Optimal Spherical Separability: Artificial Neural Networks

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Abstract. In this research paper, the concept of hyper-spherical/hyper-ellipsoidal separability is introduced. Method of arriving at the optimal hypersphere (maximizing margin) separating two classes is discussed. By projecting the quantized patterns into higher dimensional space (as in encoders of error correcting code), the patterns are made hyper-spherically separable. Single/multiple layers of spherical/ellipsoidal neurons are proposed for multi-class classification. An associative memory based on hyper-ellipsoidal neuron is proposed.

1 Introduction

In an effort to model the biological neural network, perceptron provided an important beginning. Rosenblatt proved the convergence theorem associated with the learning law, when the patterns are linearly separable.The notion of linear separability provided the conceptual basis for statistical learning theory based on support vector machines developed by V.Vapnick et. al. Specifically non-linearly separable patterns are mapped to higher dimension space where they become linearly separable by means of suitable kernel. This approach provided a method of arriving at a feature space where the classification is rendered easy. To progress the investigation, the notion of circular, spherical and hyper-spherical separability concepts are introduced. Using such concept optimal circular/spherical/hyper-spherical separating decision manifolds in 2-class case that maximizes the margin are derived. A novel method of multi-state neuron, called Spherical Neuron is proposed. It is reasoned that such a neuron enables classification of certain type of multiple classes(i.e. structured multi-class classification). Efforts are underway to train single/multi-layer networks of such neurons.

2 Circular/Spherical/Hyper-Spherical Separable Patterns: Optimal Separating Circle/Sphere/Hyper-Sphere

2.1 Motivation for spherical separability

Pattern's are said to be hyper-spherically separable if there exists a hyper-sphere which separates two classes. While, pattern's are said to be linearly separable if there exists a hyperplane which separates two classes.

A necessary condition for linear separability of pattern's belonging to two classes to imply spherical separability is that all the patterns belonging to at-least one of the classes are bounded in $(L)^2$-norm.

Lemma: Under the above condition linear separability implies spherical separability.

Proof: consider the patterns belonging to the class which is bounded.The centroid of the pattern is computed using MVEE(minimum volume enclosing ellipsoid).

Since the patterns belonging to two classes are linearly separable, there exists a hyperplane(not necessarily unique) which separates them. Using the above computed center, consider a hypersphere which is tangential to the hyperplane(in the worst case). Such a hypersphere hyper-spherically separates the patterns belonging to 2-classes.

2.2 Two class classification of circularly/spherically/hyper-spherically separable patterns in 2/3/N dimensional space

Notations used in the section are as following.

- ω_1 and ω_2: classes which are being separated.
- X and Y: data points belonging to classes ω_1 and ω_2 respectively. For N dimension case $X, Y \in \mathcal{R}^N$. Similarly for 2 dimension $X, Y \in \mathcal{R}^2$.
- Point $C(c_1, c_2, \ldots, c_N)$: center of the circle/sphere/hyper-sphere which divides the pattern in two classes. For N dimension case $C \in \mathcal{R}^N$.
- d_{max}, d_{min}: farthest and closest distances from C of points in ω_1 and ω_2 respectively.
- C is the centre of the MVEE of the class which is bounded. We use Khachiyan's algorithm [6] for the computation of MVEE.

2-D separation case Patterns are circularly separable in 2 dimension if there exists a circle which can separate both the classes.

Let ω_1, ω_2 be circularly separable. There exists a $C \in \mathcal{R}^2$ i.e. $C(c_1, c_2)$. The optimal circle which separates classes is at distance $(d_{max} + d_{min})/2$ from C. When a new data point $Z(p, q)$ is given for classification the decision is taken using following function

$$Z(p, q) = \begin{cases} \omega_1 \text{ if } (p - c_1)^2 + (q - c_2)^2 < (d_{max} + d_{min})/2 \\ \omega_2 \text{ otherwise} \end{cases} \tag{1}$$

3-D separation case Patterns are spherically separable if there exists a sphere which can separate both the classes.

Let ω_1, ω_2 be spherically separable. There exists a $C \in \mathcal{R}^3$ i.e. $C(c_1, c_2, c_3)$. The optimal sphere which separates classes is at distance $(d_{max} + d_{min})/2$ from

C. When a new data point $Z(p,q,r)$ is given for classification the decision is taken using following function

$$Z(p,q,r) = \begin{cases} \omega_1 \text{ if } (p-c_1)^2 + (q-c_2)^2 + (r-c_2)^2 < \\ \qquad (d_{max} + d_{min})/2 \\ \omega_2 \text{ otherwise} \end{cases} \quad (2)$$

N-D separation case Patterns are hyper-spherically separable if there exists a hyper-sphere which can separate both the classes.

Let ω_1, ω_2 be hyper-spherically separable. There exists a $C \in \mathcal{R}^N$ i.e. $C(c_1, c_2, \ldots, c_N)$. The optimal hyper-sphere which separates classes is at distance $(d_{max}+d_{min})/2$ from C. When a new data point $Z(z_1, z_2, \ldots, z_N)$ is given for classification the decision is taken using following function

$$Z(z_1, z_2, \ldots, z_N) = \begin{cases} \omega_1 \text{ if } (z_1-c_1)^2 + (z_2-c_2)^2 + \ldots + \\ \qquad (z_N-c_N)^2 < (d_{max} + d_{min})/2 \\ \omega_2 \text{ otherwise} \end{cases} \quad (3)$$

It is clear that if patterns belonging to two classes are linearly separable, they are hyper-spherically separable. But hyper-spherical separability does not imply linear separability(by a hyperplane). For instance, if the patterns belonging to two classes are spherically symmetric about the origin, they are clearly not linearly separable.

In the spirit of SVM, we have found the optimal hypersphere separating two classes. Training patterns belonging to classes are presented serially one class after the other, the distance from center(of one class) is varied with every training pattern. Optimal hypersphere is computed for 2-class problem. It readily applies for Multi-class case based on one against rest approach.

2.3 Multi class classification of circularly/spherically/hyper-spherically separable patterns in 2/3/N dimensional space

Notations for the section are as following.

- $\omega_1, \omega_2, \ldots, \omega_M$:$M$ classes which are being separated. Also $\omega = \omega_1 \cup \omega_2 \cup \ldots \cup \omega_M$
- X_i : data points belonging to classes $i \in (1, M)$. For N dimension case $X \in \mathcal{R}^N$.
- Point $C_i(c_{i1}, c_{i2}, \ldots, c_{iN})$: center of the circle/sphere/hyper-sphere which divides the pattern in $i \in (1, M)$ classes. For N dimension case $C \in \mathcal{R}^N$.
- A class t_i where $i \in (1, M)$ is introduced which contains all the points which lie inside circle/sphere/hyper-sphere by which ω_i is enclosed. Also $t = t_1 \cup t_2 \cup \ldots \cup t_M$
- d_{i1}, d_{i2}: farthest and closest distances from C_i of points in t_i and $t - t_i$ respectively.

2-D case Let $\omega_1, \omega_2, \ldots, \omega_M$ be M classes which are circularly separable. We use one vs rest approach to classify the data points. The optimal circle which separates classes is at distance $(d_{i1} + d_{i2})/2$ from the center. When a new data point $Z(a, b)$ is given for classification, then

$$Z(a, b) \in t_i \text{ if } (a - c_{ix})^2 + (b - c_{iy})^2 < (d_{i1} + d_{i2})/2 \quad \forall i \in (1, n) \tag{4}$$

Z(a,b) belongs to one of w_x in t_i, which can be found using distance based algorithms. Similar approach can be followed for 3-D and N-D cases.

It is important to note that, in the theory of error correcting codes, an information word is mapped to the associated codeword using an encoder. Also the coding spheres at hamming distances less than or equal to the minimum distance of the code are disjoint. Using this idea, we project quantized patterns from lower dimension space (in the spirit of SVMs), where they become spherically separable. In the following section we summarize the known results from earlier literature.

Vapnick's idea was to project non-linearly separable patterns into a higher dimensional space to render them linearly separable. This idea motivated the authors to see if certain non-hyper-spherically separable patterns can be rendered as hyper-spherically separable patterns without projecting them into a higher dimensional space. Details are provided in the following section.

3 Linear Transformation of Non-Hyper-spherically separable patterns to spherically separable patterns: Quadratic Neuron

Traditionally, single artificial neuron called perceptron was based on the concept of linear separability. Rosenblatt proposed a learning law which converges(i.e. the synaptic weights converge), when the patterns are linearly separable. The resulting hyperplane is one among various possible hyperplanes that separate the patterns into two classes.

Vapnick, by introducing the concept of margin, showed that the problem of synthesizing optimal hyperplane(i.e. a hyperplane which maximizes the margin) separating two classes can be formulated as a Quadratic optimization problem.

These two approaches remained as the basis for research related to artificial neural networks(e.g. classification problem).

The authors contemplated on the possibility of combining the logical basis of above two approaches for classification. They succeeded in such an effort by introducing hyper-spherical separability concept. The details are summarized below.

In McCulloh-Pitts neuron, the net contribution is computed using the inner product of weight vector and the vector of the inputs. This net contribution is operated on by by signum activation function, to arrive at the neuron output. Such a model of neuron is utilized to classify linearly separable patterns (by a hyperplanes). Generalizing this idea, several researchers proposed a neuron where higher order synaptic operations(e.g. quadratic synaptic operations) are utilized to arrive at the net contribution which is operated on by signum activation function[5].

In such a neuron model, the activation function is retained as signum function. It is thus clear that such models of neuron classify non-linearly separable patterns. Specifically, let W be a symmetric $M \times M$ matrix and $\bar{X}$ be a $M \times 1$ vector of inputs. The output of neurons

$$y = signum\{\bar{X}^T W \bar{X} - T_0\} \tag{5}$$

Here T_0 is a threshold value.

Assumption: W be a positive symmetric matrix. Hence by cholesky decomposition we have $W = NN^T$, where N is a

Applying it in equation (5)

$$\bar{X}^T W \bar{X} = \bar{X}^T N N^T \bar{X} = Z^T Z = \sum_{i=1}^{M} {z_i}^2 \tag{6}$$

where $Z = N^T \bar{X}$. Thus output of such a neuron is given by

$$y = signum\{\sum_{i=1}^{M} {z_i}^2 - T_0\} \tag{7}$$

Claim: The patterns arrived at by the above linear transformation are hyper-spherically separable.

Note that using above idea, first documented in research monograph [7], NP-hard problem of maximum cut computation is reduced to multi-linear objective function optimization over hypercube[9].

It is well known that homogeneous multivariate polynomial (of degree higher than two) can be expressed in terms of symmetric tensor. Using cholesky type decomposition of symmetric tensor, the results in this section can be generalized.

The approach proposed in this section naturally leads to the idea of transforming the patterns by a non-linear transformation(when they are separable by certain manifold) such that they become spherically separable(without projecting to higher dimensions.)

In the view of discussion in sections 2,3, a natural question arises whether the patterns which are not hyper-spherically separable can be projected to higher dimension where they are hyper-spherically separable(in spirit of SVM design policy).This issue is addressed in the following section. Patterns are preprocessed to ensure that they can be encoded(projected into higher dimension) into suitable codewords of an error correcting code. It is clear that the patterns in various coding spheres are hyper-spherically separable. Such a procedure ensures noise robustness for patterns classification. The following correspondence is identified between pattern classification and coding theory. Here patterns correspond to information words, class centers correspond to codewords and clusters correspond to coding spheres.

In the following section, we briefly refer to some earlier work of Bruck et.al relating associative memories to error correcting codes. Also, we generalize the concept of spherical separability resulting in spherical neuron for multiclass classification.

4 Hybrid Neural Networks: Spherical Separability : Spherical Neuron

Bruck et.al have shown that hopfield neural network is naturally associated with a graph-theoretical code in the sense that code words are associated with stable states[2]. They generalize the result to linear error correcting codes and non-linear error correcting codes. Effective code words are associated with stable states and vice-versa in the sense that they are the local/global optima of an energy function (associated with the encoder of an error correcting code). Thus effectively a one step associate memory(realized by encoder) performs clustering of data points. In [1], one of the authors proposed hybrid neural networks where encoders are cascaded with multi-layer perceptron, a feedforward network. It is clear that the patterns in different coding spheres are spherically separable. Figure 1 depicts the idea.

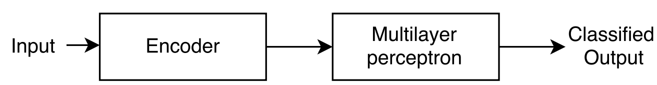

Fig. 1: Hybrid Neural Networks

The elements of pattern vectors can always be quantized such that they belong to the set $\{0, 1, 2, \ldots, p-1\}$ for a suitable chosen prime p. Such patterns constitute the information words(as in theory of error correcting codes). They are projected to a higher dimensional space by a suitable encoder to render them hyper-spherically separable. The minimum distance of the block code determines the radius of hamming sphere/ euclidean sphere around each code word that renders the codewords hyper-spherically separable. Currently we are investigating the finer details of such approach.

Spherical Neuron: Multi-class classification

In the above discussion, in two dimension circularly separable patterns(belonging to two classes) are classified. More generally, hyper spherically separable classes are classified into 2-classes in higher dimensions. Motivated by the idea of ceiling neuron [8], we introduce a novel neuron called Spherical neuron, which performs classification of patterns belonging to multiple classes with certain restrictions/structure. The details of such neuron are presented below.

The inputs belong to M classes. They are clustered around the center $(a_1, a_2, \ldots, a_N) = \bar{A}$. It could be the origin of N-dimensional euclidean space. Let an input vector be $(x_1, x_2, \ldots, x_N)$. The output class y is determined in following manner

$$y = \begin{cases} \text{class 1 if } d(\bar{X}, \bar{A}) \leq r_1 \\ \text{class 2 if } d(\bar{X}, \bar{A}) \leq r_2 \\ \vdots \\ \text{class } M \text{ if } d(\bar{X}, \bar{A}) \geq r_M \end{cases} \tag{8}$$

Here $d(\bar{X}, \bar{A})$ is the euclidean distance between the vectors $\bar{X}$ and $\bar{A}$. Note here that spherical neuron activation function has resemblance to the neurons utilized in radial basis function networks. It is multi-valued in this case.

Several such neurons are placed in one or more layers to perform fine classification of input patterns.

We can conceive of Ellipsoidal neuron, where the distance $d(\bar{X}, \bar{A})$ is computed in the following manner (with $\bar{A} = \bar{0}$).

$$d(\bar{X}, \bar{0}) = (\frac{x_1}{b_1})^2 + (\frac{x_2}{b_2})^2 + \ldots + (\frac{x_N}{b_N})^2 \tag{9}$$

Single or multiple layers of ellipsoidal neurons are utilized for fine classification of input data.

Generalizing the notion of spherical neuron for multiclass classification, we propose hyper-ellipsoidal neuron in the following section. Also, associative memory based on such a neuron in proposed.

5 Error Correcting Codes: Clustering

The problem of clustering of patterns is well studied in pattern recognition literature and various interesting algorithms such as K-means algorithm are proposed. In most of these algorithms the pattern assume values in euclidean space. Some literature exists on clustering of patterns whose coordinates/ components assume integer values (i.e. say vector space over a finite field.)

We realized that linear/nonlinear error correcting codes enable clustering of patterns after encoding in a higher dimensional space in the sense of hamming distance. We recognized that such an approach could provide insights into multiclass classification of patterns. To facilitate such an approach the components of patterns must be quantized into integer values which can always be done by choosing the integer value to be a sufficiently large prime number.

Our goal is to ensure that patterns which are not hyper-spherically separable in lower dimensional space be made hyper-spherically separable (in the hamming/euclidean distance) in a higher dimensional space by encoding. We expect that such a goal can always be achieved. There are effectively two approaches.

1. **Covering class region with hyper-spheres and clustering in pattern space:** The class region in pattern space need not be hyper-spherical.

But, it can always be covered with hyper-spheres. Using well known or new clustering algorithms, centroids of clusters/sub-clusters are determined. These centroids, which form the information words in the coding theory sense, are encoded into codewords/patterns in higher dimensional space. Using the minimum distance of error correcting code, it can always be reasoned that the classes in higher dimensional space are hyper-spherically separable under some conditions.

2. **Pattern encoding and clustering in codeword space:** Patterns in lower dimensional space constitute information words in the coding theory sense. They are encoded into codewords (by projecting into higher dimensional space) by the encoder of a suitable linear/nonlinear error correcting code. The code words are suitably clustered in such a way that the minimum distance increases. Hence, the patterns in higher dimensional space become hyper-spherically separable.

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Now, we briefly illustrate the idea of achieving hyper-spherical separability using an error correcting code. Let the pattern vector components be quantised using the alphabet $\{0, 1\}$. For the sake of example, let the pattern vector be the 1×4 row vector. Also, let the 16 possible such pattern vectors correspond to 16 different classes(i.e. centroids of classes). Now, we employ the encoder of a $(7, 4)$ hamming code to map such pattern vectors (information words) into codewords. It is well known that the minimum distance of $(7, 4)$ hamming code is 3. Hence hamming/euclidean hyper-spheres of radius one centered around the codewords are disjoint. Thus by projecting the patterns 4-dimensional euclidean space to 7-dimensional euclidean space using the encoder we made the patterns hyper-spherically separable.

In general, an (n, k) block code with minimum distance $2t + 1$ over $\{0, 1\}$ alphabet can be utilized to make k dimensional binary pattern vectors (which are not hyper-spherically separable) belonging to different 2^k classes to be hyper-spherically separable in 7-dimensional space. The euclidean spheres of radius $\sqrt{t}$(or Hamming spheres of radius t) around the codewords are disjoint.

The above approach ensures that the classification is noise tolerant/robust(enabling correction of t errors). We expect that by means of finer quantization, patterns which are not hyper-spherically separable can always be rendered hyper-spherically separable by means of a suitable encoder under some conditions. We are actively investigating this approach for pattern classification using hyper-spherical separability.

6 Hyper-Ellipsoidal Neuron: Associative Memory

Hopfield proposed an associative memory [3] based on McCulloch-Pitts neuron (which assumes $+1$ or -1 values). In literature, associative memories are proposed based on multi state neuron [4].In this research paper, we propose an associative memory based on hyper-ellipsoidal neuron. Let the state space of such an associative memory be the bounded lattice i.e. each component of the state vector , $\bar{V}(n)$ assumes values in the set $\{0, 1, 2, \ldots, M\}$. Let there be N neurons and let the symmetric synaptic weight matrix be $\bar{W}$. The i'th component of the state vector at time $n+1$ is computed in the following manner

$$V_i(n+1) = f(net) \tag{10}$$

where

$$net = w_{i1}V_1^2(n) + w_{i2}V_2^2(n) + \ldots + w_{iN}V_N^2(n)$$

$$f(net) = \begin{cases} 0 \text{ if } net < T_1, Threshold \\ 1 \text{ if } T_1 \leq net < T_2 \\ \vdots \\ M-1 \text{ if } T_{M-1} \leq net < T_M \\ M \text{ if } net \geq T_M \end{cases}$$

As in case of Hopfield associative memory, the neural network is operated in the serial mode (state of only one neuron is updated at a given time i.e. asynchronously) or fully parallel mode(state of all the neurons is updated at any given time i.e. fully synchronously)

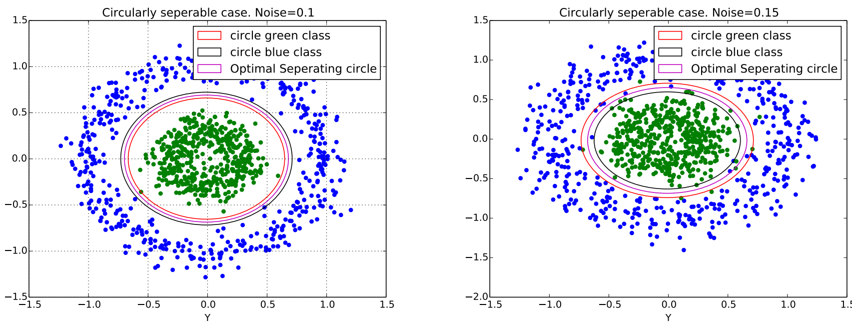
It is clear that the network dynamics is periodic (because of choice of $f(.)$). Convergence to stable state (i.e. cycle of length one) or a cycle of certain length is currently being investigated. Energy function based approach to investigate nature of dynamics is being currently pursued.

7 Experiments and Results

Following are the results for optimal circular separation case. Two circularly separable classes, having 1000 data points were generated randomly. We have compared our method against SVM with linear, polynomial and rbf kernels and K nearest neighbors algorithm with k=3. The result is repeated with different noise level(mixing of classes). Figure 2 and 3 show the graphical representation of the results.

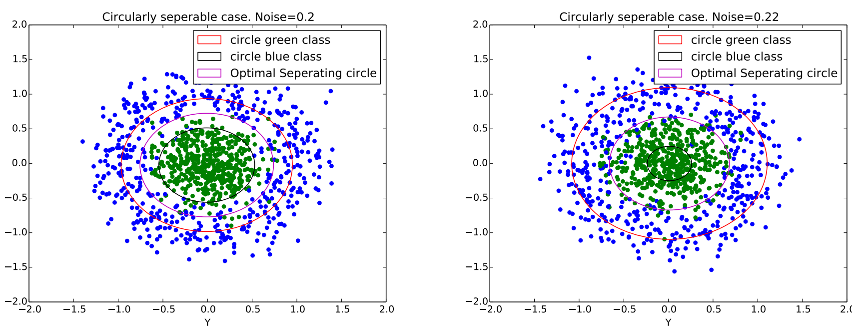
Error	**.1**	**.15**	**.2**	**.22**
Polynomial	0.5350	0.5749	0.4799	0.4774
RBF	1.0	0.9825	0.9575	0.9375
Linear	0.6474	0.4799	0.5324	0.4774
KNN	1.0	0.9825	0.9499	0.9425
Our	1.0	0.9849	0.9599	0.9425

Table 1: Comparison of classification results among SVM with polynomial, rbf and linear kernels, KNN(n=3) and our procedure. Numbers represent the accuracy at various noise levels.



(a) (b)

Fig. 2: Classification with low pattern noise



(a) (b)

Fig. 3: Classification with high pattern noise

Table 1 and figure 4 show the comparison among various methods. It is clear that our method provides competitive performance with simple computation.

8 Conclusion

In this research paper, it is reasoned that the concept of hyper-spherical separability (always implied by linear separability, when one of the classes is bounded) enables efficient classification of multiple classes of linearly separable patterns (one against the rest approach). Also, it is reasoned that certain non-spherically separable patterns can be made spherically separable by a linear transformation without projecting them into higher dimensional space. Using the results from the theory of error correcting codes, it is reasoned that hyper-spherical separability (of quantized patterns) can always be ensured by encoding (i.e. projecting

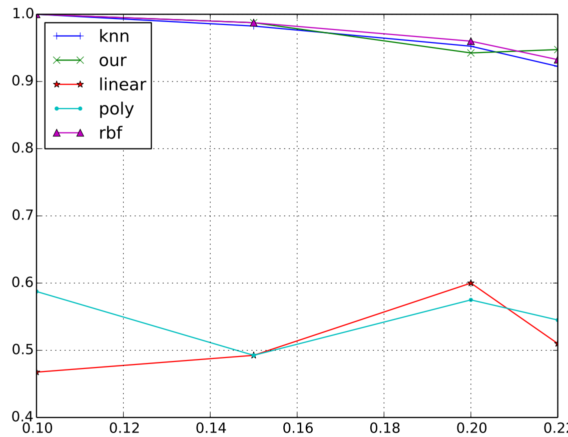


Fig. 4: Comparison of various results.

into a higher dimensional space) under some conditions. Finally, the concept of hyper-ellipsoidal neuron and an associative memory based on such a neuron is proposed.

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