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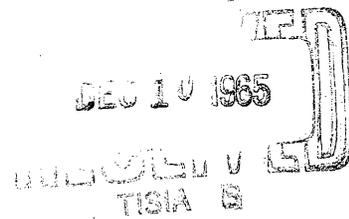


NOTES ON CLASSIFICATION CAPACITIES

T. Cover

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NOTES ON CLASSIFICATION CAPACITIES

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FOREWORD

This report was prepared under Contract AF30(602)-3448 by Stanford Research Institute, Menlo Park, California. The work was performed under Project 5581, Task 558104. The RADC Project Engineer is Mr. Charles A. Constantino.

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ABSTRACT

This is a working paper concerned with the problem of determining the information storage capacities of networks of linear threshold devices. Capacities for single element networks and low dimensional multielement networks are found, and bounds on capacities are discussed for general networks.

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NOTES ON CLASSIFICATION CAPACITIES

by

T. Cover

A. INTRODUCTION

This report is a working paper containing a series of ideas concerned with the problem of determining the capacities of networks of linear threshold devices.

Recall that the separating capacity of a single linear threshold device or threshold logic unit (TLU) is defined to be two patterns per variable weight and is well established as a natural quantity.^{1-7*} Roughly speaking, under the null hypothesis that pattern classification is uncorrelated with pattern position, a dichotomy of N patterns in d dimensions is linearly separable with high probability if $N < 2d$, and with low probability if $N > 2d$.

Now suppose that we concern ourselves with the following variations of this problem for a single threshold logic unit:

- (1) How can a TLU assign patterns to R categories? What is the associated capacity?
- (2) How many dichotomies of N points in d dimensions are there for which r or fewer errors are made?
- (3) How can a linear device assign orderings or rankings to patterns? What is the associated capacity?

* References are listed at the end of this report.

These problems will be put into a network setting in order to stake out those aspects of network capacity theorems which are well understood. Answers for general network capacity problems are still under study. It is important, in most cases, to determine which problems are theoretically possible to solve in the sense that the answer is independent of the configuration of the patterns.

B. THE NUMBER OF MAJORITY LOGIC FUNCTIONS DEFINED ON N POINTS IN THREE DIMENSIONS

In this section we shall use the fact that majority logic on regions formed by lines in 2-space is equivalent to majority logic on regions formed by corresponding planes through the origin of 3-space in order to derive an expression for the number of functions on N points in 3-space which are implementable by a bank of K parallel linear threshold devices followed by majority logic, as shown in Fig 1.

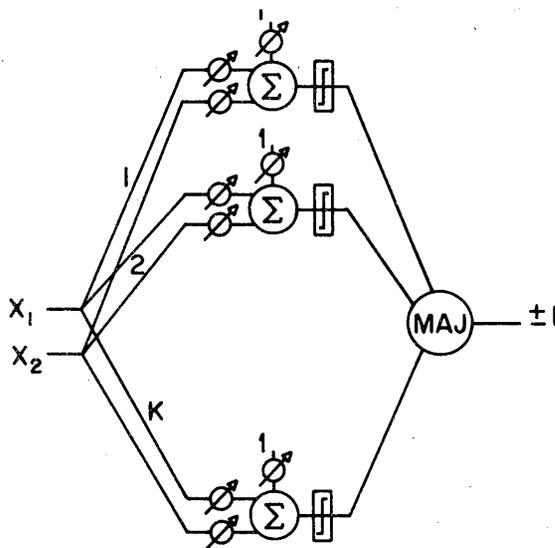


Fig. 1 A Bank of K Parallel TLU's Followed by Majority Logic

Consider a set of N points in general position in two dimensions; i.e., every set of two points is linearly independent. Consider the set of separating surfaces which consists of lines through the origin of the space. It is easily seen that precisely $2N$ dichotomies of the 2^N dichotomies of N points are homogeneously linearly separable. Moreover, it has been shown by N. J. Nilsson,⁸ based on notes by R. Singleton,⁹ and by Ablow and Kaylor,¹⁰ that a set of K lines through the origin, together with majority logic, can separate precisely $C_K(N,2)$ dichotomies of N points in general position in 2-space, where

$$C_K(N,2) = 2 \sum_{i=0}^K \binom{N-1}{i} \quad (1)$$

Note that $C_1(N,2) = 2N$ is a special case.

Let $\{x_1, x_2, \dots\}$ be dichotomized according to the assignments $\{\epsilon_1, \epsilon_2, \dots\}$, $\epsilon_i = \pm 1$. Let N be the largest integer such that $\{x_1, x_2, \dots, x_N\}$ is separable. If the ϵ_i 's are independent Bernoulli random variables with $P_r\{\epsilon = 1\} = P_r\{\epsilon = 0\} = \frac{1}{2}$, then N is a random variable having the negative binomial distribution with mean $2(K+1)$ and parameter $\frac{1}{2}$. (See, for example, Refs. 2 and 4.) We therefore define the separating capacity of majority logic in two dimensions to be (asymptotically) two patterns per separating line. Since each line requires two weights in its linear threshold unit specification, the separating capacity is one pattern per variable weight.

Consider now N points in general position in 3-space; i.e., every set of three points is linearly independent. We shall derive the number of dichotomies of a certain configuration of N points, in general position

in three dimensions, which are separable by a bank of K parallel linear threshold units followed by majority logic. Unfortunately, general position alone is not sufficient to uniquely determine the number of separable dichotomies. Note that a dichotomy is separable by the majority network if there exists a set of K open half spaces such that each point in class A, say, of the dichotomy lies in a majority of the half spaces, while each point in class B does not.

We shall treat only one of the many possible configurations. Consider the distinct vectors x_1, x_2, \dots, x_N lying on the unit circle in 2-space. Then it is easily verified that the vectors $(x_1, 1), (x_2, 1), \dots, (x_N, 1)$ lie in general position in 3-space (Fig. 2).

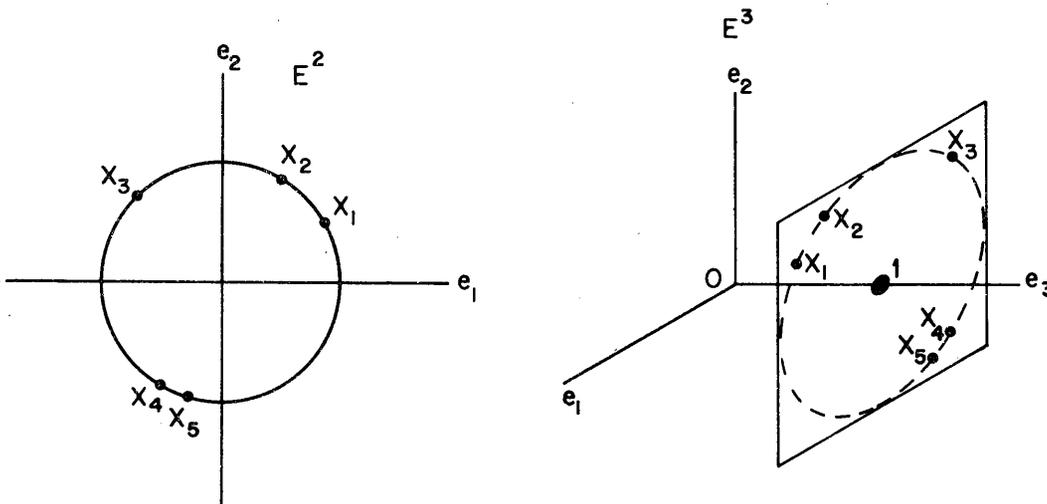


Fig. 2 A Configuration of Vectors in E^3

Any plane through the origin of E^3 corresponds to a line in E^2 . A set of K lines in E^2 cuts the unit circle in as many as $2K$ points, creating at most $2K$ intervals of alternating assignment. Let $\epsilon_1, \epsilon_2, \dots, \epsilon_N$ be the assignments of x_1, x_2, \dots, x_N to the categories 0 and 1. Let x_1, x_2, \dots, x_N be the N vectors taken in order around the circle. We claim that the assignment $\{\epsilon_1, \epsilon_2, \dots, \epsilon_N\}$ is separable by K lines with majority logic if and only if there are $2K$ or fewer runs of 0's and 1's in the sequence of ϵ 's around the circle. (There will always be an even number of runs.) The claim is easily verified by inspection of Fig. 3, for the case of three lines. It is evident

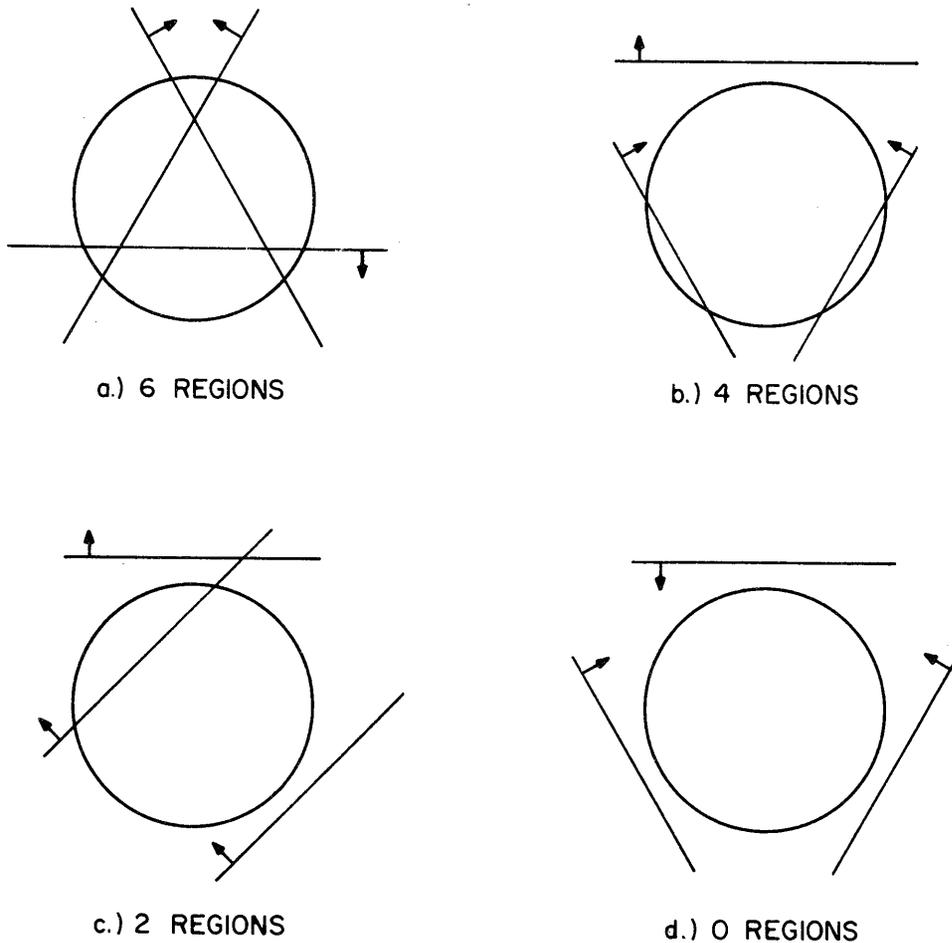


Fig. 3 Orientation of 3 Lines to Create Up to 6 Regions with Arbitrary End Points and Alternating Category

by inspection that the claim is true in general. Note that for this configuration of points in three dimensions, a majority logic second layer is equivalent to arbitrary Boolean logic.

Let us now count the number of K -majority functions of weight w . (A function of weight w on N points takes the value 1 on w points and takes the value -1 on the remaining $N-w$ points.) Using the results of Wald and Wolfowitz,¹¹ as quoted in Singleton's note,⁹ the number of ways to obtain $2K$ runs by arranging w white balls and $N-w$ black balls around a circle is

$$\frac{N}{K} \binom{w-1}{K-1} \binom{N-w-1}{K-1} \quad (2)$$

Recall that the number of runs around a circle is always even. Thus, the number of K -majority functions of weight w is given by

$$V_w = N \sum_{j=1}^K \frac{1}{j} \binom{w-1}{j-1} \binom{N-w-1}{j-1} \quad (3)$$

and the total number $C_K(N,3)$ of K -majority functions on N points is given by

$$C_K(N,3) = \sum_{w=0}^N V_w = 2 \sum_{j=0}^{2K} \binom{N-1}{j} \quad (4)$$

Hence the capacity of such a device is $2(2K+1)$ patterns, or essentially four patterns per separating plane.

C. THE NUMBER OF SEPARABLE r -CHOTOMIES OF N POINTS ON A LINE

Consider N distinct points on a line. Let each point belong to

one of r categories. Thus, there are r^N different assignments of points to categories. We shall consider two slightly different categorization schemes as follows:

Scheme 1

One selects $m-1$ boundary points defining m cells on the line. Each cell corresponds to a different category. An r -chotomy is separable according to Scheme 1 if there exist $m-1$ boundary points such that no two cells contain points of different categories and points of the same category occupy the same cell. Empty cells are allowed.

Scheme 2

One selects $m-1$ boundary points defining m cells on the line. An r -chotomy is separable according to Scheme 2 if there exist $m-1$ boundary points such that no points of different categories lie in the same cell.

Both schemes have $m-1$ variable thresholds, but Scheme 2 requires some sort of OR logic in order to combine unconnected cells into one category.

EXAMPLE: The category sequence 211333411 is separable by Scheme 2 for $m \geq 5$, but is not a separable sequence according to Scheme 1 for any m .

1. The Number of Separable r -Chotomies Under Scheme 1

Consider a sequence of $K-1$ 1's and N 0's. The 1's partition the 0's into K nonempty cells in precisely $\binom{N-1}{K-1}$ ways. The first term of the sequence must be a 0, and every 1 must be followed immediately by a 0. Thus, we have the pairings (0)0 0(10) 0(10)0 0(10)00 0, and the positions of the $K-1$ (10)'s among the $N-1$

objects may be chosen in $\binom{N-1}{K-1}$ ways. Finally, there are $r(r-1)\dots(r-K+1)$ ways to assign categories to the K nonempty cells in such a way that no two cells have the same category.

Now, $m-1$ boundary thresholds are sufficient if $K \leq m$. Hence, the number $C_{N,2}(r,m)$ of m -separable r -chotomies of N points on a line is given by

$$C_{N,2}(r,m) = \sum_{K=1}^m \binom{N-1}{K-1} \frac{r!}{(r-K)!} \quad (5)$$

or

$$C_{N,2}(r,m) = \sum_{k=0}^{m-1} \binom{N-1}{k} \frac{r!}{(r-k-1)!} \quad (6)$$

And if each of the r^N r -chotomies is equally likely, then the probability $P_{N,2}(r,m)$ that a random r -chotomy is m -separable is

$$P_{N,2}(r,m) = \left(\frac{1}{r}\right)^N \sum_{k=0}^{m-1} \binom{N-1}{k} \frac{r!}{(r-k-1)!} \quad (7)$$

We have the following remarks to make in the usual case when $m = r$, i.e., when there are a sufficient number of parameters to represent all the categories. For fixed N ,

$$\lim_{r \rightarrow \infty} P_{N,2}(r,r) = 1 \quad (8)$$

For fixed r ,

$$P_{N,2}(r,r) \sim \frac{(N-1)^{r-1}}{r^{N-1}} \rightarrow 0 \quad (9)$$

For $N > 2$, $r > 1$,

$$P_{N,2}(r,r) < 1 \quad (10)$$

2. The Number of Separable r-Chotomies Under Scheme 2

There are $r(r-1)^{K-1}$ ways to assign categories to K nonempty cells on the line in such a way that no two adjacent cells have the same category. As before, there are $\binom{N-1}{K-1}$ ways of partitioning N points into K nonempty cells. Hence, the number $C_{N,2}^*(r,m)$ of m -separable r -chotomies of N points on a line (under Scheme 2) is given by

$$C_{N,2}^*(r,m) = r \sum_{K=1}^m \binom{N-1}{K-1} (r-1)^{K-1} \quad (11)$$

or

$$C_{N,2}^*(r,m) = r \sum_{K=0}^{m-1} \binom{N-1}{K} (r-1)^K \quad (12)$$

If each of the r^N r -chotomies is equally likely, then the probability $P_{N,2}^*(r,m)$ that a random r -chotomy is m -separable is

$$P_{N,2}^*(r,m) = \sum_{K=0}^{m-1} \binom{N-1}{K} \left(1 - \frac{1}{r}\right)^K \left(\frac{1}{r}\right)^{N-K-1} \quad (13)$$

This is just the cumulative binomial distribution with parameters $N-1$, $m-1$, and $1 - \frac{1}{r}$ corresponding to the probability that one obtains $m-1$ or fewer success in $N-1$ independent tosses of a coin having probability of success $1 - \frac{1}{r}$.

The following graph (Fig. 4) illustrates the dependence of the probability of separability on the number of threshold parameters m . Let the ratio of the number of threshold parameters m to the total number of points N be fixed at α . Then,

$$\lim_{\substack{m = \alpha N \\ N \rightarrow \infty}} P_{N,2}(r,m) = \begin{cases} 1, & \alpha > (1 - \frac{1}{r}) \\ 0, & \alpha < (1 - \frac{1}{r}) \end{cases} \quad (14)$$

Roughly speaking, an m threshold device has a capacity of $\frac{rm}{r-1}$ points on a line, where each point may have one of r categories. When $r = 2$ categories, the capacity is $2m$.

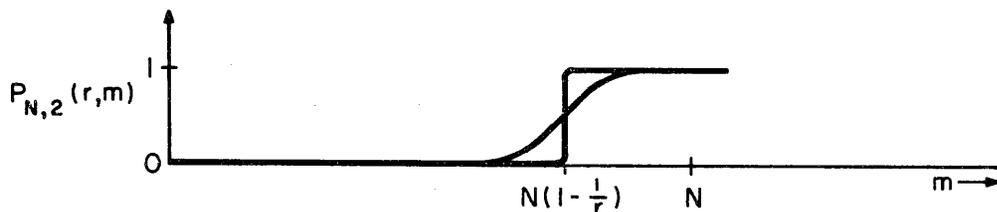


Fig. 4 Probability of Separability

D. THE NUMBER OF LINEARLY INDUCED ORDERINGS OF N POINTS IN d DIMENSIONS

In this section we shall describe the capacity of a linear threshold unit (without the threshold) as a pattern ranker (rather than a classifier). Consider a set of N vectors $X = \{x_1, x_2, \dots, x_N\}$ in Euclidean d -space E^d . We shall say that the linear weighting vector $w \in E^d$ induces the ordering

(i_1, i_2, \dots, i_N) of this set of vectors if the set of resulting inner products has the ordering $w \cdot x_{i_1} > w \cdot x_{i_2} > \dots > w \cdot x_{i_N}$. We are ordering X according to the orthogonal projections onto w . Two weights w_1 and w_2 will be said to be equivalent (with respect to X) if and only if they induce the same ordering. We shall say that the ordering (i_1, i_2, \dots, i_N) is a linearly induced ordering if there exists a $w \in E^d$ which induces this ordering. (The natural term "linear ordering" has a restricted definition in set theory.)

It is the purpose of this section to quote without proof* the fact that under simple linear independence conditions on the elements of X , the number of different linearly induced orderings of N points in E^d is given by

$$Q(N,d) = 2 \sum_{K=0}^{d-1} S_K[N-1] \quad (15)$$

where $S_K[N-1]$ is the elementary symmetric function corresponding to the coefficient of z^K in the expansion of $(1 + 2z) \dots [1 + (N-1)z]$.

In particular, it is true that

- (1) The number of linearly induced orderings of a non-degenerate collection of points is independent of the configuration of this collection of points, and
- (2) If $N \leq d+1$, then all $N!$ orderings are linearly inducible.

Incidentally, the problem of actually determining a weighting w which yields a desired possible ordering is easily disposed of. Consider without loss of generality the ordering $(1, 2, \dots, N)$, and assume

*The author is continuing work in this area. The proof and certain extensions will be presented in a forthcoming paper.

throughout that there exists a w^* which induces this ordering. To implement this ordering we wish to find a $w \in E^d$ such that

$$w \cdot x_1 > w \cdot x_2 > \dots > w \cdot x_N \quad . \quad (16)$$

Now consider the algorithm which at the k^{th} step increments the weight vector w_k by $x_i - x_j$ only if w_k incorrectly orders x_i and x_j . Specifically, for $i > j$ let

$$w_{k+1} = \begin{cases} w_k + x_i - x_j & , \quad w_k \cdot x_i \leq w_k \cdot x_j \\ w_k & , \quad w_k \cdot x_i > w_k \cdot x_j \end{cases} \quad . \quad (17)$$

Then, by the Perceptron convergence algorithm, for any sequence of pairs of vectors from x_1, x_2, \dots, x_N , the sequence of weight vectors w_k will make a finite number of mistakes. Moreover, if a sequence of pairs of vectors is presented in which each pair occurs infinitely often (for example, a cyclic sequence), then w_k converges, in a finite number of corrections, to a vector which yields the desired ordering.

If an orderly procedure like the fixed increment, relaxation, or simplex method is to be used for training, an important saving in time will be effected if only the $N-1$ extreme pattern pairs $(x_{i_1} - x_{i_2})$, $(x_{i_2} - x_{i_3})$, \dots , $(x_{i_{N-1}} - x_{i_N})$, corresponding to the ordering (i_1, i_2, \dots, i_N) , are trained on. Since all other inequalities are a consequence of these, the number of patterns in the training set can be reduced from $\binom{N}{2}$ to $N-1$.

E. SEPARATING PATTERNS WITH m OR FEWER MISTAKES

The number $C(N,d)$ of homogeneously linearly separable dichotomies of N points in E^d yields an obvious crude upper bound on $C(N,d; m)$, the number of dichotomies of N points in E^d which can be homogeneously separated with m or fewer errors.

To each separable dichotomy of N points there corresponds a set of $\binom{N}{m}$ dichotomies which differ in the assignment of precisely m points. Thus,

$$C(N,d; m) \leq \sum_{k=0}^m \binom{N}{k} C(N,d) \quad (18)$$

The crude bound

$$\sum_{k=0}^m \binom{N}{k} \leq \sum_{k=0}^m N^k \leq N^{m+1} \quad (19)$$

yields

$$C(N,d) \leq 2N^d \quad (20)$$

and

$$C(N,d; m) \leq 2N^{d+m+1} \quad (21)$$

All 2^N dichotomies of N points in E^d are separable (with m or fewer errors) only if $C(N,d; m) \geq 2^N$; i.e., only if

$$d+m+1 > \frac{N-1}{\log_2 N} \quad (22)$$

For example, suppose we are given a collection of 20,000 pattern vectors in a 100-dimensional space. We will be able to choose some very nonseparable dichotomies of this set of patterns. In fact, as a consequence of Eq. (22) with $N = 20,000$, $d = 100$, we see that there exists a dichotomy of this set of patterns for which every linear separating surface will make at least 1000 errors in classification.

Finally, we remark that there is no hope of finding a general expression for $C(N,d; m)$ for $m \neq 0$, $d > 2$, unless additional constraints on the pattern set are given, because there exist simple examples which demonstrate that this quantity depends critically on the configuration of the pattern set.

F. SUMMARY

The results of the previous sections can be summarized in the following tabular form. It will be convenient to express answers in terms of the cumulative binomial function

$$C(N,d) = 2 \sum_{K=0}^{d-1} \binom{N-1}{K}$$

1. Threshold Logic Unit (see Sec. B and Fig. 5a)

Problem:	N points in general position in d -space
Device:	Linear threshold device with d inputs, zero threshold (Fig. 1)
Dichotomies:	2^N
Separable Dichotomies:	$C(N,d)$
Capacity:	$2d$ patterns (two patterns per variable weight; two patterns per degree of freedom of the family of separating surfaces).

2. Parallel Linear Threshold Units (see Sec. B and Fig. 5b)

Problem: N points in general position in 2-space

Device: Bank of m parallel linear threshold devices, each with two inputs and threshold zero. Majority logic (no loss of generality over Boolean logic).

Dichotomies: 2^N

Separable
Dichotomies: $C(N, m+1)$

Capacity: $2(m+1)$ patterns (two patterns per separating line).

3. Parallel Linear Threshold Units (see Sec. B and Fig. 5c)

Problem: N points in general position on the surface of a cone with vertex at the origin in 3-space.

Device: Bank of m parallel linear threshold devices, each with three inputs and threshold zero. Majority logic (no loss in generality over Boolean logic).

Dichotomies: 2^N

Separable
Dichotomies: $C(N, 2m+1)$

Capacity: $4m+2$ patterns (four patterns per separating plane).

Remark: This problem is equivalent to separating N points on a circle by m lines which are not required to pass through the origin.

4. Parallel Linear Threshold Units; r Categories (see Sec. C & Fig. 5d)

Problem: N distinct points on a line

Device: Bank of m parallel linear threshold devices, each with one input and arbitrary threshold. General OR logic (also free to choose the number of modes per category).

r -Chotomies: r^N

Separable
r-Chotomies:

$$r \sum_{K=0}^{m-1} \binom{N-1}{K} (r-1)^K$$

Capacity: $\frac{rm}{(r-1)}$

5. Linear Machine (see Sec. D)

Problem: N points in general position in d-space

Device: Linear device which forms inner product

Orderings: N!

Linearly
Induceable
Orderings:

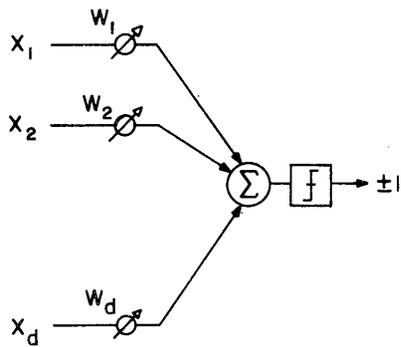
$$2 \sum_{K=0}^{d-1} S_K^{[N-1]}$$

Capacity: $\frac{N}{N - \ln N} \rightarrow 1$ patterns per dimension.

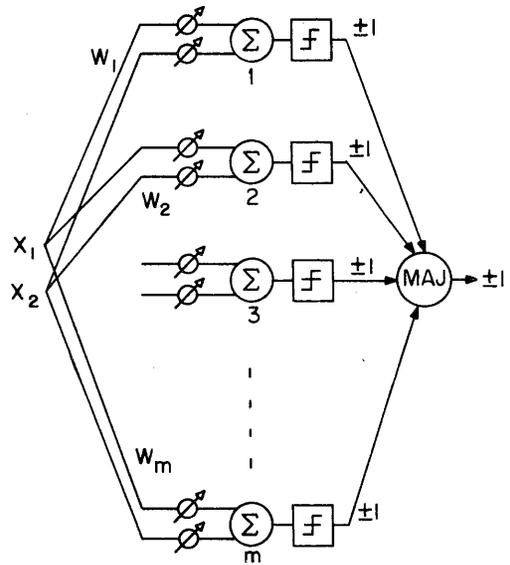
6. An Upper Bound on the Capacity of Networks (see Chapt. VII of Ref. 4)

A network of linear threshold devices in arbitrary fixed logic must contain at least $N/(1 + \log_2 N)$ variable weights in order to be able to separate every dichotomy of N pattern vectors.

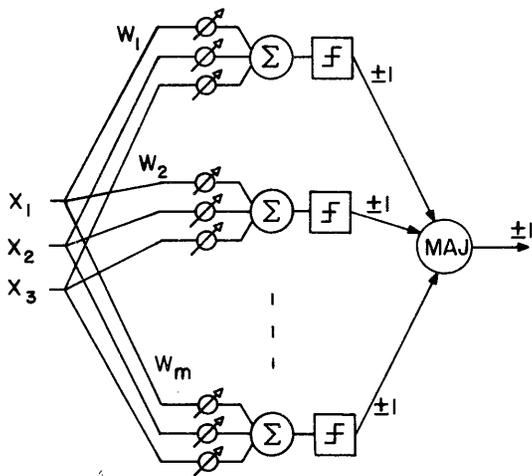
These partial results are all combinatorial in nature. It is our hope that for certain "natural" networks of linear devices the general capacities will also have combinatorial expressions independent of the precise configuration of the set of pattern vectors.



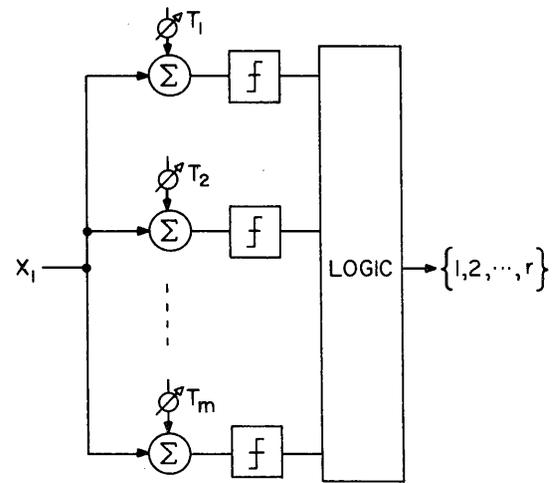
a.) LINEAR THRESHOLD UNIT



b.) BANK OF TLU's (2 DIMENSIONS)



c.) BANK OF TLU's (3 DIMENSIONS)



d.) r-CHOTOMIZER

Fig. 5 Networks of TLUs

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