# Feature Selection Via an Upper Bound (to Any Degree Tightness) on Probability of Misclassification 

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## FEATURE SELECTION VIA AN UPPER BOUND (TO ANY

DEGREE TIGHTNESS) ON PROBABILITY OF MISCLASSIFICATION

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#### Abstract

I. ABSTRACT

Currently, many techniques exist for feature selection purposes which are related but, unfortunately, in an indeterminable way to the probability of misclassification. In this paper a procedure is presented which yields an upper bound (to any degree tightness) on the probability of misclassification in sample Gaussian maximum likelihood classification between each pair of categories in p-dimensional space. The technique permits features to be selected so that the optimal $q$ ( $q \leq p$ ) features have the property that no other subset of $q$ features yield a smaller value to the upper bound on the probability of misclassification. A computer-assessible transformation is utilized which permits a multiple integral over the misclassification region in p-dimensional space to be approximated, to any degree of accuracy, by the product of $p$ iterated integrals, each over univariate space, and each of which may be obtained by a simple table-look-up procedure. Quite often, transformations are used without consideration of loss of information; however, the one utilized in this procedure results in no loss of information and leaves the standard likelihood ratio invariant in value.


## II. INTRODUCTION

There seems to be general agreement among remote sensing community personnel, and classification theorists in general, that the cost function which has applicable meaning to the user scientist is expected cost of misclassification. Any procedure, then, which is optimal for feature selection purposes should be one which minimizes this cost function. A popular (and realistic) assumption in almost all remote sensing applications is that the costs of misclassifying an individual from category $C_{i}$ as being from category $C_{j}$, $i \neq j=1,2, \ldots, m$, are equal, in which case the expected cost of misclassification reduces to probability of misclassification. Currently, many techniques exist for feature selection purposes (eigenvalue/eigenvector techniques (Chien and Fu, 1968) including factor analysis and principal components, standard regression techniques, wilk's scatter technique (Wilks, 1962), the divergence criterion (Marill and Green, 1963), Sammon's nonlinear mapping (Sammon, 1970), LaMotte-Hocking regression techniques (LaMotte and Hocking, 1970), the Battacharyya distance measure (Kailath, 1967), the Matusita distance (Matusita, 1966), the concept of equivocation (Babu, 1972), and others, including trial-and-error approaches with sets of features with varied composition) which are related but, unfortunately, in an indeterminable way to the probability of misclassification. In this paper a procedure is presented which yields an upper bound (to any degree desired tightness) on the probability of "misclassification in sample Gaussian maximum likelihood classification between each pair of categories in p-dimensional space. The technique permits features to be selected
between pairs of categories so that the optimal $q$ ( $q \leq p$ ) features have the property that no other subset of $q$ features yields a smaller value to the upper bound on the probability of misclassification. A simple, computer-assessible transformation is utilized which permits a multiple integral over the misclassification region in p-dimensional space to be approximated, to any degree of accuracy, by the product of $p$ iterated integrals, each over univariate space, and each of which may be obtained by a simple table-look-up procedure. The utility of this transformation in the classification processing phase of pattern recognition recently appeared in the literature (Minter and Hallum, 1972) and, unlike many transformations which are used without consideration of loss of information, the one utilized herein results in no loss of information and leaves the standard likelihood ratio invariant in value.

## III. TRANSFORMATION TO AN EQUIVALENT PATTERN

## RECOGNITION SPACE

Let $C_{\text {i }}$ and $C_{j}$ be two categories ( $i \neq j$ ) which have the Gaussian distribution with respective densities

$$
\begin{equation*}
P\left(X \mid C_{i}\right)=\frac{1}{(2 \pi)^{p / 2}\left|\hat{M}_{i}\right|^{1 / 2}} \exp \left\{-1 / 2\left(x-\hat{U}_{i}\right)^{T} \hat{M}_{i}^{-1}\left(x-\hat{U}_{i}\right)\right\} \tag{1}
\end{equation*}
$$

and

$$
\begin{equation*}
P\left(x \mid c_{j}\right)=\frac{1}{(2 \pi)^{\mathrm{Q}} / 2}\left|\hat{M}_{j}\right|^{1 / 2} \exp \left\{-1 / 2\left(x-\hat{U}_{j}\right)^{T} \hat{M}_{j}^{-1}\left(x-\hat{U}_{j}\right)\right\} \tag{2}
\end{equation*}
$$

where $\hat{U}_{i}$ and $\hat{U}_{j}$ are the respective sample means, $\hat{M}_{j}$ and $\hat{M}_{j}$ are the sample variancecovariance matrices. Transforming to a new space by the nonsingular transformation $Q$, where $Q$ is the matrix with the property

$$
Q^{T} \hat{M}_{i} Q=D ; \quad Q^{T} \hat{M}_{j} Q=I
$$

(D is a diagonal matrix and $I$ the identity matrix), the likelihood ratio (assuming the classification scheme is Bayes with equal a priori class probabilities and with cost matrix elements $c_{i j}=c-c \delta_{i j}$, where $c$ is a constant and $\delta_{i j}$ is the Kronecker delta) of $P\left(X \mid C_{i}\right)$ to $P\left(X \mid C_{j}\right)$ takes the form

$$
\begin{align*}
& \frac{P\left(X \mid C_{i}\right)}{P\left(X \mid C_{j}\right)}=\frac{\frac{1}{(2 \pi)^{\mathrm{P} / 2}\left|\hat{M}_{i}\right|^{1 / 2} \exp \left\{-1 / 2\left(X-\hat{U}_{i}\right)^{T} \hat{M}_{i}^{-1}\left(X-\hat{U}_{i}\right)\right.}}{\frac{1}{(2 \pi)^{p / 2}\left|\hat{M}_{j}\right|^{1 / 2} \exp \left\{-1 / 2\left(X-\hat{U}_{j}\right)^{T} \hat{M}_{j}^{-1}\left(x-\hat{U}_{j}\right)\right\}}} \\
& =\frac{\frac{1}{(2 \pi)^{\mathrm{P} / 2}\left|Q^{\mathrm{T}} \hat{\mathrm{M}}_{i} Q\right|^{1 / 2} \exp \left\{-1 / 2\left(X-\hat{U}_{i}\right)^{T}\left(Q^{T^{-1}} Q^{T} \hat{M}_{i} Q Q^{-1}\right)^{-1}\left(X-\hat{U}_{i}\right)\right\}}}{\frac{1}{(2 \pi)^{\mathrm{P} / 2}\left|Q^{T} \hat{\mathrm{M}}_{j} Q\right|^{1 / 2}} \exp \left\{-1 / 2\left(X-\hat{U}_{j}\right)^{T}\left(Q^{T}{ }^{-1} Q^{T} \hat{M}_{j} Q Q^{-1}\right)^{-1}\left(X-\hat{U}_{j}\right)\right\}}  \tag{3}\\
& \frac{1}{(2 \pi)^{\mathrm{P} / 2}|\mathrm{D}|^{1 / 2}} \exp \left\{-1 / 2\left(Q^{T} \mathrm{X}-Q^{T} \hat{U}_{i}\right)^{T} D^{-1}\left(Q^{T} X-Q^{T} \hat{U}_{i}\right)\right\} \\
& =\frac{1}{(2 \pi)^{p / 2} \exp \left\{-1 / 2\left(Q^{T} X-Q^{T} \hat{U}_{j}\right)^{T}\left(Q^{T} X-Q^{T} \hat{U}_{j}\right)\right\}}
\end{align*}
$$

$$
\begin{aligned}
& =\frac{\frac{1}{(2 \pi)^{p / 2}|D|^{1 / 2} \exp \left\{-1 / 2(z-V)^{T} D^{-1}(z-V)\right\}}}{\frac{1}{(2 \pi)^{p / 2}} \exp \left\{-1 / 2(Z-W)^{T}(Z-W)\right\}}=\frac{f\left(Z \mid C_{i}\right)}{f\left(Z \mid C_{j}\right)} \\
& =\stackrel{p}{k}_{=}^{=} \frac{p_{k i}\left(z_{k}\right)}{p_{k j}\left(z_{k}\right)}
\end{aligned}
$$

where $p_{k i}\left(z_{k}\right)$ and $p_{k j}\left(z_{k}\right)$ are the univariate normal densities

$$
\begin{align*}
& \mathrm{p}_{\mathrm{ki}}\left(\mathrm{z}_{\mathrm{k}}\right)=\frac{1}{(2 \pi)^{1 / 2} \mathrm{~d}_{\mathrm{k}}} \exp \left\{-1 / 2\left(\mathrm{z}_{\mathrm{k}}-\mathrm{v}_{\mathrm{k}}\right)^{2} / \mathrm{d}_{\mathrm{k}}^{2}\right\} ;  \tag{4}\\
& \mathrm{p}_{\mathrm{kj}}\left(\mathrm{z}_{\mathrm{k}}\right)=\frac{1}{(2 \pi)^{1 / 2} \exp \left\{-1 / 2\left(\mathrm{z}_{\mathrm{k}}-\mathrm{w}_{\mathrm{k}}\right)^{2}\right\} .} \tag{5}
\end{align*}
$$

In the above, $\alpha_{k}^{2}$ is the $k$ th diagonal element of $D ; Z_{k}, V_{k}$, and $W_{k}$ are the $k$ th coordinates of the vectors $Z=\left(Z_{1}, Z_{2}, \ldots, Z_{p}\right)^{T}=Q^{T} X, V=\left(V_{1}, V_{2}, \ldots, V_{p}\right)^{T}=$ $Q^{T} \hat{U}_{i}$, and $W=\left(W_{1}, W_{2}, \ldots, W_{p}\right)^{T}=Q^{T} \hat{U}_{j}$, respectively. The utility of the transformation $Q$ in classification processing has already appeared (Minter and Hallum, 1972) in the literature, and it needs be stressed that $Q$ needs be obtained only once for each pair of categories for a given classification situation (such as a flight-line for classification). Moreover, observe that the invariance of the likelihood ratio (note equations (3)) guarantees that pattern classification in the original and the transformed space is equivalent.

To obtain $Q$ (see Minter and Hallum, 1972 , let $Q=P^{-1}$ o where $P$ is the Cholesky (Ratishauser, 1966) factorization of $M_{j}$, i.e. $M_{j}=P^{T} P$ where $P$ is upper triangular, and $O$ is the orthogonal transformation which diagonalizes the symmetric matrix

$$
\mathrm{p}^{-1} \hat{\mathrm{M}}_{\mathrm{i}} \mathrm{P}^{-1}
$$

Routines for obtaining $P$ and $O$ have been implemented for some time and are available via the IBM Scientific Subroutine Package (IBM Corp., 1970) and the Catalog of Mathematical Routines at NASA/MSC in Houston, Texas.

## IV. A FIRST DEGREE APPROXIMATION TO THE

## PROBABILITY OF MISCLASSIFICATION

In both the transformed and the untransformed space, the boundary of the misclassification region between categories $C_{i}$ and $C_{j}$ (defined by those points satisfying $\left.P\left(X \mid C_{i}\right) / P\left(X \mid C_{j}\right)=f\left(Z \mid C_{i}\right) / f\left(Z \mid C_{j}\right)=1\right)$ is always a hyperellipsoid or a hyper-hyperboloid. In the transformed space, this boundary is specified by the quadratic equation
which is the equation of a central conic whose center is located at the point with $k$ th coordinate $\left(d_{k}^{2} W_{k}-V_{k}\right) /\left(d_{k}^{2}-1\right)$ and whose principal axes are parallel to the coordinate axes. In the forthcoming development, the center will be utilized to obtain the smallest hyper-box, with sides parallel to the coordinate axes in the transformed space, which encloses the region of misclassification. Integration, then, over the region of misclassification is approximated to "first degree approximation" (which is sufficient in a large number of cases) by integrating over this box; moreover, the manner of integration for the total probability of misclassification between $C_{i}$ and $C_{j}$ is carried out in such a manner that the result-
ing value is always greater than or equal to the probability of misclassification.
The technique for "first degree approximation" for the case of a hyperellipsoidal region of misclassification is illustrated in Fig. 1 and 2 for two dimensions. The dashed line in Fig. 1 and 2 denotes the equi-probable line between $C_{i}$ and $C_{j}$ (specified by equation (6) with $p=2$ ) and is the boundary of the region
of misclassification. Figure 2 indicates what we would see in Fig. 1 by looking down on the $Z_{1}, Z_{2}$-plane from the $y$-direction. From Fig. 1 and 2 , the probability of misclassification is given by

$$
\begin{equation*}
P=\iint_{R} f\left(z \mid c_{i}\right) d z_{1} d z_{2}+\iint_{R} f\left(z \mid c_{j}\right) d z_{1} d z_{2} \tag{7}
\end{equation*}
$$

where $\tilde{R}$ denotes the region outside of $R$. In general, the determination of the function to be integrated over $R$ is accomplished by selecting the one having minimum value at the center point $C_{R}$ of $R$, which is simply the center of the conic
specified by equation (6); the remaining function is integrated over $\widetilde{R}$. As is well-known, in p-dimensional space the integration in (7) becomes extremely difficult, if not impossible, utilizing existing techniques. However, the points $a_{11}, a_{21}, a_{12}, a_{22}$ are easily obtained; in general, for p-dimensional space, $a_{1 j}$ and $a_{2 j}$ are obtained by putting all $z_{k}$, with the exception of $z_{j}$, in (6) equal to the corresponding coordinate of the center $C_{R}$, and solving the resulting univariate quadratic in $Z_{j}$ for $Z_{j}$. Applying the quadratic formula, the resulting two values of $z_{j}$ are denoted by $a_{1 j}$ and $a_{2 j}$ and are given by

$$
\begin{equation*}
a_{l j}=C_{R j}-\sqrt{T_{j}} ; \quad a_{2 j}=C_{R j}+\sqrt{T_{j}}, j=1,2, \ldots, p \tag{8}
\end{equation*}
$$

where

$$
\begin{equation*}
c_{R j}=\frac{d_{j}^{2} w_{j}-v_{j}}{d_{j}^{2}-1} \tag{9}
\end{equation*}
$$

is the $j \frac{\text { th }}{}$ coordinate $(j=1,2, \ldots, p)$ of the center of the conic specified in equation (6) and

$$
\begin{equation*}
T_{j}=C_{R j}^{2}-\frac{d_{j}^{2}}{1-d_{j}^{2}}\left\{-\frac{c_{R j}^{2}}{d_{j}^{2}}+\sum_{k=1}^{p}\left[C_{R k}^{2}+v_{k}^{2}-d_{k}^{2}\left(W_{k}^{2}+\ln d_{k}^{2}\right)\right] / d_{k}^{2}\right\} \tag{10}
\end{equation*}
$$

An upper bound approximation to the first integral in (7) is given by integrating over the box $B$, i.e.

$$
\begin{gather*}
\iint_{R} f\left(z \mid C_{i}\right) d z_{1} d z_{2}=\iint_{R} p_{1 i}\left(z_{1}\right) p_{2 i}\left(z_{2}\right) d z_{1} d z_{2} \\
\leqslant \int_{a_{11}}^{a_{21}} p_{1 i}\left(z_{1}\right) d z_{1} \int_{a_{12}}^{a} 22 \\
p_{2 i}\left(z_{2}\right) d z_{2}  \tag{11}\\
=\left[F\left(\frac{a_{21}-v_{1}}{d_{1}}\right)-F\left(\frac{a_{11}-v_{1}}{d_{1}}\right)\right]\left[F\left(\frac{a_{22}-v_{2}}{d_{2}}\right)-F\left(\frac{a_{12}-v_{2}}{d_{2}}\right)\right]
\end{gather*}
$$

where $F$ denotes the univariate, cumulative Gaussian distribution function with mean 0 and variance 1 and whose value may be obtained at the indicated points by referring to a normal distribution table (which could easily be stored for quick reference) or by utilizing one of the several efficient techniques which are available for estimating tail probabilities under the univariate Gaussian distribution curve. Note also that the right hand side of (ll) exceeds the true value of the multiple integral over $R$ by precisely the amount

$$
\begin{equation*}
\sum_{k=1}^{4} \int_{R_{k}} f\left(z \mid c_{i}\right) d z_{1} d z_{2} \tag{12}
\end{equation*}
$$

However, a portion of this excess is eliminated in determining the total probability of misclassification between categories $C_{i}$ and $C_{j}$ by noting that the second integral in (7) may be obtained as follows:

$$
\begin{equation*}
\iint_{\widetilde{R}} f\left(z \mid C_{j}\right) d z_{1} d z_{2}=1-\iint_{R} f\left(z \mid C_{j}\right) d z_{1} d z_{2} . \tag{13}
\end{equation*}
$$

Using the similar approximation as in (11).

$$
\begin{align*}
& \iint_{R} f\left(z \mid c_{j}\right) d z_{1} d z_{2} \leqslant \int_{a_{11}}^{a_{21}} p_{1 j}\left(z_{1}\right) d z_{1} \int_{a_{12}}^{a_{22}} p_{2 j}\left(z_{2}\right) d z_{2} \\
= & {\left[F\left(a_{21}-W_{1}\right)-F\left(a_{11}-w_{1}\right)\right]\left[F\left(a_{22}-w_{2}\right)-F\left(a_{12}-W_{2}\right)\right] } \tag{14}
\end{align*}
$$

and the right-hand side of (14) exceeds the true value by precisely the amount

$$
\begin{equation*}
\sum_{k=1}^{4} \int_{R_{k}} f\left(z \mid C_{j}\right) d z_{1} d z_{2} \tag{15}
\end{equation*}
$$

However, $f\left(Z \mid C_{i}\right) \geqslant f\left(Z \mid C_{j}\right)$ for all $z$ over the regions $R_{1}, R_{2}, R_{3}$, and $R_{4}$, there-
fore the upper bound estimate to "first degree approximation" of the probability of misclassification is given by

$$
\begin{gather*}
\iint_{B} f\left(z \mid C_{i}\right) d z_{1} d z_{2}+1-\iint_{B} f\left(z \mid c_{j}\right) d z_{1} d z_{2} \\
=\left(\iint_{R} f\left(z \mid C_{i}\right) d z_{1} d z_{2}+1-\iint_{R} f\left(z \mid c_{j}\right) d z_{1} d z_{2}\right)+\varepsilon \\
=P+\varepsilon \tag{16}
\end{gather*}
$$

where $\varepsilon$ is the non-negative quantity which represents the over-estimate of the probability, $P$, of misclassification and is given by

$$
\begin{equation*}
\varepsilon=\sum_{k=1}^{4} \iint_{R_{k}}\left(f\left(z \mid C_{i}\right)-f\left(z \mid C_{j}\right)\right) d z_{1} d z_{2} \tag{17}
\end{equation*}
$$

The preceding discussion was for the case of a hyperellipsoidal region of misclassification, however the same discussion applies verbatim as well to the case of a hyper-hyperboloidal region of misclassification where, for the two-dimensional case, $R_{1}, R_{2}, R_{3}$, and $R_{4}$ are specified in Fig. 3 and $a_{11}=-\infty, a_{21}=\infty$.

In general, the misclassification region will be hyper-hyperboloidal provided $\mathrm{T}_{\mathrm{j}}<0$ in (10) for at least one value of $j=1,2, \ldots, p$, in which case, $a_{1 j}=-\infty$ and $a_{2 j}$ $=\infty$ for each such j.

Utilizing the "first-degree approximation," feature selection is easily implemented by ordering the features as follows: for $m, n \in\{1,2, \ldots, p\}$, feature $\mathrm{Z}_{\mathrm{m}}$ is preferable to feature $\mathrm{Z}_{\mathrm{n}}$ provided

$$
\begin{align*}
& {\left[F\left(\frac{a_{2 m}-V_{m}}{d_{m}}\right)-F\left(\frac{a_{1 m}-V_{m}}{d_{m}}\right)\right]+1-\left[F\left(a_{2 m}-W_{m}\right)-F\left(a_{1 m}-W_{m}\right)\right] } \\
\leqslant & {\left[F\left(\frac{a_{2 n}-v_{n}}{d_{n}}\right)-F\left(\frac{a_{1 n}-V_{n}}{d_{n}}\right)\right]+1-\left[F\left(a_{2 n}-W_{n}\right)-F\left(a_{1 n}-W_{n}\right)\right] . } \tag{18}
\end{align*}
$$

After ordering the coordinates in the above manner, denote them by ${ }^{2}(1), Z_{(2)} \ldots$. $Z_{(p)}$; if we want to achieve a probability of misclassification not to exceed a preset value $\boldsymbol{\alpha}$, we select the first $k$ ordered coordinates such that

$$
\begin{equation*}
\prod_{n=1}^{k-1} p(n)>\alpha \tag{19}
\end{equation*}
$$

but

$$
\prod_{n=1}^{k} p(n) \leqslant \alpha
$$

where

$$
\begin{aligned}
& P_{(n)}= {\left[F\left(\frac{a_{2(n)}-V_{(n)}}{d_{(n)}}\right)-F\left(\frac{a_{1(n)}-V_{(n)}}{d_{(n)}}\right)\right]+} \\
& 1-\left[F\left(a_{2(n)}-W_{(n)}\right)-F\left(a_{1(n)}-W_{(n)}\right)\right]
\end{aligned}
$$

for $n=1,2, \ldots$, If $\prod_{n=1}^{p} P(n)>\boldsymbol{\alpha}$ then the conclusion is, to the "first-degree approximation," there is reason to doubt that it is possible to classify with this probability of misclassification. We do know, however, that it is possible to distinguish, using the first $k$ ordered features, between categories $C_{i}$ and $C_{j}$ with probability of ${ }^{\circ}$ misclassification not to exceed the value of the left side of (20).

## V. AN UPPER BOUND (TO ANY DEGREE TIGHTNESS) <br> ON PROBABILITY OF MISCLASSIFICATION

The previous section summarizes the approach for a "first-degree approximation" to the probability of misclassification and provides an upper bound estimate which, in many instances, will be sufficient. The procedure may be generalized further to obtain as tight an upper bound on the probability of misclassification as one chooses. In the following, explicit expressions are given for upper bound estimates, to any degree of desired tightness, for each of the two possible regions of misclassification.

## A. A HYPERELLIPSOIDAL REGION OF MISCLASSIFICATION

In general, the region of misclassification in $p$-dimensional space will be hyperellipsoidal provided

$$
\begin{equation*}
T_{j}>0 \text { for each } j=1,2, \ldots, p, \tag{21}
\end{equation*}
$$

(or equivalently, if $d_{k}^{2}-1$ is of the same sign for all $k=1,2, \ldots, p$ ) where $T_{j}$ is given by equation (10). To aid in following the discussion below, refer to Fig. 4 for the case of two dimensions.

Utilizing the coordinates of the center of the conic of equation (6), increments along a principal axis can be made and, e.g. in two-dimensional space, the points

$$
a_{12}^{(1)}, a_{22}^{(1)}, a_{12}^{(2)}, a_{22}^{(2)}, a_{12}^{(3)}, a_{22}^{(3)}, \ldots, a_{12}^{(k)}, a_{22}^{(k)}, \ldots, a_{12}^{(N-1)}, a_{22}^{(N-1)}
$$

(e.g., in Fig. $4 \mathrm{~N}=6$ ) easily obtained by repeated application of the quadratic formula. In general, if $z_{1}, z_{2} \ldots\left(z_{q}\right.$ is a given subset of $q$ features ( $q \leqslant p$ ) of p-dimensional space, the notation $a_{i j} k_{1} \ldots, k_{q}$ will be used to represent the $i$ th of the two $j$ th coordinate values (lower coordinate value if $i=1$, upper value
if $i=2$ ) of the point on the boundary of the region of misclassification obtained after moving a distance of $k_{1} \Delta$ from $a_{11}$ to $a_{21}$, a distance of $k_{2} \Delta$ from $a_{12}$ to $a_{22}$, $\ldots$... and a distance of $k_{q} \Delta$ from $a_{l q}$ to $a_{2 q}$. The increment length $\Delta$ might, for example, be $\Delta=\max _{n}\left|a_{2 n}-a_{1 n}\right| / N$. Requiring $N$ to be an even integer in the following will simplify the problem of making certain the region over which integration is carried out completely encloses the region of misclassification. For a particular $j \in\{1,2, \ldots, q\}$, the two values (i.e. for $i=1,2$ ) of $a_{i j}^{\left(k_{1}, \ldots, k_{q}\right)}$ are obtained by replacing the $z_{k}$ 's in equation (6), with the exception of the $j$ th, by the coordinates of the point obtained after moving a distance of $k_{1} \Delta$ from $a_{11}$ toward $a_{12}$, a distance of $k_{2} \Delta$ from $a_{12}$ to $a_{22}, \ldots$, and a distance of $k_{q} \Delta$ from $a_{1 q}$ to $a_{2 q}$, and solving the resulting quadratic in $z_{j}$ for $Z_{j}$ using the quadratic for-


$$
\begin{align*}
& { }_{a_{1 j}\left(k_{1}, \ldots, k_{q}\right)}=c_{R j}-\sqrt{\left.c_{R j}^{2}-\frac{v_{j}^{2}-d_{j}^{2}\left(W_{j}^{2}+R_{j}\left(k_{1}, \ldots, k_{q}\right)\right.}{1-d_{j}^{2}}\right)}  \tag{22}\\
& { }_{\left({ }_{2 j} k_{1}, \ldots, k_{q}\right)}^{a_{2 j}}=c_{R j}+\sqrt{c_{R j}^{2}-\frac{v_{j}^{2}-d_{j}^{2}\left(W_{j}^{2}+R_{j}^{\left(k_{1}\right.}, \ldots, k_{q}\right)}{1-d_{j}^{2}}} \tag{23}
\end{align*}
$$

where

$$
\begin{gather*}
{R_{j}}_{\left(k_{1}, \ldots, k_{q}\right)=\ln \prod_{k=1}^{q} d_{k}^{2}-\sum_{i \neq j}^{q}\left[\left(\frac{a_{1 i}+k_{i}-v_{i}}{d_{i}}\right)^{2}+\left(a_{1 i}+k_{i}-w_{i}\right)^{2}\right]} \begin{array}{c}
-\left[\left(\frac{C_{R j}-v_{j}}{d_{j}}\right)^{2}-\left(C_{R j}-w_{j}\right)^{2}\right]
\end{array} . \tag{24}
\end{gather*}
$$

The ( $N$ - 1) th degree upper bound estimate of the probability of misclassification between categories $C_{i}$ and $C_{j}$ is then given by

$$
\begin{aligned}
& \sum_{k_{1}}^{N} \sum_{k_{2}=1}^{N} \cdots \sum_{k_{q}=1}^{N} \prod_{n=1}^{q} \int_{A_{n}}^{B} p_{n i}\left(z_{n}\right) d z_{n}+ \\
& 1-\sum_{k_{1}=1}^{N} \sum_{k_{2}=1}^{N} \cdots \sum_{k_{q}=1}^{N} \prod_{n=1}^{q} \int_{A_{n}}^{B_{n j}} p_{n j}\left(z_{n}\right) d z_{n} \\
&= \sum_{k_{1}}^{N} \cdots \sum_{k_{q}=1}^{N} \prod_{n=1}^{q}\left[F\left(\frac{B_{n}-v_{n}}{d_{n}}\right)-F\left(\frac{A_{n}-v_{n}}{d_{n}}\right)\right]+
\end{aligned}
$$

$$
\begin{equation*}
1-\sum_{k_{1}=1}^{N} \cdots \sum_{k_{q}=1}^{N} \prod_{n=1}^{q}\left[F\left(B_{n}-W_{n}\right)-F\left(A_{n}-W_{n}\right)\right] \tag{25}
\end{equation*}
$$

where, for each $n=1,2, \ldots, q$,

$$
B_{n}=a_{1 n}^{\left(k_{1}, \ldots, k_{q}\right)}+\left(k_{n}+1\right) \Delta+\left(a_{1 n}^{\left(k_{1}, \ldots, k_{n}+1, \ldots, k_{q}\right)-a_{1 n}\left(k_{1}, \ldots, k_{q}\right) I_{n}}\right.
$$

and

$$
A_{n}=a_{l n}\left(k_{1}, \ldots, k_{q}\right)+k_{n} \Delta+\left(a_{1 n}^{\left(k_{1}, \ldots, k_{n}+1, \ldots, k_{q}\right)}-a_{l_{n}}^{\left(k_{1}, \ldots, k_{q}\right)}\right) I_{n}
$$

where $I_{n}$ is the indicator function

$$
I_{n}= \begin{cases}1, & \text { if } k_{n}>N / 2 \\ 0, & \text { if } k_{n} \leq N / 2\end{cases}
$$

The expression in (25) is the value of the upper bound estimate over a region which encloses the region of misclassification with the property that the enclosing region squeezes down on the hyperellipsoidal region of misclassification as $N$ becomes large.

## B. A HYPER-HYPERBOLOIDAL REGION OF MISCLASSIFICATION

The region of misclassification in p-dimensional space will be hyper-hyperboloidal provided $T_{j}<0$ (of equation (10)) for one or more $j \in\{1,2, \ldots, p\}$, or equivalently, provided $d_{k}^{2}-1$ is not of the same sign for all $k=1,2, \ldots, p$. The procedure for obtaining the upper bound approximation is very similar to that for the hyperellipsoidal region. The primary difference is that of having to integrate over a region in a negative direction from $a_{0}$ and a positive direction from $a_{0}^{\prime}$ (refer to Fig. 5 for the case of two dimensions). If we let $s=\left\{j \mid T_{j}<0\right\}$ then the $j \frac{\text { th }}{\text { given by }}$ coordinates of $a_{0}$ and $a_{0}^{\prime}{ }^{\prime}$ denoted by $a_{0 j}$ and $a_{0 j}^{\prime}$, respectively, are

$$
\begin{aligned}
& a_{0 j}= \begin{cases}a_{l j^{\prime}}, & \text { if } j \in S \\
c_{R j}, & \text { if } j \in S\end{cases} \\
& a_{0 j}^{\prime}= \begin{cases}a_{2 j^{\prime}}, & \text { if } j \notin S \\
c_{R j^{\prime}}, & \text { if } j \in S\end{cases}
\end{aligned}
$$

where $a_{l j}, a_{2 j}$, and $C_{R j}$ are given by equations (8) and (9). Moreover, for the hyper-hyperboloidal region of misclassification, for each value of $i=1,2$, the quantity $a_{i j}\left(k_{1}, \ldots, k_{q}\right)$ is identical to that of equations (22) and (23) upon replacing $C_{R j}$ by $a_{0 j}$; similarly, replacing $C_{R j}$ by $a_{0 j} \operatorname{in~}_{\left(k_{1}, \ldots, k_{q}\right)}$ and (23) and $k_{i} \Delta$ by $-k_{i} \Delta$ in expression (24) for $R_{j}\left(k_{1}, \ldots, k_{q}\right)$, we obtain $a_{i j}, \ldots, k_{q}$. For larger $N$ and.
smaller $\Delta$ ( $N$ and $\Delta$ are not necessarily related and $N$ may be even or odd for the hyper-hyperboloidal case), the value of the integration over the enclosing region becomes a tighter upper bound approximation to the probability of misclassification. The explicit expression for this estimate in terms of the cumulative Gaussian distribution function $F$, with mean 0 and variance 1 , is given by

$$
\begin{aligned}
& P_{N}=\sum_{k=1}^{N} \cdots \sum_{k_{1}=1}^{N}\left[\prod_{n=1}^{q} \int_{A_{n}}^{B} p_{n i}\left(z_{n}\right) d z_{n}+\prod_{n=1}^{q} \int_{A_{n}}^{B} p_{n i}^{\prime}\left(z_{n}\right) d z_{n}\right]+ \\
& 1 \cdots \sum_{k_{1}=1}^{N} \cdots \sum_{k_{q}=1}^{N}\left[\prod_{n=1}^{q} \int_{A_{n}}^{B_{n}} p_{n j}\left(z_{n}\right) d z_{n}+\prod_{n=1}^{q} \int_{A_{n}^{\prime}}^{B_{n}^{\prime}} p_{n j}\left(z_{n}\right) d z_{n}\right] \\
& =\sum_{k=1}^{N} \cdots \sum_{k_{q}=1}^{N}\left\{\prod_{n=1}^{q}\left[F\left(\frac{B_{n}-v_{n}}{d_{n}}\right)-F\left(\frac{A_{n}-V_{n}}{d_{n}}\right)\right]+\prod_{n=1}^{q}\left[F\left(\frac{B_{n}^{\prime}-v_{n}}{d_{n}}\right)-F\left(\frac{A_{n}^{\prime}-V_{n}}{d_{n}}\right)\right]\right\}+ \\
& \left.1-\sum_{k_{1}}^{N} \cdots \sum_{k_{q}}^{N}=1 \sum_{n=1}^{N}\left[F\left(B_{n}-W_{n}\right)-F\left(A_{n}-W_{n}\right)\right]+\prod_{n=1}^{q}\left[F\left(B_{n}^{\prime}-W_{n}\right)-F\left(A_{n}^{\prime}-W_{n}\right)\right]\right\}
\end{aligned}
$$

where

$$
\begin{aligned}
& A_{n}=a_{l n}^{\left(k_{1}, \ldots, k_{q}\right)}-k_{n} \Delta ; \\
& B_{n}=a_{l_{n}}^{\left(k_{1} \ldots k_{q}\right)}-\left(k_{n}-1\right) \Delta ; \\
& A_{n}^{\prime}=a_{l n}^{\left(k_{1} \ldots k_{q}\right)}-\left(k_{n}-1\right) \Delta ; \\
& \left.B_{n}^{\prime}=a_{1 n}^{\left(k_{1}\right.} \cdots k_{q}\right)-k_{n} \Delta .
\end{aligned}
$$

## VI. CONCLUSIONS

For a given set of $q$ features, the procedure presented herein permits the calculation of as tight an upper bound estimate on the probability of misclassification in Gaussian maximum likelihood classification between each pair of categories as one chooses using these selected features. The original space is transformed to an equivalent pattern recognition space so that all calculations become univariate calculations, including the integrations. An explicit expression is given for as tight an upper bound estimate as one chooses in terms of univariate Gaussian distribution functions which are easily and accurately obtained. The procedure may be utilized to select the optimal $q$ ( $q \leqslant p$ ) features having the property that no other subset of $q$ features yield a smaller value to the upper bound on the probability of misclassification. In particular, beginning with $q=$ 1 , the technique may be applied and $q$ increased, if necessary, until the upper estimate becomes less than some preselected threshold $\alpha$, where $\alpha$ is the largest value of the probability of misclassification that can be tolerated in a given classification situation. From this set, the $q$ features yielding the smallest value less than $\alpha$ is selected.

The selected features will be those which best discriminate between categories $C_{i}$ and $C_{j}$. It is likely that for a third category, say $C_{k}$, those features which permit best discrimination between categories $C_{i}$ and $c_{k}$ will be different from those that best discriminate between $C_{i}$ and $c_{j}$ (and $C_{i}$ and $c_{k}$ ). Therefore, to achieve the degree of classification accuracy that is hoped for in the near future in remote sensing, the selection of pairwise categorical features should be significantly superior to choosing one set of features for all the categories combined.

As a final consideration, if the a priori class probabilities $q_{i}$ and $q_{j}$ are known for categories $C_{i}$ and $C_{j}$, respectively, then they may easily be incorporated into the procedure presented herein by simply replacing

$$
\ln \prod_{k=1}^{q} d_{k}^{2} \quad b y \quad \ln \frac{q_{i}}{q_{j}} \prod_{k=1}^{q} d_{k}^{2}
$$

throughout. Also, it needs be pointed out that the space in which feature selection is carried out herein is the same space in which classification processing by thresholding (see Minter and Hallum, 1972) is accomplished; consequently, the recommended procedure is to select features utilizing the technique presented herein and then perform classification processing utilizing the Minter-Hallum classification procedure.

## VII. REFERENCES

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Figure 1. The Misclassification Boundary in Two-dimensional Space Between Categories $\mathrm{C}_{\mathrm{i}}$ and $\mathrm{C}_{\mathrm{j}}$.


Figure 2. The Box Enclosing the Misclassification Region.


Figure 3. A Hyperboloidal Misclassification Region in Twodimensional Space Between Categories $C_{i}$ and $C_{j}$.


Figure 4. A Tighter Bound on the Misclassification Region


Figure 5. A Tighter Bound on the Hyperboloidal


[^0]:    Hallum, Cecil R., "Feature Selection Via an Upper Bound (to Any Degree Tightness) on Probability of Misclassification" (1973). LARS Symposia. Paper 20.
    http://docs.lib.purdue.edu/lars_symp/20

