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SUM-CONSTRAINED LINEAR MODELS

P.M.C. DE BOER AND R. HARKEMA

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ERASMUS UNIVERSITY ROTTERDAM - P.O. BOX 1738 - 3000 DR ROTTERDAM - THE NETHERLANDS

UNDERSIZED SAMPLES AND MAXIMUM LIKELIHOOD ESTIMATION OF SUM-CONSTRAINED LINEAR MODELS

by

P.M.C. de Boer and R. Harkema*

Abstract

Maximum likelihood procedures for estimating sum-constrained models like demand systems, brand choice models and so on, break down or produce very unstable estimates when the number of categories is large as compared with the number of observations available. In empirical studies this difficulty is mostly resolved by postulating the contemporaneous covariance matrix of the dependent variables at time t to equal $\sigma^2(I_n - n^{-1}\iota_n\iota_n')$. In this paper we develop a maximum likelihood procedure based on a contemporaneous covariance matrix which allows that the variances per category may be different, while the number of observations required is substantially less than the number that would be required in the case of a completely unrestricted contemporaneous covariance matrix.

Contents

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1. INTRODUCTION

Sum-constrained models, i.e., models in which subsets of the dependent variables sum to a fixed number, occur in almost every field of applied econometric research. In demand analysis the amounts spent on the categories of consumer goods and services that are distinguished add up to total expenditure, in production theory the cost shares of the various factors of production add up to unity, in marketing analysis the probabilities that a specific brand will be chosen add up to unity, in international trade the flows of exports from a specific country to different destinations add up to total exports, and so on. Sum-constrained linear models may generally be represented by means of the following system of seemingly unrelated regression equations

(1.1) $$y_i = Z_i\beta_i + u_i \qquad i = 1, \ldots, n$$

where y_i denotes a T×1 vector of observations on the i-th dependent variable, Z_i denotes a $T \times k_i$ matrix of observations on a set of k_i explanatory variables which are specific for the i-th dependent variable, β_i is a $k_i \times 1$ vector of unknown parameters to be estimated, u_i is a T×1 vector of zero-mean disturbances and n, the number of categories that are distinguished, is supposed to be larger than 2. The adding-up restrictions imply that the vectors of dependent variables y_i add up to a vector of fixed numbers m. Hence

(1.2) $$\sum_{i=1}^{n} y_i = m$$

Summing (1.1) over i and taking expectations it follows that

(1.3) $$\sum_{i=1}^{n} u_i = 0$$

and

(1.4) $$\sum_{i=1}^{n} Z_i\beta_i = m$$

Evidently, (1.3) reflects the wellknown fact that the vectors of disturbances in sum-constrained linear models are linearly dependent. The restrictions (1.4) are usually accomodated by imposing linear constraints on the vectors of parameters β_i. To give but a few examples, in the Rotterdam model (see e.g. Theil (1975)) and in the simplified version of the Almost Ideal Demand System of Deaton and Muellbauer (1980), the vectors of parameters β_i add up to the unit vector, while in the Multiplicative Competitive Interaction Model of Nakanishi and Cooper (1974) the vectors of parameters β_i are supposed to be the same for all brands.

A major difficulty in estimating sum-constrained linear models is caused by the fact that the method of maximum likelihood is very demanding with respect to the number of observations that is required. Maximum likelihood procedures frequently break down or produce very unstable estimates because of lack of data even when only a moderate number of categories is considered. Laitinen (1978), for example, has shown that the minimum number of observations required for maximum likelihood estimation of the Rotterdam model equals 2n, n denoting the number of categories that is distinguished. In applied research this problem is usually resolved by imposing far-reaching restrictions on the contemporaneous covariance matrix of the disturbances. Denoting this matrix by Ω, McGuire et al. (1968), Solari (1971), Deaton (1975), and Deaton and Muellbauer (1980), for example, impose $\Omega = \sigma^2(I_n - n^{-1}\iota_n\iota_n')$. In developing his theory of rational random behavior Theil (1971, 1974, 1980) proposes to impose $\Omega = -\sigma^2 S$, where S denotes the matrix of Slutsky-coefficients. Both approaches have in common that, apart from a constant of proportionality, the structure of the contemporaneous covariance matrix is completely specified beforehand.

The purpose of the present paper is to introduce a more flexible specification of the contemporaneous covariance matrix which allows for n parameters to be estimated freely and possesses the attractive property that the number of observations that is required need not be larger than $\max_i\{k_i + 1\}$. For the case considered by Laitinen this means that the minimum number of observations required is only n+2 instead of 2n.

The plan of the paper is as follows. In Section 2 we introduce the specification of the contemporaneous covariance matrix and derive the corresponding maximum likelihood estimators and their asymptotic distribution. In Section 3 we elaborate on the estimation procedure for the covariance matrix and in Section 4 we summarize our findings and discuss some extensions.

2. MAXIMUM LIKELIHOOD ANALYSIS

We start by rewriting (1.1) according to

$$(2.1) \qquad y_i = X_i\beta + u_i \qquad i = 1, \ldots, n$$

where y_i and u_i are as before, X_i denotes a T×k matrix containing the columns of Z_i and $k-k_i$ zero columns and β is the k×1 vector of parameters that is obtained by writing the vectors β_i in stacked form. From (1.2)-(1.4) it follows that (2.1) is subject to the following constraints

$$(2.2) \qquad \sum_{i=1}^{n} y_i = m \qquad \sum_{i=1}^{n} X_i\beta = m \qquad \sum_{i=1}^{n} u_i = 0$$

As said before, the constraints $\Sigma_{i=1}^{n} X_i\beta = m$ are usually accomodated by imposing linear constraints on the vector of parameters β. Therefore we impose[1]

$$(2.3) \qquad R\beta = r$$

where R denotes a q×k matrix of full row rank and r represents a q×1 vector. Of course, (2.3) may also represent other linear constraints like those resulting from homogeneity and symmetry conditions in linear demand systems.

As regards the vectors of disturbances u_i, we assume that the vector $u' = [u_1' \ldots u_n']$ is distributed according to a nT-variate normal distribution with zero mean and variance-covariance matrix $[\Omega_n \otimes I_T]$, Ω_n being a positive semi-definite symmetric matrix of rank (n-1). More specifically, in the present paper Ω_n will be specified as follows

$$(2.4) \qquad \Omega_n = D_n - d^{-1}\delta_n\delta_n'$$

with

1. For expository reasons all restrictions that may exist with respect to the vector of parameters β have been collected in (2.3). From a computational viewpoint, however, it may be advantageous to eliminate all restrictions right away from the start.

$$D_n = \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & \ddots & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & d_n \end{bmatrix} \qquad \delta_n' = [d_1 \ldots d_n] \qquad d = \sum_{i=1}^{n} d_i$$

In scalar notation we may write (2.4) as

$$\omega_{ii} = \mathrm{var}(u_{it}) = d_i - \frac{d_i^2}{d} \qquad i = 1, \ldots, n$$

$$\omega_{ij} = \mathrm{cov}(u_{it}, u_{jt}) = -\frac{d_i d_j}{d} \qquad i,j = 1, \ldots, n;\ i \neq j$$

The specification (2.4) originally arose from a straightforward generalization of the specification $\Omega_n = \sigma^2(I_n - n^{-1}\iota_n\iota_n')$. Recently, however, Don (1983) has shown that for $d_i > 0$ ($i = 1, \ldots, n$) the specification (2.4) corresponds to the least informative error distribution in the sense of having maximum entropy within the class of all error distributions with finite variances. Unfortunately, the condition $d_i > 0$ ($i = 1, \ldots, n$) is unduly restrictive, because it implies that the variance of each category should be smaller than the sum of the variances of all remaining categories, as may be shown as follows.

For $d_i > 0$ ($i = 1, \ldots, n$) it holds good that $(\Sigma_{i\neq k} d_i)^2 > \Sigma_{i\neq k} d_i^2$.
Dividing both sides of this inequality by $-d^{-1}$ and adding $\Sigma_{i\neq k} d_i$ yields

$$\sum_{i\neq k} d_i - \frac{1}{d}\Big(\sum_{i\neq k} d_i\Big)^2 < \sum_{i\neq k}\Big(d_i - \frac{d_i^2}{d}\Big).$$

After substituting $\Sigma_{i\neq k} d_i = d - d_k$ one obtains

$$d - d_k - \frac{1}{d}(d - d_k)^2 < \sum_{i\neq k}\Big(d_i - \frac{d_i^2}{d}\Big) \text{ or } d_k - \frac{d_k^2}{d} < \sum_{i\neq k}\Big(d_i - \frac{d_i^2}{d}\Big).$$

From (2.4) one easily verifies that $\Omega_n \iota = 0$. As a consequence the density function of the vector u will be degenerate as it should be. Barten (1969), however, has shown that this problem may be handled by simply deleting one category. Choosing without any loss of generality the last one, we delete the last row and column of Ω_n. Denoting the resulting matrix by Ω_{n-1}, straightforward matrix calculation shows that

$$(2.5)\qquad \Omega_{n-1}^{-1} = \begin{bmatrix} d_1^{-1} + d_n^{-1} & d_n^{-1} & \cdots\cdots & d_n^{-1} \\ d_n^{-1} & d_2^{-1} + d_n^{-1} & & d_n^{-1} \\ \vdots & \vdots & & \vdots \\ d_n^{-1} & d_n^{-1} & \cdots\cdots d_{n-1}^{-1} & + d_n^{-1} \end{bmatrix}$$

In addition, it is shown in Appendix A that

$$(2.6)\qquad |\Omega_{n-1}| = d^{-1} \prod_{i=1}^{n} d_i$$

and that Ω_{n-1} will be positive-definite in the following two mutually exclusive and exhaustive cases: (i) all d_i's are positive and (ii) at most one d_i is negative with d being negative as well.

From our assumptions about the distribution of the vector u, it follows that the density function of the vectors $u_1 \ldots u_{n-1}$ may be written as

$$(2.7)\qquad \begin{aligned} f(u_1 \ldots u_{n-1}) &= (2\pi)^{-T(n-1)/2} |\Omega_{n-1} \otimes I_T|^{-\frac{1}{2}} \cdot \\ &\exp\{-\tfrac{1}{2}[u_1' \ldots u_{n-1}'][\Omega_{n-1} \otimes I_T]^{-1}[u_1' \ldots u_{n-1}']'\} \end{aligned}$$

On substituting (2.1), (2.5), and (2.6) and applying some rearrangements we obtain the following likelihood function

$$(2.8)\qquad \begin{aligned} \ell(y_1 \ldots y_{n-1}) &= (2\pi)^{-T(n-1)/2} [d^{-1} \prod_{i=1}^{n} d_i]^{-T/2} \cdot \\ &\exp\{-\tfrac{1}{2}[\sum_{i=1}^{n-1} d_i^{-1}(y_i - X_i\beta)'(y_i - X_i\beta) + d_n^{-1} \sum_{i=1}^{n-1} (y_i - X_i\beta)' \sum_{j=1}^{n-1} (y_j - X_j\beta)]\} \end{aligned}$$

From the restrictions (2.2) one easily verifies that the loglikelihood function may be written as

$$(2.9)\qquad \begin{aligned} \log \ell(y_1 \ldots y_{n-1}) &= -\frac{T(n-1)}{2} \log 2\pi - \frac{T}{2} \log[d^{-1} \prod_{i=1}^{n} d_i] + \\ &- \tfrac{1}{2} \sum_{i=1}^{n} [d_i^{-1}(y_i - X_i\beta)'(y_i - X_i\beta)] \end{aligned}$$

From (2.9) it is clear that the loglikelihood function and hence the resulting maximum-likelihood estimators are invariant with respect to the category that is deleted as it should be. In order to obtain the restricted maximum-likelihood estimators, we construct the Lagrangian function

(2.10)
$$V = -\frac{T(n-1)}{2}\log 2\pi - \frac{T}{2}\log\left[d^{-1}\prod_{i=1}^{n} d_i\right] + - \tfrac{1}{2}\sum_{i=1}^{n}\left[d_i^{-1}(y_i - X_i\beta)'(y_i - X_i\beta)\right] - \lambda'(R\beta - r)$$

where λ denotes a $q\times 1$ vector of Lagrangian multipliers. Differentiating V with respect to β, λ, and d_k and putting the results equal to zero, yields the following system of equations

(2.11)
$$\sum_{i=1}^{n}(\hat{d}_i^{-1}X_i'\,y_i) - \sum_{i=1}^{n}(\hat{d}_i^{-1}X_i'X_i)\hat{\beta} - R'\hat{\lambda} = 0$$

(2.12)
$$R\hat{\beta} - r = 0$$

(2.13)
$$-\frac{T}{2\hat{d}_i} + \frac{T}{2\hat{d}} + \frac{\hat{u}_i'\hat{u}_i}{2\hat{d}_i^2} = 0 \qquad i = 1, \ldots, n$$

where $\hat{u}_i = y_i - X_i\hat{\beta}$

Eliminating $\hat{\lambda}$ from (2.11) and rewriting (2.13), the restricted maximum-likelihood estimators may be obtained from the following system of equations

(2.14)
$$\hat{\beta} = \bar{\beta} - CR'(RCR')^{-1}(R\bar{\beta} - r)$$

(2.15)
$$\hat{d}_i - \frac{\hat{d}_i^2}{\hat{d}} = \frac{\hat{u}_i'\hat{u}_i}{T} \qquad i = 1, \ldots, n$$

where[2]

$$\bar{\beta} = \left[\sum_{i=1}^{n}\hat{d}_i^{-1}X_i'X_i\right]^{-1}\left[\sum_{i=1}^{n}\hat{d}_i^{-1}X_i'y_i\right] = \left[\sum_{i=1}^{n}X_i'X_i\right]^{-1}\left[\sum_{i=1}^{n}X_i'y_i\right]$$

and

2. Note that $\bar{\beta}$ is the estimator that is obtained by writing the ordinary least-squares estimators for each separate equation in stacked form.

$$C = [\sum_{i=1}^{n} \hat{d}_i^{-1} X_i' X_i]^{-1}$$

Evidently, (2.14)-(2.15) constitutes a system of highly nonlinear equations. Apart from two very specific cases which can only occur with probability zero, it is shown in Section 3, however, that, conditional upon $\hat{u}_i'\hat{u}_i$, solving (2.15) can be accomplished by means of a numerical search procedure for the unique real root of an equation in only one variable. The full system (2.14)-(2.15) may therefore be solved by applying the following iterative procedure:

(i) Choose initial values $\hat{d}_i^0$ for d_i, for example $\hat{d}_i^0 = 1$ $(i = 1,\ldots,n)$;

(ii) Calculate $\hat{\beta}^0$ according to (2.14) and $\hat{u}_i^0$ according to $\hat{u}_i^0 = y_i - X_i\hat{\beta}^0$;

(iii) Obtain first-round estimates $\hat{d}_i^1$ by solving (2.15) conditional upon $\hat{u}_i'\hat{u}_i = (\hat{u}_i^0)'\hat{u}_i^0$;

(iv) Calculate the first-round estimates $\hat{\beta}^1$ according to (2.14) and $\hat{u}_i^1$ according to $\hat{u}_i^1 = y_i - X_i\hat{\beta}^1$ and so forth, until convergence.

Under very mild conditions, Sargan (1964) and Oberhofer and Kmenta (1974) have proved that the above procedure actually converges to a solution of the system (2.14)-(2.15). In the two specific cases referred to above, (2.15) admits of no solution. Supposing without any loss of generality that $\hat{u}_n'\hat{u}_n \geq \hat{u}_i'\hat{u}_i$ $(i = 1, \ldots, n-1)$, this occurs when in stage (iii) of the procedure either $(\hat{u}_n'\hat{u}_n)^{\frac{1}{2}} = \Sigma_{i=1}^{n-1}(\hat{u}_i'\hat{u}_i)^{\frac{1}{2}}$ or $\hat{u}_n'\hat{u}_n = \Sigma_{i=1}^{n-1}\hat{u}_i'\hat{u}_i$. In Appendix C it is shown that in the former case the likelihood function is unbounded and so one has to resort to a less flexible specification of the contemporaneous covariance matrix than the one given in (2.4); in the latter case the likelihood function attains its maximum, conditional on $\hat{u}_i'\hat{u}_i$ $(i = 1, \ldots, n)$, for $\hat{d}_n$ approaching plus or minus infinity and $\hat{d}_i = T^{-1}\hat{u}_i'\hat{u}_i$ $(i = 1, \ldots, n-1)$. For $\hat{d}_n = \pm\infty$, however, the matrix C as specified below (2.15) is no longer defined and the expression for $\hat{\beta}$ in (2.14) should be replaced by the solution of (2.11) and (2.12) in the limiting case that $\hat{d}_n = \pm\infty$. Straightforward matrix calculation shows that in this case the following estimator for $\hat{\beta}$ obtains

(2.14a) $$\hat{\beta} = \bar{\beta}_a - C_a R_a' \begin{bmatrix} A & R_n \\ R_n' & 0 \end{bmatrix}^{-1} (R_a\bar{\beta}_a - r_a)$$

with

$$\bar{\beta}_a' = [\bar{\beta}_1' \ \ldots \ \bar{\beta}_{n-1}' \ \ 0_{k_n}]$$

$$C_a = \begin{bmatrix} \hat{d}_1(Z_1'Z_1)^{-1} & \cdots & 0 & 0 \\ \vdots & \ddots & & \vdots \\ 0 & \cdots & \hat{d}_{n-1}(Z_{n-1}'Z_{n-1})^{-1} & 0 \\ 0 & \cdots & 0 & I_{k_n} \end{bmatrix}$$

$$R_a = \begin{bmatrix} R_1 & \cdots\cdots & R_{n-1} & 0 \\ 0 & \cdots\cdots & 0 & I_{k_n} \end{bmatrix}$$

$$A = \sum_{i=1}^{n-1} \hat{d}_i R_i (Z_i' Z_i)^{-1} R_i'$$

and

$$r_a' = [r' \quad 0_{k_n}]$$

where R_i $(i = 1, \ldots, n)$ contains the columns of R that correspond to the i-th category.

Under suitable regularity conditions, it follows from standard arguments that $\hat{\beta}$ and $\hat{d}_i$ are consistent estimators for β and d_i and that $\sqrt{T}(\hat{\beta} - \beta)$ is asymptotically distributed according to a k-variate normal distribution with zero mean and variance-covariance matrix PQP where

$$\text{(2.16)} \quad \begin{aligned} P &= \operatorname*{plim}_{T\to\infty} T[C - CR'(RCR')^{-1}RC] \\ Q &= \operatorname*{plim}_{T\to\infty} T^{-1}[C^{-1} - \hat{d}^{-1} \sum_{i=1}^{n} \sum_{j=1}^{n} X_i' X_j] \end{aligned}$$

when $\hat{\beta}$ is given by (2.14), or

$$\text{(2.16a)} \quad \begin{aligned} P &= \operatorname*{plim}_{T\to\infty} T\left\{\begin{bmatrix} C_r & 0 \\ 0 & 0_{k_n} \end{bmatrix} - C_a R_a' \begin{bmatrix} A & R_n \\ R_n' & 0 \end{bmatrix}^{-1} R_a \begin{bmatrix} C_r & 0 \\ 0 & 0_{k_n} \end{bmatrix}\right\} \\ Q &= \operatorname*{plim}_{T\to\infty} T^{-1} \begin{bmatrix} C_r^{-1} & 0 \\ 0 & 0 \end{bmatrix} \end{aligned}$$

with

$$C_r = \begin{bmatrix} \hat{d}_1 (Z_1' Z_1)^{-1} & \cdots\cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots\cdots & \hat{d}_{n-1} (Z_{n-1}' Z_{n-1})^{-1} \end{bmatrix}$$

when the final-round estimate of $\hat{\beta}$ is given by (2.14a).

Finally, it should be noted that the assumption of normal disturbances is not crucial for establishing the above asymptotic results. Under appropriate conditions $\hat{\beta}$ and $\hat{d}_i$ may also be interpreted as quasi-maximum likelihood estimators without affecting these results.

3. ESTIMATING THE COVARIANCE MATRIX

In this section we elaborate on how to obtain the estimates $\hat{d}_i$ for the covariance parameters in stage (iii) of the iterative procedure as described in Section 2. Without any loss of generality we assume that $T^{-1}\hat{u}_n'\hat{u}_n \equiv \hat{\alpha}_n \geq T^{-1}\hat{u}_i'\hat{u}_i \equiv \hat{\alpha}_i$ $(i = 1, \ldots, n-1)$. From (2.9) it follows that, conditional on $\hat{\alpha}_i$, the estimates $\hat{d}_i$ are obtained by minimizing

$$(3.1) \qquad f(d_1 \ldots d_n) = \log\left(d^{-1} \prod_{i=1}^{n} d_i\right) + \sum_{i=1}^{n} d_i^{-1}\hat{\alpha}_i$$

In Appendix A it is shown that Ω_{n-1} will be positive-definite if and only if either all d_i's are positive or at most one d_i is negative with d being negative as well. Take any admissible vector $(d_1 \ldots d_n)$ with d_k $(k \neq n)$ being negative. As $\hat{\alpha}_n \geq \hat{\alpha}_i$ $(i = 1, \ldots, n-1)$ the value of f will certainly not increase when the values of d_k and d_n are interchanged. Therefore we can restrict the analysis to the set of vectors $S = S_1 \cup S_2$ with S_1 and S_2 being defined by

$$(3.2) \qquad \begin{aligned} S_1 &= \left\{(d_1 \ldots d_n) \in R^n \mid d_i > 0 \ \forall\ 1 \leq i \leq n\right\} \\ S_2 &= \left\{(d_1 \ldots d_n) \in R^n \mid d_i > 0 \ \forall\ 1 \leq i \leq n-1;\ d = \sum_{i=1}^{n} d_i < 0\right\} \end{aligned}$$

In Appendix B we prove that f has a unique stationary point in S_1 when $\hat{\alpha}_n < \Sigma_{i=1}^{n-1}\hat{\alpha}_i$ and no stationary points in S_1 when[3] $\Sigma_{i=1}^{n-1}\hat{\alpha}_i \leq \hat{\alpha}_n \leq \left(\Sigma_{i=1}^{n-1}\hat{\alpha}_i^{\frac{1}{2}}\right)^2$, while f has a unique stationary point in S_2 when $\Sigma_{i=1}^{n-1}\hat{\alpha}_i < \hat{\alpha}_n < \left(\Sigma_{i=1}^{n-1}\hat{\alpha}_i^{\frac{1}{2}}\right)^2$ and no stationary points in S_2 when $\hat{\alpha}_n \leq \Sigma_{i=1}^{n-1}\hat{\alpha}_i$ or $\hat{\alpha}_n = \left(\Sigma_{i=1}^{n-1}\hat{\alpha}_i^{\frac{1}{2}}\right)^2$. The infimum of f with respect to S may now be found by means of the following theorem which is proved in Appendix C.

3. As shown in Appendix B, $\hat{\alpha}_n$ can not become larger than $\left(\Sigma_{i=1}^{n-1}\hat{\alpha}_i^{\frac{1}{2}}\right)^2$ because of the adding-up restriction on the vectors $\hat{u}_i$ $(i = 1, \ldots, n)$.

THEOREM 1: Let f be as defined in (3.1) and S_1 and S_2 as defined in (3.2). Then we have:

A.

$$\inf_{x \in S_1} f(x) = \begin{cases} f(x^0) & \text{if } \hat{\alpha}_n < \sum_{i=1}^{n-1} \hat{\alpha}_i \\ \sum_{i=1}^{n-1} \log \hat{\alpha}_i + n-1 = \lim_{d_n \to \infty} f(\hat{\alpha}_1, \ldots, \hat{\alpha}_{n-1}, d_n) & \text{if } \sum_{i=1}^{n-1} \hat{\alpha}_i \le \hat{\alpha}_n \le \left(\sum_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}}\right)^2 \end{cases}$$

where x^0 denotes the unique stationary point of f in S_1 when $\hat{\alpha}_n < \Sigma_{i=1}^{n-1} \hat{\alpha}_i$.

B

$$\inf_{x \in S_2} f(x) = \begin{cases} \sum_{i=1}^{n-1} \log \hat{\alpha}_i + n-1 = \lim_{d_n \to -\infty} f(\hat{\alpha}_1, \ldots, \hat{\alpha}_{n-1}, d_n) & \text{if } \hat{\alpha}_n \le \sum_{i=1}^{n-1} \hat{\alpha}_i \\ f(x^1) & \text{if } \sum_{i=1}^{n-1} \hat{\alpha}_i < \hat{\alpha}_n < \left(\sum_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}}\right)^2 \\ -\infty = \lim_{\lambda \downarrow 0} f\left(\lambda \hat{\alpha}_1^{\frac{1}{2}}, \ldots, \lambda \hat{\alpha}_{n-1}^{\frac{1}{2}}, -\lambda \sum_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}} - \lambda^2\right) & \text{if } \hat{\alpha}_n = \left(\sum_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}}\right)^2 \end{cases}$$

where x^1 denotes the unique stationary point of f in S_2 when $\Sigma_{i=1}^{n-1} \hat{\alpha}_i < \hat{\alpha}_n < (\Sigma_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}})^2$.

From Theorem 1 it follows that four cases should be distinguished, <u>viz</u>., $\hat{\alpha}_n < \Sigma_{i=1}^{n-1} \hat{\alpha}_i$, $\hat{\alpha}_n = \Sigma_{i=1}^{n-1} \hat{\alpha}_i$, $\Sigma_{i=1}^{n-1} \hat{\alpha}_i < \hat{\alpha}_n < (\Sigma_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}})^2$, and $\hat{\alpha}_n = (\Sigma_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}})^2$. In Appendix B, however, where it is shown that the stationary points may be found by means of a numerical search procedure for the unique real root of an equation in only one variable, it appears that the case $\hat{\alpha}_n < \Sigma_{i=1}^{n-1} \hat{\alpha}_i$ should be subdivided once more into three different cases. So we have to distinguish six cases, which are mutually exclusive and exhaustive. Five of them yield a unique solution, while in one case f becomes unbounded.

Below, we summarize all cases. First, we define

$$(3.3) \qquad f_1(d) = \sum_{i=1}^{n} \left(1 - \frac{4\hat{\alpha}_i}{d}\right)^{\frac{1}{2}} - (n-2) \qquad \text{for } d \ge 4\hat{\alpha}_n$$

$$(3.4) \qquad f_2(d) = \sum_{i=1}^{n-1} \left(1 - \frac{4\hat{\alpha}_i}{d}\right)^{\frac{1}{2}} - \left(1 - \frac{4\hat{\alpha}_n}{d}\right)^{\frac{1}{2}} - (n-2) \quad \text{for } d \ge 4\hat{\alpha}_n \text{ or } d < 0$$

and

$$(3.5) \qquad \hat{\gamma} = f_1(4\hat{\alpha}_n) = f_2(4\hat{\alpha}_n) = \sum_{i=1}^{n-1} \left(1 - \frac{\hat{\alpha}_i}{\hat{\alpha}_n}\right)^{\frac{1}{2}} - (n-2).$$

Then, we have

<u>Case 1</u>: $\hat{\alpha}_n < \sum_{i=1}^{n-1} \hat{\alpha}_i$ and $\hat{\gamma} < 0$

We have to solve on $(4\hat{\alpha}_n, \infty)$

$$f_1(\hat{d}) = 0$$

In Appendix B it is shown that the graph of $f_1(d)$ looks as follows

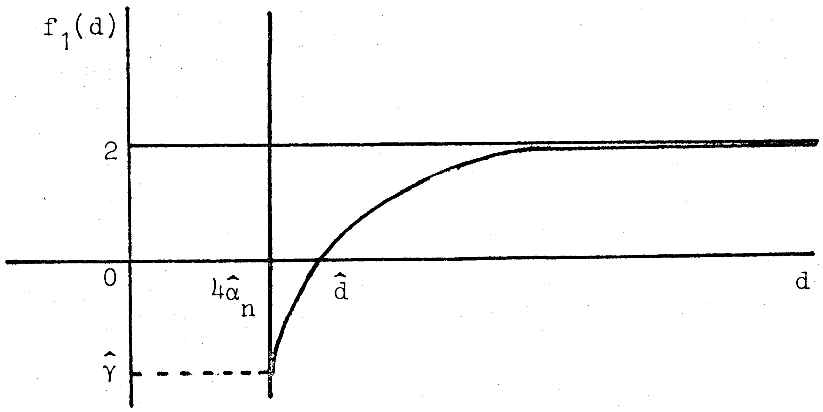

Figure 1

The solution $\hat{d}$ has to be substituted into

$$\hat{d}_i = \frac{\hat{d}}{2} - \frac{\hat{d}}{2}\left(1 - \frac{4\hat{\alpha}_i}{\hat{d}}\right)^{\frac{1}{2}} \qquad i = 1, \ldots, n$$

in order to obtain the solution in terms of the covariance parameters $\hat{d}_i$, which are all positive.

Case 2: $\hat{\alpha}_n < \sum_{i=1}^{n-1} \hat{\alpha}_i$ and $\hat{\gamma} > 0$

We have to solve on $(4\hat{\alpha}_n, \infty)$

$$f_2(\hat{d}) = 0$$

Graphically, the shape of the function $f_2(d)$ looks as follows

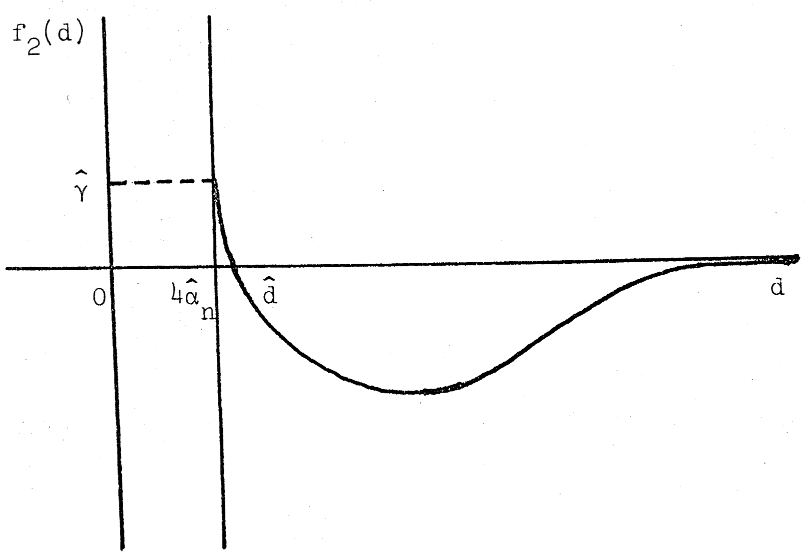

Figure 2

The solution $\hat{d}$ should be substituted into

$$\hat{d}_i = \frac{\hat{d}}{2} - \frac{\hat{d}}{2}\left(1 - \frac{4\hat{\alpha}_i}{\hat{d}}\right)^{\frac{1}{2}} \qquad i = 1, \ldots, n-1$$

$$\hat{d}_n = \frac{\hat{d}}{2} + \frac{\hat{d}}{2}\left(1 - \frac{4\hat{\alpha}_n}{\hat{d}}\right)^{\frac{1}{2}}$$

in order to find the solution in terms of the parameters $\hat{d}_i$, which are all positive again.

Case 3: $\hat{\alpha}_n < \sum_{i=1}^{n-1} \hat{\alpha}_i$ and $\hat{\gamma} = 0$

In this case the solution is

$$\hat{d} = 4\hat{\alpha}_n$$

$$\hat{d}_i = \frac{\hat{d}}{2} - \frac{\hat{d}}{2}\left(1 - \frac{4\hat{\alpha}_i}{\hat{d}}\right)^{\frac{1}{2}} \qquad i = 1, \ldots, n-1$$

$$\hat{d}_n = \frac{\hat{d}}{2}$$

Evidently, this is a border case to Cases 1 and 2 with all $\hat{d}_i$ being positive once again.

Case 4: $\sum_{i=1}^{n-1} \hat{\alpha}_i < \hat{\alpha}_n < \left(\sum_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}}\right)^2$

We have to solve on $(-\infty, 0)$

$$f_2(\hat{d}) = 0$$

In this case the graph of the function $f_2(d)$ looks as follows

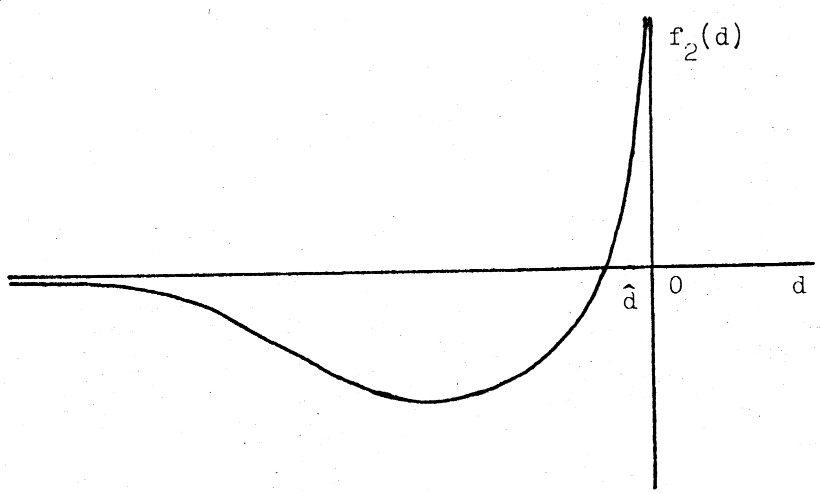

Figure 3

The solution $\hat{d}$ should be substituted into

$$\hat{d}_i = \frac{\hat{d}}{2} - \frac{\hat{d}}{2}\left(1 - \frac{4\hat{\alpha}_i}{\hat{d}}\right)^{\frac{1}{2}} \qquad i = 1, \ldots, n-1$$

$$\hat{d}_n = \frac{\hat{d}}{2} + \frac{\hat{d}}{2}\left(1 - \frac{4\hat{\alpha}_n}{\hat{d}}\right)^{\frac{1}{2}}$$

in order to obtain the solution in terms of the parameters $\hat{d}_i$. Obviously, $\hat{d}_i$ ($i = 1, \ldots, n-1$) is positive, $\hat{d}_n$ is negative, with $\hat{d}$ being negative as well.

Case 5: $\hat{\alpha}_n = \sum_{i=1}^{n-1} \hat{\alpha}_i$

In this case, which can only occur with probability zero, the estimates of the variances are such that the largest one is equal to the sum of the remaining ones. The solution is given by

$$\hat{d}_i = \hat{\alpha}_i \qquad i = 1, \ldots, n-1$$

$$\hat{d}_n = \pm\infty$$

and leads to the following estimates for the elements of the covariance matrix Ω_n

$$\lim_{\hat{d}_n \to \pm\infty} \left(\hat{d}_i - \frac{\hat{d}_i^2}{\hat{d}}\right) = \hat{\alpha}_i \qquad i = 1, \ldots, n-1$$

$$\lim_{\hat{d}_n \to \pm\infty} - \frac{\hat{d}_i \hat{d}_j}{\hat{d}} = 0 \qquad i,j = 1, \ldots, n-1;\ i \neq j$$

$$\lim_{\hat{d}_n \to \pm\infty} - \frac{\hat{d}_i \hat{d}_n}{\hat{d}} = -\hat{\alpha}_i \qquad i = 1, \ldots, n-1$$

$$\lim_{\hat{d}_n \to \pm\infty} \left(\hat{d}_n - \frac{\hat{d}_n^2}{\hat{d}}\right) = \lim_{\hat{d}_n \to \pm\infty} \frac{\hat{d}_n}{\hat{d}} \sum_{i=1}^{n-1} \hat{d}_i = \sum_{i=1}^{n-1} \hat{\alpha}_i = \hat{\alpha}_n$$

Hence, in this specific case, the estimate of the covariance matrix becomes as follows

$$\hat{\Omega}_n = \begin{bmatrix} \hat{\alpha}_1 & \cdots & 0 & -\hat{\alpha}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \hat{\alpha}_{n-1} & -\hat{\alpha}_{n-1} \\ -\hat{\alpha}_1 & \cdots & -\hat{\alpha}_{n-1} & \hat{\alpha}_n \end{bmatrix}$$

<u>Case 6:</u> $\hat{\alpha}_n = \left(\sum_{i=1}^{n-1} \hat{\alpha}_i^{\frac{1}{2}} \right)^2$

In this case, which once again can only occur with probability zero, the estimates of the variances are such that the largest standard deviation is equal to the sum of the remaining ones. It follows from Theorem 1 that f is unbounded and so one has to resort to a less flexible specification of the contemporaneous covariance matrix like, for example, the specification $\Omega_n = \sigma^2(I_n - n^{-1}\iota_n\iota_n')$.

4. CONCLUSION

In the present paper a new specification is introduced for the contemporaneous covariance matrix of the error structure of sum-constrained linear models. In applied research one usually specifies this covariance matrix either to be restricted only by logical constraints or to be equal to $\sigma^2(I_n - n^{-1}\iota_n\iota_n')$, n denoting the number of categories. The former specification is the most flexible one but suffers from the drawback that it is very demanding with respect to the number of observations when the number of categories is large. The latter specification is the most rigid one that can be thought of but requires only a small number of observations even when the number of categories is large. The specification that we propose is intermediate in the sense that it allows for n covariance parameters to be estimated freely, while it possesses the attractive property of not requiring too many observations. Apart from one very specific case, which gives rise to a likelihood function that is unbounded, the estimates involved may be obtained by a simple iterative scheme. In each stage of this scheme one numerical search procedure has to be carried out in order to determine the unique real root of an equation in only one variable. Therefore, it may be expected that the costs associated with the newly proposed estimation procedure will not be much higher than those associated with the estimation procedure under the most rigid specification.

In this paper we have restricted ourselves to linear models. However, the estimation procedure can easily be extended so as to include nonlinear models like the linear expenditure system or the Almost Ideal Demand System in its extensive form. Actually, nonlinearities will not affect the estimation procedure for the covariance parameters, but only the estimation procedure for the parameters of the deterministic part of the model. In a similar way, the present approach can easily be extended so as to apply to sum-constrained simultaneous equations models as well. Finally, it would be useful to generalize the estimation procedure to models with serially correlated errors in order to be able to test for dynamic misspecifications. We hope to address this question as well as the problem of testing the present specification against alternative ones in the near future.

Appendix A: Conditions for Ω_{n-1} to be Positive-Definite

The first principal minor of $|\Omega_{n-1}|$ (c.f. (2.4)) is

$$|\Omega_1| = d_1 - \frac{d_1^2}{d} = \frac{\sum_{i=2}^{n} d_i}{d} d_1$$

Suppose that the r-th principal minor (r < n-1) is

$$(A.1) \qquad |\Omega_r| = \frac{\sum_{i=r+1}^{n} d_i}{d} \prod_{i=1}^{r} d_i$$

If we prove that

$$|\Omega_{r+1}| = \frac{\sum_{i=r+2}^{n} d_i}{d} \prod_{i=1}^{r+1} d_i$$

it follows from induction that*

$$(A.2) \qquad |\Omega_{n-1}| = \frac{d_n}{d} \cdot \prod_{i=1}^{n-1} d_i = \frac{\prod_{i=1}^{n} d_i}{d}$$

PROOF: The ratio $|\Omega_r|/|\Omega_{r+1}|$ is equal to element (r+1, r+1) of

$$\Omega_{r+1}^{-1} = [D_{r+1} - \frac{\delta_{r+1}\delta'_{r+1}}{d}]^{-1} =$$

$$D_{r+1}^{-1} - \iota_{r+1}[\iota'_{r+1}\delta_{r+1} - d]^{-1}\iota'_{r+1}$$

Hence

$$\frac{|\Omega_r|}{|\Omega_{r+1}|} = d_{r+1}^{-1} + (\sum_{i=r+2}^{n} d_i)^{-1} = \frac{\sum_{i=r+1}^{n} d_i}{d_{r+1} \sum_{i=r+2}^{n} d_i}$$

or

$$|\Omega_{r+1}| = \frac{d_{r+1} \sum_{i=r+2}^{n} d_i}{\sum_{i=r+1}^{n} d_i} |\Omega_r| = \frac{\sum_{i=r+2}^{n} d_i}{d} \prod_{i=1}^{r+1} d_i$$

* (A.2) can be proved alternatively by using the results of Appendix A6 of Dhrymes (1970) - as pointed out by Mr. Ten Cate of the Netherlands Central Bureau of Statistics - but since we need (A.1) in the sequel we prefer to give the full proof.

after substitution of (A.1). This completes the proof.

It is obvious from (A.1) and (A.2) that a sufficient condition for Ω_{n-1} to be positive-definite is that all d_i's are positive; consequently, $d = \Sigma_{i=1}^{n} d_i$ is positive as well.

Secondly, we prove that Ω_{n-1} is positive-definite if at most one d_i is negative with d being negative as well. Suppose 2 d_i's are negative and take without any loss of generality d_{n-1} and d_n. It follows from (A.2) that $|\Omega_{n-1}|$ can only be positive when $d > 0$. But then it follows from (A.1) that $|\Omega_{n-2}|$ is negative and consequently Ω_{n-1} would not be positive-definite. Suppose 3 d_i's are negative, say d_{n-2}, d_{n-1}, and d_n. $|\Omega_{n-1}|$ can only be positive when $d < 0$, but then $|\Omega_{n-2}|$ is negative. The argument can easily be extended to more than 3 d_i's. Consequently, at most one d_i may be negative. Then, it follows from (A.1) and (A.2) that for Ω_{n-1} to be positive-definite, d should be negative as well.

Appendix B: Solving the First-Order Conditions.*

In this appendix we consider the stationary points of f in S and show that they can be obtained by means of a numerical search procedure for the unique real root of an equation in only one variable. As said before we assume without any loss of generality that $\alpha_n \geq \alpha_i$ (i = 1, ..., n-1). Of course, it may happen that multiple maxima occur, but these can easily be handled by choosing arbitrarily one of them to be α_n.

The stationary points of f in S are obtained by solving the following system of first-order conditions (compare (2.15))

$$(B.1) \qquad d_i \sum_{j \neq i} d_j = \alpha_i d \qquad i = 1, \ldots, n$$

Summing (B.1) over i ≠ n and subtracting (B.1) for i = n, one easily verifies that a stationary point can only exist when

$$(B.2) \qquad 2\sum_{1 \leq j < i \leq n-1} d_j d_i = d\left(\sum_{i=1}^{n-1} \alpha_i - \alpha_n\right)$$

From the definition of S_1 and S_2 in (3.2) it follows that $d_i > 0$ for i ≠ n. Therefore a stationary point of f in S_1 can only exist when $\alpha_n < \Sigma_{i=1}^{n-1} \alpha_i$ and likewise a stationary point of f in S_2 can only exist when $\alpha_n > \Sigma_{i=1}^{n-1} \alpha_i$.

After substituting $\Sigma_{j \neq i} d_j = d - d_i$, we obtain the following solution for (B.1) in terms of α_i and d

$$(B.3) \qquad d_i = \frac{d}{2} \pm \frac{d}{2}\left(1 - \frac{4\alpha_i}{d}\right)^{\frac{1}{2}} \qquad i = 1, \ldots, n$$

with $d \geq 4\alpha_n$ or $d < 0$ because we are only interested in real-valued solutions.

For stationary points in S_1, it is certainly true that

$$d_i = \frac{d}{2} - \frac{d}{2}\left(1 - \frac{4\alpha_i}{d}\right)^{\frac{1}{2}} \qquad \text{for } i \neq n$$

For suppose that for some j ≠ n, it would be true that

$$d_j = \frac{d}{2} + \frac{d}{2}\left(1 - \frac{4\alpha_j}{d}\right)^{\frac{1}{2}}$$

* As no confusion can arise in this appendix, we drop the "hats" for reasons of notational convenience.

Then it follows that

$$d = \sum_{i=1}^{n} d_i \geq \sum_{i \neq j,n} d_i + d + \frac{d}{2} \left[\left(1 - \frac{4\alpha_j}{d}\right)^{\frac{1}{2}} - \left(1 - \frac{4\alpha_n}{d}\right)^{\frac{1}{2}} \right] > d$$

because $\alpha_j \leq \alpha_n$ for $j \neq n$ and $d_k > 0$ ($k = 1, \ldots, n$). Consequently, we have to consider two possible solutions in S_1, viz., either

(B.4) $$d_i = \frac{d}{2} - \frac{d}{2} \left(1 - \frac{4\alpha_i}{d}\right)^{\frac{1}{2}} \qquad i = 1, \ldots, n$$

or

(B.5) $$d_i = \frac{d}{2} - \frac{d}{2} \left(1 - \frac{4\alpha_i}{d}\right)^{\frac{1}{2}} \qquad i = 1, \ldots, n-1$$

$$d_n = \frac{d}{2} + \frac{d}{2} \left(1 - \frac{4\alpha_n}{d}\right)^{\frac{1}{2}}$$

For $d < 0$, it is certainly true that $(1 - 4\alpha_i d^{-1})^{\frac{1}{2}} > 1$. Therefore, we have to consider only one possible solution in S_2, viz.,

(B.6) $$d_i = \frac{d}{2} - \frac{d}{2} \left(1 - \frac{4\alpha_i}{d}\right)^{\frac{1}{2}} \qquad i = 1, \ldots, n-1$$

$$d_n = \frac{d}{2} + \frac{d}{2} \left(1 - \frac{4\alpha_n}{d}\right)^{\frac{1}{2}}$$

because all other possibilities generate wrong signs.

It should be noted that in the case of multiple maxima, a solution must be of the form (B.4). For suppose that $\alpha_j = \alpha_n$ for some $j \neq n$. Evidently, $\alpha_n < \Sigma_{i=1}^{n-1} \alpha_i$ and so a solution must be of the form (B.4) or (B.5). Summing (B.5) over i, we obtain

$$d = \sum_{i=1}^{n} d_i = \sum_{i \neq j,n} d_i + d > d$$

Consequently, if a solution exists, it must be of the form (B.4). In the analysis of (B.5) and (B.6) we may confine ourselves therefore to the case where the strict inequality sign holds true

(B.7) $$\alpha_n > \alpha_i \qquad i = 1, \ldots, n-1$$

Let us now first consider (B.4). Summing over i and applying some rearrangements yields

$$(B.8) \qquad f_1(d) = \sum_{i=1}^{n} \left(1 - \frac{4\alpha_i}{d}\right)^{\frac{1}{2}} - (n-2) = 0$$

It is easy to show that $f_1(d)$ has the following properties

(i) $\lim_{d \to \infty} f_1(d) = 2$

(ii) $f_1'(d) > 0$

Evidently, there is a unique solution to (B.8) provided that

$$(B.9) \qquad f_1(4\alpha_n) = \sum_{i=1}^{n-1} \left(1 - \frac{\alpha_i}{\alpha_n}\right)^{\frac{1}{2}} - (n-2) \overset{\text{def}}{=} \gamma \leq 0$$

Note that in the case of multiple maxima, (B.9) is always met with.

If $\gamma < 0$, we have to solve (B.8) numerically; this is Case 1 of Section 3 where $f_1(d)$ is depicted in Figure 1. If $\gamma = 0$, the solution of (B.8) is $d = 4\alpha_n$; this is Case 3 of Section 3, where we called this a border case to Case 1. The solution for d should be substituted into (B.4) in order to obtain the solution for $d_1, \ldots, d_n$.

Next, consider (B.5). Summing (B.5) over i leads to

$$(B.10) \qquad f_2(d) = \sum_{i=1}^{n-1} \left(1 - \frac{4\alpha_i}{d}\right)^{\frac{1}{2}} - \left(1 - \frac{4\alpha_n}{d}\right)^{\frac{1}{2}} - (n-2) = 0$$

It is easily seen that

$$(B.11) \qquad \lim_{d \to \infty} f_2(d) = 0$$

Let us now define the following functions

$$c_i(d) = \frac{\left(1 - \frac{4\alpha_n}{d}\right)^{\frac{1}{2}}}{\left(1 - \frac{4\alpha_i}{d}\right)^{\frac{1}{2}}} \qquad i = 1, \ldots, n-1$$

which have the properties (see (B.7))

(B.12)
$$0 \le c_i(d) < 1$$
$$\lim_{d\to\infty} c_i(d) = 1$$

and

(B.13)
$$c_i'(d) > 0$$

The derivative of $f_2(d)$ with respect to d is easily shown to be equal to

(B.14)
$$f_2'(d) = \frac{2}{d^2\left(1 - \frac{4\alpha_n}{d}\right)^{\frac{1}{2}}}\left[\sum_{i=1}^{n-1} c_i(d)\alpha_i - \alpha_n\right]$$

From $\alpha_n < \Sigma_{i=1}^{n-1}\ \alpha_i$, (B.12), and (B.13) it follows that there exists only one $d_0 \in [4\alpha_n, \infty)$ such that

$$\sum_{i=1}^{n-1} c_i(d_0) - \alpha_n = 0$$

or, by virtue of (B.14), that

$$f_2'(d_0) = 0$$

Obviously, $f_2'(d) < 0$ for $d < d_0$ and $f_2'(d) > 0$ for $d > d_0$. The latter implies that $\lim_{d\to\infty} f_2(d) = 0$ from below. Consequently, there is a unique solution to (B.10) provided that

(B.15)
$$f_2(4\alpha_n) = \gamma \ge 0$$

If $\gamma > 0$, we have to solve (B.10) numerically; this is Case 2 of Section 3 where we depicted $f_2(d)$ in Figure 2. If $\gamma = 0$, the solution is $d = 4\alpha_n$. This is Case 3 of Section 3 where we called this a border case to Case 2. The solution for d should be substituted into (B.5) in order to obtain the solution for $d_1, \ldots, d_n$.

Finally, we consider (B.6). Summing over i, we once again obtain (B.10), but now

(B.16)
$$\lim_{d\to-\infty} f_2(d) = 0$$

Of course, the derivative of $f_2(d)$ with respect to d is given by (B.14) as before, but now the functions $c_i(d)$ have the following properties (see (B.7))

$$\text{(B.17)}\qquad \begin{aligned} &1 < c_i(d) < (\alpha_n/\alpha_i)^{\frac{1}{2}} \\ &\lim_{d\to-\infty} c_i(d) = 1 \text{ and } \lim_{d\to 0} c_i(d) = (\alpha_n/\alpha_i)^{\frac{1}{2}} \end{aligned}$$

and once again

$$\text{(B.18)}\qquad c_i'(d) > 0$$

From (B.17) it follows that

$$\text{(B.19)}\qquad \sum_{i=1}^{n-1} \alpha_i - \alpha_n < \sum_{i=1}^{n-1} c_i(d)\alpha_i - \alpha_n < \sum_{i=1}^{n-1} (\alpha_n\alpha_i)^{\frac{1}{2}} - \alpha_n$$

By virtue of the inequality of Cauchy-Schwarz it holds true that

$$\text{(B.20)}\qquad T^{-1}u_i'u_n \geq -T^{-1}\{(u_n'u_n)(u_i'u_i)\}^{\frac{1}{2}} = -(\alpha_n\alpha_i)^{\frac{1}{2}}$$

Summing (B.20) over i = 1, ..., n-1 and substituting $\Sigma_{i=1}^{n-1} u_i' = -u_n'$, we obtain

$$\text{(B.21)}\qquad \alpha_n \leq \sum_{i=1}^{n-1} (\alpha_n\alpha_i)^{\frac{1}{2}}$$

Let us first consider the case $\alpha_n = \Sigma_{i=1}^{n-1}(\alpha_n\alpha_i)^{\frac{1}{2}}$ or $\alpha_n = (\Sigma_{i=1}^{n-1}\alpha_i^{\frac{1}{2}})^2$. From (B.19) it follows that

$$\sum_{i=1}^{n-1} c_i(d)\alpha_i - \alpha_n < 0$$

and hence from (B.14) that $f_2'(d) < 0$. Together with (B.16) this implies that in this case no stationary point exists.

Next, consider the case $\alpha_n < \Sigma_{i=1}^{n-1} (\alpha_n\alpha_i)^{\frac{1}{2}}$. From $\alpha_n > \Sigma_{i=1}^{n-1} \alpha_i$, (B.19), and (B.18) it follows that there is only one $d_0 \in (-\infty, 0)$ such that

$$\sum_{i=1}^{n-1} c_i(d_0)\alpha_i - \alpha_n = 0$$

entailing according to (B.14) that $f_2'(d_0) = 0$. Obviously, $f_2'(d) < 0$ for $d < d_0$ and $f_2'(d) > 0$ for $d > d_0$. From the definition of the functions $c_i(d)$ we derive that

$$f_2(d) = \left(1 - \frac{4\alpha_n}{d}\right)^{\frac{1}{2}} \left[\sum_{i=1}^{n-1} \{c_i(d)\}^{-1} - 1\right] - (n-2)$$

$$> \left(1 - \frac{4\alpha_n}{d}\right)^{\frac{1}{2}} \frac{1}{\alpha_n} \left[\sum_{i=1}^{n-1} (\alpha_n \alpha_i)^{\frac{1}{2}} - \alpha_n\right] - (n-2)$$

because of (B.17). Since the term between brackets is positive, it follows that

$$\lim_{d \to 0} f_2(d) = \infty$$

Together with (B.16) this implies that there is a unique solution to (B.10). This is Case 4 of Section 3 where we depicted $f_2(d)$ in Figure 3. The solution for d should be substituted into (B.6) in order to obtain the solution for $d_1, \ldots, d_n$.

Summarizing, we have proved that f has a unique stationary point in S_1 when $\alpha_n < \Sigma_{i=1}^{n-1} \alpha_i$ and no stationary points in S_1 when

$\Sigma_{i=1}^{n-1} \alpha_i \leq \alpha_n \leq (\Sigma_{i=1}^{n-1} \alpha_i^{\frac{1}{2}})^2$, while f has a unique stationary point in S_2 when

$\Sigma_{i=1}^{n-1} \alpha_i < \alpha_n < (\Sigma_{i=1}^{n-1} \alpha_i^{\frac{1}{2}})^2$ and no stationary points in S_2 when $\alpha_n \leq \Sigma_{i=1}^{n-1} \alpha_i$

or $\alpha_n = (\Sigma_{i=1}^{n-1} \alpha_i^{\frac{1}{2}})^2$.

Appendix C: Proof of Theorem 1*

We start by proving part A of the theorem. Choose any number $M > 1$ such that $\forall\, x \notin [\frac{1}{M}, M]$

$$\text{(C.1)} \qquad \log x + \frac{\alpha_1}{x} > \max\{f(1, \ldots, 1), 0\} + \log n + \sum_{j=1}^{n} |\log \alpha_j|$$

and

$$\text{(C.2)} \qquad \frac{1}{M} < \alpha_1$$

Let the set B_R be defined by

$$\text{(C.3)} \qquad B_R = \{(d_1, \ldots, d_n) \in R^n \mid \frac{1}{R} \leq d_j \leq R \quad \forall\, 1 \leq j \leq n\}$$

and let C_R be such that

$$\text{(C.4)} \qquad f(C_R) = \min_{x \in B_R} f(x)$$

From the continuity of f on the compact set B_R, it follows that C_R always exists, though it need not be unique.

LEMMA 1: If $R > M$, then either C_R is a stationary point of f or $C_R = (C_{R1}, \ldots, C_{Rn})$ can be taken such that $C_{Rj} \in [\frac{1}{M}, M]$ $(j = 1, \ldots, n-1)$ and $C_{Rn} = R$.

PROOF: If C_R is not a stationary point, it must be a boundary point. Evidently, C_R can be taken such that C_{Rn} is at least as large as C_{Rj} $(j \neq n)$. For suppose that $C_{Rj} > C_{Rn}$ for some $j \neq n$. Then the value of f will certainly not increase when the values of C_{Rj} and C_{Rn} are interchanged. Hence, C_R can be taken such that $C_{Rn} \geq C_{Rj}$ $(j \neq n)$. Suppose now $C_{Rn} \neq R$. Then it must be true that $C_{Rj} = R^{-1}$ for some $j \neq n$. From (3.1), however, one easily verifies that

$$\frac{\partial f}{\partial d_j} = \frac{d_j - \alpha_j}{d_j^2} - \frac{1}{d} = \frac{R^{-1} - \alpha_j}{R^{-2}} - \frac{1}{d} < 0$$

* Without any loss of generality, we assume in this appendix that $\alpha_1 \leq \alpha_2 \leq \ldots \leq \alpha_{n-1} \leq \alpha_n$; moreover, we once again drop the "hats" for reasons of notational convenience.

because of (C.2). Consequently, an infinitesimal increase of C_{Rj} would give rise to a smaller value of f. Hence, $C_{Rn} = R$.
Finally, suppose that $C_{Rj} \notin [\frac{1}{M}, M]$ for some $j \neq n$. Obviously,

(C.5) $$\log d_i + \frac{\alpha_i}{d_i} \geq \min_{d_i}\{\log d_i + \frac{\alpha_i}{d_i}\} = \log \alpha_i + 1 \qquad \forall\ d_i \in (0,\infty)$$

Substituting (C.5) into (3.1), we obtain

$$f(C_R) = \sum_{i=1}^{n} \left(\log C_{Ri} + \frac{\alpha_i}{C_{Ri}}\right) - \log\left(\sum_{i=1}^{n} C_{Ri}\right)$$

$$\geq \sum_{i\neq j,n} (\log \alpha_i + 1) + \log C_{Rj} + \frac{\alpha_j}{C_{Rj}} + \log R + \frac{\alpha_n}{R} - \log nR$$

$$> \sum_{i\neq j,n} (\log \alpha_i + 1) + \log R + \frac{\alpha_n}{R} - \log nR +$$

$$+ \max\{f(1, \ldots, 1), 0\} + \log n + \sum_{j=1}^{n} |\log \alpha_j|$$

$$> \max\{f(1, \ldots, 1), 0\} + n - 2 > f(1, \ldots, 1)$$

where the first strict inequality sign follows from (C.1). Consequently, C_R can not give rise to a minimum of f and hence $C_{Rj} \in [\frac{1}{M}, M]$ for all $j \neq n$. This completes the proof of Lemma 1.

Letting m run through the set of positive integers larger than M, we obtain sequences $\{C_m\}$ and $\{f(C_m)\}$. As $\{f(C_m)\}$ is a nonincreasing sequence and for every point $x \in S_1$ there exists a positive integer m_0 such that $x \in B_m$ for all $m \geq m_0$, it certainly holds true that

(C.6) $$\lim_{m\to\infty} f(C_m) = \inf_{x\in S_1} f(x)$$

In Appendix B, we have proved that f can only have one stationary point in S_1.

So there are two possibilities for the sequence $\{C_m\}$, viz.,
(i) from certain N onwards $C_m = x^0$, the unique stationary point of f in S_1, and obviously

$$\inf_{x \in S_1} f(x) = \lim_{m\to\infty} f(C_m) = f(x^0)$$

(ii) from certain N onwards C_m is always a boundary point.
In the latter case, it follows from Lemma 1 that $C_{mj} \in [\frac{1}{M}, M]$ for $j \neq n$.
Therefore, the sequence $\{C_m\}$ has a subsequence $\{C_{m'}\}$ such that

$$\lim_{m'\to\infty} C_{m'j} = C'_j \in [\frac{1}{M}, M] \qquad \text{for } j \neq n$$

because of the compactness of $[\frac{1}{M}, M]$.
Hence,

$$\lim_{m\to\infty} f(C_m) = \lim_{m'\to\infty} f(C_{m'}) = \lim_{m'\to\infty} f(C_{m'1}, \ldots, C_{m'n}) =$$

$$= \lim_{m'\to\infty} f(C'_1, \ldots, C'_{n-1}, m') = \sum_{i=1}^{n-1} \left(\log C'_i + \frac{\alpha_i}{C'_i}\right)$$

From (C.5) it follows that the last expression is minimized for $C'_i = \alpha_i$ $(i = 1, \ldots, n-1)$ and consequently (C.6) implies

$$\inf_{x \in S_1} f(x) = \lim_{m\to\infty} f(C_m) = \sum_{i=1}^{n-1} \log \alpha_i + n - 1$$

Finally, we have to determine whether

$$\inf_{x \in S_1} f(x) = f(x^0) \text{ or } \inf_{x \in S_1} f(x) = \sum_{i=1}^{n-1} \log \alpha_i + n - 1$$

In Appendix B, we have proved that f does not have stationary points in S_1 when $\alpha_n \geq \Sigma_{i=1}^{n-1} \alpha_i$. Therefore,

(C.7) $$\inf_{x \in S_1} f(x) = \sum_{i=1}^{n-1} \log \alpha_i + n - 1 \quad \text{if } \sum_{i=1}^{n-1} \alpha_i \leq \alpha_n \leq \left(\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}}\right)^2$$

When $\alpha_n < \sum_{i=1}^{n-1} \alpha_i$, we have

$$f\left(\alpha_1, \ldots, \alpha_{n-1}, \frac{\alpha_n \sum_{i=1}^{n-1} \alpha_i}{\sum_{i=1}^{n-1} \alpha_i - \alpha_n}\right) =$$

$$= \sum_{i=1}^{n-1} \log \alpha_i + n - 1 + \log\left(\frac{\alpha_n}{\sum_{i=1}^{n-1} \alpha_i}\right) + 1 - \frac{\alpha_n}{\sum_{i=1}^{n-1} \alpha_i} < \sum_{i=1}^{n-1} \log \alpha_i + n - 1$$

Consequently, $\Sigma_{i=1}^{n-1} \log \alpha_i + n - 1$ can not be the infimum of f in S_1 and so we have

$$\text{(C.8)} \qquad \inf_{x \in S_1} f(x) = f(x^0) \qquad \text{if } \alpha_n < \sum_{i=1}^{n-1} \alpha_i$$

This completes the proof of part A of the theorem.

In order to prove part B of the theorem, we first restrict ourselves to the case $\alpha_n < (\Sigma_{i=1}^{n-1} \alpha_i^{\frac{1}{2}})^2$. Choose $\gamma_i = \alpha_i - \xi_i$ $(i = 1, \ldots, n-1)$ such that

$$\text{(C.9)} \qquad \xi_i > 0 \text{ and } \left(\sum_{i=1}^{n-1} \gamma_i^{\frac{1}{2}}\right)^2 > \alpha_n$$

and choose any number $M > n+1$ such that $\forall R \in [M, \infty)$

$$\text{(C.10)} \qquad - R^2\alpha_1 + 2R < 0$$

and such that $\forall x \notin [\frac{1}{M}, M]$

$$\text{(C.11)} \quad \log x + \frac{\alpha_1}{x} > \max\{f(1, \ldots, 1, -n-1), 0\} + \alpha_n + \sum_{j=1}^{n} |\log \alpha_j|$$

and

$$\text{(C.12)} \quad \log x + \frac{\xi_i}{x} > \max\{f(1, \ldots, 1, -n-1), 0\} + \sum_{j=1}^{n-1} |\log \xi_j|$$

$$i = 1, \ldots, n-1$$

Let the set B_R' be defined by

$$B'_R = \{(d_1, \ldots, d_n) \in R^n \mid \frac{1}{R} \leq d_j \leq R \quad \text{(C.13)}$$
$$\forall\, 1 \leq j \leq n-1,\ |d_n| \leq R,\ \sum_{j=1}^{n} d_j \leq -\frac{1}{R}\}$$

and let C_R be such that

$$f(C_R) = \min_{x \in B'_R} f(x) \quad \text{(C.14)}$$

LEMMA 2: If $R > M$, then either C_R is a stationary point of f or $C_R = (C_{R1}, \ldots, C_{Rn})$ is such that $C_{Rj} \in [\frac{1}{M}, M]$ $(j = 1, \ldots, n-1)$ and $C_{Rn} = -R$ or $\Sigma_{j=1}^{n} C_{Rj} = -\frac{1}{R}$.

PROOF: If C_R is not a stationary point, it must be a boundary point. Suppose $C_{Rn} > -R$ and $\Sigma_{j=1}^{n} C_{Rj} < -R^{-1}$. Because $C_{Rn} > -R$, it is certainly true that $C_{Rj} < R$ $(j = 1, \ldots, n-1)$ and hence C_R must be a boundary point such that $C_{Rj} = R^{-1}$ for some $j \neq n$. From (3.1), however, it is easily seen that

$$\frac{\partial f}{\partial d_j} = \frac{d_j - \alpha_j}{d_j^2} - \frac{1}{d} = \frac{R^{-1} - \alpha_j}{R^{-2}} - \frac{1}{\sum_{j=1}^{n} C_{Rj}} < -R^2\alpha_1 + 2R < 0$$

because of (C.10). Consequently, an infinitesimal increase of C_{Rj} would give rise to a smaller value of f without violating the restriction $\Sigma_{j=1}^{n} C_{Rj} \leq -R^{-1}$. Hence, $C_{Rn} = -R$ or $\Sigma_{j=1}^{n} C_{Rj} = -R^{-1}$.

Suppose next that $C_{Rn} = -R$ and $C_{Rj} \notin [\frac{1}{M}, M]$ for some $j \neq n$. As in the proof of Lemma 1, we obtain

$$f(C_R) = \sum_{i \neq j,n} \left(\log C_{Ri} + \frac{\alpha_i}{C_{Ri}}\right) + \log C_{Rj} + \frac{\alpha_j}{C_{Rj}} + \log\left(\frac{C_{Rn}}{\sum_{j=1}^{n} C_{Rj}}\right) + \frac{\alpha_n}{C_{Rn}}$$

$$\geq \sum_{i \neq j,n} (\log \alpha_i + 1) + \log C_{Rj} + \frac{\alpha_j}{C_{Rj}} + \log\left(\frac{C_{Rn}}{\sum_{j=1}^{n} C_{Rj}}\right) + \frac{\alpha_n}{C_{Rn}}$$

$$> \sum_{i \neq j,n} (\log \alpha_i + 1) + \log C_{Rj} + \frac{\alpha_j}{C_{Rj}} - \frac{\alpha_n}{R}$$

$$> \sum_{i \neq j,n} (\log \alpha_i + 1) - \frac{\alpha_n}{R} + \max\{f(1, \ldots, 1, -n-1), 0\} +$$

$$+ \alpha_n + \sum_{j=1}^{n} |\log \alpha_j|$$

$$> \max\{f(1, \ldots, 1, -n-1), 0\} + n - 2 > f(1, \ldots, 1, -n-1)$$

where the first strict inequality sign follows from $C_{Rn}(\Sigma_{j=1}^{n} C_{Rj})^{-1} > 1$ and the second one from (C.11). Consequently, C_R can not give rise to a minimum of f and hence $C_{Rj} \in [\frac{1}{M}, M]$ for all $j \neq n$.

Before proceeding, we first prove the following lemma, that will be used in the sequel.

LEMMA 3: Let g be defined by

$$g(x_1, \ldots, x_{n-1}, \theta) = \sum_{i=1}^{n-1} \frac{\alpha_i}{x_i} - \frac{\alpha_n}{\sum_{i=1}^{n-1} x_i + \theta}$$

and let $\alpha_n < (\Sigma_{i=1}^{n-1} \alpha_i^{\frac{1}{2}})^2$. Then $g > 0$ for all $(x_1, \ldots, x_{n-1}, \theta) \in R_+^n$.

PROOF: Choose any point $(x_1^0, \ldots, x_{n-1}^0, \theta^0) \in R_+^n$ and let $\mu = \Sigma_{i=1}^{n-1} x_i^0 + \theta^0$. Define the set L_μ by

$$L_\mu = \{(x_1, \ldots, x_{n-1}) \in R_+^{n-1} | \sum_{i=1}^{n-1} x_i + \theta^0 = \mu\}$$

Applying Lagrange's method, one easily verifies that $g(x_1, \ldots, x_{n-1}, \theta^0)$ attains its minimum in L_μ when

(C.15) $$x_i = \frac{(\mu - \theta^0)\alpha_i^{\frac{1}{2}}}{(\sum_{j=1}^{n-1} \alpha_j^{\frac{1}{2}})} \qquad i = 1, \ldots, n-1$$

Substituting (C.15) into $g(x_1, \ldots, x_{n-1}, \theta^0)$, we obtain

(C.16) $$\min_{x \in L_\mu} g(x_1, \ldots, x_{n-1}, \theta^0) = \frac{(\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}})^2}{\mu - \theta^0} - \frac{\alpha_n}{\mu} > 0$$

As $(x_1^0, \ldots, x_{n-1}^0) \in L_\mu$, it certainly holds true that $g(x_1^0, \ldots, x_{n-1}^0, \theta^0) > 0$, which proves the lemma.

In order to complete the proof of Lemma 2, suppose $\Sigma_{j=1}^{n} C_{Rj} = -R^{-1}$ and $C_{Rj} \notin [\frac{1}{M}, M]$ for some $j \neq n$. From the definition of γ_i ($i = 1, \ldots, n-1$) just above (C.9), it follows that

$$f(C_R) = \sum_{i \neq j,n} \left(\log C_{Ri} + \frac{\xi_i}{C_{Ri}}\right) + \log C_{Rj} + \frac{\xi_j}{C_{Rj}} +$$

$$+ \sum_{i=1}^{n-1} \frac{\gamma_i}{C_{Ri}} - \frac{\alpha_n}{\sum_{i=1}^{n-1} C_{Ri} + R^{-1}} + \log \left(\frac{C_{Rn}}{\sum_{i=1}^{n} C_{Ri}}\right)$$

$$> \sum_{i \neq j,n} \left(\log C_{Ri} + \frac{\xi_i}{C_{Ri}}\right) + \log C_{Rj} + \frac{\xi_j}{C_{Rj}} + \log\left(\frac{C_{Rn}}{\sum_{i=1}^{n} C_{Ri}}\right)$$

$$> \sum_{i \neq j,n} (\log \xi_i + 1) + \log C_{Rj} + \frac{\xi_j}{C_{Rj}}$$

$$> \sum_{i \neq j,n} (\log \xi_i + 1) + \max\{f(1, \ldots, 1, -n-1), 0\} +$$

$$+ \sum_{j=1}^{n-1} |\log \xi_j|$$

$$> \max\{f(1, \ldots, 1, -n-1), 0\} + n - 2 > f(1, \ldots, 1, -n-1)$$

where the first inequality sign follows from the application of Lemma 3, the second one from $C_{Rn}(\Sigma_{i=1}^{n} C_{Ri})^{-1} > 1$ and (C.5), and the third one from (C.12). Consequently, C_R can not give rise to a minimum of f and hence $C_{Rj} \in [\frac{1}{M}, M]$ for all $j \neq n$. This completes the proof of Lemma 2.

As in the proof of part A of the theorem, we may construct sequences $\{C_m\}$ and $\{f(C_m)\}$ by letting m run through the set of positive integers larger than M. In Appendix B, we have proved that f can only have one stationary point in S_2. So, once again, there are two possibilities for the sequence $\{C_m\}$, viz.,

(i) from certain N onwards $C_m = x^1$, the unique stationary point of f in S_2, and obviously

$$\inf_{x \in S_2} f(x) = \lim_{m \to \infty} f(C_m) = f(x^1)$$

(ii) from certain N onwards C_m is always a boundary point.

If C_m is a boundary point, it follows from Lemma 2 that $C_{mj} \in [\frac{1}{M}, M]$ $(j = 1, \ldots, n-1)$ and $C_{mn} = -m$ or $\Sigma_{j=1}^{n} C_{mj} = -m^{-1}$. In the latter case, however, we have

$$f(C_m) = \sum_{i=1}^{n-1} \left(\log C_{mi} + \frac{\alpha_i}{C_{mi}}\right) - \frac{\alpha_n}{\sum_{i=1}^{n-1} C_{mi} + m^{-1}} +$$

$$+ \log\left(\sum_{i=1}^{n-1} C_{mi} + m^{-1}\right) + \log m$$

and hence $\lim_{m \to \infty} f(C_m) = \infty$.

Consequently, from certain N onwards a boundary point C_m with $\Sigma_{j=1}^{n} C_{mj} = -m^{-1}$ can not give rise to a minimum of f. So we may restrict our attention to boundary points with $C_{mn} = -m$. In exactly the same way as in the proof of part A of the theorem, it then follows that

$$\inf_{x \in S_2} f(x) = \lim_{m \to \infty} f(C_m) = \sum_{i=1}^{n-1} \log \alpha_i + n - 1$$

In Appendix B, we have proved that f does not have stationary points in S_2, when $\alpha_n \leq \Sigma_{i=1}^{n-1} \alpha_i$. Therefore

(C.17) $$\inf_{x \in S_2} f(x) = \sum_{i=1}^{n-1} \log \alpha_i + n - 1 \qquad \text{if } \alpha_n \leq \sum_{i=1}^{n-1} \alpha_i$$

When $\Sigma_{i=1}^{n-1} \alpha_i < \alpha_n < (\Sigma_{i=1}^{n-1} \alpha_i^{\frac{1}{2}})^2$, we observe as in part A of the theorem that

$$f\left(\alpha_1, \ldots, \alpha_{n-1}, \frac{\alpha_n \sum_{i=1}^{n-1} \alpha_i}{\sum_{i=1}^{n-1} \alpha_i - \alpha_n}\right) < \sum_{i=1}^{n-1} \log \alpha_i + n - 1$$

Consequently, $\Sigma_{i=1}^{n-1} \log \alpha_i + n - 1$ can not be the infimum of f in S_2 and so we have

(C.18) $$\inf_{x \in S_2} f(x) = f(x^1) \qquad \text{if } \sum_{i=1}^{n-1} \alpha_i < \alpha_n < \Big(\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}}\Big)^2$$

Finally, consider the case $\alpha_n = \Big(\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}}\Big)^2$. For $\lambda > 0$, we have

$$f\Big(\lambda\alpha_1^{\frac{1}{2}}, \ldots, \lambda\alpha_{n-1}^{\frac{1}{2}}, -\lambda \sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}} - \lambda^2\Big) =$$

$$= \sum_{i=1}^{n-1} \Big(\log \lambda\alpha_i^{\frac{1}{2}} + \frac{\alpha_i^{\frac{1}{2}}}{\lambda}\Big) - \frac{\alpha_n}{\lambda \sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}} + \lambda^2} + \log \Big(\frac{\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}} + \lambda}{\lambda}\Big)$$

$$= (n-2)\log \lambda + \sum_{i=1}^{n-1} \log \alpha_i^{\frac{1}{2}} + \log\Big(\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}} + \lambda\Big) + \frac{\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}}}{\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}} + \lambda}$$

Consequently,

$$\lim_{\lambda \downarrow 0} f\Big(\lambda\alpha_1^{\frac{1}{2}}, \ldots, \lambda\alpha_{n-1}^{\frac{1}{2}}, -\lambda \sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}} - \lambda^2\Big) = -\infty$$

and so we have

(C.19) $$\inf_{x \in S_2} f(x) = -\infty \qquad \text{if } \alpha_n = \Big(\sum_{i=1}^{n-1} \alpha_i^{\frac{1}{2}}\Big)^2$$

This completes the proof of Theorem 1.

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