

A Slow Caratheodory Implementation

Algorithm 8 CARATHEODORY(P, u)

Input : A weighted set (P, u) of n points in \mathbb{R}^d .
Output: A Caratheodory set (S, w) for (P, u) in $O(n^2 d^2)$ time.

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1 if  $n \leq d + 1$  then
2   | return  $(P, u)$ 
3 Identify  $P = \{p_1, \dots, p_n\}$ 
4 for every  $i \in \{2, \dots, n\}$  do
5   |  $a_i := p_i - p_1$ 
6  $A := (a_2 \mid \dots \mid a_n) \ // \ A \in \mathbb{R}^{d \times (n-1)}$ 
7 Compute  $v = (v_2, \dots, v_n)^T \neq 0$  such that  $Av = 0$ .

8  $v_1 := -\sum_{i=2}^n v_i$ 
9  $\alpha := \min \left\{ \frac{u_i}{v_i} \mid i \in \{1, \dots, n\} \text{ and } v_i > 0 \right\}$ 
10  $w_i := u_i - \alpha v_i$  for every  $i \in \{1, \dots, n\}$ .
11  $S := \{p_i \mid w_i > 0 \text{ and } i \in \{1, \dots, n\}\}$ 
   | if  $|S| > d + 1$  then
12   |  $(S, w) := \text{CARATHEODORY}(S, w)$ 
13 return  $(S, w)$ 

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Overview of Algorithm 8 and its correctness. The input is a weighted set (P, u) whose points are denoted by $P = \{p_1, \dots, p_n\}$. We assume $n > d + 1$, otherwise $(S, w) = (P, u)$ is the desired coresot. Hence, the $n - 1 > d$ points $p_2 - p_1, p_3 - p_1, \dots, p_n - p_1 \in \mathbb{R}^d$ must be linearly dependent. This implies that there are reals v_2, \dots, v_n , which are not all zeros, such that

$$\sum_{i=2}^n v_i (p_i - p_1) = 0. \quad (2)$$

These reals are computed in Line 7 by solving system of linear equations. This step dominates the running time of the algorithm and takes $O(nd^2)$ time using e.g. SVD. The definition

$$v_1 = -\sum_{i=2}^n v_i \quad (3)$$

in Line 8, guarantees that

$$v_j < 0 \text{ for some } j \in [n], \quad (4)$$

and that

$$\sum_{i=1}^n v_i p_i = v_1 p_1 + \sum_{i=2}^n v_i p_i = \left(-\sum_{i=2}^n v_i \right) p_1 + \sum_{i=2}^n v_i p_i = \sum_{i=2}^n v_i (p_i - p_1) = 0, \quad (5)$$

where the second equality is by (3), and the last is by (2). Hence, for every $\alpha \in \mathbb{R}$, the weighted mean of P is

$$\sum_{i=1}^n u_i p_i = \sum_{i=1}^n u_i p_i - \alpha \sum_{i=1}^n v_i p_i = \sum_{i=1}^n (u_i - \alpha v_i) p_i, \quad (6)$$

where the first equality holds since $\sum_{i=1}^n v_i p_i = 0$ by (5). The definition of α in Line 9 guarantees that $\alpha v_{i^*} = u_{i^*}$ for some $i^* \in [n]$, and that $u_i - \alpha v_i \geq 0$ for every $i \in [n]$. Hence, the set S that is defined in Line 11 contains at most $n - 1$ points, and its set of weights $\{u_i - \alpha v_i\}$ is non-negative. Notice that if $\alpha = 0$, we have that $w_j = u_j > 0$ for some $j \in [n]$. Otherwise, if $\alpha > 0$, by (4) there is $j \in [n]$ such that $v_j < 0$, which yields that $w_j = u_j - \alpha v_j > 0$. Hence, in both cases there is $w_j > 0$ for some $j \in [n]$. Therefore, $|S| \neq \emptyset$.

The sum of the positive weights is thus the total sum of weights,

$$\sum_{p_i \in S} w_i = \sum_{i=1}^n (u_i - \alpha v_i) = \sum_{i=1}^n u_i - \alpha \cdot \sum_{i=1}^n v_i = 1,$$

where the last equality hold by (3), and since u sums to 1. This and (6) proves that (S, w) is a Caratheodory set of size $n - 1$ for (P, u) ; see Definition 2.1. In Line 12 we repeat this process recursively until there are at most $d + 1$ points left in S . For $O(n)$ iterations, the overall time is thus $O(n^2 d^2)$.

B Faster Caratheodory Set

Theorem B.1 (Theorem 3.1). *Let (P, u) be a weighted set of n points in \mathbb{R}^d such that $\sum_{p \in P} u(p) = 1$, and $k \geq d + 2$ be an integer. Let (C, w) be the output of a call to FAST-CARATHEODORY-SET(P, u, k); See Algorithm 1. Let $t(k, d)$ be the time it takes to compute a Caratheodory Set for k points in \mathbb{R}^d , as in Theorem 2.2. Then (C, w) is a Caratheodory set of (P, u) that is computed in time*

$$O\left(nd + t(k, d) \cdot \frac{\log n}{\log(k/d)}\right).$$

Proof. We use the notation and variable names as defined in Algorithm 1 from Section 3.

First, at Line 1 we remove all the points in P which have zero weight, since they do not contribute to the weighted sum. Therefore, we now assume that $u(p) > 0$ for every $p \in P$ and that $|P| = n$. Identify the input set $P = \{p_1, \dots, p_n\}$ and the set C that is computed at Line 9 of Algorithm 1 as $C = \{c_1, \dots, c_{|C|}\}$. We will first prove that the weighted set (C, w) that is computed in Lines 9–11 at an arbitrary iteration is a Caratheodory set for (P, u) , i.e., $\sum_{p \in P} u(p) \cdot p = \sum_{p \in C} w(p) \cdot p$, $\sum_{p \in P} u(p) = \sum_{p \in C} w(p)$ and $|C| \leq (d + 1) \cdot \lceil \frac{n}{k} \rceil$.

Let $(\tilde{\mu}, \tilde{w})$ be the pair that is computed during the execution the current iteration at Line 8. By Theorem 2.2 and Algorithm 8, the pair $(\tilde{\mu}, \tilde{w})$ is a Caratheodory set of the weighted set $(\{\mu_1, \dots, \mu_k\}, u')$. Hence,

$$\sum_{\mu_i \in \tilde{\mu}} \tilde{w}(\mu_i) = 1, \quad \sum_{\mu_i \in \tilde{\mu}} \tilde{w}(\mu_i) \mu_i = \sum_{i=1}^k u'(\mu_i) \cdot \mu_i \text{ and } |\tilde{\mu}| \leq d + 1. \quad (7)$$

By the definition of μ_i , for every $i \in \{1, \dots, k\}$

$$\sum_{i=1}^k u'(\mu_i) \cdot \mu_i = \sum_{i=1}^k u'(\mu_i) \cdot \left(\frac{1}{u'(\mu_i)} \cdot \sum_{p \in P_i} u(p) \cdot p \right) = \sum_{i=1}^k \sum_{p \in P_i} u(p) p = \sum_{p \in P} u(p) p. \quad (8)$$

We now have that

$$\begin{aligned} \sum_{p \in C} w(p) p &= \sum_{\mu_i \in \tilde{\mu}} \sum_{p \in P_i} \frac{\tilde{w}(\mu_i) u(p)}{u'(\mu_i)} \cdot p = \sum_{\mu_i \in \tilde{\mu}} \tilde{w}(\mu_i) \sum_{p \in P_i} \frac{u(p)}{u'(\mu_i)} p = \sum_{\mu_i \in \tilde{\mu}} \tilde{w}(\mu_i) \mu_i \\ &= \sum_{i=1}^k u'(\mu_i) \cdot \mu_i = \sum_{p \in P} u(p) p, \end{aligned} \quad (9)$$

where the first equality holds by the definitions of C and w , the third equality holds by the definition of μ_i at Line 5, the fourth equality is by (7), and the last equality is by (8).

The new sum of weights is equal to

$$\sum_{p \in C} w(p) = \sum_{\mu_i \in \tilde{\mu}} \sum_{p \in P_i} \frac{\tilde{w}(\mu_i) u(p)}{u'(\mu_i)} = \sum_{\mu_i \in \tilde{\mu}} \frac{\tilde{w}(\mu_i)}{u'(\mu_i)} \cdot \sum_{p \in P_i} u(p) = \sum_{\mu_i \in \tilde{\mu}} \frac{\tilde{w}(\mu_i)}{u'(\mu_i)} \cdot u'(\mu_i) = \sum_{\mu_i \in \tilde{\mu}} \tilde{w}(\mu_i) = 1, \quad (10)$$

where the last equality is by (7).

Combining (9) and (10) yields that the weighted (C, w) computed before the recursive call at Line 13 of the algorithm is a Caratheodory set for the weighted input set (P, u) . Since at each iteration we either return such a Caratheodory set (C, w) at Line 13 or return the input weighted set (P, u) itself at Line 3, by induction we conclude that the output weighted set of a call to FAST-CARATHEODORY-SET(P, u, k) is a Caratheodory set for the original input (P, u) .

By (7) we have that C contains at most $(d + 1)$ clusters from P and at most $|C| \leq (d + 1) \cdot \lceil \frac{n}{k} \rceil$ points. Hence, there are at most $\log_{\frac{k}{d+1}}(n)$ recursive calls before the stopping condition in line 2 is satisfied. The time complexity of each iteration is $n' + t(k, d)$ where $n' = |P| \cdot d$ is the number of points in the current iteration. Thus the total running time of Algorithm 1 is

$$\sum_{i=1}^{\log_{\frac{k}{d+1}}(n)} \left(\frac{nd}{2^{i-1}} + t(k, d) \right) \leq 2nd + \log_{\frac{k}{d+1}}(n) \cdot t(k, d) \in O \left(nd + \frac{\log n}{\log(k/(d+1))} \cdot t(k, d) \right).$$

□

Theorem B.2 (Theorem 3.2). *Let $A \in \mathbb{R}^{n \times d}$ be a matrix, and $k \geq d^2 + 2$ be an integer. Let $S \in \mathbb{R}^{(d^2+1) \times d}$ be the output of a call to CARATHEODORY-MATRIX(A, k); see Algorithm 2. Let $t(k, d)$ be the computation time of CARATHEODORY given k point in \mathbb{R}^{d^2} . Then S satisfies that $A^T A = S^T S$. Furthermore, S can be computed in $O(nd^2 + t(k, d^2) \cdot \frac{\log n}{\log(k/d^2)})$ time.*

Proof. We use the notation and variable names as defined in Algorithm 2 from Section 3.

Since (C, w) at Line 5 of Algorithm 2 is the output of a call to FAST-CARATHEODORY-SET(P, u, k), by Theorem 3.1 we have that: (i) the weighted means of (C, w) and (P, u) are equal, i.e.,

$$\sum_{p \in P} u(p) \cdot p = \sum_{p \in C} w(p) \cdot p, \quad (11)$$

(ii) $|C| \leq d^2 + 1$ since $P \subseteq \mathbb{R}^{(d^2)}$, and (iii) C is computed in $O(nd^2 + \log_{\frac{k}{d^2+1}}(n) \cdot t(k, d^2))$ time.

Combining (11) with the fact that p_i is simply the concatenation of the entries of $a_i a_i^T$, we have that

$$\sum_{p_i \in P} u(p_i) a_i a_i^T = \sum_{p_i \in C} w(p_i) \cdot a_i a_i^T. \quad (12)$$

By the definition of S in Line 6, we have that

$$S^T S = \sum_{p_i \in C} (\sqrt{n \cdot w(p_i)} \cdot a_i) (\sqrt{n \cdot w(p_i)} \cdot a_i)^T = n \cdot \sum_{p_i \in C} w(p_i) \cdot a_i a_i^T. \quad (13)$$

We also have that

$$A^T A = \sum_{i=1}^n a_i a_i^T = n \cdot \sum_{p_i \in P} (1/n) a_i a_i^T = n \cdot \sum_{p_i \in P} u(p_i) a_i a_i^T, \quad (14)$$

where the second derivation holds since $u \equiv 1/n$. Theorem 3.2 now holds by combining (12), (13) and (14) as

$$S^T S = n \cdot \sum_{p_i \in C} w(p_i) \cdot a_i a_i^T = n \cdot \sum_{p_i \in P} u(p_i) a_i a_i^T = A^T A.$$

Running time: Computing the weighted set (P, u) at Lines 1–4 takes $O(nd^2)$ time, since it takes $O(d^2)$ time to compute each of the n points in P .

By Theorem 3.1, Line 5 takes $O(nd^2 + t(k, d^2) \cdot \frac{\log n}{\log(k/d^2)})$ to compute a CARATHEODORY for the weighted set (P, u) , and finally Line 6 takes $O(d^3)$ for building the matrix S . Hence, the overall running time of Algorithm 2 is $O(nd^2 + t(k, d^2) \cdot \frac{\log n}{\log(k/d^2)})$. □