpha_p/\sigma_p]^T, \tag{14}$$

and

$$\boldsymbol{\eta}_2 = [\beta_1/\sigma_1, \beta_2/\sigma_2, \ldots, \beta_p/\sigma_p]^T. \tag{15}$$

By definition, $\mathbf{W}$ can be expressed in terms of its principal components, $\mathbf{Y}$, as (Mardia *et al.*, 1979, pp. 214, 215):

$$\mathbf{W} = \boldsymbol{\Gamma} \cdot \mathbf{Y} + \boldsymbol{\mu}_w, \tag{16}$$

where $\boldsymbol{\Gamma}$ is an orthogonal matrix ($\boldsymbol{\Gamma}\boldsymbol{\Gamma}^T = \mathbf{I}$) whose columns are the normalised eigenvectors corresponding to the eigenvalues of $\boldsymbol{\Sigma}_w$. Since there are only r non-zero eigenvalues, $\boldsymbol{\Gamma}$ is a $(p \times r)$ matrix, while $\mathbf{Y}$ is an $(r \times 1)$ column vector (*i.e.*, $Y_{r+1} = Y_{r+2} = \cdots = Y_p = 0$). An additional property of the principal components is that they

are independent and the ith component is normally distributed with zero mean and variance λ_i. This can be expressed as:

$$\mathbf{Y} \sim N_r(\mathbf{0}, \mathbf{\Lambda}), \tag{17}$$

where

$$\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_r). \tag{18}$$

The principal components can be used to further express $\mathbf{W}$ in terms of standard normal random variables, $\mathbf{Z}$, by defining:

$$\mathbf{Y} = \mathbf{\Lambda}^{1/2} \cdot \mathbf{Z}, \tag{19}$$

where

$$\mathbf{\Lambda}^{1/2} = \operatorname{diag}\left(\lambda_1^{1/2}, \lambda_2^{1/2}, \ldots, \lambda_r^{1/2}\right), \tag{20}$$

and hence $\mathbf{Z} \sim N_r(\mathbf{0}, \mathbf{1})$. Substituting (19) into (16) then gives:

$$\mathbf{W} = \mathbf{\Delta} \cdot \mathbf{Z} + \boldsymbol{\mu}_w, \tag{21}$$

where

$$\mathbf{\Delta} = \mathbf{\Gamma} \cdot \mathbf{\Lambda}^{1/2}. \tag{22}$$

Using (21), the desired probability (13) is equivalently given by the r-dimensional integral:

$$\text{Prob} = \int_{\{\mathbf{z}:\boldsymbol{\eta}_1 \le \mathbf{\Delta}\cdot\mathbf{z}+\boldsymbol{\mu}_w \le \boldsymbol{\eta}_2\}} f(\mathbf{Z})\, d\mathbf{Z}, \tag{23}$$

$$= \int_{Z_1^{\min}}^{Z_1^{\max}} \int_{Z_2^{\min}(Z_1)}^{Z_2^{\max}(Z_1)} \cdots \int_{Z_r^{\min}(Z_1, Z_2, \ldots, Z_{r-1})}^{Z_r^{\max}(Z_1, Z_2, \ldots, Z_{r-1})} f(\mathbf{Z})\, dZ_r \cdots dZ_2\, dZ_1, \tag{24}$$

where, from (3), the integrand is given by:

$$f(\mathbf{z}) = \frac{1}{(2\pi)^{r/2}} \exp\left[-\frac{1}{2}\sum_{j=1}^{r} Z_j^2\right], \tag{25}$$

and where $Z_j^{\min}(Z_1, Z_2, \ldots, Z_{j-1})$ and $Z_j^{\max}(Z_1, Z_2, \ldots, Z_{j-1}), j = 1, \ldots, r$, are variable lower and upper bounds of parameter Z_j that are evaluated at the parameter values $Z_1, Z_2, \ldots, Z_{j-1}$. These bounds

define the boundary of the integration region; since this region is defined through the set of linear inequalities $\{\mathbf{Z}: \boldsymbol{\eta}_1 \leq \boldsymbol{\Delta} \cdot \mathbf{Z} + \boldsymbol{\mu}_w \leq \boldsymbol{\eta}_2\}$, it corresponds to an r-dimensional convex polyhedron. In the next section, we show how linear programming can be used to enable computation of the integral (24).

3. A LINEAR PROGRAMMING-BASED PROCEDURE

3.1. General Description

The potential difficulty with evaluating (24) is that the limits of integration for each parameter depend on the limits of lower-dimensional parameters. For integrals of this form, however, the following procedure can be used (Straub and Grossmann, 1993). Firstly, the maximum and minimum values of Z_1, $Z_1^{\max}$ and $Z_1^{\min}$ respectively, are determined by solving the linear program (LP):

$$\begin{aligned}
&\max \quad (Z_1^{\max} - Z_1^{\min}),\\
\text{s.t.} \quad &\frac{\alpha_i}{\sigma_i} \leq \delta_{i1} Z_1^{\max} + \sum_{k=2}^{r} \delta_{ik} Z_k^{a,1} + \kappa_i \leq \frac{\beta_i}{\sigma_i}, \quad i = 1, \ldots, p,\\
&\frac{\alpha_i}{\sigma_i} \leq \delta_{i1} Z_1^{\min} + \sum_{k=2}^{r} \delta_{ik} Z_k^{b,1} + \kappa_i \leq \frac{\beta_i}{\sigma_i}, \quad i = 1, \ldots, p,\\
&Z^L \leq Z_1^{\min} \leq Z_1^{\max} \leq Z^U,\\
&Z^L \leq Z_k^{a,1}, Z_k^{b,1} \leq Z^U, \quad k = 2, \ldots, r, \qquad (26)
\end{aligned}$$

where δ_{ij} refers to the element of $\boldsymbol{\Delta}$ in the ith row and jth column; κ_i is the ith element of $\boldsymbol{\mu}_w$; $Z_k^{a,1}$ and $Z_k^{b,1}$ reflect the fact that different values of Z_k, $k = 2, \ldots, r$, must be chosen in order to calculate the maximum and minimum values of Z_1; and Z^L and Z^U are used to ensure that there is a closed (definite) region of integration, and so to prevent potential difficulties with a numerical integration scheme. Typical values for Z^L and Z^U might be -4 and $+4$ respectively, since 99.994% of the standard normal distribution is contained within ± 4. Note that (26) can be solved using any of several well-established methods such as the simplex algorithm (Hillier and Lieberman, 1986) or interior point methods (Marsten *et al.*, 1990).

Once the bounds, $Z_1^{\max}$ and $Z_1^{\min}$, have been determined, the next step is to discretise over this range according to a specific quadrature formula (*e.g.*, Gauss-Legendre). For each of these Q_1 discrete points, $Z_1^{q_1}$, $q_1 = 1, \ldots, Q_1$, the maximum and minimum values of Z_2 are determined by solving the LP:

$$\max \quad (Z_2^{\max q_1} - Z_2^{\min q_1}),$$

$$\text{s.t.} \quad \frac{\alpha_i}{\sigma_i} \leq \delta_{i1} Z_1^{q_1} + \delta_{i2} Z_2^{\max q_1} + \sum_{k=3}^{r} \delta_{ik} Z_k^{a,2,q_1} + \kappa_i \leq \frac{\beta_i}{\sigma_i}, \quad i = 1, \ldots, p,$$

$$\frac{\alpha_i}{\sigma_i} \leq \delta_{i1} Z_1^{q_1} + \delta_{i2} Z_2^{\min q_1} + \sum_{k=3}^{r} \delta_{ik} Z_k^{b,2,q_1} + \kappa_i \leq \frac{\beta_i}{\sigma_i}, \quad i = 1, \ldots, p,$$

$$Z^L \leq Z_2^{\min q_1} \leq Z_2^{\max q_1} \leq Z^U,$$

$$Z^L \leq Z_k^{a,2,q_1}, Z_k^{b,2,q_1} \leq Z^U, \quad k = 3, \ldots, r. \tag{27}$$

Quadrature points are then placed for Z_2, bounds are determined for Z_3, and so on, until Z_r has been discretised. The value of the integral (24) can then be estimated. Figure 2 illustrates the points that would be obtained for the case $r = 2$, with three quadrature points in both dimensions.

The procedure described above has the advantage that all the quadrature points are placed within the region of integration, which would not be the case if a hyper-rectangular method such as Monte Carlo sampling was used. This enhances the efficiency of the Gaussian quadrature scheme in accurately estimating the integral (24). Notice also that no assumption has been made about the structure of the variance-covariance matrix (6).

3.2. Algorithm 1

Based on the above theory, the steps of the proposed algorithm for the computation of a general, two-sided SMVN probability such as (4) can be summarised as follows. Given a p-dimensional random vector $\mathbf{X} \sim N_p(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, a vector of means (5) and a singular variance-covariance matrix (6) of arbitrary structure and rank r:

Step 1 Calculate $\boldsymbol{\mu}_w$ from (9); $\boldsymbol{\Sigma}_w$ from (10); the eigenvalues and associated eigenvectors of $\boldsymbol{\Sigma}_w$; hence $\boldsymbol{\Lambda}^{1/2}$ from (20), $\boldsymbol{\Gamma}$, which is the

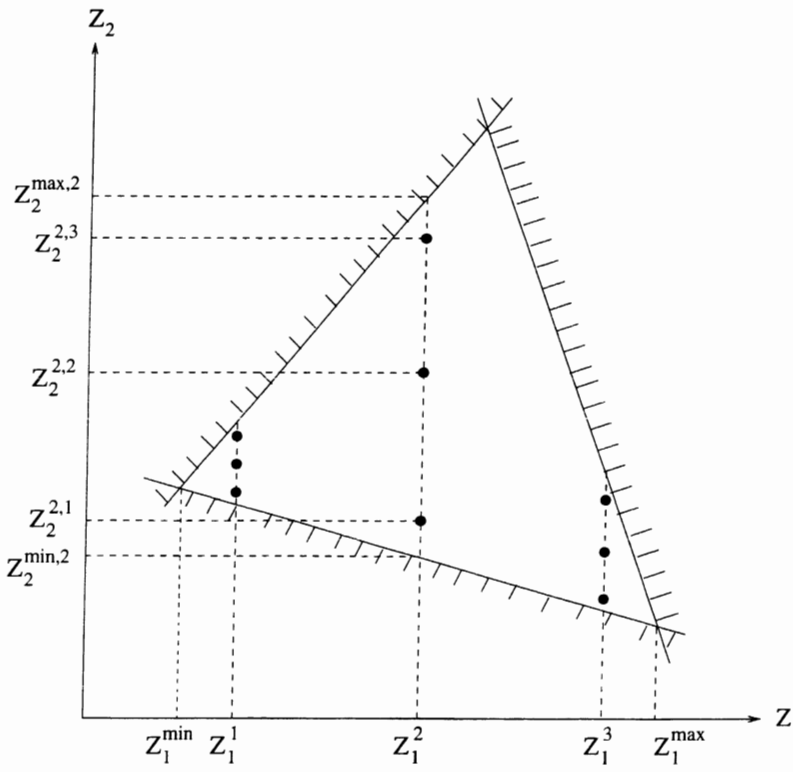

FIGURE 2 Illustration of quadrature point placement for rank $(\boldsymbol{\Sigma}) = 2$ case.

matrix whose columns are the normalised eigenvectors, and $\boldsymbol{\Delta}$ from (22); $\boldsymbol{\eta_1}$ from (14); and $\boldsymbol{\eta_2}$ from (15).

Step 2 For $j = 1$ to r:

(i) Solve the $Q_1 Q_2 \ldots Q_{j-1}$ LPs:

$$\max \left(Z_j^{\max q_1 \ldots q_{j-1}} - Z_j^{\min q_1 \ldots q_{j-1}} \right),$$

$$\text{s.t.} \quad \frac{\alpha_i}{\sigma_i} \leq \sum_{l=1}^{j-1} \delta_{il} Z_l^{q_1 \ldots q_{j-1}} + \delta_{ij} Z_j^{\max q_1 \ldots q_{j-1}} + \sum_{k=j+1}^{r} \delta_{ik} Z_k^{a,j,q_1 \ldots q_{j-1}} + \kappa_i \leq \frac{\beta_i}{\sigma_i}, \quad i = 1, \ldots, p,$$

$$\frac{\alpha_i}{\sigma_i} \le \sum_{l=1}^{j-1} \delta_{il} Z_l^{q_1 \dots q_{j-1}} + \delta_{ij} Z_j^{\min q_1 \dots q_{j-1}} + \sum_{k=j+1}^{r} \delta_{ik} Z_k^{b,j,q_1 \dots q_{j-1}} + \kappa_i \le \frac{\beta_i}{\sigma_i}, \quad i = 1, \dots, p,$$

$$-4 \le Z_j^{\min q_1 \dots q_{j-1}} \le Z_j^{\max q_1 \dots q_{j-1}} \le 4,$$

$$-4 \le Z_k^{a,j,q_1 \dots q_{j-1}}, Z_k^{b,j,q_1 \dots q_{j-1}} \le 4, \qquad k = j+1, \dots, r, \quad \forall q_1, \dots, \forall q_{j-1}. \tag{28}$$

(ii) Determine the $Q_1 Q_2 \dots Q_j$ quadrature points, $Z_j^{q_1 \dots q_j}$, in terms of the locations of Gauss-Legendre quadrature points in the $[-1, 1]$ interval (Carnahan *et al.*, 1969; Engels, 1980), $\nu_j^{q_j}$, from:

$$Z_j^{q_1 \dots q_j} = \frac{1}{2}[Z_j^{\max q_1 \dots q_{j-1}}(1 + \nu_j^{q_j}) + Z_j^{\min q_1 \dots q_{j-1}}(1 - \nu_j^{q_j})], \quad \forall q_1, \dots, \forall q_j. \tag{29}$$

Step 3 Evaluate the joint *p.d.f.* and the required probability from:

$$f(Z_{j(j=1,\dots,r)}^{q_1 \dots q_j}) = \frac{1}{(2\pi)^{r/2}} \exp\left[-\frac{1}{2}\sum_{j=1}^{r}(Z_j^{q_1 \dots q_j})^2\right], \quad \forall q_1, \dots, \forall q_j, \tag{30}$$

and

$$\text{Prob} = \frac{Z_1^{\max} - Z_1^{\min}}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{Z_2^{\max q_1} - Z_2^{\min q_1}}{2} \dots \sum_{q_{r-1}=1}^{Q_{r-1}} w_{r-1}^{q_{r-1}} \frac{Z_r^{\max q_1 \dots q_{r-1}} - Z_r^{\min q_1 \dots q_{r-1}}}{2} \sum_{q_r=1}^{Q_r} w_r^{q_r} f(Z_{j(j=1,\dots,r)}^{q_1 \dots q_j}), \tag{31}$$

respectively. In (31), $w_j^{q_j}$, $j = 1, \dots, r$, are the weights of the Gauss-Legendre quadrature points (Carnahan *et al.*, 1969; Engels, 1980).

3.3. Examples

In the following examples to demonstrate the application of Algorithm 1, the matrix manipulations in Step 1 of the algorithm were carried out

in a matter of milliseconds using MATLAB^{TM} (The Math Works, Inc., 1992). The LPs in Step 2 were solved using GAMS/CPLEX (Brooke *et al.*, 1992), with GAMS also used to perform the function evaluations in Step 3. All the computations were implemented on a Sun ULTRA 60 work station.

3.3.1. Example 1: 4-variate, Rank (Σ) = 3

Consider the heat exchanger network problem discussed in Section 1. The aim is to find

$$\text{Prob} = P(\mathbf{X} \leq \mathbf{0}),$$

where $\mathbf{X} \sim N_4(\boldsymbol{\mu}, \boldsymbol{\Sigma})$,

$$\boldsymbol{\mu} = [-19, -14, -10, -5]^T,$$

$$\text{and} \quad \boldsymbol{\Sigma} = \begin{bmatrix} 112.75875 & 78.06375 & 34.695 & 0 \\ 78.06375 & 130.10625 & -86.7375 & -34.695 \\ 34.695 & -86.7375 & 173.475 & 52.0425 \\ 0 & -34.695 & 52.0425 & 17.3475 \end{bmatrix}.$$

Step 1

$$\boldsymbol{\mu}_w = [-1.7893, -1.2274, -0.7592, -1.2005]^T, \tag{32}$$

$$\boldsymbol{\Sigma}_w = \begin{bmatrix} 1 & 0.6445 & 0.2481 & 0 \\ 0.6445 & 1 & -0.5774 & -0.7303 \\ 0.2481 & -0.5774 & 1 & 0.9487 \\ 0 & -0.7303 & 0.9487 & 1 \end{bmatrix}, \tag{33}$$

$$\boldsymbol{\Lambda}^{1/2} = \text{diag}(1.5944, 1.1926, 0.1883), \tag{34}$$

$$\boldsymbol{\Gamma} = \begin{bmatrix} -0.1418 & -0.8160 & 0.2326 \\ -0.5533 & -0.3869 & -0.4941 \\ 0.5558 & -0.3838 & 0.3792 \\ 0.6039 & -0.1930 & -0.7470 \end{bmatrix}, \tag{35}$$

$$\Delta = \begin{bmatrix} -0.2261 & -0.9731 & 0.0438 \\ -0.8823 & -0.4615 & -0.0930 \\ 0.8862 & -0.4577 & 0.0714 \\ 0.9629 & -0.2301 & -0.1407 \end{bmatrix}, \tag{36}$$

$$\eta = [0, \quad 0, \quad 0, \quad 0]^T. \tag{37}$$

Steps 2 and 3 In order to illustrate the type of LP that must be solved in Step 2(i), consider $j = 3$:

$$\max \ (Z_3^{\max q_1 q_2} - Z_3^{\min q_1 q_2}),$$

$$\begin{aligned}
\text{s.t.} \quad & -0.2261 Z_1^{q_1} - 0.9731 Z_2^{q_1 q_2} + 0.0438 Z_3^{\max q_1 q_2} - 1.7893 \le 0, \\
& -0.8823 Z_1^{q_1} - 0.4615 Z_2^{q_1 q_2} - 0.0930 Z_3^{\max q_1 q_2} - 1.2274 \le 0, \\
& 0.8862 Z_1^{q_1} - 0.4577 Z_2^{q_1 q_2} + 0.0714 Z_3^{\max q_1 q_2} - 0.7592 \le 0, \\
& 0.9629 Z_1^{q_1} - 0.2301 Z_2^{q_1 q_2} - 0.1407 Z_3^{\max q_1 q_2} - 1.2005 \le 0, \\
& -0.2261 Z_1^{q_1} - 0.9731 Z_2^{q_1 q_2} + 0.0438 Z_3^{\min q_1 q_2} - 1.7893 \le 0, \\
& -0.8823 Z_1^{q_1} - 0.4615 Z_2^{q_1 q_2} - 0.0930 Z_3^{\min q_1 q_2} - 1.2274 \le 0, \\
& 0.8862 Z_1^{q_1} - 0.4577 Z_2^{q_1 q_2} + 0.0714 Z_3^{\min q_1 q_2} - 0.7592 \le 0, \\
& 0.9629 Z_1^{q_1} - 0.2301 Z_2^{q_1 q_2} - 0.1407 Z_3^{\min q_1 q_2} - 1.2005 \le 0, \\
& -4 \le Z_3^{\min q_1 q_2} \le Z_3^{\max q_1 q_2} \le 4, \quad \forall q_1, \forall q_2.
\end{aligned} \tag{38}$$

The results of applying Steps 2 and 3 of Algorithm 1 are shown in Table I for different numbers of quadrature points, together with the numbers of LPs solved and associated computation times. It can be seen that the SMVN probability converges to 0.6632 (correct to 4

TABLE I SMVN probability evaluation for Example 1 using Algorithm 1

Q_j, $j = 1,2,3$	*Prob*	*No. of LPs*	*CPU(s)*
8	0.6650	73	0.4
16	0.6621	273	1.5
32	0.6632	1057	6.1
64	0.6632	4161	24.4

d.p.), which corresponds to the lower bound predicted by the analysis of Pistikopoulos and Mazzuchi (1990).

3.3.2. Example 2: 5-variate, Rank (Σ) = 4

Consider the problem of evaluating

$$\begin{aligned}\text{Prob} = P[&(-41 \le X_1 \le 1) \cap (-35 \le X_2 \le 2) \cap (-3 \le X_3 \le 30) \\ &\cap (-16 \le X_4 \le 0.4) \cap (2.7 \le X_5 \ge 50)],\end{aligned}$$

where $\mathbf{X} \sim N_5(\boldsymbol{\mu}, \boldsymbol{\Sigma})$,

$$\boldsymbol{\mu} = [-19, -14, -10, -5, 10]^T,$$

and

$$\boldsymbol{\Sigma} = \begin{bmatrix} 112.75875 & 78.06375 & 34.695 & 0 & 0 \\ 78.06375 & 130.10625 & -86.7375 & -34.695 & -104.085 \\ 34.695 & -86.7375 & 173.475 & 52.0425 & 156.1275 \\ 0 & -34.695 & 52.0425 & 17.3475 & 52.0425 \\ 0 & -104.085 & 156.1275 & 52.0425 & 158.9031 \end{bmatrix}.$$

Applying Algorithm 1 gives the results shown in Table II, leading to Prob = 0.1832.

3.3.3. Example 3: 7-variate, Rank (Σ) = 5

Consider the evaluation of

$$\begin{aligned}\text{Prob} = P[&(-41 \le X_1 \le 1) \cap (-35 \le X_2 \le 2) \cap (-30 \le X_3 \le 3) \\ &\cap (-10 \le X_4 \le 4) \cap (-5 \le X_5 \le 20) \\ &\cap (-6 \le X_6 \le 40) \cap (-8 \le X_7 \le 7)],\end{aligned}$$

TABLE II SMVN probability evaluation for Example 2 using Algorithm 1

Q_j, $j = 1,2,3,4$	*Prob*	*No. of LPs*	*CPU(s)*
8	0.1819	585	3.2
16	0.1835	4369	25.4
32	0.1832	33825	209
48	0.1832	112945	769

where $\mathbf{X} \sim N_7(\boldsymbol{\mu}, \boldsymbol{\Sigma})$,

$$\boldsymbol{\mu} = [-19, -14, -10, -5, 10, 25, -1.2]^T,$$

and

$$\boldsymbol{\Sigma} = \begin{bmatrix} 112.75875 & 78.06375 & 34.695 & 0 & 0 & 0 & -149.1885 \\ 78.06375 & 130.10625 & -86.7375 & -34.695 & -104.085 & -173.475 & -79.7985 \\ 34.695 & -86.7375 & 173.475 & 52.0425 & 156.1275 & 260.2125 & -69.39 \\ 0 & -34.695 & 52.0425 & 17.3475 & 52.0425 & 86.7375 & 0 \\ 0 & -104.085 & 156.1275 & 52.0425 & 158.9031 & 265.7637 & 0 \\ 0 & -173.475 & 260.2125 & 86.7375 & 265.7637 & 444.7899 & 0 \\ -149.1885 & -79.7985 & -69.39 & 0 & 0 & 0 & 302.5404 \end{bmatrix}.$$

Table III summarises the results. In this case, Algorithm 1 converges to Prob = 0.2053.

3.3.4. Example 4: 10-variate, Rank (Σ) = 6

In this example, the desired probability is

$$\text{Prob} = P(X_1 \leq 1 \cap X_2 \leq 1 \cap X_3 \leq 3 \cap X_4 \leq 4 \cap X_5 \geq -5 \cap X_6 \geq -6 \cap X_7 \leq 7 \cap X_8 \leq 8 \cap X_9 \leq 9 \cap X_{10} \leq 10),$$

where $\mathbf{X} \sim N_{10}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$,

$$\boldsymbol{\mu} = [-19, -14, -10, -5, 10, 25, -1.2, -21.8, -17.3, -6.19]^T,$$

and

TABLE III SMVN probability evaluation for Example 3 using Algorithm 1

Q_j, $j = 1, \ldots, 5$	*Prob*	*No. of LPs*	*CPU(s)*
8	0.2094	4681	27.4
12	0.2064	22621	140
16	0.2054	69905	436
24	0.2053	346201	2360

$$\boldsymbol{\Sigma} = \begin{bmatrix} 112.75875 & 78.06375 & 34.695 & 0 & 0 & 0 & -149.1885 & 58.80803 & 58.80803 & -6.2451 \\ 78.06375 & 130.10625 & -86.7375 & -34.695 & -104.085 & -173.475 & -79.7985 & -45.27698 & -10.58198 & 27.756 \\ 34.695 & -86.7375 & 173.475 & 52.0425 & 156.1275 & 260.2125 & -69.39 & 138.78 & 86.7375 & -51.00165 \\ 0 & -34.695 & 52.0425 & 17.3475 & 52.0425 & 86.7375 & 0 & 34.695 & 17.3475 & -17.00055 \\ 0 & -104.085 & 156.1275 & 52.0425 & 158.9031 & 265.7637 & 0 & 101.3094 & 49.2669 & -41.28705 \\ 0 & -173.475 & 260.2125 & 86.7375 & 265.7637 & 444.7899 & 0 & 167.9238 & 81.1863 & -65.57355 \\ -149.1885 & -79.7985 & -69.39 & 0 & 0 & 0 & 302.5404 & -134.6166 & -134.6166 & 14.98824 \\ 58.80803 & -45.27698 & 138.78 & 34.695 & 101.3094 & 167.9238 & -134.6166 & 213.64487 & 178.94987 & -41.21766 \\ 58.80803 & -10.58198 & 86.7375 & 17.3475 & 49.2669 & 81.1863 & -134.6166 & 178.94987 & 161.60237 & -24.21711 \\ -6.2451 & 27.756 & -51.00165 & -17.00055 & -41.28705 & -65.57355 & 14.98824 & -41.21766 & -24.21711 & 59.65458 \end{bmatrix}.$$

TABLE IV SMVN probability evaluation for Example 4 using Algorithm 1

$Q_j, j=1,\ldots,6$	*Prob*	*No. of LPs*	*CPU(s)*
8	0.4195	37449	244
16	0.4198	1118481	7618

Algorithm 1 gives Prob = 0.420, as indicated in Table IV.

3.4. Remarks on Algorithm 1

The examples presented above demonstrate the potential of the algorithm for accurately evaluating one- and two-sided SMVN probabilities in systems with large numbers of variates. A potential drawback, however, is that the number of LPs that must be solved in Step 2(i) increases exponentially with the rank of $\mathbf{\Sigma}$, r, and the number of quadrature points used for each parameter Z_j (if the same number of quadrature points, Q, is used for each parameter, as in the examples above, then the number of LPs that must be solved is $\sum_{j=1}^{r} Q^{j-1}$). Since the solution of the LPs is *the* computationally expensive step in the algorithm, the computation times also increase exponentially with r and Q, as displayed in Tables I to IV.

In order to diminish the computational effort associated with Algorithm 1, use can be made of the fact that the individual LPs for each parameter are independent. This then allows the LPs for each parameter to be solved *in parallel*, *i.e.*, one could solve the first LP for Z_1, then the next Q LPs for Z_2 in parallel, then the next Q^2 LPs for Z_3 in parallel, and so on. Alternatively, the number of optimization subproblems that need to be solved can be greatly reduced by utilising a procedure based on multi-parametric linear programming, as explained in the following section.

4. MULTI-PARAMETRIC LINEAR PROGRAMMING PROCEDURE

4.1. General Description

Consider an optimization problem of the form

$$\psi(\boldsymbol{\theta}) = \max_{\mathbf{v}} \ \mathbf{c}^T \cdot \mathbf{v},$$

$$\begin{aligned} \text{s.t.} \quad & \mathbf{A} \cdot \mathbf{v} \leq \mathbf{b} + \mathbf{F} \cdot \boldsymbol{\theta}, \\ & \boldsymbol{\theta}^L \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^U, \\ & \mathbf{v} \geq \mathbf{0}, \end{aligned} \tag{39}$$

where $\mathbf{v}$ is a vector of search variables; $\boldsymbol{\theta}$ is a vector of uncertain parameters; $\mathbf{A}$ and $\mathbf{F}$ are matrices of constants; and $\mathbf{b}$ and $\mathbf{c}$ are vectors of constants. (39) corresponds to a multi-parametric linear program (mp-LP) which can be solved using algorithms already reported in the literature (*e.g.*, that of Gal and Nedoma, 1972 outlined in Appendix A) to give: (i) a set of expressions for $\mathbf{v}$, and hence for ψ, which are linear in $\boldsymbol{\theta}$; and (ii) a corresponding set of regions, defined by linear inequalities in $\boldsymbol{\theta}$, in which these solutions are optimal. The principal advantage of such an approach is that by solving a single mp-LP, the objective function ψ can be evaluated for different realisations of $\boldsymbol{\theta}$ through simple function evaluations rather than by having to solve a large number of LPs.

Now consider the LPs (28) in Step 2(i) of Algorithm 1. By defining a new set of variables, $\hat{Z}_j = Z_j + \bar{Z}$, $j = 1, \ldots, r$, where $\bar{Z} \geq 4$, and re-arranging, (28) can be written as:

$$\begin{aligned} & \psi\left(\hat{Z}_{l(l=1,\ldots,j-1)}^{q_1 \ldots q_{j-1}}\right) = \max\left(\hat{Z}_j^{\max q_1 \ldots q_{j-1}} - \hat{Z}_j^{\min q_1 \ldots q_{j-1}}\right), \\ \text{s.t.} \quad & -\delta_{ij}\hat{Z}_j^{\max q_1 \ldots q_{j-1}} - \sum_{k=j+1}^{r} \delta_{ik}\hat{Z}_k^{a,j,q_1 \ldots q_{j-1}} \leq -\frac{\alpha_i}{\sigma_i} - \bar{Z}\sum_{j=1}^{r}\delta_{ij} + \kappa_i \\ & \qquad + \sum_{l=1}^{j-1}\delta_{il}\hat{Z}_l^{q_1 \ldots q_{j-1}}, \quad i = 1, \ldots, p, \\ & \delta_{ij}\hat{Z}_j^{\max q_1 \ldots q_{j-1}} + \sum_{k=j+1}^{r} \delta_{ik}\hat{Z}_k^{a,jq_1 \ldots q_{j-1}} \leq \frac{\beta_i}{\sigma_i} + \bar{Z}\sum_{j=1}^{r}\delta_{ij} - \kappa_i \\ & \qquad - \sum_{l=1}^{j-1}\delta_{il}\hat{Z}_l^{q_1 \ldots q_{j-1}}, \quad i = 1, \ldots, p, \\ & -\delta_{ij}\hat{Z}_j^{\min q_1 \ldots q_{j-1}} - \sum_{k=j+1}^{r} \delta_{ik}\hat{Z}_k^{b,j,q_1 \ldots q_{j-1}} \leq -\frac{\alpha_i}{\sigma_i} - \bar{Z}\sum_{j=1}^{r}\delta_{ij} + \kappa_i \\ & \qquad + \sum_{l=1}^{j-1}\delta_{il}\hat{Z}_l^{q_1 \ldots q_{j-1}}, \quad i = 1, \ldots, p, \\ & \delta_{ij}\hat{Z}_j^{\min q_1 \ldots q_{j-1}} + \sum_{k=j+1}^{r} \delta_{ik}\hat{Z}_k^{b,j,q_1 \ldots q_{j-1}} \leq \frac{\beta_i}{\sigma_i} + \bar{Z}\sum_{j=1}^{r}\delta_{ij} - \kappa_i \\ & \qquad - \sum_{l=1}^{j-1}\delta_{il}\hat{Z}_l^{q_1 \ldots q_{j-1}}, \quad i = 1, \ldots, p, \end{aligned} \tag{40}$$

$$\overline{Z} - 4 \leq \hat{Z}_j^{\min q_1 \ldots q_{j-1}} \leq \hat{Z}_j^{\max q_1 \ldots q_{j-1}} \leq \overline{Z} + 4,$$
$$\overline{Z} - 4 \leq \hat{Z}_k^{a,j,q_1 \ldots q_{j-1}}, \hat{Z}_k^{b,j,q_1 \ldots q_{j-1}} \leq \overline{Z} + 4, \quad k = j+1, \ldots, r,$$
$$\overline{Z} - 4 \leq \hat{Z}_l^{q_1 \ldots q_{j-1}}, \overline{Z} + 4, \quad l = 1, \ldots, j-1.$$

(40) is now in exactly the same form as (39), where

$$\mathbf{v} = \left[\hat{Z}_j^{\max q_1 \ldots q_{j-1}}, \hat{Z}_j^{\min q_1 \ldots q_{j-1}}, \hat{Z}_{k(k=j+1,\ldots,r)}^{a,j,q_1 \ldots q_{j-1}}, \hat{Z}_{k(k=j+1,\ldots,r)}^{b,j,q_1 \ldots q_{j-1}}\right]^T; \tag{41}$$

$$\boldsymbol{\theta} = \left[\hat{Z}_{l(l=1,\ldots,j-1)}^{q_1 \ldots q_{j-1}}\right]^T; \tag{42}$$

$$\mathbf{A} = \begin{bmatrix}
-\delta_{1j} & 0 & -\delta_{1k(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
\vdots & \vdots & \vdots & \vdots \\
-\delta_{pj} & 0 & -\delta_{pk(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
\delta_{1j} & 0 & \delta_{1k(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
\vdots & \vdots & \vdots & \vdots \\
\delta_{pj} & 0 & \delta_{pk(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
0 & -\delta_{1j} & 0_{(k=j+1,\ldots,r)} & -\delta_{1k(k=j+1,\ldots,r)} \\
\vdots & \vdots & \vdots & \vdots \\
0 & -\delta_{pj} & 0_{(k=j+1,\ldots,r)} & -\delta_{pk(k=j+1,\ldots,r)} \\
0 & \delta_{1j} & 0_{(k=j+1,\ldots,r)} & \delta_{1k(k=j+1,\ldots,r)} \\
\vdots & \vdots & \vdots & \vdots \\
0 & \delta_{pj} & 0_{(k=j+1,\ldots,r)} & \delta_{pk(k=j+1,\ldots,r)} \\
0 & -1 & 0_{(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
-1 & 1 & 0_{(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
1 & 0 & 0_{(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
 & & (r-j-1) \text{ rows of :} & \\
0 & 0 & -1_{(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
 & & (r-j-1) \text{ rows of :} & \\
0 & 0 & 1_{(k=j+1,\ldots,r)} & 0_{(k=j+1,\ldots,r)} \\
 & & (r-j-1) \text{ rows of :} & \\
0 & 0 & 0_{(k=j+1,\ldots,r)} & -1_{(k=j+1,\ldots,r)} \\
 & & (r-j-1) \text{ rows of :} & \\
0 & 0 & 0_{(k=j+1,\ldots,r)} & 1_{(k=j+1,\ldots,r)}
\end{bmatrix}; \tag{43}$$

$$\mathbf{F} = \begin{bmatrix} \delta_{1l(l=1,\ldots,j-1)} \\ \vdots \\ \delta_{pl(l=1,\ldots,j-1)} \\ -\delta_{1l(l=1,\ldots,j-1)} \\ \vdots \\ -\delta_{pl(l=1,\ldots,j-1)} \\ \delta_{1l(l=1,\ldots,j-1)} \\ \vdots \\ \delta_{pl(l=1,\ldots,j-1)} \\ -\delta_{1l(l=1,\ldots,j-1)} \\ \vdots \\ -\delta_{pl(l=1,\ldots,j-1)} \\ 4r-4j-1 \text{ rows of } 0_{(l=1,\ldots,j-1)} \end{bmatrix}; \tag{44}$$

$$\mathbf{b} = \begin{bmatrix} -\frac{\alpha_1}{\sigma_1} - \bar{Z}\sum_{j=1}^{r}\delta_{1j} + \kappa_1 \\ \vdots \\ -\frac{\alpha_p}{\sigma_p} - \bar{Z}\sum_{j=1}^{r}\delta_{pj} + \kappa_p \\ \frac{\beta_1}{\sigma_1} + \bar{Z}\sum_{j=1}^{r}\delta_{1j} - \kappa_1 \\ \vdots \\ \frac{\beta_p}{\sigma_p} + \bar{Z}\sum_{j=1}^{r}\delta_{pj} - \kappa_p \\ -\frac{\alpha_1}{\sigma_1} - \bar{Z}\sum_{j=1}^{r}\delta_{1j} + \kappa_1 \\ \vdots \\ -\frac{\alpha_p}{\sigma_p} - \bar{Z}\sum_{j=1}^{r}\delta_{pj} + \kappa_p \\ \frac{\beta_1}{\sigma_1} + \bar{Z}\sum_{j=1}^{r}\delta_{1j} - \kappa_1 \\ \vdots \\ \frac{\beta_p}{\sigma_p} + \bar{Z}\sum_{j=1}^{r}\delta_{pj} - \kappa_p \\ -\bar{Z}+4 \\ 0 \\ \bar{Z}+4 \\ r-j-1 \text{ rows of } -\bar{Z}+4 \\ r-j-1 \text{ rows of } \bar{Z}+4 \\ r-j-1 \text{ rows of } -\bar{Z}+4 \\ r-j-1 \text{ rows of } \bar{Z}+4 \end{bmatrix}; \tag{45}$$

$$\mathbf{c}^T = [1,\ -1,\ 2(r-j-1) \text{ elements of } 0]. \tag{46}$$

This means that (40) can be solved as an mp-LP to give a set of linear expressions and associated regions of optimality for $\hat{Z}_j^{\max q_1 \ldots q_{j-1}}$ and $\hat{Z}_j^{\min q_1 \ldots q_{j-1}}$ in terms of $\hat{Z}_{l(l=1,\ldots,j-1)}^{q_1 \ldots q_{j-1}}$. Thus, once (26) has been solved as an LP to give values for $Z_1^{\max}$ and $Z_1^{\min}$, (40) can be solved as an mp-LP for $j = 2$ to give $\hat{Z}_2^{\max q_1}$ and $\hat{Z}_2^{\min q_1}$, and hence $Z_2^{\max q_1}$ and $Z_2^{\min q_1}$ in terms of $Z_1^{q_1}$; then it can be solved again for $j = 3$ to give $Z_3^{\max q_1 q_2}$ and $Z_3^{\min q_1 q_2}$ in terms of $Z_1^{q_1}$ and $Z_2^{q_1 q_2}$; and so on, and so forth. The quadrature points $Z_1^{q_1}$ can be calculated from the values of $Z_1^{\max}$ and $Z_1^{\min}$; these can be substituted into the expressions for $Z_2^{\max q_1}$ and $Z_2^{\min q_1}$; the quadrature points $Z_2^{\min q_1 q_2}$ can then be calculated; these can be substituted together with $Z_1^{q_1}$ to give the values of $Z_3^{\max q_1 q_2}$ and $Z_3^{\min q_1 q_2}$; and so on.

4.2. Algorithm 2

The steps of a multi-parametric linear programming-based algorithm for the computation of an SMVN probability such as (4) can now be summarised as follows:

Step 1 As in Algorithm 1.

Step 2 Solve the LP (26) to give the values of $Z_1^{\max}$ and $Z_1^{\min}$.

Step 3 For $j = 2$ to r:

(i) Formulate the mp-LP (40) using $\hat{Z} = Z + \bar{Z}$ ($\bar{Z} \geq 4$) for all the variables;

(ii) Solve the mp-LP (40), using the algorithm of Gal and Nedoma (1972) outlined in Appendix A, to obtain a set of linear expressions and associated regions of optimality for $\hat{Z}_j^{\max q_1 \ldots q_{j-1}}$ and $\hat{Z}_j^{\min q_1 \ldots q_{j-1}}$ in terms of $\hat{Z}_{l(l=1,\ldots,j-1)}^{q_1 \ldots q_{j-1}}$;

(iii) Substitute $\hat{Z} = Z + \bar{Z}$ back into the expressions and regions of optimality obtained in Step 3(i). This will give a new set of linear expressions and associated regions of optimality for $Z_j^{\max q_1 \ldots q_{j-1}}$ and $Z_j^{\min q_1 \ldots q_{j-1}}$ in terms of $Z_{l(l=1,\ldots,j-1)}^{q_1 \ldots q_{j-1}}$.

Step 4

(i) For $j = 1$ to r, successively determine the quadrature points, $Z_j^{q_1 \ldots q_j}$, using (29) and the results from Steps 2 and 3.

(ii) As in Step 3 of Algorithm 1.

4.3. Remarks on Algorithm 2

The benefit of this algorithm is that instead of having to solve $\sum_{j=1}^{r} Q^{j-1}$ LPs, as in Algorithm 1, here, one can solve a *much* smaller number of optimization sub-problems (1 LP and $(r-1)$ mp-LPs). Furthermore, in contrast to Algorithm 1, where the number of sub-problems increases *exponentially* with r, in Algorithm 2 the number of sub-problems (and associated computation time) only increases *linearly* with r, making it particularly amenable to the evaluation of SMVN probabilities in systems with large values of r. In addition to this, the information given by the solution of the mp-LPs in Algorithm 2 means that the desired integral (24) can be computed for different numbers of quadrature points by simply carrying out different series of function evaluations (Step 4). This contrasts with Algorithm 1 where one has to re-apply Steps 2 and 3 of the algorithm every time one wishes to evaluate the SMVN probability for a new number of quadrature points.

4.4. Example 1 Re-visited

Here, the heat exchanger network example studied earlier is used to demonstrate the application and advantages of Algorithm 2. All the steps of the algorithm were implemented in MATLAB^{TM}.

Step 1 See (32) to (37).

Step 2 Solving the LP (26) gives $Z_1^{\max} = 2.6665$ and $Z_1^{\min} = -3.9051$.

Step 3 Appendix B illustrates how the mp-LP algorithm of Gal and Nedoma (1972) works for $j=3$. Here, only the final expressions and regions of optimality (denoted by CR to indicate "critical regions" in parametric programming parlance) are given for $j=2$ and $j=3$.

For $-3.9051 \leq Z_1^{q_1} \leq -1.0762$:

$$Z_2^{\max q_1} = 4,$$
$$Z_2^{\min q_1} = -1.9119 Z_1^{q_1} - 3.4661.$$

For $-1.0762 \leq Z_1^{q_1} \leq 0.0985$:

$$Z_2^{\max q_1} = 4,$$
$$Z_2^{\min q_1} = -0.5389 Z_1^{q_1} - 1.9886.$$

For $0.0985 \leq Z_1^{q_1} \leq 0.1218$:

$$Z_2^{\max q_1} = 4,$$
$$Z_2^{\min q_1} = -0.2324 Z_1^{q_1} - 2.0188.$$

For $0.1218 \leq Z_1^{q_1} \leq 0.2174$:

$$Z_2^{\max q_1} = 4,$$
$$Z_2^{\min q_1} = 1.9364 Z_1^{q_1} - 2.2829.$$

For $0.2174 \leq Z_1^{q_1} \leq 2.6665$:

$$Z_2^{\max q_1} = 4,$$
$$Z_2^{\min q_1} = 2.3935 Z_1^{q_1} - 2.3823.$$

$$\begin{aligned} Z_3^{\max q_1 q_2} &= 4, \\ Z_3^{\min q_1 q_2} &= -4, \end{aligned} \tag{47}$$

$$CR = \begin{cases} Z_2^{q_1 q_2} \geq 1.9364 Z_1^{q_1} - 1.0349 \\ Z_2^{q_1 q_2} \geq 4.1846 Z_1^{q_1} - 2.7717 \\ Z_2^{q_1 q_2} \geq -1.9119 Z_1^{q_1} - 1.8534 \\ Z_2^{q_1 q_2} \leq 4. \end{cases}$$

$$\begin{aligned} Z_3^{\max q_1 q_2} &= -12.4128 Z_1^{q_1} + 6.4101 Z_2^{q_1 q_2} + 10.6339, \\ Z_3^{\min q_1 q_2} &= -4, \end{aligned} \tag{48}$$

$$CR = \begin{cases} Z_2^{q_1 q_2} \leq 1.9364 Z_1^{q_1} - 1.0349 \\ Z_2^{q_1 q_2} \geq 4.1846 Z_1^{q_1} - 2.7717 \\ Z_2^{q_1 q_2} \geq -1.9119 Z_1^{q_1} - 1.8534 \\ Z_2^{q_1 q_2} \geq -1.1119 Z_1^{q_1} - 1.9116. \end{cases}$$

$$\begin{aligned} Z_3^{\max q_1 q_2} &= 4, \\ Z_3^{\min q_1 q_2} &= -9.4836 Z_1^{q_1} - 4.9604 Z_2^{q_1 q_2} - 13.1933, \end{aligned} \tag{49}$$

$$CR = \begin{cases} Z_2^{q_1q_2} \geq 1.9364Z_1^{q_1} - 1.0349 \\ Z_2^{q_1q_2} \leq -1.9119Z_1^{q_1} - 1.8534 \\ Z_2^{q_1q_2} \geq -0.2324Z_1^{q_1} - 1.6587. \end{cases}$$

$$\begin{aligned} Z_3^{\max q_1q_2} &= 4, \\ Z_3^{\min q_1q_2} &= 6.8458Z_1^{q_1} - 1.6360Z_2^{q_1q_2} - 8.5345, \end{aligned} \tag{50}$$

$$CR = \begin{cases} Z_2^{q_1q_2} \geq 1.9364Z_1^{q_1} - 1.0349 \\ Z_2^{q_1q_2} \leq 4.1846Z_1^{q_1} - 2.7717 \\ Z_2^{q_1q_2} \leq 4. \end{cases}$$

$$\begin{aligned} Z_3^{\max q_1q_2} &= -12.4128Z_1^{q_1} + 6.4101Z_2^{q_1q_2} + 10.6339, \\ Z_3^{\min q_1q_2} &= 6.8458Z_1^{q_1} - 1.6360Z_2^{q_1q_2} - 8.5345, \end{aligned}$$

$$CR = \begin{cases} Z_2^{q_1q_2} \leq 1.9364Z_1^{q_1} - 1.0349 \\ Z_2^{q_1q_2} \leq 4.1846Z_1^{q_1} - 2.7717 \\ Z_2^{q_1q_2} \geq 2.3935Z_1^{q_1} - 2.3823 \\ Z_2^{q_1q_2} \leq 4. \end{cases}$$

$$\begin{aligned} Z_3^{\max q_1q_2} &= 5.1632Z_1^{q_1} + 22.2172Z_2^{q_1q_2} + 40.8514, \\ Z_3^{\min q_1q_2} &= -4, \end{aligned}$$

$$CR = \begin{cases} Z_2^{q_1q_2} \geq 1.9364Z_1^{q_1} - 2.2829 \\ Z_2^{q_1q_2} \geq -1.9119Z_1^{q_1} - 1.8534 \\ Z_2^{q_1q_2} \leq -1.1119Z_1^{q_1} - 1.9116 \\ Z_2^{q_1q_2} \geq -0.2324Z_1^{q_1} - 2.0188. \end{cases}$$

$$\begin{aligned} Z_3^{\max q_1q_2} &= -12.4128Z_1^{q_1} + 6.4101Z_2^{q_1q_2} + 10.6339, \\ Z_3^{\min q_1q_2} &= -9.4836Z_1^{q_1} - 4.9604Z_2^{q_1q_2} - 13.1933, \end{aligned}$$

$$CR = \begin{cases} Z_2^{q_1q_2} \leq 1.9364Z_1^{q_1} - 1.0349 \\ Z_2^{q_1q_2} \leq -1.9119Z_1^{q_1} - 1.8534 \\ Z_2^{q_1q_2} \geq -1.1119Z_1^{q_1} - 1.9116. \end{cases}$$

$$\begin{aligned} Z_3^{\max q_1q_2} &= 5.1632Z_1^{q_1} + 22.2172Z_2^{q_1q_2} + 40.8514, \\ Z_3^{\min q_1q_2} &= -9.4836Z_1^{q_1} - 4.9604Z_2^{q_1q_2} - 13.1933, \end{aligned}$$

$$CR = \begin{cases} Z_2^{q_1 q_2} \leq -1.9119 Z_1^{q_1} - 1.8534 \\ Z_2^{q_1 q_2} \leq -1.1119 Z_1^{q_1} - 1.9116 \\ Z_2^{q_1 q_2} \geq 0.5389 Z_1^{q_1} - 1.9886. \end{cases}$$

Step 4 The results of the function evaluations using the expressions above are shown in Table V. As one would expect, the SMVN probabilities obtained are identical to those computed using Algorithm 1 (see Tab. I). Table V also compares the number of sub-problems that have to be solved using the two algorithms and the associated computation times. It can be seen that the computational savings given by the multi-parametric programming approach are very large. In order to generate the four probability values in the table using Algorithm 2 requires the solution of 1 LP and 2 mp-LPs, with a total CPU time of approximately 0.7 *s* (plus the time taken for function evaluations). This contrasts sharply with Algorithm 1, where a total of 5564 LPs must be solved, taking 32.4 *s* CPU.

Note that the computational benefits demonstrated above will become even greater for problems with larger values of r. Also, as with Algorithm 1, the speed of Algorithm 2 can be further improved through parallelisation since the LP in Step 2 of the algorithm and the $(r-1)$ mp-LPs in Step 3 are all independent of each other.

4.5. Extension for Calculating Percentage Points

The two-sided $100(1-a)$ percentage point, h_a^p, of the standardised p-variate normal distribution is defined by:

$$P\left[\bigcap_{i=1}^{p}(|X_j| \leq h_a^p)\right] = 1 - a, \tag{51}$$

TABLE V Comparison of Algorithms 1 and 2 for Example 1

		Number of sub-problems		*CPU(s)*	
Q_j, $j = 1,2,3$	*Prob*	*Algorithm* 1	*Algorithm* 2	*Algorithm* 1	*Algorithm* 2
8	0.6650	73 LPs	↑	0.4	↑
16	0.6621	273 LPs	1 LP+	1.5	approx.
32	0.6632	1057 LPs	2 mp-LPs	6.1	0.7
64	0.6632	4161 LPs	↓	24.4	↓

where $\mu_i = 0$, $i = 1, \ldots, p$ and $\sigma_{ij} = 1$, $i = 1, \ldots, p, j = 1, \ldots, p$, such that $\boldsymbol{\Sigma} = \mathbf{C}$, as defined in (7). Kwong and Iglewicz (1996) developed an approach for evaluating h_a^p but only for special, equicorrelated and product correlation singular structures of $\boldsymbol{\Sigma}$. Algorithm 2, however, can be elegantly extended for the determination of the two-sided percentage points when $\boldsymbol{\Sigma}$ has an arbitrary singular structure.

Consider problem (40) with $\alpha_i = \beta_i = h_a^p$, $i = 1, \ldots, p$. In this case, instead of fixing a value for h_a^p, it can be treated as another "uncertain" parameter which is added to the vector (42) and thus removed from (45). Step 2 of Algorithm 2 will then correspond to solving a single-parameter linear program (p-LP) in order to give a set of linear expressions and associated regions of optimality for $Z_1^{\max}$ and $Z_1^{\min}$ in terms of h_a^p. Similarly, the results of Step 3(ii) will be expressions for $Z_j^{\max\, q_1 \ldots q_{j-1}}$ and $Z_j^{\min\, q_1 \ldots q_{j-1}}$ in terms of $Z_{l(l=1,\ldots,j-1)}^{q_1 \ldots q_{j-1}}$ and h_a^p. The quadrature points, $Z_j^{q_1 \ldots q_{j-1}}$, in Step 4(i) will then depend on h_a^p also. Finally, in Step 4(ii), the value of a can be fixed and a set of non-linear equations solved to find the corresponding value of h_a^p.

4.5.1. Example 5

The approach described above does not rely on any assumption about the structure of $\boldsymbol{\Sigma}$. Nevertheless, we choose to illustrate its application for an example that has already been studied by Kwong and Iglewicz (1996). Consider the trivariate case with singular negative equicorrelated structure, where $\rho_{ij} = -1/2$, $i \neq j$, and $r = 2$. Applying the modified form of Algorithm 2 leads to the following expressions over the whole range $1.0 \leq h_a^3 \leq 3.5$:

$$1 - a = \frac{Z_1^{\max} - Z_1^{\min}}{2} \sum_{q_1=1}^{Q_1} w_1^{q_1} \frac{Z_2^{\max\, q_1} - Z_2^{\min\, q_1}}{2} \sum_{q_2=1}^{Q_2} w_2^{q_2} f(Z_1^{q_1}, Z_2^{q_1 q_2}), \quad (52)$$

$$f(Z_1^{q_1}, Z_2^{q_1 q_2}) = \frac{1}{2\pi} \exp\left\{ -\frac{1}{2}[(Z_1^{q_1})^2 + (Z_2^{q_1 q_2})^2] \right\}, \quad \forall q_1, q_2, \quad (53)$$

$$Z_1^{q_1} = \frac{1}{2}[Z_1^{\max}(1 + \nu_1^{q_1}) + Z_1^{\min}(1 - \nu_1^{q_1})], \quad \forall q_1, \quad (54)$$

$$Z_2^{q_1 q_2} = \frac{1}{2}[Z_2^{\max q_1}(1+\nu_2^{q_2}) + Z_2^{\min q_1}(1-\nu_2^{q_2})], \quad \forall q_1, q_2, \tag{55}$$

$$Z_1^{\max} = 1.0147 h_a^3, \tag{56}$$

$$Z_1^{\min} = -1.0147 h_a^3. \tag{57}$$

For $-4 \le Z_1^{q_1} \le -0.9846$:

$$Z_2^{\max q_1} = 1.1727 h_a^3 + 0.6126 Z_1^{q_1}, \tag{58}$$

$$Z_2^{\min q_1} = -38.4285 h_a^3 - 38.4155 Z_1^{q_1}. \tag{59}$$

For $-0.9846 \le Z_1^{q_1} \le -0.03005$:

$$Z_2^{\max q_1} = 1.1727 h_a^3 + 0.6126 Z_1^{q_1}, \tag{60}$$

$$Z_2^{\min q_1} = -1.1380 h_a^3 - 0.5432 Z_1^{q_1}. \tag{61}$$

For $-0.03005 \le Z_1^{q_1} \le 0.03005$:

$$Z_2^{\max q_1} = 1.1380 h_a^3 - 0.5432 Z_1^{q_1}, \tag{62}$$

$$Z_2^{\min q_1} = -1.1380 h_a^3 - 0.5432 Z_1^{q_1}. \tag{63}$$

For $0.03005 \le Z_1^{q_1} \le 0.9846$:

$$Z_2^{\max q_1} = 1.1380 h_a^3 - 0.5432 Z_1^{q_1}, \tag{64}$$

$$Z_2^{\min q_1} = -1.1727 h_a^3 + 0.6126 Z_1^{q_1}. \tag{65}$$

For $0.9846 \le Z_1^{q_1} \le 4$:

$$Z_2^{\max q_1} = 38.4285 h_a^3 - 38.4155 Z_1^{q_1}, \tag{66}$$

$$Z_2^{\min q_1} = -1.1727 h_a^3 + 0.6126 Z_1^{q_1}. \tag{67}$$

The set of Eqs. (52) to (67) can now be solved at different values of a to give h_a^3.

TABLE VI Two-sided percentage points for Example 5

a	h_a^3	a	h_a^3	a	h_a^3
0.50	1.1227	0.15	1.8615	0.05	2.3437
0.40	1.2914	0.10	2.0523	0.04	2.4303
0.35	1.3826	0.09	2.0991	0.03	2.5378
0.30	1.4811	0.08	2.1503	0.02	2.6823
0.25	1.5898	0.07	2.2069	0.01	2.9135
0.20	1.7137	0.06	2.2705	0.005	3.1284

This was carried out very efficiently using the software package *gPROMS* (Process Systems Enterprise Ltd., 1999). Table VI shows the results using 64-point Gauss-Legendre quadrature for many different values of a. Note that the values of h_a for $a = 0.25$, 0.1, 0.05, 0.01 and 0.005, which are the cases studied by Kwong and Iglewicz (1996), agree very closely with their results.

5. CONCLUDING REMARKS

This paper has demonstrated how principal components theory and techniques from mathematical programming can be used to overcome the previously unresolved problem of computing general, one- and two-sided probabilities for multivariate normal distributions with singular variance-covariance matrices of arbitrary structure. The performance of both the algorithms presented can be enhanced through the implementation of computer parallelisation strategies, as discussed in the paper, although Algorithm 2 would still appear to offer the better potential for solving very large problems since the number of sub-problems to be solved only increases linearly with the rank of the variance-covariance matrix. Ongoing research is aimed at developing efficient, automated software implementations of the algorithms to facilitate this.

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References

Acevedo, J. and Pistikopoulos, E. N. (1997) A multiparametric programming approach for linear process engineering problems under uncertainty. *Ind. Eng. Chem. Res.*, **36**, 717–728.

Bland, R. P. and Owen, D. B. (1966) A note on singular normal distributions. *Ann. Inst. Stat. Math.*, **18**(1), 113–116.

Brooke, A., Kendrick, D. and Meeraus, A. (1992) *GAMS Release 2.25: A User's Guide.* The Scientific Press.

Bunch, D. S., Gay, D. M. and Welsch, R. E. (1993) Algorithm 717: subroutines for maximum likelihood and quasi-likelihood estimation of parameters in nonlinear regression models. *ACM Trans. Math. Software*, **19**(1), 109–130.

Carnahan, B., Luther, H. A. and Wilkes, J. O. (1969) *Applied Numerical Methods.* pp. 101–105. John Wiley & Sons.

David, F. N. (1953) A note on the evaluation of the multivariate normal integral. *Biometrika*, **40**, 458–459.

Drezner, Z. (1992) Computation of the multivariate normal integral. *ACM Trans. Math. Software*, **18**(4), 470–480.

Engels, H. (1980) *Numerical Quadrature and Cubature.* pp. 321–322, Academic Press.

Evans, M. and Swartz, T. (1988) Monte carlo computation of some multivariate normal probabilities. *J. Statist. Comput. Simul.*, **30**, 117–128.

Gal, T. (1995) *Postoptimal Analyses, Parametric Programming, and Related Topics.* 2nd edn., de Gruyter.

Gal, T. and Nedoma, J. (1972) Multiparametric linear programming. *Management Science*, **18**, 406–422.

Genz, A. (1992) Numerical computation of multivariate normal probabilities. *J. Comput. Graph. Statist.*, **1**(1), 141–149.

Genz, A. and Kahaner, D. K. (1986) The numerical evaluation of certain multivariate normal integrals. *J. Comput. Applied Math.*, **16**(2), 255–258.

Gupta, S. S. (1963a) Bibliography on the multivariate normal integrals and related topics. *Ann. of Math. Statist.*, **34**, 829–838.

Gupta, S. S. (1963b) Probability integrals of multivariate normal and multivariate t^1. *Ann. of Math. Statist.*, **34**, 792–828.

Hillier, F. S. and Lieberman, G. J. (1986) *Introduction to Operations Research*, pp. 58–150, 305–307, 5th edn., McGraw-Hill.

Joe, H. (1995) Approximations to multivariate normal rectangle probabilities based on conditional expectations. *J. Amer. Stat. Assoc.*, **90**(431), 957–964.

Johnson, R. A. and Wichern, D. W. (1988) *Applied Multivariate Statistical Analysis.* p. 122, 2nd edn., Prentice-Hall International.

Kshirsagar, A. M. (1972) *Multivariate Analysis.* pp. 433–436. Marcel Dekker, Inc.

Kwong, K. S. (1995) Evaluation of one-sided percentage points of the singular multivariate normal distribution. *J. Statist. Comput. Simul.*, **51**, 121–135.

Kwong, K. S. (1998) On sample size and quick simultaneous confidence interval estimations for multinomial proportions. *J. Comput. Graph. Statist.*, **7**(2), 212–222.

Kwong, K. S. and Iglewicz, B. (1996) On singular multivariate normal distribution and its applications. *Comput. Statist. Data Analysis*, **22**, 271–285.

Lohr, S. L. (1993) Multivariate normal probabilities for star-shaped regions. *Applied Statistics*, **42**(3), 576–582.

Mardia, K. V., Kent, J. T. and Bibby, J. M. (1979) *Multivariate Analysis*. Academic Press.
Marsten, R., Saltzman, M., Lustig, J. and Shanno, D. (1990) Interior point methods for linear programming: Just Call Newton, Lagrange and Fiacco and McCormick. *Interfaces*, **20**(4), 105–116.
Milton, R. C. (1972) Computer evaluation of the multivariate normal integral. *Technometrics*, **14**(4), 881–889.
NAG (1998) *NAG Fortran Library Introductory Guide: Mark* 18.
Nelson, P. R. (1991) Numerical evaluation of multivariate normal integrals with correlations $\rho_{ij} = -\alpha_i\alpha_j$. In: *The Frontiers of Statistical Scientific Theory and Industrial Applications*. pp. 97–114. American Sciences Press, Inc.
Pistikopoulos, E. N. and Mazzuchi, T. A. (1990) A novel flexibility analysis approach for processes with stochastic parameters. *Comput. Chem. Eng.*, **14**(9), 991–1000.
Plackett, R. L. (1954) A reduction formula for multivariate normal integrals. *Biometrika*, **41**, 351–360.
Process, Systems Enterprise Ltd. (1999) *gPROMS Advanced User's Guide*. London.
Rudolfer, S. M. and Watson, P. C. (1993) Evaluation of orthant probabilities for singular bi- and trivariate normal distributions. *J. Statist. Comput. Simul.*, **48**, 219–232.
Schervish, M. J. (1984) Algorithm AS195: multivariate normal probabilities with error bound. *Applied Statistics*, **33**, 81–94.
Schervish, M. J. (1985) Corrections. Algorithm AS195: multivariate normal probabilities with error bound. *Applied Statistics*, **34**, 103–104.
Soong, W. C. and Hsu, J. C. (1997) Using complex integration to compute multivariate normal probabilities. *J. Comput. Graph. Statist.*, **6**(4), 397–415.
Straub, D. A. and Grossmann, I. E. (1993) Design optimization of stochastic flexibility. *Comput. Chem. Eng.*, **17**(4), 339–354.
The Math Works, Inc. (1992) *MATLAB™ Reference Guide*.
Wang, Y. C. J. (1997) Multivariate Normal Integrals and Contingency Tables with Ordered Categories. *Psychometrika*, **62**(2), 267–284.

APPENDIX A: AN ALGORITHM FOR mp-LP PROBLEMS

An algorithm for the solution of non-degenerate mp-LPs is given by Gal and Nedoma (1972), and is fully described in Chapter 4 of Gal (1995), and summarised by Acevedo and Pistikopoulos (1997). Here, the fundamental steps of the algorithm are outlined and later illustrated with an example.

Phase 1: Finding an Initial Optimal Basis

1. Solve the LP (39) with θ as a variable in order to obtain a feasible point $(\mathbf{v}_1, \theta_1)$. If no feasible point is found, then the algorithm is terminated.
2. Fix $\theta = \theta_1$ and solve (39) as an LP using the Simplex algorithm. As part of the Simplex algorithm, slack variables are added to the

inequalities. This converts systems such as (39) into the following form:

$$\begin{aligned} \psi(\boldsymbol{\theta}) &= \min_{\tilde{\mathbf{v}}} \mathbf{c}^T \cdot \tilde{\mathbf{v}} \\ \text{s.t.} \quad \tilde{\mathbf{A}} \cdot \tilde{\mathbf{v}} &= \mathbf{b} + \mathbf{F} \cdot \boldsymbol{\theta}, \\ \boldsymbol{\theta}^L \le \boldsymbol{\theta} &\le \boldsymbol{\theta}^U, \\ \tilde{\mathbf{v}} &\ge \mathbf{0}, \end{aligned} \tag{68}$$

where the vector $\tilde{\mathbf{v}}$ now incorporates the original vector $\mathbf{v}$ and slack variables.

The Simplex tableau will give the optimal basis, $\mathbf{B}_1$, associated with the solution. This basis is formed from the columns of $\tilde{\mathbf{A}}$ and reflects which elements of $\tilde{\mathbf{v}}$ are non-zero at the optimal solution. For the region in $\boldsymbol{\theta}$-space that this basis is optimal:

$$\tilde{\mathbf{v}}^1(\boldsymbol{\theta}) = \mathbf{B}_1^{-1} \cdot (\mathbf{b} + \mathbf{F} \cdot \boldsymbol{\theta}), \tag{69}$$

and hence the associated objective function is $\psi^1(\boldsymbol{\theta}) = \mathbf{c}^T \cdot \tilde{\mathbf{v}}^1(\boldsymbol{\theta})$.

The region in which the basis is optimal, or "critical region", CR^1, is uniquely defined by the conditions $\tilde{\mathbf{v}}^1(\boldsymbol{\theta}) \ge \mathbf{0}$ and $\boldsymbol{\theta}^L \le \boldsymbol{\theta} \le \boldsymbol{\theta}^U$, *i.e.*, from:

$$-\mathbf{B}_1^{-1} \cdot \mathbf{F} \cdot \boldsymbol{\theta} \le \mathbf{B}_1^{-1} \cdot \mathbf{b}, \quad \text{and} \tag{70}$$

$$\boldsymbol{\theta}^L \le \boldsymbol{\theta} \le \boldsymbol{\theta}^U. \tag{71}$$

Note that some of the constraints in (70) and (71) may be redundant. These can be identified by adding a positive slack variable to each constraint and then minimising the value of each slack variable subject to the constraints in (70) and (71). If the minimum value of a slack variable is positive, then the associated constraint is strongly redundant and can be dropped from the definition of CR^1. Conversely, if the minimum value is zero, then the associated constraint is either binding or weakly redundant and is kept in the definition.

Phase 2: Finding All Other Optimal Bases

CR^1 is a closed, convex, polyhedral set, and each of the constraints in (70) and (71) defines a "face" of this region. Another optimal basis is

said to be a neighbour of $\mathbf{B}_1$ along its ith face if, and only if, the associated ith constraint from (70) and (71) is non-redundant *and* it is possible to pass from $\mathbf{B}_1$ to this other basis by one dual (pivot) step (and *vice versa*). For the latter condition to be possible, the corresponding ith row of the matrix $\mathbf{B}_1^{-1} \cdot \tilde{\mathbf{A}}$, which appears in the Simplex tableau from Phase 1, Step 2, must have at least one negative element. Phase 2 thus consists of identifying which non-redundant rows of $\mathbf{B}_1^{-1} \cdot \tilde{\mathbf{A}}$ have negative elements; pivoting; finding the next optimal basis, its associated objective function, region of optimality and neighbours; and then repeating until the whole $\boldsymbol{\theta}$-space, for which finite optimal solutions to (39) exist, has been covered.

APPENDIX B: ILLUSTRATION OF THE mp-LP ALGORITHM

Consider the mp-LP (40) for the heat exchanger network example for $j=3$ with $\bar{Z} = 10$ (see (38) also):

$$\psi(\hat{Z}_1^{q_1}, \hat{Z}_2^{q_1 q_2}) = \max\left(\hat{Z}_3^{\max q_1 q_2} - \hat{Z}_3^{\min q_1 q_2}\right),$$

$$\begin{aligned}
\text{s.t.}\quad 0.0438\hat{Z}_3^{\max q_1 q_2} &\le -9.7653 + 0.2261\hat{Z}_1^{q_1} + 0.9731\hat{Z}_2^{q_1 q_2},\\
-0.0930\hat{Z}_3^{\max q_1 q_2} &\le -13.1403 + 0.8823\hat{Z}_1^{q_1} + 0.4615\hat{Z}_2^{q_1 q_2},\\
0.0714\hat{Z}_3^{\max q_1 q_2} &\le 5.7590 - 0.8862\hat{Z}_1^{q_1} + 0.4577\hat{Z}_2^{q_1 q_2},\\
-0.1407\hat{Z}_3^{\max q_1 q_2} &\le 7.1221 - 0.9629\hat{Z}_1^{q_1} + 0.2301\hat{Z}_2^{q_1 q_2},\\
0.0438\hat{Z}_3^{\min q_1 q_2} &\le -9.7653 + 0.2261\hat{Z}_1^{q_1} + 0.9731\hat{Z}_2^{q_1 q_2},\\
-0.0930\hat{Z}_3^{\min q_1 q_2} &\le -13.1403 + 0.8823\hat{Z}_1^{q_1} + 0.4615\hat{Z}_2^{q_1 q_2},\\
0.0714\hat{Z}_3^{\min q_1 q_2} &\le 5.7590 - 0.8862\hat{Z}_1^{q_1} + 0.4577\hat{Z}_2^{q_1 q_2},\\
-0.1407\hat{Z}_3^{\min q_1 q_2} &\le 7.1221 - 0.9629\hat{Z}_1^{q_1} + 0.2301\hat{Z}_2^{q_1 q_2},\\
-\hat{Z}_3^{\min q_1 q_2} &\le -6,\\
-\hat{Z}_3^{\max q_1 q_2} + \hat{Z}_3^{\min q_1 q_2} &\le 0,\\
\hat{Z}_3^{\max q_1 q_2} &\le 14,\\
6 \le \hat{Z}_1^{q_1}, \hat{Z}_2^{q_1 q_2} &\le 14,\\
\hat{Z}_3^{\min q_1 q_2} &\ge 0.
\end{aligned} \tag{72}$$

Phase 1

1. Solving (72) as an LP gives an initial solution $\boldsymbol{\theta} = [9.7873, 8.5533]^T$, where $\boldsymbol{\theta} = \left[\hat{Z}_1^{q_1}, \hat{Z}_2^{q_1 q_2}\right]^T$.
2. With the addition to slack variables to each of the first eleven inequality constraints (denoted by s_i, $i = 1, \ldots, 11$), (72) can be written in the form of (68), where:

$$\tilde{\mathbf{v}} = \left[\hat{Z}_3^{\max q_1 q_2}, \hat{Z}_3^{\min q_1 q_2}, s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8, s_9, s_{10}, s_{11}\right]^T,$$

$$\tilde{\mathbf{A}} = \begin{bmatrix}
0.0438 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.0930 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.0714 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-0.1407 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.0438 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & -0.0930 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0.0714 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & -0.1407 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
-1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix},$$

$$\mathbf{b} = [-9.7653,\ -13.1403,\ 5.7590,\ 7.1221,\ -9.7653,\ -13.1403,\ 5.7590,\ 7.1221,\ -6,\ 0,\ 14]^T.$$

$$\mathbf{c}^T = [1, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0],$$

$$\mathbf{F} = \begin{bmatrix}
0.2261 & 0.9731 \\
0.8823 & 0.4615 \\
-0.8862 & 0.4577 \\
-0.9629 & 0.2301 \\
0.2261 & 0.9731 \\
0.8823 & 0.4615 \\
-0.8862 & 0.4577 \\
-0.9629 & 0.2301 \\
0 & 0 \\
0 & 0 \\
0 & 0
\end{bmatrix}.$$

Solving this at θ_1 using the Simplex algorithm shows that the optimal basic variables are $\{\hat{Z}_3^{\max q_1 q_2}, \hat{Z}_3^{\min q_1 q_2}, s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8, s_{10}\}$. The optimal basis $\mathbf{B}_1$ is thus formed from all except the 11th and 13th columns of $\mathbf{A}$. From (69), the following expressions are then obtained:

$$\tilde{\mathbf{v}}^1 = \begin{bmatrix} 14 \\ 6 \\ -10.3785 \\ -11.8378 \\ 4.7594 \\ 9.0914 \\ -10.0281 \\ -12.5821 \\ 5.3306 \\ 7.9661 \\ 8 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0.2261 \\ 0.8823 \\ -0.8862 \\ -0.9629 \\ 0.2261 \\ 0.8823 \\ -0.8862 \\ -0.9629 \\ 0 \end{bmatrix} \hat{Z}_1^{q_1} + \begin{bmatrix} 0 \\ 0 \\ 0.9731 \\ 0.4615 \\ 0.4577 \\ 0.2301 \\ 0.9731 \\ 0.4615 \\ 0.4577 \\ 0.2301 \\ 0 \end{bmatrix} \hat{Z}_2^{q_1 q_2}.$$

$Z_3^{\max q_1 q_2}$ and $Z_3^{\min q_1 q_2}$ are given by the first and second rows of the vector $\tilde{\mathbf{v}}^1$, while the region of optimality for $\mathbf{B}_1$ is defined by $\tilde{\mathbf{v}}^1 \geq 0$ and the lower and upper bounds on $\hat{Z}_1^{q_1}$ and $\hat{Z}_2^{q_1 q_2}$. After removal of the redundant constraints, the following solution is obtained:

$$Z_3^{\max q_1 q_2} = 14,$$
$$Z_3^{\min q_1 q_2} = 6,$$

$$CR^1 = \begin{cases} 4.7594 - 0.8862\hat{Z}_1^{q_1} + 0.4577\hat{Z}_2^{q_1 q_2} \geq 0 \\ -12.5821 + 0.8823\hat{Z}_1^{q_1} + 0.4615\hat{Z}_2^{q_1 q_2} \geq 0 \\ 7.9661 - 0.9629\hat{Z}_1^{q_1} + 0.2301\hat{Z}_2^{q_1 q_2} \geq 0 \\ Z_2^{q_1 q_2} \leq 14. \end{cases}$$

Substituting $\hat{Z} = Z + 10$ into the above and re-arranging, then gives (47).

Phase 2 Since the three non-redundant constraints describing CR^1 above come from the 5th, 8th and 10th rows of $\tilde{\mathbf{v}}^1$, only these rows need to be examined in the matrix $\mathbf{B}_1^{-1}\tilde{\mathbf{A}}$ for negative elements. All three of these rows have negative elements. The 5th row has a negative element of -0.0714 in its 13th column, thus indicating that s_3 is replaced by s_{11} in this neighbouring optimal basic solution. Repeating

the calculations from Phase 1, Step 2 for the new set of optimal basic variables leads to the solution (48). The 8th row has a negative element of -0.0930 in its 11th column, thus indicating that s_6 is replaced by s_9 in this neighbouring optimal basic solution. Repeating the calculations from Phase 1, Step 2 for this set of optimal basic variables leads to the solution (49). The 10th row of $\mathbf{B}_1^{-1}\tilde{\mathbf{A}}$ has a negative element of -0.1407 in its 11th column, indicating that another neighbouring optimal basic solution has s_8 replaced by s_9. This leads to the solution (50). Each of these three new solutions is then investigated in a similar manner for neighbours until all the optimal solutions have been found.