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Discovering the structure of complex networks: Implementation and Complexity of the heuristic MACH

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Getting a labeling of vertices close to the structure of the graph has been proven to be of interest in many applications e.g., to follow signals indexed by the vertices of the network. This question can be related to a graph labeling problem known as the cyclic bandwidth sum problem. It consists in finding a labeling of the vertices of an undirected and unweighted graph with distinct integers such that the sum of (cyclic) difference of labels of adjacent vertices is minimized. Although theoretical results exist that give optimal value of cyclic bandwidth sum for standard graphs, there are neither results in the general case, nor explicit methods to reach this optimal result. In addition to this lack of theoretical knowledge, only a few methods have been proposed to approximately solve this problem. This report describes the implementation and the complexity of the heuristic MACH, developed to find an approximate solution for the cyclic bandwidth sum problem, by following the structure of the graph. The heuristic is a two-step algorithm: the first step consists of traversing the graph to find a set of paths which follow the structure of the graph, using a similarity criterion based on the Jaccard index to jump from one vertex to the next one. The second step is the merging of all obtained paths, based on a greedy approach that extends a partial solution by inserting a new path at the position that minimizes the cyclic bandwidth sum.

1 Description of the heuristic MACH

The aim of the heuristic, introduced in [1], is to build a labeling by traversing the graph to discover its structure.

The heuristic we propose consists of a two-step algorithm. The first step performs local searches in order to find a collection of independent paths with respect to the local structure of the graph, while the second step determines the best way to arrange the paths such that the objective function of the Cyclic Bandwidth Sum is minimized.

1.1 Step 1: Guiding the search towards locally similar vertices

The first step consists in finding a collection of paths in the graph, that is to say some sequences of vertices consecutively connected. The algorithm performs a depth-first search in which the next vertex is chosen among the neighbors of the current vertex, in order to preserve the connectivity of the path, based on its similarity with the current vertex. This similarity depends on the intersection of the two vertex neighborhoods: the more the neighborhoods of the two vertices intersect, the closer their labels are. Concretely the search is executed as follows: Starting from a vertex, the algorithm jumps to the most similar neighbor not yet labeled, and so on until there are no more accessible vertices. Then, the algorithm starts a new path from a vertex which has not been yet inserted in a path, and then continues to build paths until all the vertices are in a path. At the end of this step, a collection of paths is obtained that partitions the graph vertex set.
Initialization  
Any vertex not yet inserted in a path can be used as starting node. However, to favor the 
computation of longer paths, vertices that are at the periphery of the graph are preferred. The incentive behind 
this choice lies in the fact that the path should start at one of the extremity of the graph if there is one. For 
example, let us consider a simple path graph: Starting from a vertex in the middle of the path will generate two 
paths, although it is obvious that the graph can be traversed using a single path. There are several measures to 
determine the centrality of a vertex, that can also be used to find vertices that are at the periphery of the graph. 
We chose the simplest one, to minimize the computational cost, by namely using the degree of the vertices: the 
vertex with the smallest degree is selected to start the path.

Construction of a path  
A path is obtained by performing a depth-first search where the next adjacent vertex 
is the one that (1) is not labeled and (2) has a neighborhood that is the most similar to the one of the current 
vertex. The neighborhood similarity of two vertices is evaluated based on the Jaccard index, a quantity used 
to compare the similarity between two sets by looking at the total number of common elements over the total 
total number of elements. Let \( \text{Adj}(u) \) be the adjacent vertices of the vertex \( u \), i.e. the neighborhood of \( u \), including 
the vertex \( u \). The similarity index between the vertex \( u \) and \( v \), denoted \( J(u,v) \), is defined by:

\[
J(u,v) = \frac{|\text{Adj}(u) \cap \text{Adj}(v)|}{|\text{Adj}(u) \cup \text{Adj}(v)|}
\]

This measure is equal to 1 if the two vertices are connected and have the same adjacent vertices, otherwise it 
is strictly lower than 1. A value close to 0 means that the total number of vertices in the two neighborhoods is 
much higher than the number of common neighbors.

It is preferable that the adjacent vertices of degree 1 that are only adjacent, to the current vertex, are not 
chosen as the following vertices, despite their high similarity, because it would end up the path. These vertices 
are immediately inserted after their unique neighbor to guarantee that the vertices are as close in the labeling 
as they are in the graph. However, we let the traversal continue.

End of the search  
The search for a path ends when all the neighbors of the current vertex have been inserted 
in a path. The algorithm starts a new path using the remaining vertices, until all the vertices belong to a path.

1.2 Step 2: Greedy merger of paths

The second step of the algorithm aims at aggregating the paths obtained in Step 1 in a unique labeling. The 
results of this step is a list of vertices, where the position of the vertex in the list gives its label. The merging 
is performed using the following process: From an empty list, the paths are sequentially added in such a way 
that at each iteration, the value of CBS is locally minimized. More precisely, for a given partial labeling and a 
given path, the position in which the path is inserted in the current labeling, as well as the direction in which 
the path is inserted (i.e. if the path is reversed or not), are chosen such that the value of CBS, computed over 
the vertices in the partial labeling and in the path, is minimized. The paths are selected in turns according to 
their length, the largest one being selected first. The rational behind this choice is so that to broadly explore 
the space of solutions.

Incremental computing of the CBS  
Evaluating the CBS is demanding computationally, as it requires considering every edge of the graph. For each insertion of path, the current CBS is computed twice (ordered and 
reverse ordered) for each possible insertion index of the current labeling. If the partial labeling has \( n \) vertices, 
there are \( n + 1 \) possible indices in which the path can be inserted, and then \( 2(n + 1) \) computations of the value 
of CBS required to select the best index. It is thus very costly, but can be largely alleviated by observing that, 
from an index to the next one, many edges have the same contribution in the total CBS value. From this 
perspective, we propose an incremental update of the CBS to take into account the state before the shift: At 
each update, only the edges whose adjacent vertex labels have been modified are considered.

We adopt the following notations: at a given iteration, the partial ordering is denoted \( O \) and contains \( n_o \) 
vertices while the path is denoted \( P \) and contains \( n_p \) vertices. Let \( i \) be the index of insertion, with \( i \in \{0, \ldots, n_o \} \). 
The partial ordering is decomposed into three parts: the first part is denoted \( O_1 \) and is made of the vertices 
located before \( i \). The vertex right after the position \( i \) is denoted \( k \), while the remaining vertices compose the 
third part called \( O_2 \). With these notations, the insertion of the path \( P \) in the current labeling \( O \) at the index \( i \) 
means that the resulting labeling is composed of the list \( O_1 \) followed by the path \( P \), the vertex \( k \) and terminated 
by the list \( O_2 \). Likewise, the insertion of the path \( P \) in the current labeling \( O \) at the index \( i + 1 \) means that the 
resulting labeling is composed of the list \( O_1 \) followed by the vertex \( k \), the path \( P \), and terminated by the list 
\( O_2 \).

Using this representation, it is clear that the positions in the partial ordering and then the corresponding 
labels change only for the vertices in \( P \) and the vertex \( k \). Let \( \pi_{i}[u] \) be the label of vertex \( u \) when \( P \) is inserted
at index \( i \), i.e. after the vertex at the \( r \)th position in the partial labeling. The changes in the labels for each group of vertices are the following:

\[
\pi_{i+1}[k] = \pi_i[k] - n_p \\
\forall u \in P, \pi_{i+1}[u] = \pi_i[u] + 1 \\
\forall u \in O_1, \pi_{i+1}[u] = \pi_i[u] \\
\forall u \in O_2, \pi_{i+1}[u] = \pi_i[u]
\] (2) (3) (4) (5)

We denote by \( CBS^{(i)} \) the value of the cyclic bandwidth sum when \( P \) is inserted at index \( i \). The computation of \( CBS^{(i)} \) can be decomposed according to the different groups of vertices defined above:

\[
CBS^{(i)} = CBS^{(i)}(O_1, O_1) + CBS^{(i)}(O_2, O_2) + CBS^{(i)}(O_1, O_2) + CBS^{(i)}(P, P) + CBS^{(i)}(k, O_1) + CBS^{(i)}(k, O_2) + CBS^{(i)}(k, k) + CBS^{(i)}(P, O_1) + CBS^{(i)}(P, O_2)
\] (6)

where \( CBS^{(i)}(X, Y) = \sum_{u \in X, v \in Y} d_C(\pi_i[u], \pi_i[v]) \) is the value of CBS when only the edges of the graph between the two sets \( X \) and \( Y \) are considered, with \( d_C(\pi_i[u], \pi_i[v]) \) defined by:

\[
d_C(\pi_i[u], \pi_i[v]) = \min\{|\pi_i[u] - \pi_i[v]|, n - |\pi_i[u] - \pi_i[v]|\}
\] (7)

The definition of the distance \( d_C \) shows trivially that if the labels of the endpoint vertices of an edge are not shifted or are shifted equally, then the value of \( d_C \) remains the same:

\[
CBS^{(i+1)}(O_1, O_1) = CBS^{(i)}(O_1, O_1) \\
CBS^{(i+1)}(O_2, O_2) = CBS^{(i)}(O_2, O_2) \\
CBS^{(i+1)}(O_1, O_2) = CBS^{(i)}(O_1, O_2) \\
CBS^{(i+1)}(P, P) = CBS^{(i)}(P, P)
\] (8) (9) (10) (11)

When the labels of endpoint vertices are not shifted equally, it is necessary to consider not only the changes induced by the shift, but also which terms between \(|\pi_i[u] - \pi_i[v]|\) and \( n_o - |\pi_i[u] - \pi_i[v]| \) is the minimum, both at index \( i \) and \( i + 1 \), as it can vary. We prove in the following the results when the endpoint vertices are \( k \) and a vertex in \( O_1 \). The other results follow the same reasoning.

**Theorem 1.1.** (Edges between \( k \) and the vertices of \( O_1 \))
Let \( u \in O_1 \) and \( \Delta = \pi_i[k] - \pi_i[u] \). We have:

1. if \( \Delta \leq \frac{n}{2} \) then \( CBS^{(i+1)}(k, u) = CBS^{(i)}(k, u) - n_p \).
2. if \( \Delta \geq \frac{n}{2} + n_p \) then \( CBS^{(i+1)}(k, u) = CBS^{(i)}(k, u) + n_p \).
3. if \( \frac{n}{2} + n_p > \Delta > \frac{n}{2} \) then \( CBS^{(i+1)}(k, u) = CBS^{(i)}(k, u) + 2\Delta - (n_o + n_p) \)

### 1.3 Detailed algorithm

The whole algorithm MACH comprises the consecutive execution of two steps, introduced in the previous Section. For readability, the algorithm of each step is described separately, respectively in Algorithms 1 and 2.

From a connected, unweighted, and undirected graph \( G = (V, E) \) with \( n \) vertices, the algorithm outputs a one-to-one mapping \( \pi \) from \( V \) to \( \{0, \ldots, n - 1\} \). We consider in the following a List as a list of elements with the associated functions List-Insert(\( A, a, idx \)) which inserts the element \( a \) in the list \( A \) at the index \( idx \) (if \( idx \) is not given, the element \( a \) is inserted at the end of the list), List-Remove(\( A, a \)) which removes the element \( a \) from the list \( A \), Length(\( A \)) which returns the number of elements of the list \( A \), and the function Reverse(\( A \)), which returns the list \( A \) in the reverse order. The function Degree(\( u \)) returns the degree of the vertex \( u \) in the graph \( G \), i.e. the number of vertices adjacent to the vertex \( u \). Finally Adj(\( u \)) returns the adjacent vertices of \( u \).

Algorithm 1 computes the first step of the heuristic as described in Section 1.1. It consists in building a collection of paths containing the vertices of the graph, each path traversing the graph following its structure. Line 1 initializes a list \( S \) containing all the vertices of the graph, while Line 2 initializes an empty list which will contain the paths. The search of paths (Lines 3 to 26) is then performed until all vertices are included in a path. A vertex of \( S \) minimum degree value is considered (Line 4). The selected vertex, noted \( u_0 \), is removed from \( S \) (Line 5) and is the starting vertex of the search from Line 8 to Line 24. The path is defined as a sequence of vertices added in a list \( P \) (Line 7) and is closed when there are no more successors available to extend the
Algorithm 1 Step 1: Guiding the search towards locally similar vertices

Require: \( G = (V, E) \)

Ensure: Paths

1: \( S = \text{List}(V) \)
2: Paths \( \leftarrow \text{List}() \)
3: \textbf{while} \( S \) is not empty \textbf{do} 
4: \( u_0 \leftarrow \arg \min_{u \in S} \text{Degree}(u) \)
5: \text{List-Remove}(S, u_0) 
6: \text{exist_successors} \leftarrow \text{True} 
7: \( P \leftarrow \text{List}() \)
8: \textbf{while} \( \text{exist_successors} \) \textbf{do} 
9: \text{List-Insert}(P, u_0) 
10: \( H \leftarrow \text{List}() \)
11: \textbf{for all} \( v \in \text{Adj}(u_0) \cap S \) \textbf{do} 
12: \text{if} \ \text{Degree}(v) = 1 \text{ then} 
13: \text{List-Insert}(P, v) 
14: \text{List-Remove}(S, v) 
15: \text{else} 
16: \text{List-Insert}(H, v) 
17: \text{end if} 
18: \textbf{end for} 
19: \textbf{if} \( H \) is not empty \textbf{then} 
20: \( u_0 \leftarrow \arg \max_{w \in H} \text{Similarity Index}(u, w) \)
21: \text{else} 
22: \text{exist_successors} \leftarrow \text{False} 
23: \text{end if} 
24: \textbf{end while} 
25: \text{List-Insert}(\text{Paths}, P) 
26: \textbf{end while} 

path or when the depth-first search ends. The first step of this loop consists of adding the vertex \( u_0 \) to the path \( P \) (Line 9). A new list \( H \) is then initialized (Line 10) and will contain the potential successors of \( u_0 \). These successors are selected among the adjacent vertices of \( u_0 \) which are still in the list \( S \), i.e. which have not been included in a path beforehand (Line 11). For each of the successors, noted \( v \), if the degree of \( v \) is equal to 1, i.e. the vertex \( v \) has only the vertex \( u_0 \) as adjacent vertex, then \( v \) is directly added in the path (Lines 12 to 14). Otherwise, it is added to the list \( H \) (Line 16). When all the potential successors have been either added to \( P \) or \( H \), the next vertex to be considered is chosen according to Eq. 1 and given by the function Similarity Index. The heuristic then loops using the updated value of \( u_0 \). If \( H \) is empty, exist_successors is set to False (Line 22) and the path is inserted in the list of paths (Line 25). If \( S \) is not empty, then \( u_0 \) is updated using the procedure described in Line 4 and the search of a path from this vertex is repeated. When \( S \) is empty, the first step is completed.

Algorithm 2 computes the second step of the heuristic as described in Section 1.2. A list Order is first initialized as the path in Paths with the highest number of elements (Line 1). This path is then removed from the list Paths, and the algorithm inserts all the remaining path in the list Order using a loop from Line 3 to Line 12. The path with the highest number of elements is selected (Line 4). The function Incremental CBS returns the index and the direction of insertion of \( P \) that minimizes the CBS. Depending on the value of the boolean variable reverse, the path \( P_0 \) is inserted reversed (Line 7) or not (Line 9). The path is then removed from the list of paths Paths and the heuristic loops until all the paths have been inserted in Order. As the result, the mapping \( \pi \) is built using the vertices as keys and the index of the vertices in the list Order as values.

1.4 Worst-case complexity of the algorithm

We now examine the worst-case time complexity of the algorithm MACH described in the previous section, when applied on a graph \( G(V, E) \) with \( |V| = n \) and \( |E| = m \).

We first examine the complexity of Algorithm 1. The set \( S \) initialized Line 1 can be implemented as a min-priority queue with a binary min-heap. The time to build the binary min-heap is \( O(n) \). Lines 4 and 5 can be done using the EXTRACT-MIN function that takes time \( O(\log n) \). Similarly, the set Paths can be implemented as a max-priority queue with a binary max-heap and Line 13 takes in the worst case a time proportional to the logarithm of the number of paths, that is in the worst case \( O(\log n) \). Using aggregate analysis, the \textbf{while} loop in Line 8 is executed at most once for each vertex of \( V \), since the vertex \( u_0 \) is removed from \( S \) (Line 5).
Algorithm 2 Step 2: Greedy merge of paths

Require: Paths
1: Order $\leftarrow \arg \max_{P \in \text{Paths}} \text{Length}(P)$
2: List-Remove(Paths, Order)
3: while Paths is not empty do
4: $P_0 \leftarrow \arg \max_{P \in \text{Paths}} \text{Length}(P)$
5: $\text{idx, reverse} \leftarrow \text{Incremental\_CBS(Order, } P_0\text{)}$
6: if reverse is True then
7: Insert-List(Order, Reverse($P_0$), idx)
8: else
9: Insert-List(Order, $P_0$, idx)
10: end if
11: List-Remove(Paths, $P_0$)
12: end while
13: $i \leftarrow 0$
14: for $i = 0 : (n - 1)$ do
15: $\pi[\text{Order}[i]] \leftarrow i$
16: end for
17: return $\pi$

function List-Insert is in constant time. The set $H$ of vertices that are adjacent to $u$ and in $S$ is implemented as a max-priority queue using a binary heap data structure that makes possible to run MAX\_HEAP\_INSERT, that inserts a new element into $H$ (Line 16) while maintaining the heap property of $H$ in $O(\log(|H|))$, that is in the worst case in $O(\log(|\text{Adj}[u]|))$. Thus, the loop on Lines 8-18 is executed $|\text{Adj}[u]|$ times and at each iteration (1) the similarity index computation takes time $O(\min(|\text{Adj}[u]|, |\text{Adj}[v]|))$, and (2) MAX\_HEAP\_INSERT takes time $O(\log(|\text{Adj}[u]|))$. Therefore, the loop on Lines 8-18 is in $O(|\text{Adj}[u]|^2)$. Line 20 can be done using EXTRACT\_MAX in time $O(\log(|\text{Adj}[u]|))$ and the total complexity of Lines 8-24 is in $O(|\text{Adj}[u]|^2)$. Consequently, the total time is $O(\sum_{u \in V}(|\text{Adj}[u]|^2))$. As K. Das established in [2] that

$$\sum_{u \in V} |\text{Adj}[u]|^2 \leq m \left( \frac{2m}{n - 1} + n - 2 \right)$$

we can conclude that the total cost of Algorithm [1] is in $O(n \log n + mn) = O(mn)$.

We can also use an aggregate analysis to evaluate the time taken by the Algorithm [2]. Lines 2 and 5 are in $O(n)$, when almost all the vertices have already been merged in Order. Incremental\_CBS runs through (1) all the edges between the vertices of the current path $P$ and the ones of Order and (2) between the vertex of Order at position Position and the other vertices of Order $\cup P$.

- Step (1) takes $O(mn)$ since all the edges of the graph are examined when aggregating the analysis over the all paths: the adjacency list of each vertex is examined once. Furthermore, for each of these $m$ edges, the $n$ positions of Order are evaluated.

- Step (2) is also in $O(mn)$ since aggregating the adjacency lists of the vertices of Order leads to the $m$ edges of the graph that are evaluated for each of the at most $n$ paths.

The other instructions of the loop are executed in constant time. Therefore, the total time spent in Algorithm [2] is $O(mn)$.

Finally, we have that the whole algorithm has a worst case complexity in $O(mn)$.

References
