Balanced K-Means Clustering on an Adiabatic Quantum Computer

Applied Quantum Machine Learning Project

Politecnico di Milano

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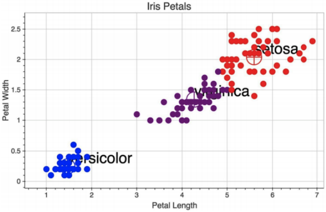
Outline

Advantages over classical approaches

- Better targets the global solution of the training problem
- Better theoretic scalability on large datasets



Outline

- QUBO formulation and theoretical analysis
- Empirical Analysis
- Conclusions and considerations

Lloyd's algorithm

- Complexity $O(Nkdi)$ [13]
    - N number of data points
    - k number of clusters
    - d number of features
    - i number of iterations before the algorithm converges

Scikit-learn implementation

- Complexity $O(Nkd)$ [18]

[13] J. A. Hartigan and M. A. Wong, "Algorithm AS 136: A K-Means clustering algorithm" Applied Statistics

[18] "Scikit-learn: Machine learning in python," J. Mach. Learn. Res.

Malinen et al.

- Complexity $O(N^3)$ [13]

Algorithm 1. Balanced k-means
Input: dataset X, number of clusters k
Output: partitioning of dataset.

```
Initialize centroid locations C^0.
t ← 0
repeat
   Assignment step:
         Calculate edge weights.
         Solve an Assignment problem.
   Update step:
         Calculate new centroid locations C^{t+1}
   t ← t + 1
until centroid locations do not change.
Output partitioning.
```

[21] Malinen, Mikko. (2014). Balanced K-Means for Clustering.

QUBO formulation

$$\min_{z \in \mathbb{B}^M} z^T A z$$

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$$X = \{x_1, x_2, \ldots, x_N\}$$

$$\Phi = \{\phi_1, \phi_2, \ldots, \phi_k\}.$$

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Distance matrix: D

Assignment matrix: $\hat{W}$

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$$\sum_{x,y \in \phi_j} \|x - y\|^2 = \hat{w}_j'^T D \hat{w}_j'$$

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$$\min_{\Phi} \sum_{j=1}^{k} \sum_{x,y \in \phi_j} \|x - y\|^2$$

Distance matrix: D
Assignment matrix: $\hat{W}$

$$\sum_{x,y \in \phi_j} \|x - y\|^2 = \hat{w}_j'^{\,T} D \hat{w}_j'$$

$$\min_{\hat{w}} \hat{w}^T \left(I_k \otimes D\right) \hat{w}$$

Penalties

$$\alpha \left(\hat{w}_j'^T \hat{w}_j' - N/k \right)^2$$

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$$\hat{w}_j'^T \alpha F \hat{w}_j'$$

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$$F = 1_N - \frac{2N}{k} I_N$$

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$$F = 1_N - \frac{2N}{k} I_N$$

$$\min_{\hat{w}} \hat{w}^T\left(I_k \otimes \left(D + \alpha F\right)\right)\hat{w}$$

Penalties

$$\alpha\left(\hat{w}_j'^T\hat{w}_j' - N/k\right)^2$$

$$\beta\left(\hat{w}_i^T\hat{w}_i - 1\right)^2$$

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$$\hat{w}_j'^T\alpha F\hat{w}_j'$$

$$\hat{w}_i^T\beta G\hat{w}_i$$

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$$F = 1_N - \frac{2N}{k} I_N$$

$$G = 1_k - 2 I_k$$

$$\min_{\hat{w}} \hat{w}^T \left(I_k \otimes \left(D + \alpha F \right) \right) \hat{w}$$

Penalties

$$\alpha\left(\hat{w}_j'^T\hat{w}_j' - N/k\right)^2$$

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$$\min_{\hat{w}}\hat{w}^T\left(I_k \otimes \left(D + \alpha F\right)\right)\hat{w}$$

$$\hat{w}^T Q^T\left(I_N \otimes \beta G\right)Q\hat{w}$$

$$\alpha\left(\hat{w}_j'^T\hat{w}_j' - N/k\right)^2 \qquad \beta\left(\hat{w}_i^T\hat{w}_i - 1\right)^2$$

$$\hat{w}_j'^T\alpha F\hat{w}_j' \qquad \hat{w}_i^T\beta G\hat{w}_i$$

$$F = 1_N - \frac{2N}{k}I_N \qquad G = 1_k - 2I_k$$

$$\min_{\hat{w}}\hat{w}^T\left(I_k\otimes(D+\alpha F)\right)\hat{w} \qquad \hat{w}^TQ^T\left(I_N\otimes\beta G\right)Q\hat{w}$$

$$\min_{\hat{w}}\hat{w}^T\left(I_k\otimes(D+\alpha F)+Q^T\left(I_N\otimes\beta G\right)Q\right)\hat{w}$$

Hyper-parameters tuning

$$\min_{\hat{w}} \hat{w}^T \left(I_k \otimes (D + \alpha F) + Q^T (I_N \otimes \beta G) Q \right) \hat{w}$$

$$\alpha = \frac{\max(D)}{2(N/k) - 1} \qquad \beta = \max(D)$$

Converting equation into a QUBO

$$\min_{\hat{w}} \hat{w}^T \left(I_k \otimes (D + \alpha F) + Q^T (I_N \otimes \beta G) Q\right) \hat{w}$$

$$\min_W \sum_{l=1}^{k} \sum_{j=1}^{N} \sum_{i=1}^{N} \sum_{m=1}^{d} w_{il} (x_{im} - x_{jm})^2 w_{jl}$$

$$+\alpha \sum_{l=1}^{k} \sum_{j=1}^{N} \sum_{i=1}^{N} w_{il} f_{ij} w_{jl} + \beta \sum_{l=1}^{N} \sum_{j=1}^{k} \sum_{i=1}^{k} w_{li} g_{ij} w_{lj}$$

- Complexity $O(N^2 kd)$

Malinen et al.

- Complexity $O(N^3)$

Scikit-learn implementation

- Complexity $O(Nkd)$

Algorithms used for comparisons

- balanced quantum k-means (case study)
- balanced classical k-means (authors implementation)
- classical k-means scikit-learn implementation

classical version of the k-means (non balanced) is used since, due to the structure of the dataset, constitute a valid comparison.

Adjusted Rand Index (ARI)

- compare the similarity of two partitions of a dataset
- range from −1 to 1 (high values indicates the two partitions are similar)
- used to compare the target partitions to the partitions produced by clustering

Total Computing time in quantum approach

$$t = t_{QUBO_convertion} + t_e + t_a + t_{postprocessing} \tag{1}$$

- $t_{QUBOconvertion}$ time to convert the problem in QUBO
- t_e time to embed the QUBO on hardware
- t_a time to solve the QUBO (anealing time)
- $t_{postprocessing}$ extract clustering from binary solution

synthetic classification datasets created with *make_classification* (Scikit-learn)

Datasets structure

- **N** points
- **k** classes
- **1** cluster per class
- **d** features
- clusters centered on a d-dimensional hypercube (with side length 2.0)
- points generated from a normal dist. about their cluster center (std 1.0)
- each class made of $\frac{N}{k}$ points

Hardware Configuration

Classical Machine

- 2.7 GHz Dual-Core Intel i5
- 8 GB 1.867 MHz DDR3 memory

Quantum Machine

- D-Wave 2000Q quantum computer
- 2048 qubits, 5600 inter-qubit connections

Technical Aspects

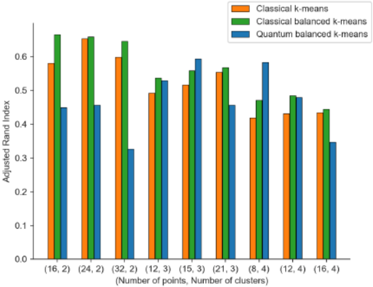
- quantum approach pre/post-processing done via the above classical machine
- quantum anealing operation perfomed 100 times for each experiment
- only ground state is used

Experiments Setup

- clustering quality of the 3 algorithms is compared
- each algorithm evaluated on different **problem types**
  - total of 9 problem types
  - defined by *(num. of points, num. of clusters)*
- for each problem type:
  - all the 3 algorithm evaluated on 50 **synthetic datasets**

Commenting Results for Quantum Approach

- performances drop for $k = 2$
  - less way to cluster means a local solution is more likely to be the correct one
- performances drop as the problem size increase
  - reflection of the quantum hardware



Limitations faced

- **Variable limitation** D-Wave 2000Q qubit limitation for problems $Nk > 64$ var.
- **Qubit connectivity** limitation => higher embedding time

Approximations

- Quantum run time for larger problems ($Nk > 64$)
  - used to evaluate scalability of the Quantum Approach
  - measure $t_{QUBO_convertion}$ (measurable)
  - estimate embedding time t_e (from smaller problems)
  - estimate annealing time t_a (constant, averaging smaller problems)
  - measure $t_{postprocessing}$

According to the embedding algorithms chosen by authors which scales quadratically in the number of binary variables of the QUBO

$$t_e = 1.887 \times 10^{-6}(Nk)^2 + 4.632 \times 10^{-6}(Nk) + 4.022 \times 10^{-4} \quad (2)$$

$$t_a = 0.03481 \pm 0.00008 \quad (3)$$

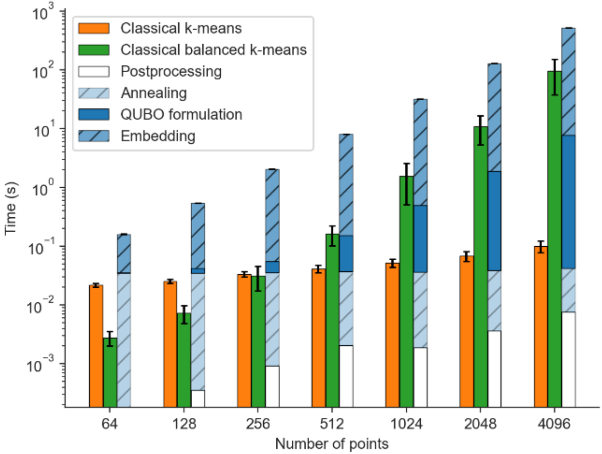
Experiments to assess scalability

- baselines evaluated on the three variables:
  - N data points
  - k clusters
  - d features
- $\forall$ **problem type** baselines runned on 50 **synthetic datasets**

Setup and Considerations

- baselines evaluated on increasing **data points**
- fixed cluster $k = 4$ and features $d = 2$
- considerations:
  - quantum is outperformed (due to embedding time)
  - future embedding time improvements may surpass classical balanced ($N \geq 1024$)
  - classical k-means scales the best expected since its **time complexity** $O(Nkd)$ vs quantum balanced $O(N^2kd)$

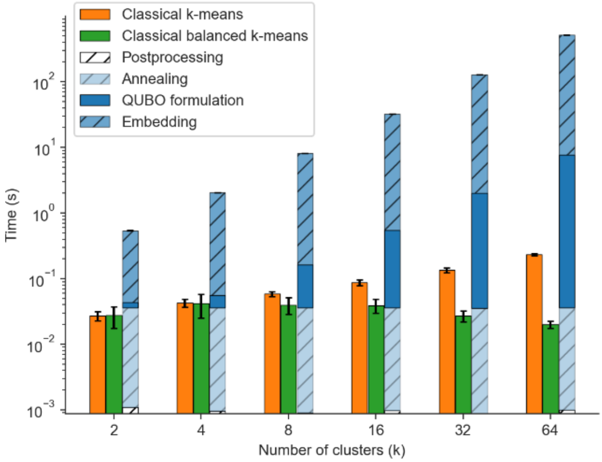
Scalability w.r.t. points (N) II



Setup and Considerations

- baselines evaluated on increasing **cluster size**
- fixed data points $N = 256$ and features $d = 8$
- considerations:
  - quantum scales worse on cluster size w.r.t. to other approaches
  - expected: third term on QUBO has $O(Nk^2)$ time complexity

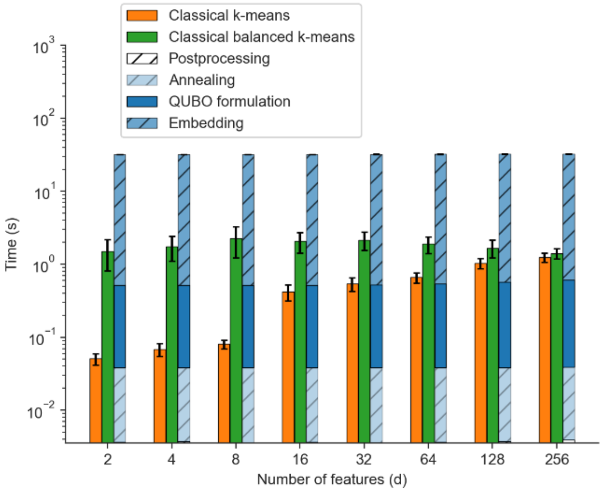
Scalability w.r.t. clusters (k) II



Setup and Considerations

- baselines evaluated on increasing **features number**
- fixed data points $N = 1024$ and cluster $k = 4$
- considerations:
  - quantum is the worse on time
  - quantum is promising in a future perspective, depending on embedding process optimizations
  - quantum approach scales better w.r.t. to classical *k-means* on d
  - expected: QUBO formulation only requires one comput. related to the dimension of the dataset
  - *classical balanced k-means* scales better in d w.r.t. to quantum approach
  - expected: *quantum balanced* $O(N^2kd)$ vs *classical balanced* $O(N^3)$

Scalability w.r.t. features (d) II



The Iris Dataset

- Reduced due to qubit limitations on modern hardware
- Pick N/k points from $2 \leq k \leq 3$ of the data set's classes

Experiments Run

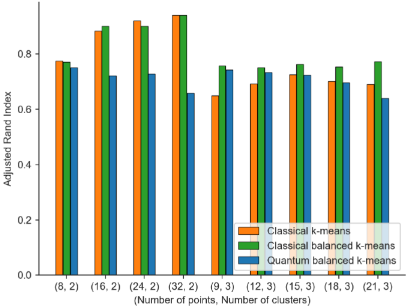
- All the 3 clustering algorithms were tested
- Experiments are run on 50 subsets of the dataset

Results

- $k = 2$
    - Trivial case, points are linearly separable
    - Classical algorithms perform better than quantum
    - Evident as the number of binary variables (Nk) increases

Clustering a Benchmark Data Set II

- $k = 3$
  - Similar performance to **classical balanced** k-means
  - Outperforms **Scikit-Learn** implementation
  - Performance of the QA degrades as the problem size increases



- Enhancements provided by adiabatic computers for solving **NP**-Hard or **NP**-Complete problems
- Promising result for Quantum Machine Learning
- The approach targets the global solution of the training problem **better** than the classic alternatives
- The **D-Wave 2000Q** machine
- Quantum approach partitions data with similar accuracy to the classical approaches
- The approach assumes viability as the quantum hardware improves

Future Works

- Bring the QUBO formulation to the generic k-means training problem
- Use elements of the approach to formulate quantum algorithms for similar clustering models
  - k-medoids clustering
  - fuzzy C-means clustering
- Cluster larger datasets

How complex is to construct the QUBO ?

$$\min_{\Phi} \sum_{j=1}^{k} \sum_{x,y \in \phi_j} \|x - y\|^2$$

$$\Downarrow$$

$$\min_{\hat{w}} \hat{w}^T \left(I_k \otimes (D + \alpha F) + Q^T \left(I_N \otimes \beta G \right) Q \right) \hat{w}$$

Complexity: $O(N^2 kd)$
Since $kd < N$:

- **Better** than classical balanced k-means: $O(N^3)$
- **Worse** than Scikit Learn implementation: $O(Nkd)$

Critical View II

Hyperparameter α allows to make considerations in the data preparation phase of the clustering algorithm:

- **Completely unbalanced** $\Longrightarrow$ use Scikit-Learn implementation
- **Fairly Balanced** $\Longrightarrow$ tuning on α and use Quantum Balanced implementation
- **Balanced** $\Longrightarrow$ use Quantum Balanced implementation with $\alpha < \beta$

Tuning α

- Modifies the curvature of the quadratic function to optimize
- By making α looser we change the position of the optimum allowing to cluster datasets that are not completely balanced
- Tuning α allows to prepare the algorithm on how much balanced the dataset will be

Variables and Density of the QUBO

- In the QUBO formulation we introduce k binary variables for each variable in the original problem

$$O(Nk)\ \textbf{variables}$$

- Efficient embedding algorithms [30] allow for a density of

$$O(N^2k^2)\ \textbf{qubits}$$

TABLE I
NUMBER OF BINARY VARIABLES AND AVERAGE NUMBER OF QUBITS USED IN THE QUANTUM APPROACH.

(N, k)	(16, 2)	(24, 2)	(32, 2)	(12, 3)	(15, 3)	(21, 3)	(8, 4)	(12, 4)	(16, 4)
Variables	32	48	64	36	45	63	32	48	64
Qubits	185	429	794	244	381	743	209	456	806

[30] P. Date, R. Patton, C. Schuman, and T. Potok, "Efficiently embedding qubo problems on adiabatic quantum computers," Quantum Information Processing, vol. 18, no. 4, p. 117, 2019.

Critical View IV

Can we cluster larger datasets on Advantage?

D-Wave 2000Q

- 2048 qubits
- 6,016 couplers
- 128,472 JJs

Advantage

- 5640 qubits
- 40,484 couplers
- 1,030,000 JJs

Thanks for your Attention