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# Exact enumeration of local minima for k-medoids clustering in a 2D Pareto Front

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**Abstract** K-medoids clustering is solvable by dynamic programming in  $O(N^3)$  time for a 2D Pareto Front (PF). A key element is a interval clustering optimality. This paper proves this property holds also for local minima for k-medoids. It allows to enumerate the local minima of k-medoids with the same complexity than the computation of global optima for  $k=2$  ou  $k=3$ . A pseudo-polynomial enumeration scheme is designed, for small values of  $k$ . This allows to understand results obtained by local search approaches in a 2D PF.

**Keywords:**

Local minimums, k-medoids, clustering, Pareto Front,

## 1. Problem statement, notation

**Definition 1.** A 2D PF is defined as a set  $E$  of  $N$  points in  $\mathbb{R}^2$ , indexed with  $E = \{(x_k, y_k)\}_{k \in \llbracket 1, N \rrbracket}$  such that  $k \in \llbracket 1, N \rrbracket \mapsto x_k$  is increasing and  $k \in \llbracket 1, N \rrbracket \mapsto y_k$  is decreasing.

Let  $\Pi_K(E)$  the set of partitions of  $E$  in  $K$  subsets.  $K$ -medoids clustering is a combinatorial optimization problem indexed by  $\Pi_K(E)$ . It minimizes the sum for all the  $K$  clusters of the dissimilarity measure minimizing the sum of the squared distances from one chosen point of  $P$ , the *medoid*, to the other points of  $P$  :

$$\min_{\pi \in \Pi_K(E)} \sum_{P \in \pi} \min_{c \in P} \sum_{x \in P} \|x - c\|^2 \quad (1)$$

Combinatorial optimization problem (1) defines global optimums. For this paper, local minima are defined using neighborhoods of the PAM (Partitioning Around Medoids) heuristic for k-medoids, adaptation of seminal Lloyd's heuristic for the k-means problem [6].

**Definition 2** (Local minima of  $K$ -medoids). *For all  $K \in \mathbb{N}^*$ , local minima of  $K$ -medoids (for PAM) are characterized by the encoding of partitioning subsets  $P_1, \dots, P_K$  and their respective medoids  $c_1, \dots, c_K$ , with the property:*

$$\forall k \in \llbracket 1; K \rrbracket, \forall p \in P_k, \forall k' \neq k, \quad \|p - c_k\| \leq \|p - c_{k'}\| \quad (2)$$

## 2. Local optimality and interval clustering

A global minimum of optimization problem (1) can be computed in a 2D PF by dynamic programming in  $O(N^3)$  time [1]. A key element is a necessary condition: interval optimality as in 1D clustering problems [3, 5]. The interval clustering property holds also for local minima for k-medoids:

**Theorem 3.** *We suppose that points  $(x_i)$  are sorted as in Definition 1. Each local minimum of  $K$ -Medoids in a 2dPF is only composed of clusters  $\mathcal{C}_{i,i'} = \{x_j\}_{j \in \llbracket i, i' \rrbracket} = \{x \in E \mid \exists j \in \llbracket i, i' \rrbracket, x = x_j\}$ . As a consequence, there is at most  $\binom{N}{K}$  local optima for  $K$ -Medoids in a 2d PF of size  $N$ .*

Note that this optimality property is specific for k-medoids clustering. For k-center problems, global minima exist with nested clusters [2]. For the k-means problem, we can give a counter example of local minima which do not fulfill the interval clustering property.

## 3. Enumeration algorithms of local optima

Theorem 3 allows to enumerate the  $\binom{N}{K}$  possible local minimums. Lemmas help to decrease the complexity of such operation. Enumeration schemes require to prove that a candidate solution is a local minimum fulfilling 2, which can be checked easily using properties related to interval clustering:

**Lemma 4.** *Interval clustering  $\mathcal{C}_{1,f_1}, \mathcal{C}_{f_1+1,f_2}, \dots, \mathcal{C}_{f_{K-2}+1,f_{K-1}}, \mathcal{C}_{f_{K-1}+1,N}$  with medoids  $c_1, \dots, c_K$  is a local minimum if and only if both properties are fulfilled:*

$$\forall k \in \llbracket 1; K-1 \rrbracket, \quad \|z_{f_k} - c_k\| \leq \|z_{f_k} - c_{k+1}\| \quad (3)$$

$$\forall k \in \llbracket 1; K-1 \rrbracket, \quad \|z_{1+f_k} - c_{k+1}\| \leq \|z_{1+f_k} - c_k\| \quad (4)$$

For enumeration schemes, it requires to compute the medoids  $c_{j,j'}$  for each cluster  $\mathcal{C}_{j,j'}$  with  $j \leq j'$ . Lemmas 5 and 6 allows to do it efficiently for our enumeration schemes:

**Lemma 5.** *Computing medoids (and costs) of clusters  $\mathcal{C}_{j',j}$  for all  $j' \in \llbracket 1; j \rrbracket$  for a given  $j \in \llbracket 1; N \rrbracket$  runs in  $O(j^2)$  time and uses  $O(j)$  memory space.*

**Lemma 6.** *Computing medoids (and costs) of clusters  $\mathcal{C}_{j,j'}$  for all  $j' \in \llbracket j; N \rrbracket$  for a given  $j \in \llbracket 1; N \rrbracket$  runs in  $O((N - j)^2)$  time and uses  $O(N - j)$  memory space.*

For  $K = 2$  and  $K = 3$ , straightforward enumeration of local minima has the same complexity than computing only a global optimum:

**Proposition 7.** *Enumerating the  $O(N)$  local minima of 2-Medoids in a 2d PF of size  $N$  runs in  $O(N^2)$  time using  $O(N)$  additional memory space.*

**Proposition 8.** *Enumerating the  $O(N^2)$  local minima of 3-Medoids in a 2d PF of size  $N$  runs in  $O(N^3)$  time using  $O(N)$  additional memory space.*

For a general algorithm, we use  $O(N^2)$  additional memory space, computing first the medoids  $c_{j,j'}$  of each interval cluster  $\mathcal{C}_{j,j'}$  in  $O(N^3)$  time. Then, a backtracking algorithm enumerates only partial feasible solutions for Lemma 4: if  $\mathcal{C}_{1,f_1}, \mathcal{C}_{f_1+1,f_2}, \dots, \mathcal{C}_{f_{k-2}+1,f_{k-1}}, \mathcal{C}_{f_{k-1}+1,f_k}$  with medoids  $c_1, \dots, c_k$  partially fulfills (3) and (4), the next point  $f_{k+1} > f_k$  induces a new medoid  $c_{f_{k-1}+1,f_k}$  such that  $\|z_{f_k} - c_{f_{k-1}+1,f_k}\| \leq \|z_{f_k} - c_{f_k+1,f_{k+1}}\|$  and  $\|z_{1+f_k} - c_{f_k+1,f_{k+1}}\| \leq \|z_{1+f_k} - c_{f_{k-1}+1,f_k}\|$ . The following recursive algorithm calls `ENUMLOCALMIN(0, [], [], 0)` to print all the local minimums. We use functional programming notations, as in OCaml,  $x :: l$  pop first element  $x$  in top of list  $l$ ,  $l' = x :: l = (\text{hd } l') :: (\text{tl } l')$ ,  $[]$  is empty list.

## 4. Conclusions and perspectives

If  $k$ -medoids clustering in a 2D PF is solvable by dynamic programming in  $O(N^3)$  time with an interval clustering property, this paper proves that this property holds also for local minima for  $k$ -medoids. It allows to enumerate the local minima of  $k$ -medoids with the same complexity than the computation of global optima for  $k = 2$  ou  $k = 3$ . A pseudo-polynomial enumeration scheme is designed, for small values of  $k$ . Perspectives are to understand results obtained by local search approaches in a 2D PF and why local minima of a poor quality can be found by PAM local search in a 2D PF [4]. This problem and these properties are also an interesting for landscape analysis approaches.

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**Algorithm : Exhaustive search of Local Minima of  $K$ -Medoids**


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**Input:**  $N$  points of a 2D PF,  $E = \{z_1, \dots, z_N\}$ ,  $K \leq N$

The medoids  $c_{j,j'}$  of each interval cluster  $C_{j,j'}$  are computed in pre-processing

```

ENUMLOCMIN(last, ptList, medList, k)
  if k ==  $K - 1$ 
    c := hd medList
    if  $\|z_{last} - c\| \leq \|z_{last} - c_{last+1,N}\| \ \&\& \ \|z_{1+last} - c_{last+1,N}\| \leq \|z_{1+last} - c\|$ 
      then print(ptList)
    end if
  else
    for next =  $1 + last$  to  $N - K + k + 1$ 
      c' :=  $c_{1+last,next}$ 
      if k == 0 then ENUMLOCMIN (next, next::[], c'::[], 1)
      else
        c := hd medList
        if  $\|z_{last} - c\| \leq \|z_{last} - c'\| \ \&\& \ \|z_{1+last} - c'\| \leq \|z_{1+last} - c\|$ 
          then ENUMLOCMIN (next, next::ptList, c'::medList,  $1 + k$ )
        end if
      end if
    end for
  end if
end

```

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