cliquematch: Finding correspondence via cliques in large graphs

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Abstract

The maximum clique problem finds applications in computer vision, bioinformatics, and network analysis, many of which involve the construction of correspondence graphs to find similarities between two given objects. cliquematch is a Python package designed for this purpose: it provides a simple framework to construct correspondence graphs, and implements an algorithm to find and enumerate maximum cliques in C++, that can process graphs of a few million edges on consumer hardware, with comparable performance to publicly available methods.

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1 Introduction

Given an undirected graph $G$, a subgraph $H$ of $G$ is a clique if an edge exists between any two vertices in $H$. A clique in $G$ is a maximum clique if there exist no cliques of a larger size. The maximum clique problem (Bonze et al., 1999) is a special case of the maximal clique problem: a clique is maximal if it is not properly contained in any other clique, therefore all maximum cliques are also maximal. It is also related to the problem of clique enumeration.

Finding cliques in a graph is applicable to a variety of domains, such as bioinformatics, robotics, forensics, image analysis etc. (Conte et al., 2004). The applications transform into a clique problem in two general ways. In (Pradalier and Sekhavat, 2003), vertices of the graph refer to elements of a dataset, and an edge indication function computes a relationship between every pair of elements. Alternatively, in (Horaud and Skordas, 1989), a correspondence graph is constructed to find similar substructures between two different objects; vertices correspond to potential mappings between similar elements of the two objects, and edges reinforce the mappings.

cliquematch is a Python package designed to construct correspondence graphs and find maximum cliques. It implements a modified version of a well-known maximum clique algorithm (Pat-tabiraman et al., 2015) in C++, and uses template programming to provide a simple framework for constructing correspondence graphs. cliquematch makes use of the pybind11 library to provide Python bindings. The remainder of this section provides a simple example using cliquematch. Section 2 describes the algorithm used by cliquematch when finding maximum cliques, Section 3 shows how problems of data association can be converted into finding maximum cliques in a graph. Section 4 provides examples showcasing how cliquematch can be used to solve such kinds of problems. Section 5 summarizes the properties of cliquematch and discusses future directions.

1.1 Basic Usage

The core functionality of cliquematch involves loading an undirected graph and finding a clique. The graph can be loaded from edge lists, adjacency matrices, adjacency lists, and text files that follow the Matrix Market Coordinate Text File format. 

```
import cliquematch
G = cliquematch.Graph.from_file("cond-mat-2003.mtx")
print(G) # cliquematch.core.Graph object at 0x559e7da730c0
# (n_vertices=31163, n_edges=120029, lower_bound=1, upper_bound=4294967295,
# time_limit=1, use_heuristic=False, use_dfs=True, search_done=False)
G.get_max_clique()
# [9986, 9987, 10066, 10068, 10071, 10072, 10074, 10076,
# 10077, 10078, 10079, 10080, 10081, 10082, 10083, 10085,
# 10287, 10902, 10903, 10904, 10905, 10906, 10907, 10908, 10909]
```

The search for a clique can be modified by: (a) setting the bounds on clique size (via lower_bound and upper_bound), (b) choosing to use the heuristic method, the depth-first search, or both (via use_heuristic and use_dfs), and (3) setting a time limit for the search (via time_limit).

The search for maximum cliques can be resumed and interrupted intermittently using search.done and get_max_clique() in a loop, which is useful for incremental searching in the case of dense graphs. reset_search() resets the search for maximum cliques in case different bounds are required.

```
G.reset_search()
while not G.search_done:
    answer = G.get_max_clique(
        lower_bound=1, upper_bound=1729,
        use_heuristic=True, use_dfs=True,
        time_limit=100, continue_search=True
    )
```

1https://github.com/ahgamut/cliquematch
2https://math.nist.gov/MatrixMarket/formats.html
The all_cliques() method can be used to obtain all cliques of a particular size from the graph G. all_cliques() does not find all the cliques at once; the cliques are discovered upon the user's repeated requests.

```python
import cliquematch
G = cliquematch.Graph.from_file("cond-mat-2003.mtx")
for clique in G.all_cliques(size=24):
    print(clique)
```

2 The Maximum Clique Problem - A Literature Review

The maximum clique problem is NP-Hard (Garey and Johnson, 1979), and many algorithms for computing an exact solution have been discovered. These usually involve a possible optimal vertex ordering, fast heuristic bounds on the maximum clique size, followed by branch-and-bound: performing a depth-first search from each vertex to find cliques, and pruning the search space to avoid unnecessary calculations. The earliest such algorithm (Carraghan and Pardalos, 1990) sorts vertices in ascending order of degree, with search steps being pruned if they cannot beat the current maximum. Ostergård, 2002 sorts vertices in descending order, and processes them in a defined sequence for better performance. MCQ (Tomita and Seki, 2003) first sorts vertices in descending order, and uses an approximate coloring for additional sorting of the vertices, which also helps pruning in the clique. A later version (Tomita, Sutani, et al., 2010) improves on the approximate coloring used so as to maximize pruning.

More recent algorithms for finding maximum cliques focus on massive sparse graphs; these may require specialized hardware, and attempt to use the parallel nature of the problem. FMC (Pattabiramam et al., 2015) prunes vertices with degree less than the current maximum clique size as early as possible, and ignores vertices that have already been processed; it also provides a degree-based heuristic method to obtain a lower bound on the maximum clique size. PMC (Rossi, Gleich, and Gebremedhin, 2015) uses the core-number (Seidman, 1983) of a vertex instead of the degree, which provides a tight lower and upper bound, thereby pruning the search space more effectively, and provides a parallel-friendly implementation based on OpenMP (Dagum and Menon, 1998). BBMC (San Segundo, Rodriguez-Losada, and Jimenez, 2011) uses bitstrings of 64-bit machine words to encode the adjacency matrix and vertex sets, to benefit from bit-parallelism in set operations. BBMCSP (San Segundo, Lopez, and Pardalos, 2016) defines a sparse encoding for bitstrings; it also unrolls the initial search step to avoid unnecessary recursive calls. It is interesting to note that pruning methods based on heuristics are not optimal for some kinds of real-world graphs; RMC (Lu et al., 2017) describes a probabilistic algorithm for finding maximum cliques, with examples and benchmarks showcasing potential limitations in heuristic-based methods.

The algorithm used in cliquematch is mostly similar to FMC: the depth-first search and the heuristic method both filter out vertices based on degree, and the search space is pruned based on potential to beat the current maximum. cliquematch also uses bitstrings compressed into 32-bit machine words, similar to BBMC, to represent the vertex sets during the clique search. However, cliquematch differs from FMC in three ways:

- Instead of filtering out completed vertices (FMC Pruning 2) and neighbors of a vertex \(v\) with lesser degree than the current maximum clique size (FMC Pruning 3), cliquematch filters out all neighbors of \(v\) of lesser degree than \(d(v)\), the degree of \(v\). This means that every maximum clique is now found using the vertex of least degree and the search is now amortized over all the vertices, which reduces reliance on vertex ordering.
- The heuristic method returns a clique instead of just the lower bound. This helps users to obtain a clique quickly in case the branch-and-bound method is too slow.
- The branch-and-bound method is repurposed to also provide clique enumeration. This allows to find all cliques of a given size, as there might be multiple maximum cliques. The clique enumeration is done in a lazy manner; new cliques are found incrementally upon request.

The performance of cliquematch on various benchmark graphs is comparable to existing C++ implementations, see Appendix A.
3 Correspondence Graphs

Finding maximum cliques in graphs can be applied to data association problems, where the aim is to find similarity between two objects by comparing their components. Such problems are found in bioinformatics (Gardiner, Artymiuk, and Willett, 1997), robotics (Pradalier and Sekhavat, 2003), forensics (Tu and Hartley, 1999), image analysis (Horaud and Skordas, 1989) etc. These problems can be solved by constructing a correspondence graph, a general form of the association graph (Kozen, 1978) used for subgraph isomorphism. Given two given objects $P$ and $Q$, the correspondence graph $G_{P,Q}$ constructs the largest possible correspondence between $P$ and $Q$ by extending mappings in a pairwise manner.

![Figure 1: A sample correspondence graph for sets of points in two dimensions. The corresponding points are marked in red, green, blue, and purple. The vertices of the correspondence graph $G$ which refer to these are marked with the same colors. Note that the edges between the colored vertices form a maximum clique, and the configurations of the corresponding points (thicker lines) are the same in both $P$ and $Q.}$](image)
Definition 1 (Correspondence Graph). Let $P = \{p_1, p_2, ..., p_M\}$ and $Q = \{q_1, q_2, ..., q_N\}$ be two sets of elements of length $M$ and $N$ respectively. Let $G(V, E)$ be an undirected graph, where $V = P \times Q$. An edge $e \in E$ is drawn between $v_1(p_{i_1}, q_{j_1})$ and $v_2(p_{i_2}, q_{j_2}) \in V$ if for a given boolean function $f : (P \times P \times Q \times Q) \rightarrow \{0, 1\}$

$$(v_1, v_2) \in E \iff f(p_{i_1}, p_{i_2}, q_{j_1}, q_{j_2}) = 1; \quad i_1 \neq i_2, j_1 \neq j_2$$ (1)

Finding a maximum clique $H$ in $G$ is equivalent to finding the largest correspondence between $P$ and $Q$ as shown in the following step by step argument.

(a) $V_H \subset V_G = P \times Q$.
(b) Let $P' \subset P$, and $Q' \subset Q$ be such that

$$(p_i, q_j) \in V_H \iff p_i \in P', q_j \in Q'.$$

(c) $H$ is a clique, so there exists an edge between every pair of vertices in $V_H$. Remember that an edge can be drawn only if Equation 1 is satisfied, therefore

$$f(p_{i_1}, p_{i_2}, q_{j_1}, q_{j_2}) = 1, \quad i_1 \neq i_2, j_1 \neq j_2 \; \forall \; (v_1(p_{i_1}, q_{j_1}), v_2(p_{i_2}, q_{j_2})) \in V(H)$$

$$\Rightarrow f(p_{i_1}, p_{i_2}, q_{j_1}, q_{j_2}) = 1, \quad i_1 \neq i_2, j_1 \neq j_2 \; \forall \; p_{i_1}, p_{i_2} \in P', \forall \; q_{j_1}, q_{j_2} \in Q'$$

because every vertex in $V_H$ is a pair of elements, one from $P'$ and the other from $Q'$.

Hence, there exists a correspondence between $P'$ and $Q'$.

(d) $H$ is a maximum clique, so there exists no clique in $G$ that is larger than $H$. Thus, $P'$ and $Q'$ are subsets of $P$ and $Q$ having the largest possible correspondence.

Note that $f$ requires two pairs of elements $p_{i_1}, p_{i_2}, q_{j_1}, q_{j_2}$, when constructing an edge of the correspondence graph, and thus there is a pairwise correspondence between elements of $P'$ and $Q'$. $f$ can be optimized to benefit from properties of $P$ and $Q$. A common use case is if $P$ and $Q$ are point-clouds in an $n$-dimensional space (see Figure 1), the function $f$ can be:

$$f(p_{i_1}, p_{i_2}, q_{j_1}, q_{j_2}) = 1 \iff ||d_P(p_{i_1}, p_{i_2}) - d_Q(q_{j_1}, q_{j_2})|| \leq \epsilon$$

where $d_P$ is a distance metric on $P$, $d_Q$ is a distance metric on $Q$, and $\epsilon$ is a small positive real number. Therefore, the edge construction rule in Equation 1 is modified to:

$$(v_1, v_2) \in E \iff ||d_P(p_{i_1}, p_{i_2}) - d_Q(q_{j_1}, q_{j_2})|| \leq \epsilon \; i_1 \neq i_2, j_1 \neq j_2$$ (2)

4 Applications

cliquematch can construct correspondence graphs where $P, Q$ are either 2D numpy arrays or Python lists, via the below classes:

- A2AGraph, where $P$ and $Q$ are numpy arrays
- L2LGraph, where $P$ and $Q$ are lists of arbitrary objects, and
- A2LGraph and L2AGraph, for cases that may require mapping a list of objects to numpy arrays of related data.

The user is required to define the function $f$ or the metrics $(d_P, d_Q)$ for cliquematch to perform the construction of the graph. cliquematch uses pybind11 for Python wrappers, so one can define $d_P$, $d_Q$, and $f$ as regular Python functions or Callable objects for fast prototyping. Note that accessing elements of $P$ and $Q$ is done only within these functions.

```python
1  def euclidean(P, i1, i2):
2    return sqrt(sum((P[i1] - P[i2]) ** 2))
3
4  class MyCustomCondition(object):
5    def __call__(P, i1, i2, Q, j1, j2):
6      if my_condition_works:
7        return True
8      return False
```

5
Once $G$ has been constructed as per the given conditions, \texttt{cliquematch} searches for cliques – the search parameters can be defined as per Subsection 1.1 – and returns the subsets with largest correspondence, as seen in the following examples.

### 4.1 Image Registration and Matching using interest points

Image registration can be converted into point-cloud registration by selecting a suitable function to obtain interest points, following which simple distance metrics can be used to construct a correspondence graph as in Equation 2. Once a maximum clique has been found, the sets of corresponding points can be used obtain a matching score, or perform a registration of the image.

CCMM (San Segundo and Artieda, 2015) performs feature matching for color images by computing SURF descriptors (Bay, Tuytelaars, and Van Gool, 2006) to obtain interest points. The algorithm to construct a correspondence graph $G$ can be described as follows:

- $P, Q$ are the sets of SURF keypoints in the first and second images.
- $d_P$ and $d_Q$ are the Euclidean metrics.
- Additionally, apply a condition function $f$ that allows an edge from $(p_{i1}, q_{j1})$ to $(p_{i2}, q_{j2})$ if and only if $q_{j1}$ is one of the top $k$ SURF descriptor matches of $p_{i1}$ and $q_{j2}$ is one of the top $k$ SURF descriptor matches of $p_{i2}$; where $k$ is some integer.
- The correspondence graph $G$ is constructed using the distance metrics and $f$, for some appropriate values of $k$ and $\epsilon$.

![Figure 2: The CCMM algorithm tested on images from the Dinosaur dataset (University of Oxford Visual Geometry Group Multi-View Datasets 2020). The points in red are the corresponding points.](image)

An implementation of the above steps using the \texttt{cliquematch.A2AGraph} and \texttt{OpenCV} is available on Github,\(^3\) a sample result is shown in Figure 2. A similar procedure can be followed for registering or matching a pair of images, based on the kinds of interest points extracted:

- (Tu and Hartley, 1999) compares fingerprint images by selecting corresponding pairs of minutia: the vertices of the correspondence graph are mappings of minutia, and edges are drawn with respect to a function computing angle, distance, and ridge counts.
- (Park and Carriquiry, 2020) extracts SURF points and computes maximum cliques on a correspondence graph to perform alignment of footwear outsole impressions.
- (Theiler, Schindler, et al., 2012) performs registration of laser scans by computing tie points, and uses description vectors for each point along with the Euclidean distance metric to ensure construction of a sparse graph. The correspondence computed via finding maximum cliques is used to register the scans.

\(^3\)https://github.com/ahgamut/cliquematch/blob/master/examples/ccmm.py
4.2 Matching of Molecular Structures

The structure of molecules can be represented as an attributed graph, and therefore matching the 3-D structures of two different molecules can be converted into finding a clique in their correspondence graph. (Gardiner, Artymiuk, and Willett, 1997) provides a procedure for structure matching of molecules via correspondence graph, which can be described as follows:

- $P, Q$ are the sets of atoms in the first and second molecules to be matched.
- $d_P$ and $d_Q$ are the Euclidean metrics to measure inter-atomic distances.
- Additionally, apply a condition function $f$ that allows an edge if and only if a bond exists between the pairs of atoms being mapped.
- The correspondence graph $G$ is constructed using the distance metrics and $f$, for some appropriate value of $\epsilon$. $f$ can be modified to account for additional properties (e.g. match ring bonds to ring bonds, valence).

![Figure 3: Molecule structure matching using inter-atomic distances. The molecules were obtained from the datasets provided in (Sutherland, O’brien, and Weaver, 2003).]

An illustrative example using cliquematch is shown in Figure 3. A similar procedure is followed for matching protein molecules using their secondary structure elements (SSEs). (Butenko and Wilhelm, 2006) gives an overview of applying clique-based methods in biochemistry.

4.3 Subgraph Isomorphism

Finding a subgraph isomorphism between two graphs can be solved by constructing a correspondence graph as described in (Kozen, 1978):

- Let $G_P(P, E_P)$ and $G_Q(Q, E_Q)$ be simple, unweighted, undirected graphs such that $G_Q$ is isomorphic to a subgraph of $G_P$. The vertices of the graphs are sets $P$ and $Q$.
- Define a correspondence graph $G^*(V, E)$ where $V = P \times Q$.
- Define a boolean condition function $f$ to construct edges in $G^*$ as below:
  \[
f(P, i_1, i_2, Q, j_1, j_2) = 1 \iff (q_{j_1}, q_{j_2}) \in E_Q \implies (p_{i_1}, p_{i_2}) \in E_P
  \]
- Once $G^*$ has been constructed, finding a maximum clique will give the vertices of the isomorphic subgraphs.

cliquematch provides an IsoGraph class which encapsulates the above functionality.

\*Implementation available at https://github.com/ahgamut/cliquematch/blob/master/examples/molecule.py
5 Conclusions and Future Work

I have described the capabilities of cliquematch, a Python package that finds maximum cliques in large sparse graphs and shown that its performance is comparable to other publicly available methods. I also provided examples showing that the implementation of cliquematch can be used to in solving data association problems in different domains, by constructing a correspondence graph and finding a maximum clique.

Multiple aspects of cliquematch can be developed further: the core search algorithm can be modified to find maximum cliques in a weighted graph. The computation time can improved with better heuristics, like vertex coreness and approximate coloring. The construction of correspondence graphs is applicable to many problem domains. There is also scope for clique augmentation or lenient matching methods (para-cliques) using the cliquematch design, and for providing GPU or streaming-specific implementations.

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A Performance

| Graph          | | | | | | | | | |
|----------------|---|---|---|---|---|---|---|---|---|
|                | $|V|$ | $|E|$ | $\omega$ | $t_{cm}$ | $t_{fmc}$ | $t_{pmc}$ | $t_{cm-heur}$ | $t_{fmc-heur}$ | $t_{pmc-heur}$ |
| Erdos02        | 6927 | 8472 | 7 | 0.0003 | 0.0013 | 0.0022 | 0.0002 | 6 | 0.0009 | 7 |
| Erdos972       | 5488 | 7085 | 7 | 0.0002 | 0.0007 | 0.0015 | 0.0002 | 7 | 0.0002 | 6 |
| Erdos982       | 5822 | 7375 | 7 | 0.0004 | 0.0005 | 0.0015 | 0.0002 | 7 | 0.0002 | 7 |
| Erdos992       | 6100 | 7515 | 8 | 0.0002 | 0.0004 | 0.0017 | 0.0002 | 8 | 0.0002 | 8 |
| Fault_639      | 638802 | 14626683 | 18 | 21.3265 | 14.456 | - | 1.2731 | 18 | 2.4945 | 18 |
| brock200_2     | 200 | 9876 | 12 | 0.4408 | 0.6408 | 0.0018 | 0.0031 | 10 | 0.0023 | 9 |
| c-fat200-5     | 200 | 8473 | 58 | 0.1485 | 0.4204 | 0.0003 | 0.0004 | 58 | 0.0106 | 58 |
| ca-AstroPh     | 18772 | 198110 | 57 | 0.0024 | 0.0802 | 0.0016 | 0.0045 | 239 | 0.2589 | 239 |
| ca-CondMat     | 23133 | 93497 | 26 | 0.0001 | 0.0048 | 0.0083 | 0.0002 | 26 | 0.0004 | 26 |
| ca-GrQc        | 5242 | 14496 | 44 | 0.0002 | 0.0005 | 0.0018 | 0.0002 | 44 | 0.0011 | 44 |
| ca-HepPh       | 12008 | 118521 | 239 | 0.0041 | 0.0138 | 0.0016 | 0.0045 | 239 | 0.2589 | 239 |
| ca-HepTh       | 9877 | 25998 | 32 | 0.0002 | 0.0007 | 0.0036 | 0.0001 | 32 | 0.0001 | 32 |
| caidaRouterLevel | 192244 | 609066 | 17 | 0.0672 | 0.2193 | 0.0784 | 0.0258 | 17 | 0.0723 | 15 |
| coPapersCiteseer | 434102 | 16036720 | 845 | 0.028 | 0.8812 | 1.8326 | 0.0501 | 845 | 16.2965 | 845 |
| com-Youtube    | 1134890 | 2987624 | 17 | 2.467 | 10.6184 | - | 0.2301 | 16 | 0.3597 | 13 |
| cond-mat-2003 | 31163 | 120029 | 25 | 0.0024 | 0.013 | 0.0104 | 0.0032 | 25 | 0.0054 | 25 |
| cti            | 16840 | 48232 | 3 | 0.0283 | 0.0052 | 0.0002 | 0.0058 | 3 | 0.0014 | 3 |
| hamming6-4     | 64 | 704 | 4 | 0.0018 | 0.0005 | 6.1989 | 0.0001 | 4 | 6.6042 | 4 |
| johnson8-4-4   | 70 | 1855 | 14 | 0.6535 | 0.1582 | 0.0003 | 0.0005 | 14 | 0.0005 | 14 |
| keller4        | 171 | 9435 | 11 | 10.8767 | 15.7847 | - | 0.0022 | 9 | 0.0027 | 9 |
| loc-Brightkite | 58228 | 214078 | 37 | 7.0798 | 2.9293 | 0.0271 | 0.0077 | 36 | 0.0155 | 31 |

Table 1: Comparing cliquematch performance on some benchmark graphs. $|V|$ and $|E|$ denote the number of nodes and edges in the graph. $\omega$ denotes the size of the maximum clique found. All the branch-and-bound methods agreed on the maximum clique size in every benchmark. $t_{cm}$, $t_{fmc}$, and $t_{pmc}$ denote the time taken by cliquematch, FMC, and PMC respectively in the branch-and-bound search: the least time is in bold text. $w_{cm-heur}$, $t_{cm-heur}$ denote the size of clique and time taken by the heuristic method in cliquematch; and similarly for $w_{fmc-heur}$ and $t_{fmc-heur}$. A minus sign (-) indicates that the program returned an error without completing the calculation.

The benchmark graphs were obtained from the Stanford SNAP collection (Leskovec and Krevl, 2014), the University of Florida Sparse Matrix collection (Davis and Hu, 2011), and the DIMACS Challenges (Johnson and Trick, 1996, Bader et al., 2011). I thank the authors of FMC for making their source code publicly available.

I used gcc 7.5.0 to compile the programs at optimization level -O3. For cliquematch I set the BENCHMARKING flag to 1 before compilation. I compiled and tested the programs on a 64-bit Ubuntu 18.04 system with Intel(R) Core(TM) i5-4200U CPU @ 1.60GHz and 4GB RAM. The following command line parameters were used:

- fmc -t 0 -p was used to run the FMC branch-and-bound algorithm.
- pmc -t 1 -r 1 -a 0 -h 0 -d (single CPU thread, reduce wait time of 1 second, full algorithm, skip heuristic, search in descending order) was used to run the PMC branch-and-bound algorithm.
- fmc -t 1 was used to run the FMC heuristic algorithm.
- A small python script similar to the code block in Subsection 1.1 was used to run the cliquematch algorithms.

5http://cucis.ece.northwestern.edu/projects/MAXCLIQUE/download.html
6https://github.com/ryanrossi/pmc