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Constellation Queries over Big Data

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Abstract. *A geometrical pattern is a set of points with all pairwise distances (or, more generally, relative distances) specified. Finding matches to such patterns has applications to spatial data in seismic, astronomical, and transportation contexts. Finding geometric patterns is a challenging problem as the potential number of sets of elements that compose shapes is exponentially large in the size of the dataset and the pattern. In this paper, we propose algorithms to find patterns in large data applications. Our methods combine quadtrees, matrix multiplication, and bucket join processing to discover sets of points that match a geometric pattern within some additive factor on the pairwise distances. Our distributed experiments show that the choice of composition algorithm (matrix multiplication or nested loops) depends on the freedom introduced in the query geometry through the distance additive factor. Three clearly identified blocks of threshold values guide the choice of the best composition algorithm.*

Resumo. *Um padrão geométrico é definido por um conjunto de pontos e todos os pares de distâncias entre estes pontos. Encontrar casamentos de padrões geométricos em datasets tem aplicações na astronomia, na pesquisa sísmica e no desenho de áreas urbanas. A solução do problema impõe um grande desafio, considerando-se o número exponencial de candidatos, potencialmente função do número de elementos no dataset e número de pontos na forma geométrica. O método aqui apresentado inclui: quadtrees, multiplicação de matrizes e junções espaciais para encontrar conjuntos de pontos que se aproximem do padrão fornecido, com um erro admissível. Apresentamos uma implementação distribuída reveladora de que a escolha do algoritmo (multiplicação de matrizes ou junções espaciais) depende da liberdade introduzida por um fator de erro aditivo na geometria do padrão. Identificamos três regiões baseadas nos valores de erro tolerados que determinam a escolha do algoritmo.*

1. Introduction

The availability of large datasets in science, web and mobile applications enables new interpretations of natural phenomena and human behavior. Consider the following use

case: **Scenario 1.** An astronomy catalog is a table holding billions of sky objects from a region of the sky, captured by telescopes. An astronomer may be interested in identifying the effects of *gravitational lensing* in quasars, as predicted by Einstein's General Theory of Relativity [Einstein 2015]. According to this theory, massive objects like galaxies bend light rays that travel near them just as a glass lens does. Due to this phenomenon, an earth telescope would receive two or more virtual images of the lensed quasar leading to a composed new object (Figure 1), such as the Einstein cross [Overbye 2015].

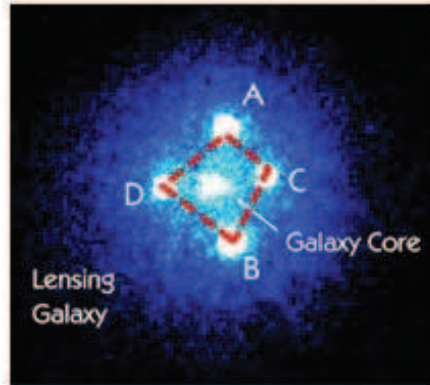


Figure 1. Einstein Cross identification from astronomic catalogs

In the scenario above, constellations, such as the Einstein cross, are obtained from compositions of individual elements in large datasets in some spatial arrangement with respect to one another. Thus, extracting constellations from large datasets entails matching geometric pattern queries against sets of individual data observations, such that each set obeys the geometric constraints expressed by the pattern query.

Solving a constellation query in a big dataset is hard due to the sheer number of possible compositions from billions of observations. In general, for a big dataset D and a number k of elements in the pattern, an upper bound for candidate combinations $\binom{|D|}{k}$ is the number of ways to choose k items from D . This paper focuses primarily on *pure constellation queries* (when all pairwise distances are specified up to an additive factor). We develop parallel algorithms that reduce the number of possible candidate sets by applying local and global constraints.

The remainder of this paper is organized as follows. Section 2 formalizes the constellation query problem. Section 3 presents our techniques to process constellation queries. In section 4, we present our algorithms. Section 5 discusses our experimental environment and discusses the evaluation results, followed by section 6 that discusses related work. Finally, section 7 concludes.

2. Problem Formulation

In this section, we introduce the problem of answering pure Constellation Queries on a dataset of objects. A Dataset D defined as a set of elements (or objects) $D = \{e_1, e_2, \dots, e_n\}$, in which each e_i , $1 \leq i \leq n$, is an element of a domain Dom . Furthermore, $e_i = \langle atr_1, atr_2, \dots, atr_m \rangle$, such that atr_j ($1 \leq j \leq m$) is a value describing a characteristic of e_i .

A constellation query $Q_k = \{q_1, q_2, \dots, q_k\}$ is (i) a sequence of k elements of domain Dom , (ii) the distances between the centroids of each pair of query elements that define the query shape and size with an additive allowable factor ϵ , and (iii) an element-wise function $f(e, q)$ that computes the similarity (e.g. in brightness at a certain wavelength) between elements e and q up to a threshold θ .

A sequence s of elements of length k in D *property matches* query Q if every element $s[i]$ in s satisfies $f(e(s[i], q_i))$ up to a threshold θ and for every $i, j \leq k$: (i) the distance between elements $s[i]$ and $s[j]$ is within an additive factor ϵ of the distance between q_i and q_j , which is referred to as *distance match*. The solutions obtained using *property match* and *distance match* to solve a query Q are referred to as *pure constellations*.

3. Pure Constellation Queries

Applying *pure constellation* to find patterns such as the Einstein cross over an astronomy catalog requires efficient query processing techniques as the catalog may hold billions of sky objects.

In this context, efficiently answering pure constellation queries involves constraining the huge space of candidate sets (i.e. subsets of the catalog with the same number of stars as the query).

The next sections describe in detail the query processing techniques.

3.1. Reducing Data Complexity using a Quadtree

A constellation query looks for patterns in large datasets, such as the 2MASS catalog. Computing constellation queries involves matching each star to all neighboring stars with respect to the distances in the query, a costly procedure in large catalogs. To reduce this cost, we adopt a filtering process that eliminates space regions where solutions cannot exist.

The filtering process is implemented on top of a quadtree [Samet 1990], constructed over the entire input dataset. The quadtree splits the 2-dimensional catalog space into successively refined quadrangular regions.

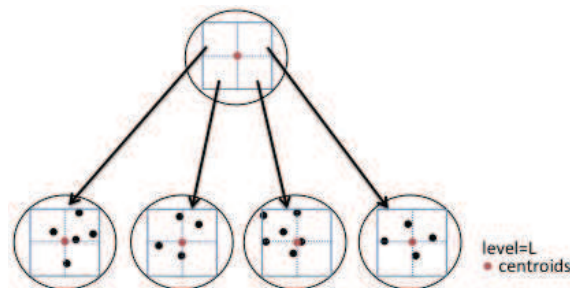


Figure 2. Quadtree node representation

A node in the tree is associated to a spatial quadrant. The geometric center of the quadrant is the node centroid and is used as a representative for all stars located in that quadrant, for initial distance matching evaluation. The quadtree data structure includes: a root node, at level $L = 0$; a list of intermediary nodes, with level $1 \leq L \leq tree_height -$

1; and leaf nodes. To avoid excessive memory usage, data about individual stars are stored only in leaf nodes, Figure 2.

The algorithm begins by determining the level of the quadtree L_e at which the ϵ error bound exceeds the diameter of the node. If we make the reasonable assumption that ϵ is less than the minimum distance between elements in the query ($minq$), then at height L_e no two stars would be covered by a single quadtree node.

Given a star s that will correspond to the centroid q_0 of the pattern being matched, the first step is to eliminate all parts of the quadtree that could not be relevant. The algorithm finds the node at level L_e containing s . That is called the query anchor node. The algorithm finds the nodes that lie within a radius ρ of the query anchor node, where ρ is the maximum distance plus the additive error bound ϵ between the centroid of the query pattern and any other query element. As depicted in Figure 3, in (a) a query Q has an anchor element q_0 and the largest distance to the remaining query elements $d_{0,2}$. In (b), a star is picked as an anchor and all neighboring stars within distance $d_{0,2} + \epsilon$ are preliminary candidates for distance matching.

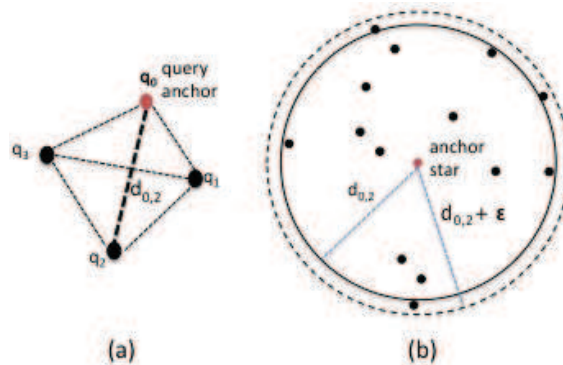


Figure 3. (a) Pure constellation query with anchor and maximum distance (b) Neighboring elements of anchor element

Next the algorithm determines for each pattern element q_i , which stars are at distance $dist(q_0, q_i)$ from s within an additive factor of ϵ . Such stars might correspond to q_i in the case where s corresponds to q_0 . For each pair of nodes $n1$ and $n2$, where $n1$ contains s and $n2$ may contain stars that correspond to q_i for some i , the algorithm checks whether the distance between the centroids of $n1$ and $n2$ matches $dist(q_0, q_i)$, taking into account both the diameter of the nodes and the error bound. This procedure filters out all node pairs at that level for which no matching could possibly occur.

If $n2$ has not been filtered out, then a simple test determines whether going one level down the tree is cost effective as opposed to testing pairs of individual stars in the two nodes. That test consists of determining whether any pair of children of $n1$ and $n2$ will be eliminated from consideration based on a distance test to the centroids of those children. If so, then the algorithm goes down one level. The same matching procedure is applied to the children nodes of $n1$ and $n2$ respectively. If not, then the stars for $n1$ and $n2$ are fetched and any star in $n2$ that lies within an ϵ additive bound of s is put into bucket B_i .

3.2. Composition algorithms

In this section, we discuss approaches to join the buckets produced by the filtering step. As we will observe in section 5, composition algorithms are the most time consuming operation in processing constellation queries. A given anchor node may generate buckets containing thousands of elements. Thus, finding efficient composition algorithms is critical to efficient overall processing.

3.2.1. Buckets Nested Loop (Bucket-NL)

An intuitive way to produce constellations for a given anchor element is by directly joining the buckets of candidate elements considering the corresponding pairwise distances between query elements as the join predicate. In this approach, each bucket is viewed as a relation, having as a schema their spatial coordinates and an id, $B_i(starid, ra, dec)$. A solution is obtained whenever a tuple is produced having one neighbor element from each bucket, such that the distances between each element in the solution *distance-match* those among respective query elements, $\pm \epsilon$. Bucket-NL assumes a nested loop algorithm to traverse the buckets of candidate elements and checks for the distance predicates. Thus, applying a *distance-match* constraint corresponds to applying a cyclic join among all buckets in the bucket set followed by a filter among non-neighbors in the cycle. For example, Bucket-NL would find pairs (t1, t2) where t1 is from B_i with and t2 from B_{i+1} if $dist(t1, t2)$ is within $dist(p_i, p_{i+1}) \pm \epsilon$. Then given these pairs for buckets 1 and 2, buckets 2 and 3, buckets 3 and 4, etc, Bucket-NL will join these cyclically and then for any k-tuple of stars s_1, s_2, \dots, s_k that survive the join, Bucket-NL will also check the distances of non-neighbor stars (e.g. check that $dist(s_2, s_5) = dist(p_2, p_5) \pm \epsilon$).

3.2.2. Matrix Multiplication based approaches

The Matrix Multiplication (*MM*) based approaches precede the basic *Bucket-NL* algorithm by filtering out candidate elements. Here are the details: recall that bucket B_i holds elements for the candidate anchor that correspond to $dist(q_0, q_i) \pm \epsilon$. Compute the matrices: $M1(B_1, B_2), M2(B_2, B_3), M3(B_3, B_1)$ where $Mi(B_i, B_{i+1})$ has a 1 in location j, k if the j th star in B_i and the k th star in B_{i+1} is within $dist(p_i, p_{i+1}) \pm \epsilon$. The product of matrices indicates the possible existence of solutions for a given anchor element, as long as the resulting matrix contains at least a one in its diagonal. The MM approach can be implemented with fast matrix multiplication algorithms [R. Bank 1993][U. Zwick 2005] and enables quick elimination of unproductive bucket elements.

3.2.3. MMM Filtering

Matrix multiplication may be applied multiple times to eliminate stars that cannot be part of any join. The idea is to apply k matrix multiplications, each with a sequence of matrices starting with a different matrix (i.e. a B_i bucket appears in the first and last matrices of a sequence, for $1 \leq i \leq k$). The resulting matrix diagonal cells having zeros indicate that the corresponding element is not part of any solution and can be eliminated. For example, for buckets B_1, B_2, B_3 and matrices $M1(B_1, B_2), M2(B_2, B_3), M3(B_3, B_1)$, we would

run $\langle M1 \cdot M2 \cdot M3 \rangle$; $\langle M2 \cdot M3 \cdot M1 \rangle$ and $\langle M3 \cdot M1 \cdot M2 \rangle$. For the multiplication starting with say $M1$, elements in bucket B_1 with zeros in the resulting matrix diagonal are deleted from B_1 , reducing the size of the full join.

3.2.4. Matrix Multiplication Compositions

The matrix multiplication filtering is coupled with a composition algorithm leading to *MM_Composition* algorithms. The choices explore the tradeoff between filtering more by applying the *MMM* filtering strategy or not.

The *MMM_NL* strategy uses the *MMM* filtering strategy to identify the elements of each bucket that do not contribute to any solutions and can be eliminated from their respective buckets. Next, the strategy applies *Bucket_NL* to join the buckets with elements that do contribute to solutions.

The *MM_NL* considers a single bucket ordering with the anchor node bucket at the head of the list. Thus, once the multiplication has been applied, elements in the anchor node bucket that appear with zero in the resulting matrix diagonal are filtered out from its bucket. Next, the strategy applies *Bucket_NL* to join the buckets with anchor elements that do contribute to solutions.

4. Algorithms for Pure Constellation Queries

To compute *Pure Constellation Queries*, the overall algorithm implements *property matching* and finds matching pairs, whereas the composition algorithms implement *distance matching* as discussed above.

4.1. Main Algorithm

The Constellation Algorithm depicts the essential steps needed to process a Constellation query. The main function is called *ExecuteQuery*. It receives as input a query q , dataset D , element predicate fe , similarity threshold θ , and error bound ϵ . At step 1, a quadtree entry level L_e is computed. Next, a quadtree qt is built covering all elements in D and having height L_e . Figure 2.a illustrates a typical quadtree built on top of heterogeneously distributed spatial data. The quadtree nodes at level L_e become the representatives of stars for initial distance matching. Considering the list of nodes at level L_e , an iteration picks each node, takes it as an anchor node, and searches qt to find neighbors. The geometric centroid of the node quadrant is used as a reference to the node position and neighborhood computation. Next, each pair (anchor node, neighbor) is evaluated for distance matching against one of the query pairs: (query anchor, query element) and additive factor ϵ . Matching nodes contribute with stars for distance matching or can be further split to eliminate non-matching children nodes. Matching stars are placed in a bucket holding matches for the corresponding query element.

The *Compose Function*, applies a composition algorithm, described in the previous section, between buckets $B = \{B_1, B_2, \dots, B_k\}$, for $q.size = k + 1$, to see which $k+1$ -tuples match the pure constellation query. The composition algorithm builds a query execution plan to join buckets in B . The distance matching of elements in buckets B_i and B_j , $i \neq j$, and $i, j \neq anchor$, is applied by checking their pairwise distances $\pm \epsilon$, with respect to the corresponding distances between q_i and q_j , in q .

The choice between running *Bucket_NL* or a *MM_filtering* algorithm to implement element composition, as our experiments in section 5 will show, is related to the size of the partial join buckets. For dense datasets and queries with an error bound close to the average distance among stars, lots of candidate pairs are produced and *MM_filtering* improves composition performance, see Figure 4.b.

5. Experimental Evaluation

In this section, we start by presenting our experimental setup. Next, we assess the different components of our implementation for Constellation Queries.

5.1. Set Up

5.1.1. Dataset Configuration

The experiments focus on the Einstein cross constellation query and are based on an astronomy catalog dataset obtained from the Sloan Digital Sky Survey (SDSS), a seismic dataset, as well as synthetic datasets. The SDSS catalog, published as part of the data release DR12, was downloaded from the project website link (<http://skyserver.sdss.org/CasJobs/>).

We consider a projection of the dataset including attributes (*objID, ra, dec, u, g, r, i, z*). The extracted dataset has a size of 800 MB containing around 6.7 million sky objects. The submitted query to obtain this dataset follows:

```
Select objID, ra, dec, u, g, r, i, z
From PhotoObjAll into MyTable
```

From the downloaded dataset, some subsets were extracted to produce datasets of different size. Additionally, in order to simulate very dense regions of the sky, we built synthetic datasets with: 1000, 5000, 10000, 15000, and 20000 stars. The synthetic dataset includes millions of scaled solutions in a very dense region. Each solution is a multiplicative factor from a base query solution chosen uniformly within an interval of scale factors $s = [1.00000001, 1.00000009]$.

5.1.2. Calibration

We calibrated constellation query techniques using the SDSS dataset described above and a 3D seismic dataset from a region on the North Sea: Netherlands Offshore F3 Block Complete ¹. The procedure aimed at finding the *Einstein Cross* in the astronomy catalog and a seismic dome within the North Sea dataset, using our constellation query answering techniques. In both cases, the techniques succeeded in spotting the right structures among billions of candidates.

5.1.3. Computing Environment

The Constellation Query processing is implemented as an Apache Spark dataflow running on a shared nothing cluster. The Petrus.Incc.br cluster is composed of 6 DELL PE R530

¹<https://opendtect.org/osr/pmwiki.php>

servers running CENTOS v. 7.2, kernel version 3.10.0327.13.1 .el7.x86_64. Each cluster node includes a 2 Intel Xeon E5-2630 V3 2.4GHz processors, with 8 cores each, 96 GB of RAM memory, 20MB cache and 2 TB of hard disk. We are running Hadoop/HDFS v2.7.3, Spark v2.0.0 and Python v2.6. Spark was configured with 50 executors each running with 5GB of RAM memory and 1 core. The driver module was configured with 80GB of RAM memory. The implementation builds the quadtree at the master node, at the driver module, and distributes the list of nodes at the tree entry level. Each worker node then runs the *property_matching* and *distance_matching* algorithms. Finally, answers are collected in a single solution file.

5.2. The Effectiveness of the Descent Tree algorithm

The quadtree structure enables reducing the cost of constellation query processing by restricting composition computation to stars in pairs of nodes whose spatial quadrants match in distance. Selected matching pair nodes are evaluated for further splitting, according to cost model. In this section, we investigate the efficiency of the algorithm. We compare the cost of evaluating the stars matching at the tree entry level with one that descends based on the cost model.

We ran the *buildQuadtree* function with dense datasets and measured the difference in elapsed-time in both scenarios. In terms of number of comparisons for 1 million stars, the cost model saves approximately 1.9x, leading to an order of magnitude on execution time savings.

5.3. Composition Algorithm Selection

In this section, we discuss the characteristics of the proposed composition algorithms.

In the first experiment a constellation query based on the Einstein cross elements is run for each composition algorithm and their elapsed-times are compared. The elapsed-time values correspond to the average of 10 runs measuring the maximum among all parallel execution nodes in each run.

The geometric nature of constellation queries and the density of astronomical catalogs make the distance additive factor ϵ a very important element in query definition. As our experiments have shown, variations in this parameter may change a null result set to one with million of solutions. The experiments evaluate two classes of composition algorithms. In one class, we use the *Bucket_NL* algorithm and, in the second one, we include the adoption of various *Matrix Multiplication* filtering strategies.

The experiment results are depicted in Figures 4.a and 4.b. In these plots, the horizontal axis presents different error tolerance values ϵ , while the vertical axis shows the elapsed-time of solving the constellation query using one of the composition algorithms.

Figure 4.a shows basically two scenarios. For very small ϵ , $\leq 10^{-6}$, the number of candidate elements in buckets is close to zero, leading to a total of 32 anchor elements to be selected and producing 52 candidate shapes. In this scenario, the choice of a composition algorithms is irrelevant, with a difference in elapsed-time of less than 10% among them. It is important to observe, however, that such a very restrictive constraint may eliminate interesting sets of stars. Unless the user is quite certain about the actual shape of its constellation, it is better to loosen the constraint.

The last blocks of runs involving the composition algorithms in Figure 4.a shows that the results are different when increasing ϵ by up to a factor of 100. Considering $\epsilon = 2,0 \times 10^{-5}$, we obtain 522,578 productive anchor elements and an average of close to one element per bucket. The total number of candidate shapes rises to 12.6 million. In this setting, *Bucket_NL* is very fast, as it loops over very few elements in the buckets to discover solutions. The overhead of computing matrix multiplication is high, so *Bucket_NL* is a clear winner. This scenario continues to hold up to $\epsilon = 2 \times 10^{-4}$, see Figure 4.a. In this range, *Bucket_NL* is faster than *MM_NL* and *MMM_NL* by 214% and 240%, respectively.

Figure 4.b highlights the behavior of algorithms under additive error tolerance values. The flexibility introduced by $\epsilon = 6 \times 10^{-3}$ generates 6.7 million productive anchor elements and a total of 7.1 billion solutions, with average elements per bucket of 10. In this scenario, eliminating non-productive anchor elements, close to 300,000, by filtering using matrix multiplication eliminates the need of computing nested loops over approximately 405 candidate elements in buckets. Thus, running fast matrix multiplication as a pre-step to nested-loop becomes beneficial.

Figure 5 shows the point at which matrix multiplication becomes beneficial: when $\epsilon = 6.0 \times 10^{-3}$ matrix multiplication starts to efficiently filter out anchor nodes and so the reduction in nested-loop time compensates for the cost of performing matrix multiplication. The gains observed by running matrix multiplication algorithms as a pre-filtering step before nested loop for ϵ in range 6×10^{-3} and 9×10^{-3} are up to 45.6% for *MM_NL* and 34.6% for *MMM_NL*.

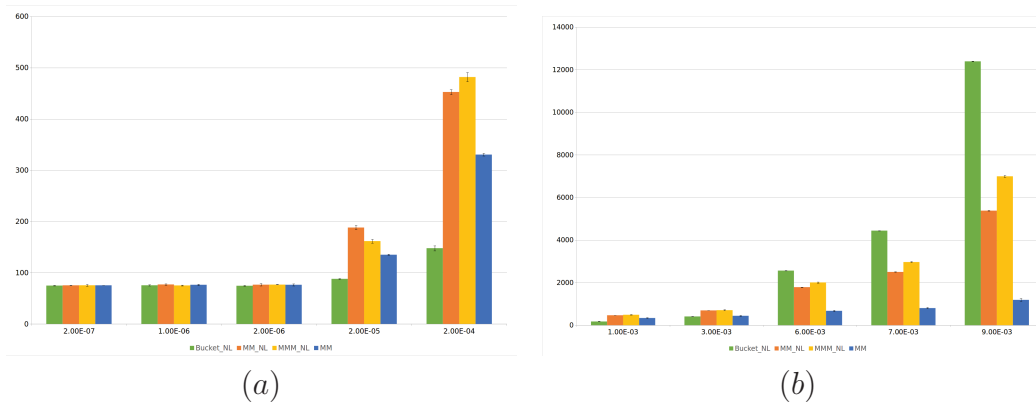


Figure 4. Low Additive Error Tolerance ϵ (a) High Additive Error Tolerance ϵ (b)

Figures 5.a and 5.b zoom in on the *Matrix Multiplication* algorithms. The former shows the results with thresholds not less than 1×10^{-3} . In this range, we can observe an inversion in performance between *MM_NL* and *MMM_NL*. The inflexion point occurs after $\epsilon \geq 2 \times 10^{-3}$. Threshold values below the inflexion point include anchor nodes with very few elements in buckets. In this scenario, computing multiple matrix multiplication is very fast. Moreover, elements that appear with zeros in the resulting matrix diagonal can be looked up in buckets and deleted, before the final nested-loop. The result is a gain of up to 14% in elapsed-time with respect to *MM_NL*. From the inflexion point on, *Matrix_Multiplication_NL* is the best choice with gains up to 30% with respect to *MMM_NL*. The selection among composition algorithms is summarized in Table 1,

according to the results on the SDSS dataset.

Table 1. Composition Algorithms Selection

Threshold-Range	Best Choice Composition Algorithm
≤ 0.003	<i>Bucket_NL</i>
> 0.003	<i>MM_NL</i>

Finally, the matrix multiplication *MM* algorithm is, as expected, a good choice for existential constellation queries which ask whether any subset of the dataset matches the query but does not ask to specify that subset. In this scenario, once the matrix multiplication indicates a resulting matrix diagonal with all zeros, the anchor element produces no candidate shape and can be eliminated from the existential query result.

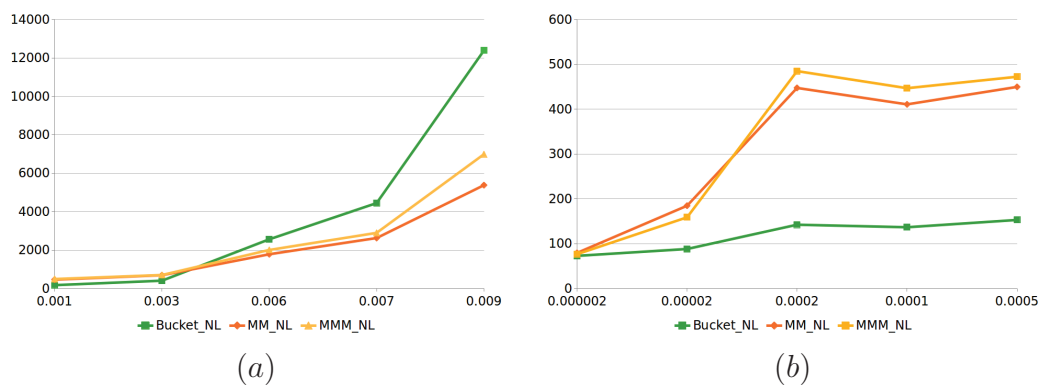


Figure 5. Zoom In on Matrix Multiplication: large threshold (a) Zoom In on Matrix Multiplication: low threshold (b)

5.4. Pure Constellation Scale-up

We investigated Pure CQ scale-up adopting the set of dense datasets (see section 5.1.1), error bound $\epsilon = 4.4 \times 10^{-6}$ and *Bucket_NL* for the composition algorithm. The execution produced solutions of size: zero, 21, 221, 1015, and 2685. The run with 1000 stars dataset produced zero solutions, which shows the relevance of tuning the error bound for a given dataset and the restrictions imposed by Pure CQ. Apart from the runs with the 15,000 stars dataset, the variations in time followed the increase in the number of solutions. This indicates that non solutions are quickly discarded and the time is mostly due to producing solutions. Figure 6 depicts the results, where time corresponds to the elapsed-time in seconds of the parallel execution.

6. Related Work

Finding collections of objects having some metric relationship of interest is an area with many applications. The problem has different names depending on the discipline, including *Object Identification* [Singla and Domingos 2005], *Graph Queries* [Zou et al. 2011], *Pattern Matching* and *Pattern Recognition* [Bishop 2006].

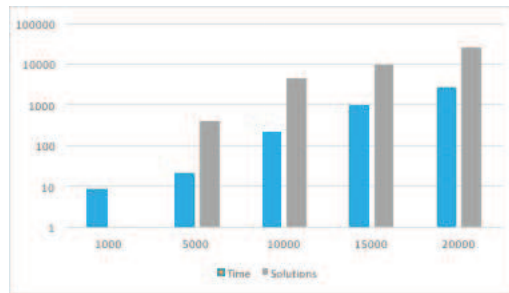


Figure 6. Pure Constellation Scale-up

Pattern recognition research focuses on identifying patterns and regularities in data [Bishop 2006]. Graphs are commonly used in pattern recognition due to their flexibility in representing structural geometric and relational descriptions for concepts, such as pixels, predicates, and objects [Jolion 2001]. In this way, problems are commonly posed as a graph query problem, such as subgraph search, shortest-path query, reachability verification, and pattern match. Among these, subgraph matching queries are related to our work.

In a subgraph query, a query is a connected set of nodes and edges (which may or may not be labeled). A match is a (usually non-induced) subgraph of a large graph that is isomorphic to the query. While the literature in that field is vast [[Zou et al. 2009], [Giugno and Shasha 2002]], the problem is fundamentally different, because there is no notion of space (so data structures like quadtrees are useless) and there is no distance notion of scale (the ϵ that plays such a big role for us).

Finally, constellation queries are a class of package queries (PQ), Brucato et al. [Brucato et al. 2016].

7. Conclusion

In this paper, we introduce *constellation queries*, specified as a geometrical composition of individual elements from a big dataset. We illustrate the application of Constellation Queries in astronomy (e.g. Einstein crosses).

We have designed procedures to efficiently compute both pure Constellation Queries. First, we reduce the space of possible candidate sets by associating to each element in the dataset neighbors at a maximum distance, corresponding to the largest distance between any two elements in the query. Next, we filtered candidates yet further into buckets through the use of a quadtree. Next, we used a bucket joining algorithm, optionally preceded by a matrix multiplication filter to find solutions.

Our experiments execute on Spark, running on the neighboring dataset distributed over HDFS. Our work shows that our filtering techniques having to do with quadtrees are enormously beneficial, whereas matrix multiplication is beneficial only in high density settings.

There are numerous opportunities for future work, especially in optimization for higher dimensions.

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