Semi-invariants of the Interclass Mahalanobis Distance

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Abstract—A new closed-form expression for the semi-invariants of the interclass Mahalanobis distance is derived. Typically, in the analysis of two multivariate Gaussian populations with different covariance matrices, simultaneous diagonalization of these matrices is required. The semi-invariants are given directly in terms of the mean vectors and inverse covariance matrices by the results established in this correspondence. In addition, a new iterative algorithm is derived for computing the moments of the interclass Mahalanobis distance from the semi-invariants.

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I. Introduction

Pattern recognition and image processing techniques based on the Mahalanobis distance have found wide applicability, ranging from nuclear reactor surveillance and automated analysis of image texture data to discrimination problems in biomedical observations [1], [2], [3].

The importance of the Mahalanobis distance classifier lies in the fact that under a Gaussian assumption it is an optimal discriminant in the Bayes sense [4]. The estimation of the probability density function (pdf) of the interclass Mahalanobis distance has been a topic of active interest for a number of years because of its direct relation to the probability of error of the Bayes classifier [5]. For Gaussian data with equal covariance matrices, the solution of this problem is straightforward [6]. When the covariance matrices are not equal, however, the problem becomes considerably more complicated, requiring the use of numerical integration techniques for computing the pdf [7].

In many applications (e.g., cluster seeking, texture analysis, and measuring spatial stationarity of multivariate data) it is often of interest to compute descriptors based on the interclass Mahalanobis distance. Two such descriptors are the moments and semi-invariants. In an earlier paper, we established that the nth moment could be expressed as a polynomial of degree n and gave a closed-form solution for computing the coefficients [17]. This procedure, however, requires that the covariance matrices of the two populations be simultaneously diagonalized.

The present work deals with the derivation of a closed-form expression for the semi-invariants of the Mahalanobis distance. This expression involves the mean vectors and inverse covariance matrices directly and does not require the diagonalization of these matrices. It is well known that the moments and semi-invariants are related by expressions that, though theoretically simple, are quite inefficient in terms of computer implementation [11]. A new, iterative algorithm that is easily implementable in a digital computer is presented in Section IV for computing the moments from a given set of semi-invariants.

II. Background

Consider two d-dimensional Gaussian vector populations $\{x\}$ and $\{y\}$ with mean vectors and covariance matrices m_x, m_y, C_x, and C_y, respectively. The *intraclass Mahalanobis distance*[1] between any member of $\{x\}$ and m_x is given by the familiar equation [1]

$$R(x,m_x) = (x - m_x)^T C_y^{-1}(x - m_x) \tag{1}$$

and similarly,

$$R(y,m_y) = (y - m_y)^T C_x^{-1}(y - m_y), \tag{2}$$

where T indicates the transpose.

As indicated in the previous section, (1) and (2) have been applied extensively in pattern recognition. In this work, we are interested in characterizing the *interclass Mahalanobis distance* between members of x and the mean m_y, which is given by

$$R(x,m_y) = (x - m_y)^T C_y^{-1}(x - m_y) \tag{3}$$

and similarly,

$$R(y,m_x) = (y - m_x)^T C_x^{-1}(y - m_x). \tag{4}$$

For any nonsingular, real transformation matrix A, it is easily shown that if

$$r = Ax \tag{5}$$

and

$$s = Ay \tag{6}$$

then r and s are Gaussian random variables with mean vectors

$$m_r = Am_x \tag{7}$$

$$m_s = Am_y \tag{8}$$

and covariance matrices

$$C_r = AC_xA^T \tag{9}$$

$$C_s = AC_yA^T. \tag{10}$$

It is also easily shown that

$$R(r,m_s) = R(x,m_y) \tag{11}$$

and

$$R(s,m_r) = R(y,m_x). \tag{12}$$

Furthermore, as described in [6] and [16], the transformation matrix A can be chosen so that

$$C_r = AC_xA^T = I \tag{13}$$

and

$$C_s = AC_yA^T = D \tag{14}$$

where I is the identity matrix and D is a diagonal matrix with elements $\gamma(i)$, $i = 1,2,\cdots,d$, along the main diagonal.[2] The elements $\gamma(i)$ are the eigenvalues of $C_x^{-1}C_y$. From (13), it is noted that the elements of r are uncorrelated which, in view of our Gaussian assumption, implies statistical independence. The same holds true for the elements of s.

Using (3), (11), and (14), it follows that

$$\begin{aligned} R(x,m_y) &= R(r,m_s) \\ &= (r - m_s)^T D^{-1}(r - m_s) \\ &= \sum_{i=1}^{d} (r_i - m_{si})^2 \gamma^{-1}(i), \end{aligned} \tag{15}$$

where r_i and m_{si}, $i = 1,2,\cdots,d$, are the components of vectors r and m_s, respectively. Since r is a Gaussian random vector and $C_r = I$, we have that the variable $z_i = (r_i - m_{si})$ is Gaussian with mean $(m_{ri} - m_{si})$ and unit variance. It then follows [9] that

$$w_i = z_i^2 = (r_i - m_{si})^2 \tag{16}$$

is a non-central chi-square variable with density

$$p(w_i) = e^{-\lambda_i} \sum_{k=0}^{\infty} \frac{\lambda_i^k w_i^{(1+2k)/2} e^{-w_i/2}}{k! 2^{(1+2k)/2} \Gamma\left(\frac{1+2k}{2}\right)} \tag{17}$$

and moment generating function

$$\phi_{w_i}(t) = e^{-\lambda_i} \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!}(1 - 2t)^{-(1+2k)/2} \tag{18}$$

where

$$\lambda_i = \frac{1}{2}(m_{ri} - m_{si})^2. \tag{19}$$

Since r_i, $i = 1,2,\cdots,d$, are statistically independent, it follows that the w_i defined in (16) are also statistically independent.

[1]This is in reality a *squared* distance. However, it has become customary to refer to this measure simply as the *Mahalanobis distance*.

[2]Although diagonalization is not required in our final results, (13) and (14) are used in proving the theorem given in the next section.

A similar development can be carried out for $R(y, m_x)$:

$$R(y, m_x) = R(s, m_r) = (s - m_r)^T I^{-1}(s - m_r) = \sum_{i=1}^{d} (s_i - m_{ri})^2. \tag{20}$$

The variable $z_i = (s_i - m_{ri})/\sqrt{\gamma(i)}$ is Gaussian with mean $(m_{si} - m_{ri})/\sqrt{\gamma(i)}$ and unit variance. As above, the variable

$$w_i = z_i^2 = \frac{1}{\gamma(i)}(s_i - m_{ri})^2 \tag{21}$$

has the density and moment generating function given in (17) and (18), but λ_i is now given by

$$\lambda_i = \frac{1}{2\gamma(i)}(m_{si} - m_{ri})^2. \tag{22}$$

III. Semi-Invariants of the Interclass Mahalanobis Distance

One of the most important properties of the semi-invariants is that the nth semi-invariant of a sum of independent random variables is equal to the sum of the n semi-invariants of the individual variables [10], [11]. As will be seen in the following discussion, this property leads to a straightforward procedure for computing the semi-invariants of the interclass Mahalanobis distance, using only the original mean vectors and inverse covariance matrices of the given populations.

A. Semi-invariants of w_i.

We first obtain the semi-invariants of w_i and then extend the results to the general case involving R. The nth semi-invariant of a random variable w_i with moment generating function $\phi_{w_i}(t)$ is defined [14] as

$$X_n(w_i) = \frac{\partial^n}{\partial t^n}\left[\ln \phi_{w_i}(t)\right]_{t=0}. \tag{23}$$

Use of (18) in this definition leads to the following result involving λ_i.

Lemma: The nth semi-invariant of w_i is given by the expression

$$X_n(w_i) = 2^{n-1}(n-1)![1 + 2n\lambda_i]. \tag{24}$$

Proof: From (18)

$$\phi_{w_i}(t) = e^{-\lambda_i} \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!}(1-2t)^{-(1+2k)/2} = e^{-\lambda_i}(1-2t)^{-1/2} \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!}(1-2t)^{-k} = e^{-\lambda_i}(1-2t)^{-1/2} \sum_{k=0}^{\infty} \frac{1}{k!}\left(\frac{\lambda_i}{1-2t}\right)^k.$$

The infinite summation is recognized as the Taylor expansion of $e^{\lambda_i/(1-2t)}$; therefore

$$\phi_{w_i}(t) = e^{-\lambda_i}(1-2t)^{-1/2} e^{\lambda_i/(1-2t)}. \tag{25}$$

Use of (23) yields

$$X_n(w_i) = \frac{\partial^n}{\partial t^n}\left[\ln e^{-\lambda_i} + \ln(1-2t)^{-1/2} + \frac{\lambda_i}{1-2t}\right]_{t=0} = \frac{\partial^n}{\partial t^n}\left[\ln(1-2t)^{-1/2}\right]_{t=0} + \frac{\partial^n}{\partial t^n}\left[\frac{\lambda_i}{1-2t}\right]_{t=0} = 2^{n-1}(n-1)! + 2^n n!\lambda_i = 2^{n-1}(n-1)![1 + 2n\lambda_i].$$

This concludes the proof.

As an illustration, the first five semi-invariants of w_i are

$$X_1(w_i) = 1 + 2\lambda_i$$
$$X_2(w_i) = 2 + 8\lambda_i$$
$$X_3(w_i) = 8 + 48\lambda_i$$
$$X_4(w_i) = 48 + 384\lambda_i$$
$$X_5(w_i) = 384 + 3840\lambda_i. \tag{26}$$

B. Semi-invariants of R

The semi-invariants of the interclass Mahalanobis distance $R(x, m_y)$ are given by the following theorem.

Theorem: The nth semi-invariants of $R(x, m_y)$ and $R(y, m_x)$ are given, respectively, by

$$X_n[R(x, m_y)] = 2^{n-1}(n-1)!\left[\operatorname{tr}\left\{\left(C_y^{-1}C_x\right)^n\right\} + n(m_x - m_y)^T C_y^{-1}\left(C_x C_y^{-1}\right)^{n-1}(m_x - m_y)\right] \tag{27}$$

and

$$X_n[R(y, m_x)] = 2^{n-1}(n-1)!\left[\operatorname{tr}\left\{\left(C_x^{-1}C_y\right)^n\right\} + n(m_y - m_x)^T C_x^{-1}\left(C_y C_x^{-1}\right)^{n-1}(m_y - m_x)\right]. \tag{28}$$

Proof: From (15) and (16)

$$R(x, m_y) = \sum_{i=1}^{d} w_i \gamma^{-1}(i).$$

Since the nth semi-invariant of a sum of independent random variables is the sum of the semi-invariants, and $X_n[w_i\gamma^{-1}(i)] = X_n(w_i)\gamma^{-n}(i)$ [10], we have

$$X_n[R(x, m_y)] = \sum_{i=1}^{d} X_n(w_i)\gamma^{-n}(i). \tag{29}$$

Then, from the lemma in Section III-A,

$$X_n[R(x, m_y)] = \sum_{i=1}^{d} 2^{n-1}(n-1)![1 + 2n\lambda_i]\gamma^{-n}(i) = 2^{n-1}(n-1)! \sum_{i=1}^{d} \gamma^{-n}(i) + 2^n n! \sum_{i=1}^{d} \lambda_i \gamma^{-n}(i). \tag{30}$$

Since $\gamma(i)$, $i = 1, 2, \cdots, d$ are the eigenvalues of $C_x^{-1}C_y$, the sum of the eigenvalues $\gamma^{-n}(i)$ for $i = 1, 2, \cdots, d$, is the trace of $(C_y^{-1}C_x)^n$. Modifying (30) by this observation, and using the definition of λ_i given in (19), yields

$$X_n[R(x, m_y)] = 2^{n-1}(n-1)! \operatorname{tr}\left\{\left(C_y^{-1}C_x\right)^n\right\} + 2^{n-1}n! \sum_{i=1}^{d} \frac{(m_{ri} - m_{si})^2}{\gamma^n(i)}. \tag{31}$$

The summation in (31) may be expressed as

$$\sum_{i=1}^{d} \frac{(m_{ri} - m_{si})^2}{\gamma^n(i)} = (m_r - m_s)^T (D^{-1})^n (m_r - m_s). \tag{32}$$

However, from (7) and (8),

$$(m_r - m_s) = A(m_x - m_y) \tag{33}$$

and, from (14),

$$(D^{-1})^n = \left[\left(AC_yA^T\right)^{-1}\right]^n = \left[(A^T)^{-1}C_y^{-1}A^{-1}\right]^n.$$

Expansion of the right side of this equation yields

$$\left[(A^T)^{-1}C_y^{-1}A^{-1}\right]^n = (A^T)^{-1}C_y^{-1}A^{-1}(A^T)^{-1}C_y^{-1}A^{-1}\cdots(A^T)^{-1}C_y^{-1}A^{-1}$$

But from (13), $A^{-1}(A^T)^{-1} = C_x$, so that

$$(D^{-1})^n = (A^T)^{-1}C_y^{-1}\left(C_xC_y^{-1}\right)^{n-1}A^{-1}. \quad (34)$$

By substituting (33) and (34) into (31) we obtain

$$\sum_{i=1}^{d}\frac{(m_{ri}-m_{si})^2}{\gamma^n(i)} = (m_x-m_y)^TC_y^{-1}\left(C_xC_y^{-1}\right)^{n-1}(m_x-m_y). \quad (35)$$

Finally, substituting this result into (31) completes the proof of (27).

The proof of (28) follows essentially the same line of reasoning, with the exception that it involves $\gamma^n(i)$ instead of $\gamma^{-n}(i)$, and the definitions of w_i and λ_i are different, as given in (21) and (22). From (20) and (21) and the distributive properties of the semi-invariants stated earlier,

$$X_n[R(y,m_x)] = \sum_{i=1}^{d}X_n(w_i)\gamma^n(i), \quad (36)$$

and, from the lemma in Section III-A,

$$X_n[R(y,m_x)] = \sum_{i=1}^{d}2^{n-1}(n-1)![1+2n\lambda_i]\gamma^n(i). \quad (37)$$

The validity of the trace portion of (28) follows directly from the fact that $\gamma^n(i)$ are eigenvalues of $(C_x^{-1}C_y)^n$. To prove the validity of the second term on the right side of (28), we note that

$$2^nn!\sum_{i=1}^{d}\lambda_i\gamma^n(i) = 2^{n-1}n!\sum_{i=1}^{d}(m_{si}-m_{ri})^2\gamma^{n-1}(i). \quad (38)$$

The summation term can be expressed as

$$\sum_{i=1}^{d}(m_{si}-m_{ri})^2\gamma^{n-1}(i) = (m_x-m_y)^TA^TD^{n-1}A(m_x-m_y). \quad (39)$$

Expansion of the matrix D^{n-1} (see (14)) gives

$$D^{n-1} = AC_yA^TAC_yA^T\cdots AC_yA^T. \quad (40)$$

However, from (13), $A^TA = C_x^{-1}$. Using this fact in (40) and (39) completes the proof.

It is important to note that the semi-invariants in (27) and (28) are given directly in terms of the original population parameters m_x, m_y, C_x, and C_y and, therefore, do not require computation of the transformation matrix A.

C. Special Cases

In this section we consider special cases involving various arrangements of mean vectors and covariance matrices of two populations.

Equal Covariance Matrices: For equal covariance matrices, $C_x = C_y = C$, it is easily shown that (27) and (28) reduce to

$$X_n\left[R(x,m_y)\right] = X_n[R(y,m_x)] = 2^{n-1}(n-1)!\cdot\left[d+n(m_x-m_y)^TC^{-1}(m_x-m_y)\right]. \quad (41)$$

Equal Mean Vectors: When $m_x = m_y$, we have from (27) and (28) that

$$X_n\left[R(x,m_y)\right] = 2^{n-1}(n-1)!\left[\mathrm{tr}\left\{\left(C_y^{-1}C_x\right)^n\right\}\right] \quad (42)$$

and

$$X_n[R(y,m_x)] = 2^{n-1}(n-1)!\left[\mathrm{tr}\left\{\left(C_x^{-1}C_y\right)^n\right\}\right]. \quad (43)$$

Equal Mean Vectors and Covariance Matrices (Intraclass Mahalanobis Distance): In this case we are considering the same Gaussian population and obtain the semi-invariants by letting $x = y$, $m_x = m_y$, $C_x = C_y$ in either (27) or (28). This results in the simple expression

$$X_n[R(x,m_x)] = 2^{n-1}(n-1)!d \quad (44)$$

which depends only on the order of the semi-invariant and the dimensionality of the vectors.

IV. Obtaining the Moments from the Semi-Invariants

The nth moment α_n of the interclass Mahalanobis distance can be obtained directly from the semi-invariants $X_1, X_2, \cdots, X_n$ by using the expression

$$\alpha_n = \sum\frac{n!}{a_1!a_2!\cdots a_n!}\prod_{r=1}^{n}[X_r/r!]^{a_r} \quad (45)$$

where the sum is taken over values of a_i such that $a_1 + 2a_2 + \cdots + na_n = n$ [11]. Equation (45) can be used to obtain the moments of either w_i or R, given the semi-invariants corresponding to one of these two variables [11]. A similar relationship exists for computing the semi-invariants given the moments [11].

As an illustration of the above relationship we have

$$\alpha_1 = X_1$$
$$\alpha_2 = X_2 + X_1^2$$
$$\alpha_3 = X_3 + 3X_1X_2 + X_1^3$$
$$\alpha_4 = X_4 + 4X_1X_3 + 3X_2^2 + 6X_1^2X_2 + X_1^4.$$

A direct implementation of (45) in a digital computer is inherently inefficient, involving, among other things, the determination of all n tuples of nonnegative integers $(a_1,\cdots,a_n)$ satisfying $a_1 + 2a_2 + \cdots na_n = n$. Fortunately, there is a very efficient recursive algorithm, described below, for computing these moments.

Let

$$Z_n = X_n/n!2^n \quad (46)$$

where X_n is given by (27) or (28), as determined by the relevant semi-invariant. Under this change of variables (45) becomes

$$\alpha_n = \sum\frac{n!}{a_1!\cdots a_n!}\prod_{r=1}^{n}(2^rZ_r)^{a_r} = n!2^n\sum\prod_{r=1}^{n}(Z_r^{a_r}/a_r!) \quad (47)$$

taken over all n tuples of nonnegative integers $(a_1,\cdots,a_n)$ satisfying $a_1 + 2a_2 + \cdots + na_n = n$. If we define a rectangular array $\beta(n,k)$ by

$$\beta(n,k) = \sum\prod_{r=1}^{n}(Z_r^{a_r}/a_r!), \qquad n \geqslant 0, \qquad k \geqslant 1 \quad (48)$$

taken over all k tuples of nonnegative integers $(a_1,\cdots,a_k)$ satisfying $a_1 + 2a_2 + \cdots + ka_k = n$, then by (47)

$$\alpha_n = n!2^n\beta(n,n), \qquad n \geqslant 1, \quad (49)$$

so that the quantities α_n may easily be computed from the

TABLE I
$\beta(n,k)$: $0 \leqslant n \leqslant 3, 1 \leqslant k \leqslant 3$

n \ k	1	2	3
0	1	1	1
1	Z_1	Z_1	Z_1
2	$Z_1^2/2$	$Z_1^2/2 + Z_2$	$Z_1^2/2 + Z_2$
3	$Z_1^3/6$	$Z_1^3/6 + Z_1 Z_2$	$Z_1^3/6 + Z_1 Z_2 + Z_3$

elements lying just below the main diagonal (the main diagonal elements of $\beta(n,k)$ are $\beta(n-1,n)$, since $n \geqslant 0$ and $k \geqslant 1$) of the arrays $\beta(n,k)$.

It is clear from (48) that

$$\beta(0,k) = 1, \qquad k \geqslant 1 \tag{50}$$

that

$$\beta(n,1) = Z_1^n/n!, \qquad n \geqslant 0 \tag{51}$$

and that

$$\beta(n,k) = \beta(n,n), \qquad k > n > 0. \tag{52}$$

The remaining elements of the array $\beta(n,k)$ are generated by the recurrence relation

$$\beta(n,k) = \sum_{j=0}^{[n/k]} \beta(n-jk, k-1) Z_k^j/j! \tag{53}$$

where $[n/k]$ denotes the greatest integer $\leqslant n/k$. Hence the elements in column k of the array $\beta(n,k)$ are just linear combinations of certain elements in column $k-1$. Equation (53) is justified by observing that the nonnegative integral solutions of $a_1 + 2a_2 + \cdots + \mathrm{k}a_k = n$ may be partitioned according to the possible values $j = 0,1,\cdots,[n/k]$ of a_k, the terms in (53) corresponding to those $[n/k]+1$ possible values of a_k. Values of $\beta(n,k)$ for $0 \leqslant n \leqslant 3$ and $1 \leqslant k \leqslant 3$ are listed in Table I.

V. Conclusion

The expressions given in (27) and (28) provide a straight-forward solution to the problem of computing the semi-invariants of the interclass Mahalanobis distance. As indicated in Section I, the semi-invariants are useful descriptions of the underlying interclass distance pdf.

Although the semi-invariants do not in general have the familiar "physical" interpretation possessed by the moments (e.g., spread, skew, and curtosis), the distributive property of the semi-invariants resulted in a computational procedure involving only the mean vectors and inverse covariance matrices of two populations, without the need for the simultaneous diagonalization required to obtain the moments [17]. The algorithm given in Section IV provides a rather simple iterative technique for computing the moments once the semi-invariants have been obtained via (27) and (28).

The semi-invariants were considerably simplified in the special cases discussed in Section III-C. In particular, the semi-invariants of the intraclass Mahalanobis distance was shown to be dependent only on the order of the semi-invariants and on the dimensionality of the vector populations.

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