

# Matching and Fusing Signal-Estimation Errors for Similarity-based Pattern Classification

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*Abstract:* Error estimation using different optimal models for signal processing has been an active research field in data analysis such as speech recognition, image analysis, geophysics, and earth science. A popular direction of research in pattern classification is to develop computational models for comparing objects being either abstract or physical based on some measure of similarity or dissimilarity. This paper explores some linear-prediction models for deriving signal estimation errors and their fusion for similarity-based pattern classification.

*Key-Words:* Linear prediction, error matching, similarity measure, information fusion, classification.

## 1 Introduction

A basic study in the broad field of pattern recognition is the selection of good features that can be effectively utilized to distinguish the identities of different objects. Typically, sufficient collection of these features are used to train classifiers that are supervised to be able to classify unknown objects based on past learning. However, there are many practical pattern-recognition problems where the availability or the sufficient amount of good features are not feasible for machine-learning purpose. These are cases when the object features involve with high dimensionalities or the datasets are limited. An alternative strategy is to classify patterns based on some measures of similarity or dissimilarity between the two objects. This type of approach has recently renewed and regained increased attention among the community of pattern-recognition researchers [1].

Metric-based measures of similarity have been conventionally applied for the design of various machine-learning methods. An alternative representation of similarity or dissimilarity is the the notion of non-metric measure known as the distortion measure which relaxes the symmetrical property of the distance measure. The central idea of a distortion measure is based on the error matching of the estimations of the two signals. This type of measure has been particularly explored and applied for solving problems in speech recognition. Its various forms are based on the the theory of linear predictive coding and still remain an important research area of digital signal processing for signal detection and signal coding [2, 3, 4, 5].

LPC has become a popular signal processing tool because 1) it is very useful for low-bit-rate coding, 2) it pro-

vides a compact and tractable presentation of the spectral properties of the signals, and 3) its computation is relatively simple. Given its advantages, the theory of LPC has not widely applied for the analysis of other types of data such as modern biomedical and biological signals including genomic, proteomic, and microarray data [6, 7, 8, 9, 10, 24]. In addition, the formulation of the LPC and LPC-based distortion measures have not been well explored to capture the spatial information which inherently exists in several domains of real data including those having described before. Besides the exploration of various sources of information for measuring similarities between objects for pattern classification, it is beneficial to take advantage of these sources by integrating the independent pieces of evidence in order to improve the recognition rate instead of solving the problem separately with different measures.

In this paper we discuss some computational procedures for estimating and matching signal errors in both time-series and spatial domains. We then design a strategy for pattern classification by decision fusion of the two distortion measures. The rest of this paper is organized as follows. To be self-contained in the technical discussion throughout this paper, Section 2 covers the basic idea of the computational principle of linear prediction. Section 3 presents the formulation of a spatial linear predictive coding. The derivations of two different distortion measures based on the notion of error matching are discussed in Section 4. Section 5 illustrates the application of the proposed approach using some real biomedical signal and image datasets. Section 6 summarizes and concludes the technical contribution of the paper and suggests some problems for further investigation.

## 2 Linear Predictive Coding

In time series analysis, a continuous-time signal  $s(t)$  is sampled to obtain a discrete-time signal  $s(nT)$ , where  $n$  is an integer variable and  $T$  is the sampling interval. For the sake of convenience, from now on we denote  $s(nT)$  as  $s(n)$  without the loss of generality.

The basic formulation of linear prediction is based on the assumption that a signal  $s_n$  is considered to be the output of some system with some unknown input  $u_n$  such that [2]

$$s_n = \sum_{k=1}^p a_k s(n-k) + G \sum_{l=0}^q b_l u(n-l) \quad (1)$$

where  $b_0 = 1$ , the terms  $\{a_k\}$  and the gain  $G$  are the parameters of the hypothesized system.

Equation (1) can be expressed in the frequency domain by taking the  $z$  transform on its both sides, which results in

$$H(z) = \frac{S(z)}{U(z)} = G \frac{1 + \sum_{l=1}^q b_l z^{-l}}{1 + \sum_{k=1}^p a_k z^{-k}} \quad (2)$$

where  $H(z)$  is the system transfer function,  $U(z)$  is the  $z$  transform of  $u(n)$ , and  $S(z)$  the  $z$  transform of  $s(n)$  which is defined as

$$S(z) = \sum_{n=-\infty}^{\infty} s(n)z^{-n} \quad (3)$$

The term  $H(z)$  expressed in (2) is called the general *pole-zero* model – the roots of the numerator are the *zeros*, and the roots of the denominator are the *poles* of the model. Thus, two special cases of the model are the all-zero and all-pole models. As the names refer, for the all-zero model:  $a_k = 0, \forall k$ ; whereas for the all-pole model:  $b_l = 0, \forall l$ . Our discussion is now focused on the all-pole model which assumes that the signal  $s(n)$  can be determined as a linear combination of the past values and some input  $u(n)$ :

$$s(n) = \sum_{k=1}^p a_k s(n-k) + Gu(n) \quad (4)$$

where  $G$  is a gain factor and the transfer function  $H(z)$  of the all-pole model simplifies to

$$H(z) = \frac{G}{1 + \sum_{k=1}^p a_k z^{-k}} \quad (5)$$

In general, the problem of the linear prediction based on the all-pole model is to determine the set of the predictor coefficients  $\{a_k\}$  and the gain  $G$ . In many applications the input  $u(n)$  is unknown. This fact further reduces the linear prediction model to

$$\hat{s}(n) = \sum_{k=1}^p a_k s(n-k) \quad (6)$$

where  $\hat{s}(n)$  is the approximation of  $s(n)$ .

The prediction error  $e(n)$  between the observed sample  $s(n)$  and the predicted value  $\hat{s}(n)$  can be defined as

$$e(n) = s(n) - \hat{s}(n) = s(n) - \sum_{k=1}^p a_k s(n-k) \quad (7)$$

Since the spectral properties of the signal can vary over time, the predictor coefficients at a given time  $n$  must be estimated from a short segment of the signal occurring around time  $n$ . Using the principle of least squares, we can find an optimal set of predictor coefficients by minimizing the mean-squared prediction error over a short segment of the whole signal.

A short-term signal,  $s_n(m)$ , and its error segment,  $e_n(m)$ , at time  $n$  can be defined as

$$s_n(m) = s(n+m) \quad (8)$$

and

$$e_n(m) = e(n+m) \quad (9)$$

The mean-squared error signal at time  $n$  to be minimized is defined as

$$E_n = \sum_m e_n^2(m) \quad (10)$$

which can be expressed in terms of  $s_n(m)$  as follows.

$$E_n = \sum_m \left[ s_n(m) - \sum_{k=1}^p a_k s_n(m-k) \right]^2 \quad (11)$$

Differentiating  $E_n$ , which is expressed in (11), with respect to each  $a_k$  and set the result to zero:

$$\frac{\partial E_n}{\partial a_k} = 0, \quad k = 1, \dots, p \quad (12)$$

giving

$$\sum_m s_n(m-i)s_n(m) = \sum_{k=1}^p a_k \sum_m s_n(m-i)s_n(m-k) \quad (13)$$

It can be noticed that the terms of the form  $\sum s_n(m-i)s_n(m-k)$  are those of the short-term covariance of  $s_n(m)$ , that is

$$\phi_n(i, k) = \sum_m s_n(m-i)s_n(m-k) \quad (14)$$

One possible way of defining the limits on  $m$  expressed in (14) is to assume that the segment,  $s_n(m)$ , is zero outside the interval  $0 \leq m \leq N-1$ , where  $N$  is the size of the short segment. This assumption is equivalent to that the

signal  $s(m+n)$  is multiplied by a finite length window,  $w(m)$ , which zero outside the range  $0 \leq m \leq N-1$ . Thus the segment for minimization can be expressed as

$$s_n(m) = \begin{cases} s(m+n)w(m) & : 0 \leq m \leq N-1 \\ 0 & : \text{otherwise} \end{cases} \quad (15)$$

where  $w(m)$  is usually a Hamming window.

Based on using the signal expressed in (15), the error signal  $e_n(m)$  is exactly zero since  $s_n(m) = 0$  for all  $m < 0$ , and for  $m > N-1+p$  the prediction error is also zero because again  $s_n(m) = 0$  for all  $m > N-1$ . Thus an optimal range of  $m$  used in defining the short segment of the sequence and the region over which the mean-squared error is minimized is from  $m = 0$  to  $m = N-1+p$  to minimize the errors at section boundaries. Using this range for  $m$ , the mean-squared error becomes [3]

$$E_n = \sum_{m=0}^{N-1+p} e_n^2(m) \quad (16)$$

and  $\phi_n(i, k)$  can be rewritten as

$$\phi_n(i, k) = \sum_{m=0}^{N-1+p} s_n(m-i)s_n(m-k), 1 \leq i \leq p, 0 \leq k \leq p \quad (17)$$

or

$$\phi_n(i, k) = \sum_{m=0}^{N-1-(i-k)} s_n(m)s_n(m+i-k), 1 \leq i \leq p, 0 \leq k \leq p \quad (18)$$

Since (18) is a function of  $(i-k)$ , the covariance function  $\phi_n(i, k)$  can be reduced to the simple autocorrelation function:

$$\phi_n(i, k) = r_n(i-k) = \sum_{m=0}^{N-1-(i-k)} s_n(m)s_n(m+i-k) \quad (19)$$

Since the autocorrelation function is symmetric, that is  $r_n(-k) = r_n(k)$ , the system of LPC equations can be expressed as

$$\sum_{k=1}^p r_n(|i-k|)a_k = r_n(i), 1 \leq i \leq p \quad (20)$$

which describes a set of  $p$  equations in  $p$  unknowns, and can be expressed in matrix form as

$$\mathbf{R} \mathbf{a} = \mathbf{r} \quad (21)$$

where  $\mathbf{R}$  is a  $p \times p$  autocorrelation matrix (Toeplitz matrix which is symmetric with all diagonal elements being

equal),  $\mathbf{r}$  is a  $p \times 1$  autocorrelation vector, and  $\mathbf{a}$  is a  $p \times 1$  vector of prediction coefficients:

$$\mathbf{R} = \begin{bmatrix} r_n(0) & r_n(1) & r_n(2) & \cdots & r_n(p-1) \\ r_n(1) & r_n(0) & r_n(1) & \cdots & r_n(p-2) \\ r_n(2) & r_n(1) & r_n(0) & \cdots & r_n(p-3) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ r_n(p-1) & r_n(p-2) & r_n(p-3) & \cdots & r_n(0) \end{bmatrix}$$

$$\mathbf{a}^T = [ a_1 \ a_2 \ a_3 \ \cdots \ a_p ]$$

and

$$\mathbf{r}^T = [ r_n(1) \ r_n(2) \ r_n(3) \ \cdots \ r_n(p) ]$$

Thus, the LPC coefficients can be obtained by solving

$$\mathbf{a} = \mathbf{R}^{-1} \mathbf{r} \quad (22)$$

### 3 Spatial Linear Predictive Coding

Having outlined the theory of linear predictive coding (LPC), we present in this section a new approach for estimating the LPC model parameters based on the theory of regionalized variables [11] and the kriging estimation procedure [12, 13]. A regionalized variable is thought to have characteristics intermediate between a random variable and a deterministic function - its values vary over space but are spatially correlated over some short distance. The degree of the spatial continuity of a regionalized variable can be expressed by a semivariogram (to be discussed later). We now describe how the theory of regionalized variables and the unbiased estimation of kriging can be used for modeling the all-pole linear prediction.

Consider a stationary random function that consists of several random variables, one for each of the available values and one for the unknown value. Let  $V(s(n-k))$ ,  $k = 1, \dots, p$ , be the random variables of  $s(n-k)$ ,  $k = 1, \dots, p$ , respectively. Let  $V(s(n))$  be the random variable for  $s(n)$ . These random variables are assumed to have the same probability distribution, and the expected value of the random variables at all locations is  $E\{V\}$ . Thus, the estimate of  $s(n)$  is also a random variable and expressed by a weighted linear combination of the random variables at  $p$  locations:

$$\hat{V}(s(n)) = \sum_{k=1}^p a_k V(s(n-k)) \quad (23)$$

And the error of estimation is

$$R(s(n)) = \hat{V}(s(n)) - V(s(n)) \quad (24)$$

Alternatively we have

$$R(s(n)) = \sum_{k=1}^p a_k V(s(n-k)) - V(s(n)) \quad (25)$$

The expected value of the error of estimate is

$$E\{R(s(n))\} = \sum_{k=1}^p a_k E\{V(s(n-k))\} - E\{V(s(n))\} \tag{26}$$

Based on the assumption that the random function is stationary, both  $E\{V(s(n-k))\}$  and  $E\{V(s(n))\}$  can be expressed as  $E\{V\}$ ; thus (26) becomes

$$E\{R(s(n))\} = \sum_{k=1}^p a_k E\{V\} - E\{V\} \tag{27}$$

If the unbiased condition is imposed, then  $E\{R(s(n))\}$  must be set to zero. Giving

$$E\{V\} \sum_{k=1}^p a_k = E\{V\} \tag{28}$$

resulting

$$\sum_{k=1}^p a_k = 1 \tag{29}$$

The variance of the random variable  $V(s(n))$  which is the result of a weighted linear combination of other  $p$  random variables is given by

$$Var\left\{\sum_{k=1}^p a_k V(s(n-k))\right\} = \sum_{k=1}^p \sum_{j=1}^p a_k a_j Cov\{V(s(n-k))V(s(n-j))\} \tag{30}$$

Recalling that  $R(s(n)) = \hat{V}(s(n)) - V(s(n))$  and using (30), the variance of the error can be expressed as either

$$Var\{R(s(n))\} = Cov\{\hat{V}(s(n))\hat{V}(s(n)) - 2Cov\{\hat{V}(s(n))V(s(n))\} + Cov\{V(s(n))V(s(n))\} \tag{31}$$

or

$$\sigma_R^2 = \sigma^2 + \sum_{k=1}^p \sum_{j=1}^p a_k a_j C_{kj} - 2 \sum_{k=1}^p a_k C_k \tag{32}$$

which defines the variance of error as a function of  $a_1, \dots, a_p$ .

An optimal choice for the predictor parameters  $a_1, \dots, a_p$  is to minimize  $\sigma_R^2$ . Introducing a Lagrange multiplier  $\beta$  into (32) we have

$$\sigma_R^2 = \sigma^2 + \sum_{k=1}^p \sum_{j=1}^p a_k a_j C_{kj} - 2 \sum_{k=1}^p a_k C_k + 2\beta \left( \sum_{k=1}^p a_k - 1 \right) \tag{33}$$

The error variance term,  $\sigma_R^2$ , can now be minimized by differentiating (33) with respect to the predictor coefficients and the Lagrange parameter, and setting each one to zero. By doing so, we obtain the following equations.

$$\sum_{j=1}^p a_j C_{kj} + \beta = C_{kn}, \forall k = 1, \dots, p. \tag{34}$$

$$\sum_{k=1}^p a_k = 1 \tag{35}$$

The above system of equations are known as the ordinary kriging system [], which can be expressed in matrix notation as

$$\mathbf{C} \mathbf{a} = \mathbf{D} \tag{36}$$

where

$$\mathbf{C} = \begin{bmatrix} C_{11} & \dots & C_{1p} & 1 \\ \vdots & \dots & \vdots & \vdots \\ \vdots & \dots & \vdots & \vdots \\ \vdots & \dots & \vdots & \vdots \\ C_{p1} & \dots & C_{pp} & 1 \\ 1 & \dots & 1 & 0 \end{bmatrix}$$

$$\mathbf{a} = [ a_k \quad \dots \quad a_p \quad \beta ]^T$$

$$\mathbf{D} = [ C_{1n} \quad \dots \quad C_{pn} \quad 1 ]^T$$

Thus the values of the spatial predictor coefficients can be obtained by solving

$$\mathbf{a} = \mathbf{C}^{-1} \mathbf{D} \tag{37}$$

The sample covariance used for the kriging estimator can be calculated as

$$C(h) = \frac{1}{N(h)} \sum_{(i,j)|h_{ij}=h} s(i)s(j) - \left( \frac{1}{n} \sum_{k=1}^n s(k) \right)^2 \tag{38}$$

in which the sample covariance is a function of the lag distance  $h$ ,  $N(h)$  is the number of pairs that  $s(i)$  and  $s(j)$  are separated by  $h$ , and  $n$  is the total number of data.

On the derivation of the error of variance, it is assumed that the random variables have the same mean and variance which lead to the development of the mathematical relationship between the variogram, denoted as  $\gamma(h)$ , and the covariance [13]

$$\gamma(h) = \sigma^2 - C(h) \tag{39}$$

where the sample  $\gamma(h)$  is defined as

$$\gamma(h) = \frac{1}{2N(h)} \sum_{(i,j)|h_{ij}=h} [s(i) - s(j)]^2 \tag{40}$$

Using the variogram, the kriging weights can be determined by solving

$$\sum_{k=1}^p a_k \gamma_{jk} - \beta = \gamma_{jn}, \quad j = 1, \dots, p \quad (41)$$

and

$$\sum_{k=1}^p a_k = 1 \quad (42)$$

The variance of the estimation residual (error) can readily be determined by

$$\sigma_R^2 = \mathbf{a}^T \mathbf{D} \quad (43)$$

Taking the square root of (43) gives the standard error of the estimate:

$$\sigma_R = (\mathbf{a}^T \mathbf{D})^{\frac{1}{2}} \quad (44)$$

#### 4 Classification by Error Matching and Fusion

To apply the results obtained from the linear prediction for classification of unknown signals, the method of vector quantization can be utilized to generate a decision logic for classification. We discuss herein the implementation of both conventional and spatial distortion measures and the fusion of the two measures for the VQ-codebook design.

A distortion measure between two vectors  $\mathbf{x}$  and  $\mathbf{y}$ , denoted as  $D(\mathbf{x}, \mathbf{y})$ , is considered to be a cost of reproducing any input vector  $\mathbf{x}$  as a reproduction of vector  $\mathbf{y}$ . Given such a distortion measure, the mismatch between two signals can be quantified by an average distortion between the input and the final reproduction. Intuitively, a match of the two patterns is good if the average distortion is small.

A popular distortion measure is the likelihood ratio (LR) distortion. The LR distortion measure,  $D_{LR}$ , is defined by [3]

$$D_{LR} = \frac{\mathbf{a}^T \mathbf{R}_s \mathbf{a}'}{\mathbf{a}^T \mathbf{R}_s \mathbf{a}} - 1 \quad (45)$$

where  $\mathbf{R}_s$  is the autocorrelation matrix of signal  $s$  associated with its LPC coefficient vector  $\mathbf{a}$ , and  $\mathbf{a}'$  is the LPC coefficient vector of signal  $s'$ .

Based on the same principle derived for the likelihood ratio distortion and using (43), the spatial distortion, denoted as  $D_S$ , can be defined as

$$D_S = \frac{\mathbf{a}^T \mathbf{D}}{\mathbf{a}'^T \mathbf{D}} - 1 \quad (46)$$

where  $\mathbf{a}$  defined in (36) is the spatial LPC vector of signal  $s$ ,  $\mathbf{D}$  is the matrix defined in (36) associated with  $s$ , and  $\mathbf{a}'$  is the spatial LPC vector of signal  $s'$ .

Based on the two different distortion measures, we can combine them in two simple ways by either summing or

multiplying the two measures in a similar fashion proposed in [14] as follows.

$$D_{Sum} = D_{LR} + D_S \quad (47)$$

or

$$D_{Prod} = D_{LR} \times D_S \quad (48)$$

It is noted that the above two distortion measures are dimensionless. The rationale for taking the sum of the two measures is that if the two features are independent then adding the values of the two measures provides more information for decision making. Whereas the rationale for combining the two measures by the multiplication rule relates to the joint probability of the occurrence of the two events. We next discuss how to implement the quantization of the LPC vectors of coefficients and limit the case to one-dimensional signal.

Now assume we have a set of  $T$  frames or subsequences of the whole signal, which are represented by the corresponding set of  $T$  LPC vectors  $\mathbf{A} = \{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_T\}$ , where  $\mathbf{a}_t = (a_{t1}, a_{t2}, \dots, a_{tp})$ . It can be seen that these LPC vectors represent a type of feature of the sequence. Let the codebook of the LPC vectors be  $\mathbf{C} = \{\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_N\}$ , where  $\mathbf{c}_n = (c_{n1}, c_{n2}, \dots, c_{np})$ ,  $n = 1, 2, \dots, N$  are codewords. Each codeword  $\mathbf{c}_n$  is assigned to an encoding region  $R_n$  in the partition  $\Omega = \{R_1, R_2, \dots, R_N\}$ . The source LPC vector  $\mathbf{a}_t$  can be represented by the encoding region  $R_n$  and expressed by

$$V(\mathbf{a}_t) = \mathbf{c}_n, \text{ if } \mathbf{a}_t \in R_n \quad (49)$$

The main idea of LPC based vector quantization (VQ) is to find an optimal codebook such that for a given training set  $\mathbf{A}$  and a codebook size  $N$ , the average distortion in representing each LPC vector  $\mathbf{a}_t$  by the closest codeword  $\mathbf{c}_n$  is minimum. In mathematical terms we express

$$D^* = \min_{\mathbf{c}_n} \left[ \frac{1}{T} \sum_{t=1}^T \min_{1 \leq n \leq N} (D(\mathbf{c}_n, \mathbf{a}_t)) \right] \quad (50)$$

where  $D$  is an LPC distortion (either  $D_{LR}$ ,  $D_S$ ,  $D_{Aver}$ , or  $D_{Prod}$ ), and  $D^*$  is the average distortion of the vector quantizer.

In general, a vector quantizer is a system that maps a sequence of continuous or discrete vectors into a digital sequence suitable for storage in a digital channel. Vector quantization has been found to be very useful for encoding LPC vectors [15]. In other words, LPC vectors coupling with vector quantization have found to be very effective for signal coding and recognition [16]. Although there are several data partitioning methods for the determination of an optimal VQ codebook. One of the most popular methods for VQ is the LBG (Linde, Buzo and Gray) algorithm [17]. The LBG-VQ method requires an initial codebook,

Table 1:  $k$ -fold cross validation results for ovarian cancer data ( $\mu_{cl}$ : control mean,  $\mu_{cr}$ : cancer mean)

$k$	SVM		$D_{LR}/D_S$		$D_{Sum}/D_{Prod}$	
	$\mu_{cl}$	$\mu_{cr}$	$\mu_{cl}$	$\mu_{cr}$	$\mu_{cl}$	$\mu_{cr}$
2	0.8930	0.9492	0.9224/0.9231	0.9637/0.9640	0.9231/0.9245	0.9643/0.9641
4	0.9058	0.9722	0.9327/0.9320	0.9811/0.9821	0.9330/0.9326	0.9832/0.9829
6	0.9094	0.9760	0.9348/0.9332	0.9825/0.9814	0.9352/0.9337	0.9842/0.9828
8	0.9098	0.9784	0.9362/0.9359	0.9852/0.9887	0.9378/0.9362	0.9859/0.9889
10	0.9096	0.9801	0.9377/0.9412	0.9885/0.9890	0.9388/0.9434	0.9892/0.9891

and iteratively bi-partitions the codevectors based on the optimality criteria of nearest-neighbor and centroid conditions until the number of codevectors is reached.

The classification system based on the LPC analysis and VQ codebook approach works as follows. The given input signal is analyzed by the LPC giving the sequence of LPC vectors. The resultant LPC vectors are quantized using the number of codebooks according to the number of different classes. The distortions with respect to each codebook are accumulated across the whole test. The average spectral distortion (dissimilarity) measure between an unknown sample and a particular known class is

$$\bar{D}(\mathbf{x}_m, \mathbf{c}^i) = \frac{1}{T} \sum_{m=1}^T \min_{1 \leq j \leq J} D(\mathbf{x}_m, \mathbf{c}_j^i) \quad (51)$$

where  $D$  is a spectral distortion measure,  $\bar{D}$  is the average distortion,  $\mathbf{x}_m$  is an LPC vector of the unknown signal,  $T$  is the number of LPC vectors of the unknown signal,  $\mathbf{c}_j^i$  is the  $j$  LPC-VQ codevector of a particular class represented by codebook  $\mathbf{C}^i$ , and  $J$  the size of  $\mathbf{C}^i$ .

The unknown signal is assigned to class  $i^*$  if the average distortion measure of its LPC feature vector  $\mathbf{x}_m$  and the LPC feature codebook  $\mathbf{C}^i$  is minimum, that is

$$i^* = \arg \min_i \bar{D}(\mathbf{x}_m, \mathbf{C}^i) \quad (52)$$

## 5 Application

The identification of biomarkers using mass spectrometry (MS) data is a challenging task which requires the combination of the contrast fields of knowledge of modern biology, signal processing, and pattern recognition. The basic problem is to classify an unknown MS signal as either the control (non-disease) group or the disease group. Figure 1 illustrates the classification system based on the LPC analysis and VQ codebook approach.

The proposed method (spatial LPC-VQ) was tested using a public ovarian high-resolution SELDI-TOF mass spectrometry dataset. Regarding the implementation of proposed method, the number of poles  $p = 8$  was specified for the LPC analysis. The codebook size of 64 code-

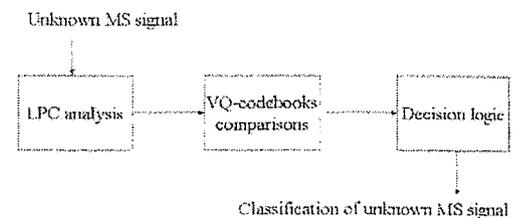


Figure 1: LPC-VQ-based MS-data classification system

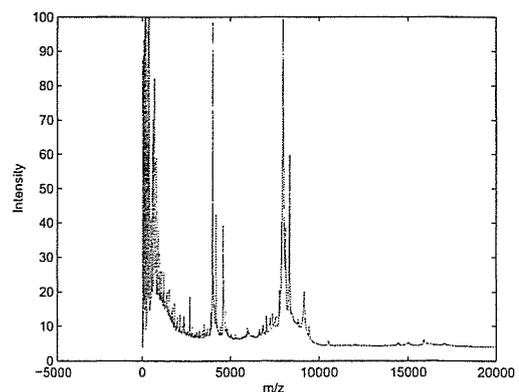


Figure 2: MS-based ovarian control data

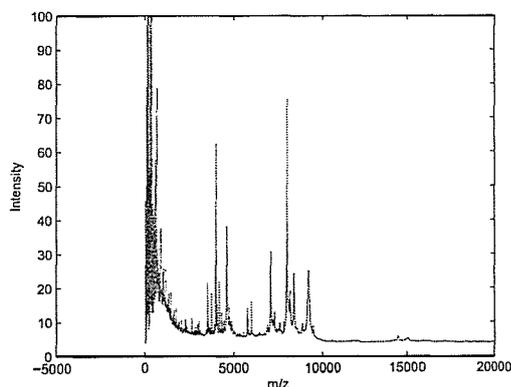


Figure 3: MS-based ovarian cancer data

vectors was used to generate the prototype for the control and cancer classes. Each MS sequence was split into multiple frames of 150 data points having 20 points overlapping between the two adjacent frames. At present, these parameters for signal processing were arbitrarily chosen and based on the experience that these values have been considered reasonable for the classification of speech signals. These parameters were also used for the conventional (non-spatial) LPC-VQ method. Figures 2-3 show the typical MS signals of ovarian control, and ovarian cancer respectively.

The ovarian high-resolution SELDI-TOF mass spectrometry dataset, which can be obtained from the FDA-NCI Clinical Proteomics Program Databank (<http://home.ccr.cancer.gov/ncifdaproteomics/ppatterns.asp>), was used to test the proposed spatial LPC-VQ based method. The dataset was generated using a non-randomized study set of ovarian cancers and control specimens on an ABI Qstar fitted with a SELDI-TOF source to study ovarian cancer case versus high-risk control. The dataset consists of 100 control samples and 170 cancer samples. The validation of the classification of the proposed approach was designed with similar strategies to those carried out in [23], who applied support vector machine (SVM) for the classification, so that comparisons can be made. The measure of performance is the  $k$ -fold cross validation where  $k = 2, 4, 8, \text{ and } 10$ , and each  $k$ -fold validation was carried out 1000 times.

It is noted that the raw ovarian high-resolution SELDI-TOF dataset used by Yu *et al.* [23] consists of 95 control samples and 121 cancer samples; while the raw ovarian high-resolution SELDI-TOF dataset we used to test the performance of the proposed approach has 100 control samples and 170 cancer samples.

Table I shows the mean classification values of the  $k$ -fold cross validation obtained from the SVM classification on the preprocessed data and the proposed method using  $D_{LR}$ ,  $D_S$ ,  $D_{Sum}$ , and  $D_{Prod}$ . The overall results obtained

for the different types of validation of the classification performance show that both the spatial and non-spatial LPC-VQ methods are more favorable for MS-based ovarian cancer identification than the other approach in two folds - feature extraction and classification methods. The spatial distortion  $D_S$  and the likelihood-ratio distortion  $D_{LR}$  are competitive and can be complementary for information fusion as shown from the improved classification rates using the two combined measures  $D_{Sum}$  and  $D_{Prod}$ .

In terms of feature extraction, the procedure for extracting the LPC-based features is more straightforward than the other feature extraction method [23] which transforms raw MS data to binned MS data, from binned MS data to Kolmogorov-Smirnov(KS)-test based feature selection, from KS-test based features to the restriction of coefficient of variation (CV), and finally from the restriction of CV to wavelet coefficients. In terms of pattern classification, the classification using the VQ-based decision rule is much simpler than the SVM-based classifier; however it is not meant that the SVM-based classifier is inferior to the VQ-based decision rule for classifying MS data. The LPC-based coefficients can be used as robust features for training different classifiers to improve the performance capable of more effective discrimination of complex patterns.

## 6 Conclusion

We have presented several distortion measures in terms of the matching of signal-estimation errors and their fusion for similarity-based pattern classification. Particularly, we have discussed a new implementation for estimating the spatial linear-prediction coefficients using the principles of the theory of regionalized variables and the unbiased kriging estimator. Based on the spatial LPC vectors and the error variance of kriging estimation, we derived a novel spatial distortion measure. We then used two simple strategies for the fusion of the two measures to determine the optimal codevectors to serve as a basis a decision logic. Information fusion is an important and interesting topic for signal detection and classification and worth further investigation. We employed a VQ method to model class prototypes. However, in case of limited data for training, the decision logic for class assignment can be directly based on the minimum of the distortion between known and unknown classes.

Most recently developed computational methods for similarity-based pattern recognition focus on the use of non-metric similarities [1]. Our proposed methodology is biased toward the standpoint of statistical signal processing including a special case of geostatistics which has recently attracted the attention of signal-processing researchers [25]. We applied the proposed method to solve an important biomedical problem for cancer classification using MS data and found the result promising.

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