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WHAT DISTINGUISHES AN INDEPENDENTLY OBSERVED VECTOR FROM AN ESTIMATED MULTIVARIATE NORMAL POPULATION?

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By

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Systems Integration Division

3 April 1972

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CONTENTS

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WHAT DISTINGUISHES AN INDEPENDENTLY OBSERVED VECTOR FROM AN ESTIMATED MULTIVARIATE NORMAL POPULATION?

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SUMMARY

Once a researcher has determined that a multivariate observation $\underline{x}_o$ is different from an estimated population, he still has an unanswered question. He wants to know, "How is it different?" A method for answering this question is considered in this report.

Two results are shown and both involve the estimated population parameters $\underline{\overline{x}}$-the estimated mean, an $\hat{\Sigma}$-the estimated covariance matrix. The first result answers the question "Which linear combinations of the elements of the difference $\underline{x}_o - \underline{\overline{x}}$ are significant?" The second answers the question "Which elements of the difference $\underline{x}_o - \underline{\overline{x}}$ are significant?" Both results are derived using S. N. Roy's Union-Intersection Principle; hence, one can set an overall α/significance/type-1 level for the totality of tests.

A brief discussion of an application is also presented.

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GLOSSARY

$\underline{x}_o$	A p-component (p by 1) vector observation, "o", independent of the vectors $\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_n$
n	The number of independent observations which are independent of the vector $\underline{x}_o$
$\bar{\underline{x}} = \frac{1}{n} \sum_{i=1}^{n} \underline{x}_i$	A p-component (p by 1) estimate of the population mean vector $\underline{\mu}$
$\underline{\mu}$	A p-variate (p by 1) population mean vector
$\underline{\Sigma}$	A p by p population covariance matrix
$\hat{\underline{\Sigma}}$	An unbiased estimate of the population covariance matrix based on m degrees of freedom
$\hat{\underline{\Sigma}}^{-1}$	The inverse of the matrix $\hat{\underline{\Sigma}}$
a	The probability that the (null) hypothesis H_0 will be rejected when it is true
H_0	The hypothesis that the vector $\underline{x}_o$ and the set of vectors $\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_n$ are from the same population
H_1	The negation of the hypothesis H_0
$N(\underline{\mu}, \underline{\Sigma})$	The multivariate normal population with parameters $\underline{\mu}$ and $\underline{\Sigma}$
m	The number of degrees of freedom of the matrix estimate $\hat{\underline{\Sigma}}$
t	A "students" t-test statistic
$\underline{c}$	A (1 by p) p-variate vector of constant coefficients

$\underline{c}^t$	The p by 1 transpose of the vector $\underline{c}$
$\underline{\tilde{c}}$	The (1 by p) p-variate vector which maximizes the function $T^2(\underline{c})$
$\underline{e}_i$	A 1 by p vector which has a 1 as the i-th element and zeros elsewhere
$\frac{\partial T^2(\underline{c})}{\partial(\underline{c})}$	A p-variate (p by 1) vector of partial derivatives whose i-th component is $\frac{\partial T^2(\underline{c})}{\partial(c_i)}$
$\underline{0}$	A p by 1 vector which has zeros for all the elements
s_i^2	An unbiased estimate of the i-th variate from $N(\underline{\mu}, \Sigma)$
D	A matrix conformal with $\underline{x}$

INTRODUCTION

In a previous report by the author (reference 1), a probability density/distribution function was developed for an observed (p by 1) vector ($\underline{x}_0$) from a multivariate normal distribution with estimated parameters (see A-1).* This result enables a researcher to ask the general question "How unlikely is it that the observation $\underline{x}_0$ arose from $N(\underline{\mu}, \Sigma)$ where $\underline{\mu}$ is estimated by $\overline{\underline{x}}$ and Σ is estimated by $\hat{\Sigma}$?" Specifically the statistic:

$$T^2 = \frac{n}{n+1} (\underline{x}_o - \overline{\underline{x}})^t \hat{\Sigma}^{-1} (\underline{x}_o - \underline{x}) \tag{1}$$

which is distributed as $\frac{mp}{m-p+1}$ F with p and m-p+1 degrees of freedom (df), can be compared with tables of the F distribution for probability of occurrence. If the probability of occurrence is less than some specified amount (α), then the hypothesis (H_0) that $\underline{x}_o$ is from the same population that generated $\overline{\underline{x}}$ could be rejected. In other words, the hypothesis (H_1) that the populations which generated $\underline{x}_o$ and $\overline{\underline{x}}$ are not the same would be accepted.

The rejection of the hypothesis that $\underline{x}_o$ and $\overline{\underline{x}}$ are from the same population (H_0) doesn't show which of the variates of $\underline{x}_o$ were significantly different. Although individual tests of significance could be constructed (e.g., t-tests), there is no control of the overall α level for the set of comparisons. The reasons for this are twofold; there are p such tests, and the variates are generally correlated. Hence an approach is needed for testing the individual variates of $\underline{x}_o$ while controlling the overall α-level. The purpose of the present development is to delineate such a procedure.

*The results A-1 and A-2 are working theorems which are given in the appendix.

APPROACH

The approach employed here uses S.N. Roy's Union-Intersection Principle (reference 2, and reference 3). This principle allows one to fix the overall significance level for the totality of tests of linear compounds of the difference $\underline{x}_o - \underline{\overline{x}}$. Operationally, this is accomplished by employing the same (α-level) criterion required for the test of the most unlikely linear compound, $\underline{\tilde{c}}(\underline{x}_o - \underline{\overline{x}})$, to all particular tests of linear compounds. Since the individual variates $x_{oi} - \underline{\overline{x}}_i$ $(i=1, \ldots, p)$ can be tested by the linear compounds $\underline{e}_i(\underline{x}_o - \underline{\overline{x}})$ $(i=1, \ldots, p)$, this procedure will yield a solution to the problem posed in the Introduction.*

Let us define the statistic $T^2(\underline{c})$ as follows:

$$T^2(\underline{c}) = \frac{n}{n+1}\left[\underline{c}(\underline{x}_o - \underline{\overline{x}})\right]^t \left[\underline{c}\,\hat{\Sigma}\,\underline{c}^t\right]^{-1}\left[\underline{c}(\underline{x}_o - \underline{\overline{x}})\right] \tag{2}$$

where $\underline{c}$ is a fixed 1 by p vector. This equation is a special case of equation (1) with the p-variate terms $\underline{x}_o, \underline{\overline{x}}$, and $\hat{\Sigma}$ replaced by the corresponding univariate terms $\underline{c}\underline{x}_o$, $\underline{c}\underline{\overline{x}}$, and $\underline{c}\,\hat{\Sigma}\,\underline{c}^t$. These univariate terms are those appropriate for linear compounds of the respective variates (see A-2). Under the hypothesis (H_0) that $\underline{x}_o$ is from the same population that generated $\underline{\overline{x}}$, equation (2) is distributed as F with 1 and m degrees of freedom. Hence, the most unlikely $T^2(\underline{c})$ value would occur for that $\underline{c}$ which maximizes (2).

DERIVATIONS

In the following, a theorem will be stated which contains both the conditions for maximizing $T^2(\underline{c})$, and a procedure for testing the significance of the totality of linear compounds with a fixed overall significance level. Consider the following:

Theorem 1.0. If $T^2(\underline{c})$ is defined as in equation (2), then its maximum value is

$$T^2(\underline{\tilde{c}}) = \frac{n}{n+1}(\underline{x}_o - \underline{\overline{x}})^t \hat{\Sigma}^{-1}(\underline{x}_o - \underline{\overline{x}}) \tag{3}$$

which is distributed as $\dfrac{mp}{m-p+1}$ F with p and m-p+1 degrees of freedom when H_0 is true. This value of $T^2(\underline{c})$ is obtained for

$$\underline{\tilde{c}} = (\underline{x}_o - \underline{\overline{x}})^t \hat{\Sigma}^{-1} \tag{4}$$

*$\underline{e}_i$ $(i=1, \ldots, p)$ is a 1 by p vector with a 1 in the i-th entry and zeros elsewhere.

Further, the totality of linear compounds of the form $\underline{c}(\underline{x}_o - \underline{\bar{x}})$ could be tested for significance at the overall α-level by the test:

$$T^2(\underline{c}) \underset{H_0}{\overset{H_1}{\gtrless}} \frac{mp}{m-p+1} F_{\alpha:p,m-p+1} \tag{5}$$

Here H_1 is accepted if $T^2(\underline{c})$ is greater than the product of (mp)/(m-p+1) and the α-level F for p and m-p+1 degrees of freedom and H_0 is accepted otherwise.

Proof. Let is first rewrite equation (2) as follows:

$$T^2(\underline{c}) = \frac{n}{n+1} \frac{\underline{c}(\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t \underline{c}^t}{\underline{c}\hat{\Sigma}\underline{c}^t} \tag{6}$$

To obtain the condition for maximizing $T^2(\underline{c})$, let us take its partial derivative with respect to $\underline{c}$ and set the resulting system equal to $\underline{0}$. From the rules of differentation, it can be seen that

$$\frac{\partial T^2(\underline{c})}{\partial \underline{c}} = \frac{n}{n+1} (\underline{c}\hat{\Sigma}\underline{c}^t)^{-2} \Big[\underline{c}\hat{\Sigma}\underline{c}^t \, [2(\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t \underline{c}^t]$$

$$- \underline{c}(\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t \underline{c}^t \, [2\hat{\Sigma}\underline{c}^t]\Big] \tag{7}$$

Setting this system equal to $\underline{0}$ and solving, one can obtain the condition:

$$[\hat{\Sigma}^{-1}(\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t - \lambda I_p]\underline{c}^t = \underline{0} \tag{8}$$

where

$$\lambda = \frac{\underline{c}(\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t \underline{c}^t}{\underline{c}\hat{\Sigma}\underline{c}^t} \tag{9}$$

It is apparent upon comparison of (9) with (6) that the maximum $T^2(\underline{c})$ would be obtained for the transposed eigenvector which corresponds to the largest eigenvalue of the matrix:

$$\frac{n}{n+1} \hat{\Sigma}^{-1} (\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t \tag{10}$$

There will be one nonzero eigenvalue of (10) since the rank of $(\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t$ is one and the product of it and any conformal nonsingular matrix (e.g., $\hat{\Sigma}^{-1}$) would have the same rank.* Since the trace (tr) of (10) equals the sum of its eigenvalues (of which there is exactly one, $T^2(\tilde{\underline{c}})$, that is nonzero), it follows that

$$T^2(\tilde{\underline{c}}) = \mathrm{tr}\left[\frac{n}{n+1}\hat{\Sigma}^{-1}(\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t\right] \tag{11}$$

This can, by the commutative laws for traces, be rewritten

$$T^2(\tilde{\underline{c}}) = \left(\frac{n}{n+1}\right) \mathrm{tr}\left[(\underline{x}_o - \underline{\bar{x}})^t\hat{\Sigma}^{-1}(\underline{x}_o - \underline{\bar{x}})\right] \tag{12}$$

$$= \left(\frac{n}{n+1}\right)(\underline{x}_o - \underline{\bar{x}})^t\hat{\Sigma}^{-1}(\underline{x}_o - \underline{\bar{x}}) \tag{13}$$

which is the first result (3) of Theorem 1.0.* The distribution of (3) or (13) is given by A-1; hence, the first result of the theorem is completed.

The second result of this theorem $(\tilde{\underline{c}})$ follows upon substitution of the value of $\tilde{\underline{c}}$ given in equation (4) for $\underline{c}$ in equation (6). This yields a $T^2(\underline{c})$ value of

$$\left(\frac{n}{n+1}\right)\frac{\left[(\underline{x}_o - \underline{\bar{x}})^t\hat{\Sigma}^{-1}\right](\underline{x}_o - \underline{\bar{x}})(\underline{x}_o - \underline{\bar{x}})^t\left[(\underline{x}_o - \underline{\bar{x}})^t\hat{\Sigma}^{-1}\right]^t}{(\underline{x}_o - \underline{\bar{x}})^t\hat{\Sigma}^{-1}(\underline{x}_o - \underline{\bar{x}})} \tag{14}$$

or equivalently

$$\left(\frac{n}{n+1}\right)(\underline{x}_o - \underline{\bar{x}})^t\hat{\Sigma}^{-1}(\underline{x}_o - \underline{\bar{x}}) \tag{15}$$

Because this corresponds to the maximum value of $T^2(\underline{c})$, equation (5) gives the desired vector.

The last portion of the theorem can be seen when one recalls the nature of the Union-Intersection principle. Specifically, by employing the significance criterion (α - level) of $T^2(\tilde{\underline{c}})$ for each test of the type $T^2(\underline{c})$, one is assured that the totality of such tests has a joint significance level of α. Since $\frac{mp}{m-p+1} F_{\alpha:p,m-p+1}$ is this criteria, as indicated by the first part of the theorem and A-1, the general test (5) follows directly.

*See reference 4 for discussion of the rank of the product of two matrices.

**Reference 4 also contains a discussion of various results concerning the traces of matrices.

Tests for the individual components can be derived from specialization of equation (5). Since testing a specific component for significance (i-th) is equivalent to testing $T^2(\underline{e}_i)$ for significance, one could substitute $\underline{e}_i$ for $\underline{c}$ in equation (5) and obtain a specialized result. This will be considered in the remainder of this section.

Substitution of $\underline{e}_i$ for $\underline{c}$ in equation (5) yields

$$T^2(\underline{e}_i) \underset{H_0}{\overset{H_1}{\gtrless}} \frac{mp}{m-p+1} F_{\alpha:p,m-p+1} \tag{16}$$

which by equation (2) is equivalent to

$$\left(\frac{n}{n+1}\right)\left[\underline{e}_i(\underline{x}_o - \overline{\underline{x}})\right]^t \left[\underline{e}_i \hat{\Sigma} \underline{e}_i^t\right]^{-1} \left[\underline{e}_i(\underline{x}_o - \overline{\underline{x}})\right] \underset{H_0}{\overset{H_1}{\gtrless}} \frac{mp}{m-p+1} F_{\alpha:p,m-p+1} \tag{17}$$

Multiplying out each of the bracketed terms,

$$\left(\frac{n}{n+1}\right)\left[x_{oi} - \overline{x}_i\right]\left[\hat{\Sigma}_{ii}\right]^{-1} \left[x_{oi} - \overline{x}_i\right] \underset{H_0}{\overset{H_1}{\gtrless}} \frac{mp}{m-p+1} F_{\alpha:p,m-p+1} \tag{18}$$

where x_{oi} is the i-th entry of $\underline{x}_o$, $\overline{x}_i$ is the i-th entry of $\overline{\underline{x}}$, and $\hat{\Sigma}_{ii}$ is the i, i-th entry of $\hat{\Sigma}$. Since in general the diagonal entries of $\hat{\Sigma}$ are variance estimates, $[\hat{\Sigma}_{ii}]^{-1}$ can be written as $\frac{1}{s_i^2}$ where s_i^2 is the estimated variance of the i-th variate. Thus equation (18) can be written:

$$\left(\frac{n}{n+1}\right)\frac{(x_{oi} - \overline{x}_i)^2}{s_i^2} \underset{H_0}{\overset{H_1}{\gtrless}} \frac{mp}{m-p+1} F_{\alpha:p,m-p+1} \tag{19}$$

which is a considerable simplification of the test equation of the theorem. This result is summarized in the following corollary:

Corollary 1.1 Let x_{oi} be the i-th entry of $\underline{x}_o$, $\overline{x}_i$ be the i-th entry of $\overline{\underline{x}}$, and s_i^2 be the i, i-th entry of $\hat{\Sigma}$. Then the set of p-variates of $\underline{x}_o$ can be individually tested for difference from $\underline{\mu}$ by

$$T^2(\underline{e}_i) = \left(\frac{n}{n+1}\right)\frac{(x_{oi} - \overline{x}_i)^2}{s_i^2} \underset{H_0}{\overset{H_1}{\gtrless}} \frac{mp}{m-p+1} F_{\alpha:p,m-p+1} \tag{20}$$

with assurance that the overall significance level for the entire set of p tests is less than α.

DISCUSSION

In the above, two results were derived which answered the question "How does the observation $\underline{x}_o$ differ from the population which generated $\underline{\bar{x}}$?" The first of these, Theorem 1.0, allows one to ask if any particular linear combination of variates $(\underline{c}\underline{x}_o)$ distinguishes $\underline{x}_o$ from the population which generated $\underline{\bar{x}}$. The second result, Corollary 1.1, allows one to ask if any particular variate distinguishes $\underline{x}_o$ from the $\underline{\bar{x}}$ generating population. Both of these results have obvious practical application. Let us briefly consider one.

In a multiple criteria experiment, an unforseen (random) event occurs which makes suspect a single observation $\underline{x}_o$. The first question which faces the research is, "Is $\underline{x}_o$ from the same population as the set of other observations $(\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_n)$ from the same condition?" This question can be answered by employing the statistic:

$$T^2 = \frac{n}{n+1} (\underline{x}_o - \underline{\bar{x}})^t \hat{\Sigma}^{-1} (\underline{x}_o - \underline{\bar{x}}) \tag{21}$$

where $\underline{\bar{x}} = \frac{1}{n} \sum_{i=1}^{n} \underline{x}_i$, $\hat{\Sigma} = \frac{1}{n-1} \sum_{i=1}^{n} (\underline{x}_i - \underline{\bar{x}})(\underline{x}_i - \underline{\bar{x}})^t$, and T^2 is distributed as $\frac{(n-1)p}{n-p}$ F with p and n-p degrees of freedom.* Given that this statistic (21) is significant, the next question is, "Which variates of $\underline{x}_o$ differ from the population which generated $\underline{\bar{x}}$ and $\hat{\Sigma}$?" This could be answered by applying Corollary 1.1 with m equaling n-1. Guided by the costs of observations and their number, the results of these tests would be useful for decisions regarding the inclusion of $\underline{x}_o$ as part of the data of the experiment.

The above does not exhaust the set of possible applications. Hopefully this application will suggest others to the reader.

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*The statistic shown in (21) is a variation of A-1. A proof for its distribution was shown in reference 1.

APPENDIX

TWO WORKING THEOREMS

The first theorem (A-1) was shown in reference 1 by the author. The second theorem (A-2) was shown by Anderson (reference 5) in 1958.

A-1

If $\underline{x}_o$ is an observed p-variate vector from $N(\underline{\mu}, \Sigma)$,

$$\overline{\underline{x}} = \frac{1}{n} \sum_{i=1}^{n} \underline{x}_i$$

is a mean vector also from $N(\mu, \Sigma)$ based on n independent observations, and $m\hat{\Sigma}$ is the sum of the matrix products of m independent $N(\underline{0}, \Sigma)$ p-variate vectors $(\underline{Z}_1, \underline{Z}_2, \ldots, \underline{Z}_m)$; i.e.,

$$m\hat{\Sigma} = \sum_{i=1}^{m} \underline{Z}_i \underline{Z}_i^t$$

then

$$T^2 = \frac{n}{n+1} (\underline{x}_o - \overline{\underline{x}})^t \hat{\Sigma}^{-1} (\underline{x}_o - \overline{\underline{x}})$$

is distributed as:

$$\frac{mp}{m - p + 1} F$$

where F has p and m - p + 1 degrees of freedom.

If x is distributed according to $N(\underline{\mu}, \Sigma)$, then $Z = D\underline{x}$ is distributed according to $N(D\underline{\mu}, D\Sigma D^t)$.

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WHAT DISTINGUISHES AN INDEPENDENTLY OBSERVED VECTOR FROM AN ESTIMATED MULTIVARIATE NORMAL POPULATION?

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13. ABSTRACT

Once a researcher has determined that a multivariate observation $\underline{x}_o$ is different from an estimated population, he still has an unanswered question. He wants to know, "How is it different?" A method for answering this question is considered in this report.

Two results are shown and both involve the estimated population parameters $\bar{\underline{x}}$-the estimated mean, and $\hat{\Sigma}$-the estimated covariance matrix. The first result answers the question "Which linear combinations of the elements of the difference $\underline{x}_o - \bar{\underline{x}}$ are significant?" The second answers the question "Which elements of the difference $\underline{x}_o - \bar{\underline{x}}$ are significant?" Both results are derived using S. N. Roy's Union-Intersection principle; hence, one can set an overall α/significance/type-1 level for the totality of tests.

A brief discussion of an application is also presented.

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(PAGE 2)

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