The Dynamic Vertex Minimum Problem and Its Application to Clustering-type Approximation Algorithms

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Abstract

The dynamic vertex minimum problem (DVMP) is to maintain the minimum cost edge in a graph that is subject to vertex additions and deletions. DVMP abstracts the clustering operation that is used in the primal-dual approximation scheme of Goemans and Williamson (GW). We present an algorithm for DVMP that immediately leads to the best-known time bounds for the GW approximation algorithm for problems that require a metric space. These bounds include time $O(n^2)$ for the prize-collecting TSP and other direct applications of the GW algorithm (for n the number of vertices) as well as the best-known time bounds for approximating the k-MST and minimum latency problems, where the GW algorithm is used repeatedly as a subroutine. Although the improvement over previous time bounds is by only a sublogarithmic factor, our bound is asymptotically optimal in the dense case, and the data structures used are relatively simple. The DVMP algorithm is also extended to an implementation of the GW clustering algorithm for sparse graphs, which is more accurate but slower than a recent algorithm of Cole et.al.[5].

1 Introduction

Many approximation algorithms are applications of the primal-dual algorithm of Goemans and Williamson (GW) [11]. (This algorithm is rooted in the approach proposed by Agrawal, Klein and Ravi [2].) This paper determines the asymptotic time complexity of the GW clustering operation on metric spaces. Although our improvement is a sublogarithmic factor, the issue is important from a theoretic viewpoint. Also our algorithm uses simple data structures that will not incur much overhead in a real implementation.

Aside from operations involving a problem-specific oracle, the only difficulty in implementing the GW algorithm is the clustering operation which determines the next components to merge. Goemans and Williamson's original implementation [11] uses time $O(n^2 \log n)$. This was improved to $O(n(n + \sqrt{m \log \log n}))$ [9] and $O(n\sqrt{m} \log n)$ [14]. Here and throughout this paper n and m denote the number of vertices and edges in the given graph, respectively. Regarding time bounds one should bear in mind that many applications of the GW algorithm are for the dense case $m = \Theta(n^2)$ (see below). We improve the above bounds to $O(n\sqrt{m})$. Cole et. al.[5] present a modified version of the GW clustering algorithm that runs in time $O(km \log^2 n)$. Here k is an arbitrary constant, and the approximation factor of the modified algorithm increases (i.e., worsens) by the small additive

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term $O(1/n^k)$. This time bound is a substantial improvement for sparse graphs. Still in the dense case this algorithm is slower than the original GW implementation (and slightly less accurate).

One reason that dense graphs arise is assumption of the triangle inequality. Because of this our algorithm gives the best known time bound $O(n^2)$ for these applications of the GW algorithm [11]: 4-approximation for the exact tree, exact path and exact cycle partitioning problems; 2-approximation algorithm for the prize-collecting TSP (see [13] for the TSP time bound); and finally the 2-approximation for minimum cost perfect matching (whose primary motivation is speed). The GW approximation algorithms for prize-collecting Steiner tree and TSP, on metric spaces, are used as subroutines in several constant factor approximation algorithms for the minimum latency problem and the k-MST problem. For minimum latency these include [3, 10] and the best-known 10.77-approximation algorithm of [7]. For k-MST they include [4], and the best-known 3-approximation of [7] for the rooted case and 2.5-approximation of [1] for the unrooted case. In all of these algorithms multiple executions of the GW algorithm dominate the running time, so our implementation improves these time bounds too (although the precise time bounds are higher).

For the approximation algorithm for survivable network design [9, 17, 8] the given graph can be sparse but there are additional quadratic computations. Our algorithm achieves time $O((\gamma n)^2)$ when the maximum desired connectivity is γ . (The bound of [9] is $O((\gamma n)^2 + \gamma n \sqrt{m \log \log n})$. For $\gamma = 2$ Cole et. al. avoid the quadratic computations and achieve time bound $O(km \log^2 n)$ for k as above.) For other applications of the GW algorithm where the time is dominated by clustering (generalized Steiner tree problem, prize-collecting Steiner tree problem, nonfixed pointto-point connection, and T-joins [11]) our bound is $O(n\sqrt{m})$, which improves the previous strict implementations of GW and improves the algorithm of Cole et. al. [5] in very dense graphs (but of course not in sparse graphs).

We obtain our results by solving the "dynamic vertex minimum problem" (DVMP). This problem is to keep track of the minimum cost edge in a graph where vertices can be inserted and deleted. Ignoring the graph structure it is obvious that $O(m \log n)$ is the best time bound possible, for m the total number of edges. Taking advantage of the graph structure we achieve time $O(n^2)$, for n the total number of vertices. This result immediately implies a time bound of $O(n^2)$ for GW clustering. It gives all the dense graph time bounds listed above. Our solution to DVMP is based on an amortized analysis of a system of binomial queues.

We apply the DVMP algorithm to implement the GW clustering algorithm on sparse graphs in time $O(n\sqrt{m})$. We actually solve the more general "merging minimum problem" (MMP). This problem is to keep track of the minimum cost edge in a graph whose vertices can be contracted. The costs of edges affected by the contraction are allowed to change, subject to a "monotonicity property." We solve the MMP using our DVMP algorithm and a grouping technique.

Section 2 gives our solution to the DVMP. This immediately implements GW clustering for dense graphs. Section 3 solves the MMP and implements GW clustering for sparse graphs.

2 Dynamic Vertex Minimum Problem

The dynamic vertex minimum problem (DVMP) concerns an undirected graph G where each edge e has a real-valued cost c[e]. The graph is initially empty. We wish to process (on-line) a sequence of operations of the following types:

$\texttt{Add_vertex}(v)$:	add v as a new vertex with no edges.
$\texttt{Add_edge}(e)$:	add edge e with cost $c[e]$.
$\texttt{Delete_vertex}(v)$:	delete vertex v and all edges incident to v .
Find_min	:	return the edge currently in G that has smallest cost.

This section shows how to support Add_vertex, Add_edge and Delete_vertex operations in O(1) amortized time, and Find_min in worst-case time linear in the number of vertices currently in G. For convenience we assume the edge costs are totally-ordered. If two edges actually have the same cost we can break the tie using lexicographic order of the vertex indices.

Our high-level approach is to store the edges incident on each vertex in a heap. Since the DVMP only involves the edge of globally minimum cost, these heaps ignore important information: An edge that is not the smallest in one of its heaps is not a candidate for the global minimum, even if it is the smallest in its other heap. We capture this principle using a notion of "active" and "inactive" edges (defined precisely below). This allows us to economize on the number of heap operations.

2.1 The Algorithm

This section presents the data structure and algorithm, and proves correctness of the implementation.

Our data structure is a collection of heaps. Our heaps are a variant of the standard binomial queue data structure [15]. As usual, each heap is a collection of heap-ordered binomial trees. However our structure differs from the standard definition in two ways. First and most importantly, one heap is allowed to contain an arbitrary number of binomial trees of a given rank. Second, a lazy strategy is used for deletion: Heap elements are marked when they get deleted (elements are initially unmarked). The root of a heap is never marked.

Throughout this section "tree" and "binomial tree" are abbreviations for "heap-ordered binomial tree." "Root" always refers to the root of a binomial tree.

The data structure consists of |V(G)| heaps, one for each vertex. We denote by H(u) the heap associated with $u \in V(G)$. Elements of H(u) correspond to edges incident on u. An edge $\{u, v\}$ appears in both H(u) and H(v); we differentiate these two elements with the notation (u, v) and (v, u), respectively. Let twin(u, v) be synonymous with (v, u). H(u) may contain marked elements (u, x) (for edges previously incident to u that have been deleted). But as already mentioned, such marked elements are never tree roots.

Each heap H(u) is a collection of binomial trees divided into two groups: the *active* trees and the *inactive* trees. We sometimes refer to a whole tree by its root. Hence an *active root* is the root of an active tree. As usual the *rank* of an element e, denoted rank(e), is the number of children it has, which is also the logarithm (base 2) of the size of the subtree rooted at e. The following invariant characterizes the active and inactive trees.

DVMP Invariant

- (i) For all elements e, $rank(e) \le rank(twin(e)) + 1$.
- (ii) Consider a tree root f. If rank(f) > rank(twin(f)) then f is inactive. If $rank(f) \le rank(twin(f))$ and f is inactive then twin(f) is either active or a nonroot.
- (iii) Consider a vertex u. H(u) contains at most one active root per rank k, denoted $r_u(k)$ if it exists. At all times $s_u(k)$ points to the element with minimum cost among $\{r_u(k), r_u(k+1), \ldots\}$.

To better understand (ii) consider elements f and twin(f) that are both roots. If the twin roots have equal rank then at least one of them is active. If the twins have unequal rank then the smaller rank element is active while the larger one is not.

Here is some motivation for the DVMP Invariant. The purpose of (i) is that the ranks of an item and its twin should not differ too much. To maintain the first part of (iii) we will sometimes merge two active trees of the same rank. This increments the rank of the resulting tree's root by one. If this happened too often the ranks of an item and its twin could differ by an arbitrary amount, violating (i). To avoid this when a root's rank is one more than that of its twin (ii) makes the root inactive. We never merge inactive trees. Hence we do not violate (i).

One consequence of the DVMP Invariant is that the minimum cost edge is easy to find:

Lemma 2.1 If $\{u, v\}$ is the edge with minimum cost in G then either $s_u(0)$ or $s_v(0)$ points to it.

Proof: Because $\{u, v\}$ is of minimum cost, (u, v) and (v, u) must be roots in H(u) and H(v), respectively. DVMP Invariant (ii) implies that either (u, v) or (v, u) is active. DVMP Invariant (iii) implies that in general, $s_u(0)$ points to the minimum element in an active tree of vertex u. Hence either $s_u(0)$ or $s_v(0)$ points to $\{u, v\}$. (The fact that nonroot elements can be marked, i.e., deleted, has no affect on this argument.)

The procedure for Find_min follows directly from Lemma 2.1. We simply take the minimum cost element pointed to by $s_u(0)$, over all $u \in V(G)$.

The Add_vertex, Add_edge and Delete_vertex operations are implemented in a lazy fashion: They perform the least amount of work necessary to restore the DVMP Invariant. Each of these operations makes use of the routines Activate(e) and Deactivate(e). The purpose of these routines is to change a tree root e = (u, v) from the inactive to the active state, or the reverse. Both these changes of state may violate DVMP Invariant (iii): Making a root e active may create two active roots of rank rank(e). Making root e active or inactive may make $r_u(rank(e))$ or $s_u(0), \ldots, s_u(rank(e))$ out-of-date. The routines Activate(e) and Deactivate(e) repair these violations, as follows.

Deactivate(e=(u,v))

It is assumed that e is an active root. Furthermore deactivating e will not violate DVMP Invariant (ii).

- 1. Move the tree rooted at e to the set of inactive trees in H(u).
- 2. If $r_u(rank(e)) = e$, set $r_u(rank(e)) =$ nil.
- 3. Update $s_u(0), \ldots, s_u(rank(e))$.

Activate(e = (u, v))

It is assumed that e is an inactive tree root and $rank(e) \leq rank(twin(e))$.

Remove the tree rooted at e from the set of inactive trees in H(u).

2. Let cur := e.

The following loop sets $r_u(rank(cur)) = cur$ unless $r_u(rank(cur)) \neq nil$, in which case merging is necessary.

3. LOOP {

1.

4. Let k := rank(cur).

- 5. If $r_u(k) = \mathbf{nil}$
- 6. Let $r_u(k) := cur$.
- 7. Update $s_u(0), ..., s_u(k)$.

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8.
             EXIT THE LOOP.
9.
         Otherwise, merge the trees rooted at cur and r_u(k), and let cur be the resulting root.
         Set r_u(k) := \mathbf{nil}.
10.
         If rank(cur) > rank(twin(cur))
11.
12.
            Deactivate(cur).
             Activate(twin(cur)) if twin(cur) is an inactive root.
13.
14.
             EXIT THE LOOP.
15.
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It is clear that Deactivate works correctly. Activate is more complicated because of the tail recursion in Step 13. Its correctness amounts to the following fact.

Lemma 2.2 Activate eventually returns with the DVMP Invariant intact.

Proof: We will prove by induction that each time Step 5 of Activate is reached,

- (i) $rank(twin(cur)) \ge k = rank(cur);$
- (ii) the only possible violation of the DVMP Invariant is part (iii), specifically, H(u) can contain two active nodes of rank k, cur and $r_u(k)$, and the values $s_u(0), \ldots, s_u(k)$ can be incorrect.

In the inductive argument we will also note that the lemma holds whenever Activate returns.

For the base case of the induction note that activating e (in Step 1) cannot introduce a violation of DVMP Invariant (i)-(ii). Hence the first time Step 5 is reached, only DVMP Invariant (iii) for ucan fail and inductive assertion (ii) holds. Assertion (i) follows from the corresponding inequality on ranks in the entry condition of Activate.

Now consider Step 5. If $r_u(k) = \text{nil}$, Steps 6-7 restore DVMP Invariant (iii). Then Activate returns with the DVMP Invariant holding, as desired. So suppose $r_u(k) \neq \text{nil}$, i.e., there is a previously existing active tree of rank k.

The inequality $rank(f) \leq rank(twin(f))$ holds for both f = cur (by inductive assumption) and $f = r_u(k)$ (by DVMP Invariant (ii)-(iii)). Step 9 merges trees cur and $r_u(k)$ and makes cur point to the new tree root, which has rank k + 1. The previous inequality (along with DVMP Invariant (i)) shows that now rank(cur) is equal to either rank(twin(cur)) or rank(twin(cur)) + 1. In the first case, since cur is active DVMP Invariant (ii) permits twin(cur) to be active or inactive. Hence the algorithm proceeds to the next execution of Step 5 with inductive assertions (i)-(ii) intact. So the first case is correct.

In the second case DVMP Invariant (ii) requires that cur be inactive and twin(cur) be active if it is a root. Step 12 makes cur inactive and **Deactivate** restores DVMP Invariant (iii). (Note the entry condition to **Deactivate** is satisfied.) The recursive call of Step 13 fixes up DVMP Invariant (ii) in its Step 1. (Again note the entry condition to **Activate** is satisfied.) Then Step 5 is reached with inductive assertions (i)-(ii) intact. This completes the induction.

It remains to show that Activate eventually returns. This is clear, since every time it reaches Step 5 the number of trees in the data structure has decreased (in the merge of Step 9). \Box

Now consider the remaining operations Add_vertex, Add_edge and Delete_vertex. Add_vertex is trivial. The routines for Add_edge and Delete_vertex are given below. Delete_vertex works in a lazy fashion: We mark heap elements when they get deleted. We keep a marked element in the heap as long as possible, i.e., until all its ancestors become marked.

Add_edge($\{u, v\}$)

- 1. Create rank 0 nodes (u, v) and (v, u).
- 2. Put (u, v) and (v, u) in the inactive sets of H(u) and H(v), respectively.
- 3. Activate(u, v).

 $Delete_vertex(u)$

- 1. For each element $e \in H(u)$, mark twin(e) as deleted.
- 2. For each tree root f = twin(e) marked in Step 1,
- 3. Deactivate(f) if it is active.
- 4. For each unmarked element g that is in the tree of f and has all its ancestors marked,
- 5. Designate g an inactive tree root (remove all marked ancestors of g).
- 6. If twin(g) is an inactive root,
- 7. If $rank(g) \le rank(twin(g))$, Activate(g)
- 8. Else Activate(twin(g)).

It is obvious that Add_edge is correct, so we turn to $\texttt{Delete_vertex}$. Step 1 can discard all the nodes of H(u) since they are no longer needed. Step 4 finds the nodes g by a top-down exploration of the tree rooted at f. Step 2 ensures that every new tree root is found. Step 5 causes DVMP Invariant (ii) to fail if twin(g) is an inactive root. In that case if g and twin(g) have equal ranks one of them should be active; if they have unequal ranks the smaller rank element should be active. However all the rest of the DVMP Invariant is preserved in Step 5. Thus Steps 6-8 restore DVMP Invariant (ii). (Note the entry conditions to Activate and Deactivate are always satisfied.) We conclude that Delete_vertex works correctly.

We close this section with the final details of the data structure. Each value twin(e) is represented by a pointer, so nodes (u, v) and (v, u) point to each other. The set of inactive trees in each heap H(u) is represented as a doubly-linked list. Now almost every step of the four routines takes constant time. The exceptions are first, the updates of s_u : Step 3 of Deactivate takes O(rank(e) + 1) time and Step 7 of Activate takes O(k + 1) time. (We compute $s_u(i)$ in O(1) time using the value of $s_u(i + 1)$). Second, the top-down search in Step 4 of Delete_vertex amounts to O(1) time for the root f plus O(1) time for each binomial tree edge that is explored (and removed).

2.2 Timing Analysis

This section proves the claimed time bounds. It is immediate that the worst-case bounds for Find_min and Add_vertex are O(n) and O(1) respectively, where n is the current number of vertices. We show below that Add_edge and Delete_vertex use O(1) amortized time.

To start off we charge each edge of G O(1) time to account for work in its creation and destruction, specifically Steps 1-2 of Add_edge plus the possible time for marking the edge in Steps 1-2 of Delete_vertex. It is easy to see that the remaining work performed by our algorithm is linear in the number of comparisons between edge costs. (Specifically, the time for Deactivate is dominated by the comparisons to update s_u in Step 3; Activate is dominated by the comparison to merge binomial trees (Step 9) and the comparisons to update s_u (Step 7); in Delete_vertex each remaining unit of work corresponds to the destruction of a binomial tree edge, i.e., a previous comparison.) It therefore suffices to bound the number of comparisons.

We do this using the accounting method of amortized analysis [6, 16]. Define 1 credit to be the work required for 1 comparison. We will maintain the following invariant after each operation:

Credit Invariant

- (i) Every heap element has C = O(1) credits.
- (ii) Every root of rank k has an additional k + 4 credits.
- (iii) Every nonroot of rank k with a marked parent has an additional 2k + 5 credits.

The precise value of the constant C will be determined below.

Note that each call Deactivate(e) uses rank(e) + 1 credits. We will require that each call Activate(e) is given rank(e) + 1 credits. Using this credit system the amortized cost of Add_edge is 2(C+4) + 1: C+4 credits per rank 0 element created plus 1 credit for the call to Activate. Thus Add_edge takes O(1) amortized time as desired.

2.2.1 Amortized Cost of Activate

When Activate(e) is called rank(e) + 1 credits are available to be spent. We maintain that at each iteration of the loop (Step 3) at least k + 1 credits are available, for k = rank(cur). This is clearly true for the first iteration.

Suppose in Step 5, $r_u(k) = \text{nil}$. The only remaining comparisons in this call to Activate are for updating $s_u(0), \ldots, s_u(k)$. We pay for these with the k + 1 available credits.

Suppose now $r_u(k) \neq \text{nil.}$ Step 9 merges *cur* and $r_u(k)$, two rank k trees, producing a rank k + 1 tree, also denoted *cur*. The merge changes one root into a nonroot, releasing k + 4 credits. We use one credit to pay for the comparison of the merge; additionally the new rank k + 1 root requires one more credit. This leaves a total of (k + 1) + (k + 2) = 2k + 3 credits available.

Suppose Steps 12-14 are executed. We pay for Deactivate(cur) in Step 12 with k + 2 credits. (Actually we could save a comparison in Deactivate, since it need not update $s_u(rank(e))$.) Since rank(twin(cur)) = k, we can pay for the call to Activate(twin(cur)) in Step 13 (if necessary) with the remaining k + 1 credits.

Finally suppose the 'If' statement in Step 11 fails. The loop returns to Step 3 with $2k+3 \ge k+2$ available credits, as called for.

2.2.2 Amortized Cost of Delete_vertex

Consider an operation $\texttt{Delete_vertex}(u)$ and an element $(u, v) \in H(u)$ with rank k. DVMP Invariant (i) ensures $rank(v, u) \leq k + 1$. When Step 1 marks (v, u) Credit Invariant (iii) requires credits to be placed on the children of (v, u). Let us temporarily assume this has been done and discuss the rest of $\texttt{Delete_vertex}$ before returning to this issue. In Step 3 a possible operation Deactivate(v, u) requires at most k + 2 credits, paid for by the k + 4 credits on (v, u).

Now consider an unmarked element g as in Step 4. The cost of discovering g and processing it in Steps 4-6 has already been associated with merge comparisons. In addition if rank(g) = j we need 2j+5 credits: Credit Invariant (ii) requires j+4 credits when g becomes a root (Step 5), plus we need at most j+1 credits to pay for the call to Activate for g or its twin (Steps 7-8). Credit Invariant (iii) for g gives the 2j+5 needed credits.

It remains only to explain how Credit Invariant (iii) is maintained when (v, u) is marked in Step 1. (v, u) has at most k + 1 children, one child of each rank i = 0, ..., k. So Credit Invariant (iii) requires a total of at most

$$\sum_{i=0}^{k} (2i+5) = (k+1)(k+5)$$

credits. We consider two cases, depending on whether or not (u, v) is a root of H(u).

H(u) contains at most $|H(u)|/2^{k+1}$ rank k nonroot elements (u, v), since the parent of such a nonroot has 2^{k+1} descendants. So the total cost associated with deleting all nonroots (u, v) of all ranks k is bounded by

$$\sum_{k=0}^{\infty} \frac{|H(u)| \cdot (k+1)(k+5)}{2^{k+1}}.$$

Recall that $\sum_{k=0}^{\infty} \frac{1}{2^k} = \sum_{k=0}^{\infty} \frac{k}{2^k} = 2$ and $\sum_{k=0}^{\infty} \frac{k^2}{2^k} = 6$. Hence the above sum is at most |H(u)|(6 + 12 + 10)/2 = 14|H(u)|. We pay for this by taking 14 credits from each element of H(u), assuming $C \ge 14$ in Credit Invariant (i).

Next consider a rank k root (u, v). The elements in the binomial tree of (u, v) now have a total of $k + 4 + (C - 14)2^k$ credits by Credit Invariant (i)-(ii). Choosing C = 18 makes this quantity at least (k + 1)(k + 5), because $k^2 + 5k + 1 \le 2^{k+2}$ for every $k \ge 0$. (This inequality follows by induction using base case $k \le 1$. For the inductive step we use the identity $2k + 6 \le 2^{k+2}$ for every $k \ge 1$.) Hence we can pay the cost associated with (u, v).

Theorem 2.3 The dynamic vertex minimum problem can be solved in amortized time O(1) for each Add_vertex, Add_edge and Delete_vertex operation and worst-case time O(n) for each Find_min when the graph contains exactly n vertices.

We close with three remarks. First, the constant C in the analysis can be lowered because the algorithm performs unnecessary comparisons. Specifically in $\texttt{Delete_vertex}(u)$ consider an element $e = (u, v) \in H(u)$ whose twin f = (v, u) is a tree root. When Steps 3-8 are executed for this edge f, the values $s_v(\cdot)$ get updated both in Step 3 by Deactivate(f) and in every call Activate(g) in Step 7. Clearly we need only update the $s_v(\cdot)$ values once, after the loop iteration for f.

Second, an actual implementation of this data structure will probably be more efficient if we modify DVMP Invariants (i)–(ii) slightly. The current requirement $rank(e) \leq rank(twin(e)) + 1$ may cause many activates and deactivates of the same tree. We can replace this by a requirement $rank(e) \leq c_1 \cdot rank(twin(e)) + c_2$, for two constants c_1, c_2 . This allows DVMP Invariant (ii) to be relaxed so there are fewer activates and deactivates. The changes do not affect Theorem 2.3.

Finally, if necessary we can ensure that the space is always O(m), for m the current number of edges. To do this we maintain counts of the number of marked and unmarked heap elements. Whenever the former exceeds the latter we discard all heaps and reconstruct the data structure using Add_edge operations. The reconstruction time is O(m), which is accounted for by charging each marked edge O(1) time.

3 GW Clustering

This section defines and solves the merging minimum problem. The solution is then used to derive an efficient algorithm for GW clustering.

The merging minimum problem (MMP) concerns an undirected graph G where each edge e has a real-valued cost c(e). We wish to process (on-line) a sequence of contraction operations on G. Specifically the operation $\text{Merge}(x_1, x_2, y, c')$ contracts vertices x_1 and x_2 to form a new vertex y, assigning cost c'(e) to each edge e incident to y. The contraction discards parallel edges, and for each vertex z only the smallest cost edge joining y and z is retained. Merge returns the edge currently in G that has smallest cost.

To make an efficient solution possible the MMP is restricted to functions c' that satisfy two properties. First, c'(e) can be computed in O(1) time. To state the second property assume that each vertex has a color, chosen from amongst O(1) possibilities. The color of a vertex originally in G is given, and each Merge specifies the color of the new vertex y. We assume a monotonicity property that says c' preserves the relative order of edges going to similarly colored vertices. More precisely:

Monotonicity Property. For c the cost function before $Merge(x_1, x_2, y, c')$, for any $i \in \{1, 2\}$ and any two edges e, f joining x_i to vertices of the same color, $c(e) \ge c(f)$ implies $c'(e) \ge c'(f)$.

We will solve the MMP in time $O(n\sqrt{m})$. The idea is to reduce the problem to DVMP on a graph H having a small number of vertices (which we will call groups). Towards this end let k be a parameter (whose value will be determined in the analysis). Let d(v) denote the degree of a vertex v in the current graph G (v may be an original or contracted vertex). For a set of vertices S the total degree of S is $d(S) = \sum_{v \in S} d(v)$.

We partition the vertices of G into sets called *groups*. A group that consists of one vertex is a *singleton*. A group with total degree < k is *short*. We maintain this invariant:

MMP Invariant

- (i) A nonsingleton group has total degree $\leq 2k$ and all its vertices are of the same color.
- (ii) Each color has at most one short group.

(ii) ensures that the total number of groups is O(m/k).

We maintain a graph H using DVMP. H has one node for each group. Hence there are O(m/k) nodes. Two nodes g and g' are joined by an edge corresponding to the edge in G of smallest cost joining two vertices in groups g and g'. H does not have any parallel edges.

An internal edge of a (nonsingleton) group g is an edge with both ends in g. For each nonsingleton group g we maintain int(g) as the internal edge of G with smallest cost.

Clearly the smallest cost edge in G is either some edge int(g) or the edge returned by Find_min on H. We now describe how H is maintained, i.e., how the groups and H are initialized and how they are updated by Merge.

The initialization begins by partitioning V into groups: Each vertex of degree $\geq k$ is a singleton. Each remaining vertex has degree $\langle k$. Partition these vertices into groups that are maximal subsets of like colored vertices of total degree at most 2k. This achieves MMP Invariant (ii).

For the rest of the initialization H starts as an empty graph. Then the following Build Step is performed for each group g:

Build Step. If g is a nonsingleton, set int(g) to the internal edge of g with smallest cost. Execute Add_vertex(g). For every node $h \neq g$ already in H, take vertices $u \in g$ and $v \in h$ such that edge $\{u, v\}$ exists and has cost c(u, v) as small as possible. Whenever $\{u, v\}$ exists execute Add_edge($\{g, h\}$) using cost c(u, v).

We turn to the algorithm for $\text{Merge}(x_1, x_2, y, c')$. Let vertex x_i belong to group g_i . The reader should bear in mind that there are several possibilities: We can have $g_1 = g_2$, or alternatively $g_1 \neq g_2$ with 0.1 or 2 of these groups being singletons. We proceed as follows.

Execute Delete_vertex (g_i) for i = 1, 2. Create a new singleton group $g = \{y\}$. Execute the Build Step for g. To achieve the desired efficiency we specify in more detail how each edge $\{u, v\}$

of the Build Step is found. For i = 1, 2 let e_i be the smallest cost edge of G joining x_i and h. If g_i is a nonsingleton find e_i by examining all the edges incident to x_i . Otherwise $(g_i$ is the singleton $\{x_i\}$) e_i is the edge that previously joined g_i and h in H. (To show this note that any two vertices in h have the same color. By Monotonicity c' preserves the relative order of edges from x_i to h.) Choose $e \in \{e_1, e_2\}$ so c'(e) is minimum. The Build Step adds edge $\{g, h\}$ to H using cost c'(e).

Next we update H for the nodes remaining in groups g_i : Delete x_i from g_i . For each $g' \in \{g_1, g_2\}$ with g' still nonempty execute the Build Step for g'. Note that before the Merge g' was a nonsingleton and so had total degree $\leq 2k$. The Build Step computes int(g') and the smallest edge joining g' to every other group by scanning all the edges incident to g'.

Finally we restore MMP Invariant (ii): If any color now has more than one short group combine these to form maximal nonsingleton groups of total degree between k and 2k, plus possibly one short group. Delete each of the original groups from H and execute the Build Step for each of the new groups.

This completes the description of the algorithm. Now we compute the total time, using Theorem 2.3, choosing the value of k in the process. First consider initialization. We add O(m/k) nodes to H. The edges of G are scanned in time O(m) and the graph H is constructed in time O(m).

Next consider a Merge. It performs O(1) Add_vertex and Delete_vertex operations. It does O(m/k) Add_edge operations, since H has that many nodes. To find the edges of H in the Build Step it examines O(k) edges incident to nonsingleton groups, spending O(1) time on each of these edges. (No extra work is done on edges incident to singleton groups.) Finally it spends O(m/k) time for Find_min, since H has that many nodes. Thus the total time for a Merge is O(1+m/k+k). Choose $k = \sqrt{m}$ to get time $O(\sqrt{m})$ for each Merge.

There are at most n merges in an MMP. Hence the total time is $O(n\sqrt{m})$.

Theorem 3.1 The MMP can be solved in time $O(n\sqrt{m})$.

We turn to GW clustering, starting with a brief review of the algorithm [11]. We are given an undirected graph G = (V, E) with a cost function $\gamma : E \to \mathbf{R}_+$. The algorithm maintains a "dual" variable d(v) for each $v \in V$. It also uses a variable t for "time" which advances monotonically. The algorithm works by repeatedly merging vertices in G. So at any point in time, each $v \in V$ belongs to exactly one current vertex of G. At any iteration each current vertex of G is either "active" or "inactive"; we classify a vertex $v \in V$ as active or inactive depending on the status of its current vertex. For vertices $u, v \in V$ adjacent in the given graph, edge $\{u, v\} \in E$ has "reduced cost"

$$\widehat{\gamma}(u, v) = \gamma(u, v) - d(u) - d(v)$$

and "addition time"

$$a(u, v) = t + \frac{\widehat{\gamma}(u, v)}{s(u) + s(v)}$$

where t is the current time and the status s(x) equals 1 if vertex x is active else 0. The addition time is infinite if u and v are both inactive.

Each iteration of the clustering algorithm chooses the edge $\{u, v\}$ with smallest addition time. It advances time by $\delta = a(u, v) - t$, increases the dual d(v) of each active vertex v by δ , and merges the vertices containing u and v. (For some versions of the GW algorithm additional merges are performed [12].)

To model this as an MMP assign each current vertex of G the color "active" or "inactive" as appropriate. To define edge costs for MMP let , be the largest given cost in the GW algorithm. At all times define edge costs by

(1)
$$c(u,v) = \begin{cases} a(u,v) & a(u,v) \neq \infty, \\ n, +\widehat{\gamma}(u,v) & a(u,v) = \infty. \end{cases}$$

When the GW algorithm merges current vertices x_1 and x_2 into a new vertex y, the MMP executes $Merge(x_1, x_2, y, c')$, for c' the new cost function defined by (1).

We show that with these definitions any algorithm for MMP correctly implements the GW clustering algorithm. Consider any GW iteration and its corresponding operation $Merge(x_1, x_2, y, c')$. The argument consists of three observations.

First note that in each GW iteration the only addition times that change are for edges incident to the new vertex y. (This uses the fact that the only vertices of V whose status can change in an iteration are those belonging to the new vertex y.) This implies that the only MMP costs c(a, b)that change are for edges incident to y (as required by MMP).

Next we verify the Monotonicity Property. Let x be x_1 or x_2 . Let c(c') be the MMP cost function before (after) the merge. Take edges $\{x, y_1\}$ and $\{x, y_2\}$, where y_1 and y_2 have the same color and $c(x, y_1) \ge c(x, y_2)$. The same color assumption means $s(y_1) = s(y_2)$. Thus the assumed inequality on c with (1) implies $\widehat{\gamma}(x, y_1) \ge \widehat{\gamma}(x, y_2)$. This in turn implies $c'(x, y_1) \ge c'(x, y_2)$.

Finally we must check that Merge returns the edge required by GW, i.e., the edge with smallest addition time. An iteration of the GW algorithm that chooses edge $\{u, v\}$ advances time by at most $\gamma(u, v)$. There are $\langle n \rangle$ iterations [11]. Thus time in the GW algorithm is always $\langle n \rangle$. This precludes any edge $\{u, v\}$ with infinite addition time from achieving the minimum cost c(u, v) in the MMP algorithm. So Merge correctly returns the edge with smallest addition time.

Theorem 3.2 The GW clustering algorithm can be implemented in time $O(n\sqrt{m})$.

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