

Quantum jet clustering with LHC simulated data

Jorge J. Martínez de Lejarza,* Leandro Cieri and Germán Rodrigo¹

Instituto de Física Corpuscular, Universitat de València - Consejo Superior de Investigaciones Científicas, Parc Científic, E-46980 Paterna, Valencia, Spain

*E-mail: Jorge.M.Lejarza@ific.uv.es, lcieri@ific.uv.es,
german.rodrigo@csic.es*

We study the case where quantum computing algorithms could improve jet clustering by considering two new quantum algorithms that might speed up classical jet clustering algorithms. The first one is a quantum subroutine to compute a Minkowski-based distance between two data points, while the second one consists of a quantum circuit to track the rough maximum into a list of unsorted data. When one or both algorithms are implemented in classical versions of well-known clustering algorithms (K-means, Affinity Propagation and k_T -jet) we obtain efficiencies comparable to those of their classical counterparts. Furthermore, in the first two algorithms an exponential speed up in dimensionality and data length can be achieved when applying the distance algorithm or the maximum search algorithm. Whereas in the k_T algorithm, a quantum version of the same order as FastJet is achieved.

41st International Conference on High Energy physics - ICHEP2022

6-13 July, 2022

Bologna, Italy

¹Disclaimer: GR currently on leave at the European Research Council Executive Agency, European Commission, BE-1049 Brussels, Belgium. The views expressed are purely those of the writer and may not in any circumstances be regarded as stating an official position of the European Commission.

*Speaker

1. Introduction

Quantum computing devices, based on the laws of quantum mechanics, offer the possibility to efficiently solve specific problems that become very complex or even unreachable for classical computers since they scale either exponentially or super-polynomially. Very recently, quantum algorithms have started to be applied in solving problems which appear in high-energy particle physics. Recent applications of quantum algorithms to HEP cover diverse subareas such as jet clustering [1–4] or multi-loop Feynman integrals [5]. For a recent review on the applications of quantum computing to data analysis in HEP we refer the reader to Ref. [6].

In the present work, which is based on Ref. [4], we address the problem of clustering and jet reconstruction from collider data, which is a nontrivial and computationally expensive task, as it often involves performing optimizations over potentially large numbers of final-state particles. In particular, we consider the possibility of using quantum algorithms to improve the velocity in jet identification. Here we focus on three well-known classical algorithms: K-means clustering [7], Affinity Propagation (AP) [8] and k_T -jet clustering in all its variants [9–12]. We propose the corresponding quantum versions of the precedents algorithms: quantum K-means clustering, quantum AP-algorithm and quantum k_T -based algorithms.

These quantum versions made use of two new quantum subroutines proposed in this work. The first one serves to compute distances satisfying Minkowski metric, whereas the second one consists of a quantum circuit to track the maximum into a list of unsorted data.

2. Quantum distance in Minkowski space

In quantum computing, it is essential to have the ability to measure quantum entanglement between two states, as in many cases it determines the possibility of obtaining a quantum advantage. We rely on the *SwapTest* method [13] to quantify the similarity of two states.

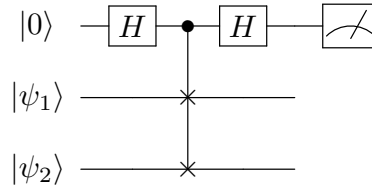


Figure 1: Quantum circuit *SwapTest*.

As it can be seen in Fig. 1, the *SwapTest* procedure makes use of one auxiliary qubit to get the inner product between two states:

$$P(|0\rangle) = \frac{1}{2} + \frac{1}{2} |\langle\psi_1|\psi_2\rangle|^2 . \quad (1)$$

The Eq. (1) displays that a distance between two quantum vectors can be obtained just measuring an ancillary qubit.

Vectors in high-energy physics are defined in a four-dimensional space-time with Minkowski metric. They have the form $x_i = (x_{i,0}, \mathbf{x}_i)$, where $x_{i,0}$ is the temporal component and \mathbf{x}_i represent

the three spatial components. In the following, we assume that the dimension of the space-time is d , where $d - 1$ is the number of spatial components. We shall define the analogue of the Euclidean classical distance in the Minkowski space corresponding to the invariant sum squared $s_{ij}^{(C)}$, which is commonly called invariant mass squared when vectors are particle four-momenta,

$$s_{ij}^{(C)} = (x_{0,i} + x_{0,j})^2 - |\mathbf{x}_i + \mathbf{x}_j|^2. \quad (2)$$

This quantity, which is Lorentz invariant, can be used as test distance to measure similarity between particle momenta. It is necessary to apply twice the *SwapTest* subroutine for computing the Minkowski-type distance through a quantum algorithm. Once for the spatial and once for the temporal component.

The spatial distance is computed using the subsidiary states:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} (|0, x_i\rangle + |1, x_j\rangle), \quad |\psi_2\rangle = \frac{1}{\sqrt{Z_{ij}}} (|\mathbf{x}_i|0\rangle - |\mathbf{x}_j|1\rangle), \quad (3)$$

where $Z_{ij} = |\mathbf{x}_i|^2 + |\mathbf{x}_j|^2$ is a normalization factor and $|0\rangle$ and $|1\rangle$ are the states of an ancillary qubit. Whereas the temporal distance is computed as a result of the overlap of the following states:

$$|\varphi_1\rangle = H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle), \quad |\varphi_2\rangle = \frac{1}{\sqrt{Z_0}} (x_{0,i}|0\rangle + x_{0,j}|1\rangle), \quad (4)$$

where $Z_0 = x_{0,i}^2 + x_{0,j}^2$. Then, applying the *SwapTest* to the states $|\psi_1\rangle, |\psi_2\rangle$ and $|\varphi_1\rangle, |\varphi_2\rangle$ one gets the relations:

$$P(|0\rangle|_{spatial}) = \frac{1}{2} + \frac{1}{2} |\langle\psi_1|\psi_2\rangle|^2, \quad P(|0\rangle|_{time}) = \frac{1}{2} + \frac{1}{2} |\langle\varphi_1|\varphi_2\rangle|^2, \quad (5)$$

where the overlaps $|\langle\psi_1|\psi_2\rangle|^2$ and $|\langle\varphi_1|\varphi_2\rangle|^2$ are given by

$$|\langle\psi_1|\psi_2\rangle|^2 = \frac{1}{2Z_{ij}} |\mathbf{x}_i - \mathbf{x}_j|^2, \quad |\langle\varphi_1|\varphi_2\rangle|^2 = \frac{1}{2Z_0} (x_{0,i} + x_{0,j})^2. \quad (6)$$

At this point, the quantum version of the invariant sum squared follows from the combination of results from Eq. (5) and Eq. (6):

$$s_{ij}^{(Q)} = 2(Z_0(2P(|0\rangle|_{time}) - 1) - Z_{ij}(2P(|0\rangle|_{spatial}) - 1)). \quad (7)$$

3. Quantum maximum search

Finding a particular element belonging to a dataset is a recurring problem in data analysis. This is a computationally very expensive task. However, quantum computing offers suitable tools to solve data query in a shorter computational time. In particular, it is well known the quadratic speed up exhibited by Grover's algorithm [14]. In this work, we present a considerably simpler algorithm that is used exclusively to find the rough maximum in a list of values.

Let $L[0, \dots, N - 1]$ be an unsorted list of N items. Solving the maximum searching problem is to find the index y such that $L[y]$ is the maximum. For clustering algorithms, $L[y]$ represents the inverse of the distance. The quantum algorithm to solve that problem using amplitude encoding proceeds in two steps:

1. The list of N elements is encoded into a $\log_2(N)$ qubits state as follows:

$$|\Psi\rangle = \frac{1}{\sqrt{L_{sum}}} \sum_{j=0}^{N-1} L[j] |j\rangle, \quad (8)$$

where $L_{sum} = \sum_{j=0}^{N-1} L[j]^2$ is a normalization constant.

2. The final state is measured.

The procedure is rerun several times to reduce the statistical uncertainty. Once done, the most repeated state gives us the rough maximum.

4. Quantum clustering algorithms

4.1 K means

K-means is an unsupervised machine learning algorithm that classifies the elements of a dataset into K groups called clusters [7]. The input for this algorithm is a set of N data points or vectors in d dimensions as well as the number of clusters K , with $K \leq N$, and its output is a set of K centroids. The main core of this algorithm is computing distances among data points and then assigning the data points to their nearest centroid. That might be speed up using the quantum algorithms explained in Sec. 2 and 3 respectively assuming the data has been loaded from a quantum Random Access Memory (qRAM). In particular, we would obtain a speed up from $O(NKd)$ in the classical version to $O(N \log K \log(d-1))$ in our quantum version, where the speed-up in the dimensionality d would be achieved when the quantum distance subroutine is applied and the speed-up number of clusters K would be achieved when the minimum is obtained by the quantum maximum search algorithm.

4.2 Affinity Propagation

The Affinity Propagation algorithm is an unsupervised machine learning algorithm that, in contrast to K-means, does not need the number of clusters K to be defined beforehand [8]. Its main ideas are that all data points are considered as exemplars (clusters) and what is called “passing messages between data points”. That is achieved calculating the responsibility matrix $R(i, k)$, that measures how well-suited k is to serve as an exemplar for i , and the availability matrix, that gauges how appropriate it would be for i to choose k as its exemplar. These matrices are computed based on the so-called similarity matrix. This matrix includes a distance as a metric to quantify the similarity among data points. This distance will be, in our study, the invariant sum squared shown in Eq. (8) and it might be computed quantumly. In fact, one would obtain a speed-up from $O(N^2Td)$ to $O(N^2T \log(d-1))$, where N is the number of data points, T is the iterations of the algorithm and d the dimensionality.

4.3 k_T jet algorithm

The inclusive variant of the generalised k_T -jet algorithm is formulated as follows:

1. For each pair of partons i, j the following distance is computed:

$$d_{ij} = \min(p_{T,i}^{2p}, p_{T,j}^{2p}) \Delta R_{ij}^2 / R^2, \quad (9)$$

with $\Delta R_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$, where $p_{T,i}$, y_i and ϕ_i are the transverse momentum (with respect to the beam direction), rapidity and azimuth of particle i . R is a jet-radius parameter usually taken of order 1. For each particle i the beam distance is $d_{iB} = p_{T,i}^{2p}$.

2. Find the minimum d_{min} amongst all the distances d_{ij} , d_{iB} . If d_{min} is a d_{ij} , the particles i and j are merged into a single particle summing their four-momenta; if d_{min} is a d_{iB} then the particle i is declared as a final jet and it is removed from the list.

3. Repeat from step 1 until there are no particles left.

The step 2 of the above flow chart might be speed up using the quantum search algorithm presented in Sec. 3. Then, the quantum k_T -jet algorithm would be $\mathcal{O}(N \log N)$ which outperforms the $\mathcal{O}(N^2)$ version of the k_T -jet algorithm and is of the same order as the FastJet version.

5. Quantum simulations

In Table 1, the quantum algorithms described above are tested with a simulated physical n -particle event produced at the LHC. The efficiency ε_c , defined as the quotient of the number of particles clustered in the same way as their classical counterpart and the total number of particles to be classified, is reasonably high for every algorithm, which evidences the success of our quantum implementations.

	Quantum K-means	Quantum Affinity Propagation	Quantum k_T , $p = 1$	Quantum anti- k_T , $p = -1$	Quantum Cam/Aachen, $p = 0$
ε_c	0.94	1.00	0.98	0.99	0.98

Table 1: Efficiencies of the different quantum algorithms in comparison with their classical counterparts.

6. Conclusions

We have considered the quantum versions of the well-known K-means, AP and k_T -jet clustering algorithms. These quantum versions, which are based on two novel quantum procedures, might speed up their classical counterparts on a quantum device with qRAM. The first one is a quantum subroutine which serves to compute distances satisfying Minkowski metric, whereas the second one consists of a quantum circuit to track the rough maximum into a list of unsorted data.

In the case of the K-means clustering algorithm, applying both quantum subroutines we would get an exponential advantage in the vector dimensionality d , as well as in the number of clusters K . In the quantum version of the Affinity Propagation method the similarity is computed with the same quantum procedure as in the K-means case. Thus, it would lead to an exponential speed-up regarding its classical counterpart in the vector dimensionality d . Finally, we have presented the quantum versions of the well-known k_T -jet clustering algorithms. On a true universal quantum device, the implementation of these algorithms would exhibit an exponential speed up in finding the minimum distance. In this way, we would obtain a quantum version of order $\mathcal{O}(N \log(N))$, which is of the same order as the fully optimal version of FastJet.

For all the clustering algorithms considered, the quantum simulations show an excellent performance and clustering efficiencies. Furthermore, the comparison with their classical counterparts displays that both classifications of the LHC simulated data are quite in agreement.

Acknowledgments

This work is supported by the Spanish Government (Agencia Estatal de Investigación MCIN/AEI/10.13039/501100011033) Grant No. PID2020-114473GB-I00, and Generalitat Valenciana Grant No. PROMETEO/2021/071. JJML is supported by Universitat de València, Atracció de Talent programme. LC is supported by Generalitat Valenciana GenT Excellence Programme (CIDEAGENT/2020/011).

References

- [1] A.Y. Wei, P. Naik, A.W. Harrow and J. Thaler, *Quantum Algorithms for Jet Clustering*, *Phys. Rev. D* **101** (2020) 094015 [1908.08949].
- [2] D. Pires, P. Bargassa, J.a. Seixas and Y. Omar, *A Digital Quantum Algorithm for Jet Clustering in High-Energy Physics*, [2101.05618](#).
- [3] A. Delgado and J. Thaler, *Quantum Annealing for Jet Clustering with Thrust*, [2205.02814](#).
- [4] J.J.M. de Lejarza, L. Cieri and G. Rodrigo, *Quantum clustering and jet reconstruction at the LHC*, *Phys. Rev. D* **106** (2022) 036021 [2204.06496].
- [5] S. Ramírez-Uribe, A.E. Rentería-Olivo, G. Rodrigo, G.F.R. Sborlini and L. Vale Silva, *Quantum algorithm for Feynman loop integrals*, *JHEP* **05** (2022) 100 [2105.08703].
- [6] A. Delgado et al., *Quantum Computing for Data Analysis in High-Energy Physics*, in *2022 Snowmass Summer Study*, 3, 2022 [2203.08805].
- [7] J. MacQueen et al., *Some methods for classification and analysis of multivariate observations*, in *Proceedings of the fifth Berkeley symposium on mathematical statistics and probability*, Oakland, CA, USA, 1967.
- [8] B.J. Frey and D. Dueck, *Clustering by passing messages between data points*, *Science* **315** (2007) 972.
- [9] S. Catani, Y.L. Dokshitzer, M. Olsson, G. Turnock and B.R. Webber, *New clustering algorithm for multi - jet cross-sections in $e^+ e^-$ annihilation*, *Phys. Lett. B* **269** (1991) 432.
- [10] S. Catani, Y.L. Dokshitzer, M.H. Seymour and B.R. Webber, *Longitudinally invariant K_t clustering algorithms for hadron hadron collisions*, *Nucl. Phys. B* **406** (1993) 187.
- [11] S.D. Ellis and D.E. Soper, *Successive combination jet algorithm for hadron collisions*, *Phys. Rev. D* **48** (1993) 3160 [hep-ph/9305266].
- [12] M. Cacciari, G.P. Salam and G. Soyez, *The anti- k_t jet clustering algorithm*, *JHEP* **04** (2008) 063 [0802.1189].
- [13] H. Buhrman, R. Cleve, J. Watrous and R. de Wolf, *Quantum fingerprinting*, *Phys. Rev. Lett.* **87** (2001) 167902.
- [14] L.K. Grover, *Quantum mechanics helps in searching for a needle in a haystack*, *Phys. Rev. Lett.* **79** (1997) 325 [quant-ph/9706033].