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

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School of Computer Science University of Birmingham Birmingham, B15 2TT, UK xxh1640student, bhan, ac, uk Max A. Little

School of Computer Science University of Birmingham Birmingham, B15 2TT, UK max10mit.edu

#### 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  $O\left(N^{K+1}\right)$  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.

#### I. 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].

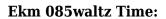
While approximate algorithms are computationally efficient and have been scaled up to large dataset sizes, because they are approximate they provide no guarantee that the exact (globally optimal) solution can be obtained. In high-stakes or safety-critical applications, where errors are unacceptable or 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 appeach 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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#### **Table of Contents Ekm 085waltz Time**

- 1. Understanding the eBook Ekm 085waltz Time
  - The Rise of Digital Reading Ekm 085waltz Time
  - Advantages of eBooks Over Traditional Books
- 2. Identifying Ekm 085waltz Time
  - Exploring Different Genres
  - Considering Fiction vs. Non-Fiction
  - Determining Your Reading Goals
- 3. Choosing the Right eBook Platform
  - Popular eBook Platforms
  - Features to Look for in an Ekm 085waltz Time
  - User-Friendly Interface
- 4. Exploring eBook Recommendations from Ekm 085waltz Time
  - Personalized Recommendations
  - Ekm 085waltz Time User Reviews and Ratings
  - Ekm 085waltz Time and Bestseller Lists

- 5. Accessing Ekm 085waltz Time Free and Paid eBooks
  - Ekm 085waltz Time Public Domain eBooks
  - Ekm 085waltz Time eBook Subscription Services
  - Ekm 085waltz Time Budget-Friendly Options
- 6. Navigating Ekm 085waltz Time eBook Formats
  - ∘ ePub, PDF, MOBI, and More
  - Ekm 085waltz Time Compatibility with Devices
  - Ekm 085waltz Time Enhanced eBook Features
- 7. Enhancing Your Reading Experience
  - Adjustable Fonts and Text Sizes of Ekm 085waltz Time
  - Highlighting and Note-Taking Ekm 085waltz Time
  - Interactive Elements Ekm 085waltz Time
- 8. Staying Engaged with Ekm 085waltz Time
  - Joining Online Reading Communities
  - Participating in Virtual Book Clubs
  - Following Authors and Publishers Ekm 085waltz Time
- 9. Balancing eBooks and Physical Books Ekm 085waltz Time
  - Benefits of a Digital Library
  - Creating a Diverse Reading Collection Ekm 085waltz Time
- 10. Overcoming Reading Challenges
  - Dealing with Digital Eye Strain
  - Minimizing Distractions
  - Managing Screen Time
- 11. Cultivating a Reading Routine Ekm 085waltz Time
  - Setting Reading Goals Ekm 085waltz Time
  - Carving Out Dedicated Reading Time
- 12. Sourcing Reliable Information of Ekm 085waltz Time
  - Fact-Checking eBook Content of Ekm 085waltz Time
  - Distinguishing Credible Sources
- 13. Promoting Lifelong Learning

- Utilizing eBooks for Skill Development
- Exploring Educational eBooks
- 14. Embracing eBook Trends
  - Integration of Multimedia Elements
  - Interactive and Gamified eBooks

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