
EKM: an exact, polynomial-time algorithm for the K -medoids problem

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Abstract

The K -medoids problem is a challenging combinatorial clustering task, widely used in data analysis applications. While numerous algorithms have been proposed to solve this problem, none of these are able to obtain an exact (globally optimal) solution for the problem in polynomial time. In this paper, we present EKM: a novel algorithm for solving this problem exactly with worst-case $O(N^{K+1})$ time complexity. EKM is developed according to recent advances in transformational programming and combinatorial generation, using formal program derivation steps. The derived algorithm is provably correct by construction. We demonstrate the effectiveness of our algorithm by comparing it against various approximate methods on numerous real-world datasets. We show that the wall-clock run time of our algorithm matches the worst-case time complexity analysis on synthetic datasets, clearly outperforming the exponential time complexity of benchmark branch-and-bound based MIP solvers. To our knowledge, this is the first, rigorously-proven polynomial time, practical algorithm for this ubiquitous problem.

1 Introduction

In machine learning (ML), K -medoids is the problem of partitioning a given dataset into K clusters where each cluster is represented by one of its data points, known as a *medoid*. A plethora of approximate/heuristic methodologies have been proposed to solve this problem, such as PAM (Partitioning Around Medoids) [Kaufman, 1990], CLARANS (Clustering Large Applications based on randomized Search) [Ng and Han, 2002], and variants of PAM [Schubert and Rousseeuw, 2021, Van der Laan et al., 2003].

While approximate algorithms are computationally efficient and have been scaled up to large dataset sizes, because they are approximate they provide no guarantee that the *exact (globally optimal) solution* can be obtained. In *high-stakes* or *safety-critical* applications, where errors are unacceptable or carry significant costs, we want the best possible partition given the specification of the clustering problem. Only an exact algorithm can provide this guarantee.

However, there are relatively few studies on exact algorithms for the K -medoids problem. The use of *branch-and-bound* (BnB) methods predominates research on this problem [Ren et al., 2022, Elloumi, 2010, Christofides and Beasley, 1982, Ceselli and Righini, 2005]. An alternative approach is to use off-the-shelf *mixed-integer programming* solvers (MIP) such as Gurobi [Gurobi Optimization, 2021] or GLPK (GNU Linear Programming Kit) [Makhorin, 2008]. These solvers have made significant achievements, for instance, [Elloumi, 2010, Ceselli and Righini, 2005]’s BnB algorithm is capable of processing medium-scale datasets with a very large number of medoids. More recently, [Ren et al., 2022] designed another BnB algorithm capable of delivering tight approximate solutions—with an

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