Clustering Geometric Objects and Applications to Layout Problems*

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ABSTRACT

This paper deals with the relationship between cluster analysis and computational geometry describing clustering strategies using a Voronoi diagram approach in general and a line separation approach to improve the efficiency in a special case. We state the following theorems:

1. The set of all centralized 2-clusterings (S_1, S_2) of a planar point set S with $|S_1| = a$ and $|S_2| = b$ is <u>exactly</u> the set of all pairs of labels of opposite Voronoi polygons $v_a(S_1, S)$ and $v_b(S_2, S)$ of $V_a(S)$ and $V_b(S)$ respectively.

2. An optimal centralized 2-clustering [centralized divisive hierarchical 2-clustering]$_3$ can be constructed in $O(n \sqrt{n} \log^2 n + U_f(n) \cdot n \sqrt{n} + P_f(n))$ $[O(n \sqrt{n} \cdot \log^3 n + U_f(n) \cdot n \sqrt{n} + P_f(n))$ respectively] steps with $P_f(n)$ and $U_f(n)$ being the time complexity to compute and update a given clustering measure f.

Applications to layout problems (design of assembly lines; VLSI-placement problems and board design) as well as image understanding problems (clustering of sets of geometric objects as points, edges, polygons etc.) will be given in the talk.

Keywords: Cluster analysis, computational geometry, image understanding, layout problem, line separation, Voronoi diagram

1. INTRODUCTION

Given a set S of n points $x_1, \ldots, x_n \in R^d$ (this paper will deal only with planar point sets - d = 2 - and Euclidian metric), a partition of S into C disjoint "natural groupings" $S_1, \ldots, S_C$ is called a "C-clustering" of S. There are several ways to specify "natural groupings". You can ask for minimization (maximization) of some "clustering measure" $f:(S_1, \ldots, S_C) \to r \in R$ (e.g. minimize the maximum diameter) or you give an algorithmic specification.

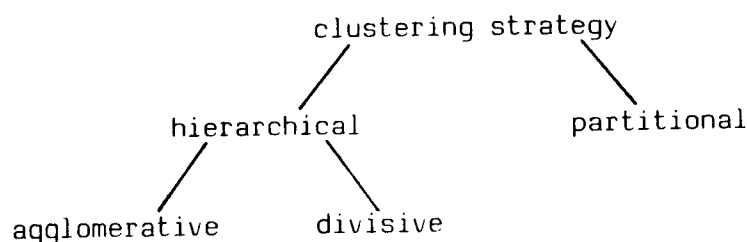Most of the proposed strategies in clustering literature can be classified according to fig. 1.

fig. 1

Agglomerative hierarchical (divisive hierarchical) algorithms produce a sequence of nested partitions with decreasing (increasing) number of clusters hoping to approach the given goal. Partitional strategies divide S into C clusters at one trying mostly to improve this partitioning in some postprocessing steps (keeping the number of clusters constant) - refer to [DE], [DJ], [M], [P], [R].
This paper will deal with the relationships between cluster analysis and computational geometry describing two divisive hierarchical clustering strategies using computational geometry methods.

2. CLUSTER CENTERS AND VORONOI DIAGRAMS

2.1 Basic definitions and properties

Several clustering methodologies (e.g. FORGY/ISODATA, see [DJ]) select C cluster centers from S assigning the remaining n-C points to their nearest cluster center (consult [DJ] for more details).
We extend this to the following

Definition 1:

(a) A cluster $S_i \subseteq S$ is called "centralized", if there exists a center center $x \in R^2$ with S_i being the set of s_i nearest neighbors of x with respect to S. (Let $s_i := |S_i|$ for the remaining of this paper.)

(b) A C-clustering $(S_1, \ldots, S_C)$ of S is called centralized, if all $S_i (1 \le i \le C)$ are centralized.

(c) A C-clustering $(S_1, \ldots, S_C)$ of S is called "balanced", if for all $1 \le i < j \le C : |s_i - s_j| \le 1$ (This is the most interesting case in practice).

Let $v_k(S_i, S)$ be the order k Voronoi polygon of some $S_i \subseteq S$ $(k=s_i)$ and $V_k(S)$ be the order k Voronoi diagram of S (see [SH] and [L]). We shall call S_i the "label" of the Voronoi polygon $v_k(S_i, S)$.

Using the notations of [SH], [L] and [D] it is easy to prove the following

Lemma 1:

1.1 $S_i \subseteq S$ is a centralized cluster if and only if S_i is the label of some Voronoi polygon $v_k(S_i, S) \ne \{\}$.

1.2 $(S_1, \ldots, S_C)$ is a centralized C-clustering if and only if all $S_i (1 \le i \le C)$ are labels of some Voronoi polygon of some Voronoi diagram $V_k(S)$ and S is the disjoint union of $S_1, \ldots, S_k$.

1.3 $(S_1, \ldots, S_C)$ is a balanced centralized C-clustering of S if and only if all $S_i (1 \le i \le C)$ are labels of some Voronoi polygon of $V_{\lfloor n/C \rfloor}(S)$ or $V_{\lceil n/C \rceil}(S)$ and S is the disjoint union of $S_1, \ldots, S_C$.

It states, that a centralized C-clustering is a selection of disjoint labels of Voronoi polygons. This leads to the idea, to use the geometric properties of Voronoi diagrams for the design of clustering methodologies.

2.2 Applications to divisive hierarchical clustering

Using our above definitions a (C-nested) <u>divisive hierarchical clustering</u> is a nested sequence of C-clusterings (which we will call clustering steps) successively decomposing S into smaller subsets as demonstrated in fig. 2.
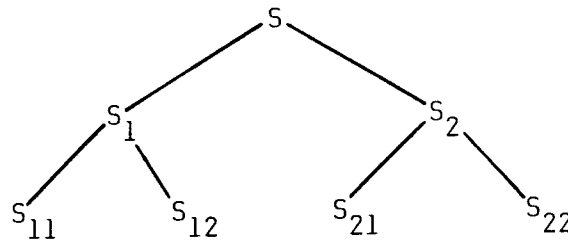
(S_1, S_2), (S_{11}, S_{12}), (S_{21}, S_{22}) is a 2-clustering of S, S_1, S_2 respectively

fig. 2

We shall call a divisive hierarchical clustering centralized (balanced), if all clustering steps are centralized (balanced).

This chapter will demonstrate the relationship between order k Voronoi diagrams and 2-nested centralized divisive hierarchical clustering.

Definition 2:

Two disjoint Voronoi polygons vp_1 and vp_2 are "<u>opposite</u>" to each other, if there are two nonparallel straight lines g and g' each containing two disjoint rays r_1, r_2 and r_1', r_2' respectively with $r_1, r_1' \subseteq vp_1$ and $r_2, r_2' \subseteq vp_2$. (Note, that opposite Voronoi polygons are always open.)

With this definition we can prove the following lemmata:

Lemma 2:

Let a,b be two positive integers with $a+b \leq n$, $a = |S_1|$, $b = |S_2|$ and $v_a(S_1, S)$, $v_b(S_2, S)$ two nonempty Voronoi polygons which are opposite, then S_1 and S_2 are disjoint.

and

Lemma 3:

Let a,b be two positive integers with $a+b = n$, $a = |S_1|$, $b = |S_2|$ and $v_a(S_1, S)$, $v_b(S_2, S)$ two Voronoi polygons with S being the disjoint union of S_1 and S_2, then $v_a(S_1, S)$ and $v_b(S_2, S)$ are open and opposite.

Summarizing this, we have

Theorem 1:
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The set of all centralized 2-clusterings (S_1, S_2) of S with $|S_1| = a$ and $|S_2| = b$ is exactly the set of all pairs of labels of opposite Voronoi polygons $v_a(S_1, S)$ and $v_b(S_2, S)$ of $V_a(S)$ and $V_b(S)$ respectively.

Because every $S_1 \subseteq S$ has exactly one complement $S_2 = S - S_1$, it follows immediately, that every open order k Voronoi polygon $v_k(S_1, S)$ has exactly one opposite order n-k Voronoi polygon, thus the four bounding rays of these polygons having pairwise exactly opposite direction.

This is an interesting property of order k Voronoi diagrams, which appears to be new.

Consider the problem of constructing an <u>optimal</u> centralized 2-clustering (S_1, S_2) of S with respect to some <u>clustering measure</u> $f(S_1, S_2) \in R$ and $|S_1| = k$, $|S_2| = n-k$. We assume a <u>given algorithm F</u>, which is able to compute $f(S_1, S_2)$ in time $P_F(n)$ and exchange exactly one element of S_1 and S_2 respectively in $U_F(n)$ steps (eventually using heraditary properties). The following steps are appropriate to solve the problem:

(1) Compute all open order k (and n-k) Voronoi polygons sorted by the angle of their bounding rays (respectively). (There are $O(n\sqrt{k})$ such polygons: see Theorem 1, Lemma 4 and [EW 1])

(2) Following exactly one revolution of a rotating line pointing at the current pair of opposite Voronoi polygons and select the optimal one with respect to f computing $O(n\sqrt{k})$ updates using F.

From the aspect of computational complexity step (1) is the most expensive one. Lee [L] has proposed an algorithm to construct an order k diagram in $O(k^2 n \log n)$ steps. With k being of order n in most cases of 2-clustering this would normally lead to an $O(n^3 \log n)$ algorithm, but [ERS] describe some methods to construct <u>all</u> Voronoi diagrams in $O(n^3)$. So current state of the art (as known by the authors) in constructing Voronoi diagrams leads to an $O(n^3 + n\sqrt{n}\ U_F(n) + P_F(n))$ algorithm to compute an optimal centralized 2-clustering.

A centralized divisive hierarchical clustering will be obtained by a successive application of this algorithm to the current partition of S. This leads to the same asymptotic time complexity.

Note, that we compute much more information than we actually need, leaving us with the problem to look for some better algorithm to construct an order k Voronoi diagram or all of its open polygons respectively. This will significantly improve the complexity of our algorithm.
For the special case of 2-clustering we will give a more efficient solution in the following chapter.

3. AN $O(n\sqrt{n}\ \log^2 n + U_F(n)\ n\sqrt{n} + P_F(n))$ ALGORITHM TO CONSTRUCT AN OPTIMAL CENTRALIZED 2-CLUSTERING

To construct an optimal centralized 2-clustering (S_1, S_2) of S with $|S_1| = k$ and $|S_2| = n-k$ we state the following

Lemma 4:

(S_1, S_2) is a centralized 2-clustering of S if and only if S_1 and S_2 are separable and S is the disjoint union of S_1 and S_2.

After constructing the k-belt of T(S) (see [EW 2]) in $O(n\sqrt{k} \log^2 n)$ steps we search along its upper and lower border, respectively, update the clustering value $f(S_1, S_2)$ and select an optimal partition. From [EW 1] and [EW 2] we know, that our dynamic updating procedure F will be executed $O(n\sqrt{k})$ times, leading to an $O(n\sqrt{n} \log^2 n + U_F(n) n\sqrt{n} + P_F(n))$ algorithm.

By a successive application of this procedure as described in 2.2 we obtain a centralized divisive hierarchical clustering in $O(n\sqrt{n} \log^3 n + U_F(n) n\sqrt{n} + P_F(n))$ steps.

So we have

Theorem 2:

An optimal centralized 2-clustering [centralized divisive hierarchical 2-clustering] can be constructed in $O(n\sqrt{n} \log^2 n + U_F(n) n\sqrt{n} + P_F(n))$ [$O(n \sqrt{n} \log^3 n + U_F(n) n\sqrt{n} + P_F(n))$ respectively] steps.

4. REMARKS

Allowing cluster centers to be points of R^2 gives us the possibility to apply the geometric structure of order k Voronoi diagrams as an interesting tool for solving clustering problems. The described Voronoi diagram approach has the additional advantage of apparently being extendible to centralized C-clustering (in contrast to chapter 3).

Clustering of sets of geometric objects as edges, polygons etc. can be reduced to the partitioning of sets of points in more general spaces respectively of sets of labelled points. Details are given in the forthcoming paper [DNZ 1], applications of these methods to image understanding are analysed in [DNZ 2].
Applications to layout problems in a wide range are obvious: VLSI-placement problems in chip design as well as placement of VLSI-components on boards.
By additionally use of Voronoi-trees [N] the design of assembly lines (in the case of poor precedence structure) can be done most efficiently.

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