

Graph Theory

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Preface

When writing this book, I mainly refer to (Bondy and Murty 1976), which covers both theoretical results and crucial applications in graph theory.

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Chapter 1 Basic Concepts of Graphs

1.1 Isomorphism

Two graphs G and H are identical, written as G=H, if all their components are the same, that is, V(G)=V(H), E(G)=E(H) and $\psi_G=\psi_H$. Identical graphs of course share the same properties. However, a graph H does not necessarily have to be exactly G to preserve all its properties. The labels of the vertices and edges are immaterial.

Definition 1.1.1

Two graphs G and H are said to be isomorphic, written as $G \cong H$, if there exist bijections $\theta: V(G) \to V(H)$ and $\phi: E(G) \to E(H)$ such that

$$\psi_G(e) = uv \implies \psi_H(\phi(e)) = \theta(u)\theta(v)$$
 (1.1)

The ordered pair (θ, ϕ) is called an **isomorphism** between G and H.

(Bondy and Murty 1976) includes the reverse direction of (1.1) in the definition, that is,

$$\psi_G(e) = uv \iff \psi_H(\phi(e)) = \theta(u)\theta(v)$$

But the reverse direction is redundant. To see this, we suppose that $\psi_H(\phi(e)) = \theta(u)\theta(v)$ and $\psi_G(e) = xy$. By (1.1), we have $\psi_H(e) = \theta(x)\theta(y)$. It then follows that $\theta(u)\theta(v) = \theta(x)\theta(y)$. We have either $\theta(u) = \theta(x)$, $\theta(v) = \theta(y)$, or $\theta(u)\theta(y)$, $\theta(v) = \theta(x)$. Because θ is a bijection, either u = x, v = y, or u = y, v = x. Either way, we have uv = xy. Therefore, $\psi_G(e) = xy = uv$, which proves the reverse direction \Leftarrow .

For simple graphs, there is no need to find a bijection between edges once the bijection θ between vertices is established.

Proposition 1.1.1

Let G and H be simple graphs. Then $G \cong H$ if and only if there exists a bijection $\theta : V(G) \to V(H)$ such that

$$uv \in E(G) \implies \theta(u)\theta(v) \in E(H)$$
 (1.2)

Proof (Necessity) Suppose that there exist θ and ϕ satisfying (1.1). If $e = uv \in E(G)$, then by (1.1), $\psi_H(\phi(e)) = \theta(u)\theta(v)$, which implies $\theta(u)\theta(v) \in E(H)$.

(Sufficiency) Define
$$\phi: E(G) \to E(H)$$
 by

$$\phi(uv) = \theta(u)\theta(v)$$

We need to show ϕ is bijective. Suppose $\phi(uv) = \phi(xy)$. We have $\theta(u)\theta(v) = \theta(x)\theta(y)$. Applying a similar argument we used in the previous comments, we will finally obtain uv = xy, which means ϕ is injective. On the other hand, for any edge $f \in H$. Write f = ij (i.e., $\psi_H(f) = ij$). Then because θ is bijective, there exist $u, v \in V(G)$ such that $\theta(u) = i$ and $\theta(v) = j$. Hence, $\phi(uv) = ij$, which implies ϕ is surjective.

If $\psi(e) = uv$, i.e., $e = uv \in E(G)$, then we have $\theta(u)\theta(v) \in E(H)$ by (1.2). Equivalently, $\psi_H(\phi(e)) = \theta(u)\theta(v)$.

A complete bipartite graph is a *simple* bipartite graph with bipartition (X,Y) in which each vertex in X is incident with each vertex in Y. That is, if $x \in X$ and $y \in Y$, then $xy \in E$. If |X| = m and |Y| = n, we often use the symbol $K_{m,n}$ to denote this complete bipartite graph. (See Figure 1.1.) Note that this implicitly implies that the complete bipartite graph is unique in some way since we can represent it with a common symbol. Indeed, it is unique up to isomorphism, as we will show in the next proposition.

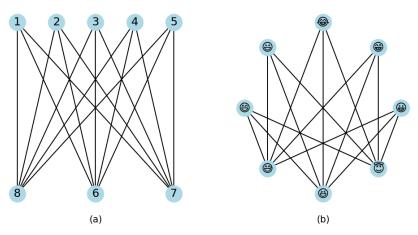


Figure 1.1: Both (a) and (b) are $K_{5,3}$.

Proposition 1.1.2

Let G[X,Y] and H[U,V] be two complete bipartite graphs with |X| = |U| and |Y| = |V|. Then $G \cong H$. In other words, a complete bipartite graph is unique up to isomorphism if the sizes of its two vertex sets in bipartition are determined.

Proof Since |X| = |U| and |Y| = |V|, we can find a bijection $\theta : V(G) \to V(H)$ in such a way that θ maps each point in X onto U, and each point in Y onto V. Then for an edge $xy \in E(G)$, we have $\theta(x)\theta(y) \in E(H)$ since there has to be an edge connecting $\theta(x) \in U$ and $\theta(y) \in V$ by the definition of complete bipartite graphs. This proves $G \cong H$ by Proposition 1.1.1.

1.2 Vertex Degrees

1.3 Paths and Connection

A walk in a graph is a sequence of edges $e_1 \cdots e_k$ joining a *nonempty* sequence of vertices $v_0 v_1 \cdots v_k$, which is denoted by

$$v_0 e_1 v_1 \cdots e_k v_k \tag{1.3}$$

with each edge written after one of its end and followed by its other end. Note that though the sequence of vertices in a walk is required to be nonempty, the sequence of edges may be empty. And in that

case, the walk contains only one vertex, say v_0 , and it is called the **trivial walk**.



Note The term **sequence** in mathematics often means an infinite sequence, which is essentially a function defined on \mathbb{N}^* . However, in graph theory, we usually refer to sequence as a **finite** list of ordered elements.

We call a walk W from v_0 to v_k a (v_0, v_k) -walk. The vertices v_0 and v_k are referred to as the **origin** and the **terminus** of that walk, respectively.

It should be emphasized that neither the edges nor the vertices in a walk are necessarily distinct. However, if all edges of walk W are distinct, we call W a **trail**. And if all vertices in W are distinct, it is then called a **path**. Of course, all edges in a path are also distinct since the vertices are.

Two vertices are said to be **connected** if there exists a path joining them. Otherwise, they are **disconnected**.

The length of a path P, written as |P|, is defined as the number of edges along it. Note that the length of a trivial path is zero since there are no edges.

If G is a simple graph, then we may write a walk simply as a sequence of vertices since there is one and only one edge joining each pair of consecutive vertices in the walk. For example, we write the (v_0, v_k) -walk in (1.3) as

$$v_0v_1\cdots v_k$$

with edges dropped.

Proposition 1.3.1

If there is a (u, v)-walk in G, then there is also a (u, v)-path in G.

•

This can be proved easily using the following algorithm (Algorithm 1).

Algorithm 1: Extracting a Path From a Walk

```
Input: A walk W = v_0 e_1 v_1 \cdots e_k v_k

Output: A path P

1 initialize P as a sequence containing just one vertex v_0;

2 for i = 1, \dots, k do

3 | if v_i is not in P then

4 | append e_i and v_i to P;

5 | else

6 | remove all the vertices and edges after the vertex v_i from P;

7 | end

8 end
```

Proposition 1.3.2

The number (v_i, v_j) -walks of length k in G is the (i, j)-th entry of the k-th power of the adjacency matrix A, i.e., A^k .

Proof

1.4 Cycles

One simple yet useful observation of a particular longest path in a graph is that all the neighbors of the terminus must occur along the path. To be specific, if $P = v_0 e_1 v_1 \cdots e_k v_k$ is one of the longest paths in G then P must contain all vertices in $N(v_k)$. To prove this, we assume P does not contain $v_{k+1} \in N(v_k)$. (Suppose $\psi(e_{k+1}) = v_k v_{k+1}$.) Then the path $P + e_{k+1} v_{k+1}$ is clearly longer than P, which leads to a contradiction. Figure 1.2 depicts such an example. Note that if 8 were a neighbor of 7, then path 12345678 would be longer.

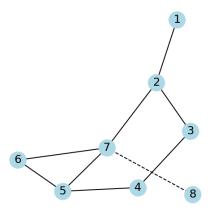
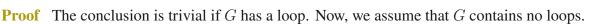


Figure 1.2: Path 1234567 is one of the longest paths.

Proposition 1.4.1

If $\delta(G) > 2$, then we can find a cycle starting from each vertex of G.



Note Note that there are cases where G has no paths if we allow it to have loops. For example, if every vertex of G is incident with just exactly one loop, then G still satisfies the hypothesis. But there are no paths in G.

Let $P = v_0 e_1 v_1 \cdots e_{k-1} v_{k-1} e_k v_k$ be one of the longest paths in G. Since $\deg(v_k) \geq 2$ and v_k has no loops, v_k has a neighbor, say u, other than v_{k-1} . As noted before, u must occur in P. Therefore, there exists a cycle from u to u.

In fact, we have an algorithm to find a cycle without knowing the longest path in G.

Proof We need to show that Algorithm 2 works correctly.

Initialization: Firstly, note that line 7 is possible since v_0 has no loops and $deg(v_0) \ge 2$.

We claim the loop invariants are

- 1. P has j vertices assuming that we are to execute the j-th iteration,
- 2. P has no duplicated vertices, i.e., P is a path, and
- 3. edge e is incident with v.

Maintenance: Suppose we are in the j-th iteration. After line 9, P remains a path. Because $deg(v) \ge 2$, there exists an edge f other than e that is incident with v. Hence, line 10 works correctly.

Algorithm 2: Finding a Cycle in G With $\delta(G) > 2$

```
Input: G with \delta(G) \geq 2
   Output: A cycle C
1 if G has a loop e from v to v then
       C \leftarrow vev:
       return C;
4 end
5 pick a vertex v_0;
6 P \leftarrow v_0;
7 pick v \in N(v_0) and let e be the corresponding edge, i.e., \psi(e) = v_0 v;
8 while v \notin P do
       P \leftarrow Pev;
       pick u \in N(v) such that there exists an edge f satisfying \psi(f) = vu and f \neq e;
11
       e \leftarrow f;
12
13 end
14 remove from P all vertices and edges before v;
15 C \leftarrow Pev;
```

After executing line 12, we find that the number of vertices in P is increased by one, i.e., j + 1, P is still a path and e is incident with v.

Termination: We can complete at most n-1 iterations since P can hold at most as many vertices as there are in G. Upon termination, we find v is in P and e is incident with v. By removing from P all vertices and edges before v and then append to it edge e and vertex v, we will obtain a cycle from v to itself.

Theorem 1.4.1



The **girth** of a graph is defined as the length of its shortest cycle. We say the girth of G is infinity if it contains no cycles. Apparently, if G has girth 1, then it contains a loop. If it has girth 2, then there must be a parallel edge. But it has no loops. And if the girth of G is greater than or equal to 3, then it must be a simple graph.

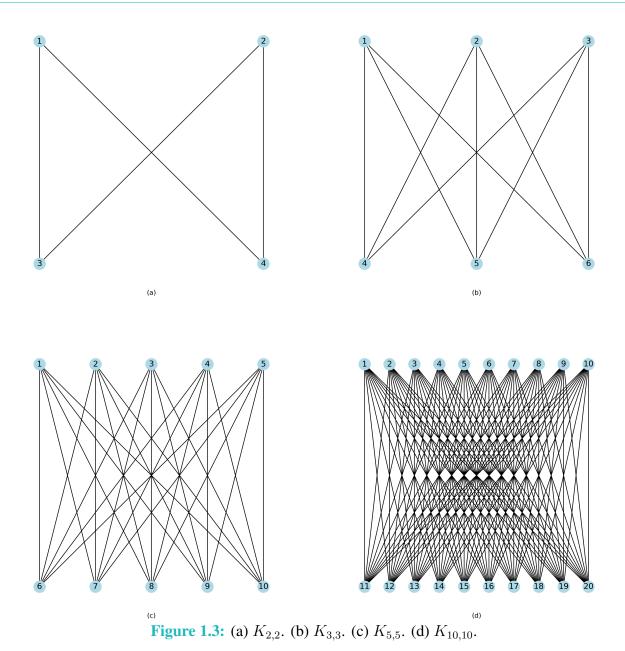
Proposition 1.4.2

A k-regular graph with girth 4 has at least 2k vertices. Moreover, if it has exactly 2k vertices, then it must be $K_{k,k}$, i.e., a complete bipartite graph with both sides of the bipartition having the same size k. Conversely, $K_{k,k}$ is a k-regular graph with girth 4.

Figure 1.3 depicts several $K_{k,k}$ graphs.

Proof Take a pair of incident vertices u and v in G. We have $N(u) \cap N(v) = \emptyset$. Otherwise, a triangle would appear. Because the degrees of u and v are both k, equivalently, the sizes of their neighbors are k, G must has at least 2k vertices having these two disjoint sets N(u) and N(v).

Suppose |V|=2k. Pick a pair of incident vertices u and v as before. From the previous proof, we know |N(u)|=|N(v)|=k and they are disjoint. Since G now only has 2k vertices, V is composed of



these two neighbor sets, i.e., $V = N(u) \uplus N(v)$. Observe that each pair of vertices in N(u) cannot be joined with each other for there are no triangles. The same conclusion also holds for N(v). Therefore, every vertex in N(u) is joined with every vertex in N(v) because the degree of every vertex is k. This shows that G is $K_{k,k}$.

We also need to show $K_{k,k}$ is a k-regular graph with girth 4. Clearly, it is k-regular. It contains no cycles with length 1 or 3 by Theorem 1.4.1. Of course, it does have any parallel edges, hence no 2-cycles. And we can easily find a 4-cycle in it. For example, if we suppose $X = \{x_1, \ldots, x_k\}$ and $Y = \{y_1, \ldots, y_k\}$ form a bipartition of $K_{k,k}$, then $x_1y_1x_2y_2x_1$ is a 4-cycle.

1.5 Shortest Paths and Dijkstra's Algorithm

With every edge e in graph G, we can associate a real number w(e), usually positive, which we shall call the **weight** of that edge. As we will see, to unify our notations for some special cases, it is convenient to define the weight of a nonexistent edge between two non-incident vertices as infinity ∞ .

We can now extend our former definition of the length of a path by

$$|P| := \sum_{e \in P} w(e)$$

Note that if all the edges are assigned to unit weights, then |P| is just the number of edges in it, which reduces to the former definition. Notice also that the length of a trivial path is also zero since the sum of nothing in the above equation, by convention, is zero.

Given a map, the cities can be regarded as vertices, and for each pair of adjacent cities, we can draw an edge in between them. In this example, it is reasonable to define the weight of edge uv as the distance between cities u and v. Then the problem of finding a shortest path from u_0 to v arises quite naturally if we want to travel from city u_0 (where we live) to every other city v at the minimum cost.

Formally, for all $u, v \in V$, the length of the shortest path from u to v is defined as

$$d(u,v) := \begin{cases} \min \left\{ |P| \mid P \text{ is a } (u,v)\text{-path} \right\}, & \text{if } u \text{ and } v \text{ are connected} \\ \infty, & \text{if } u \text{ and } v \text{ are disconnected} \end{cases}$$

Given a proper subset S of V and a source $u_0 \in S$ in it, it is natural to define the distance from u_0 to the complement S^{\complement} as the minimum distance from u_0 to every $v \in S^{\complement}$, that is,

$$d(u_0, S^{\complement}) := \min_{v \in S^{\complement}} d(u_0, v)$$

Of course, if $d(u_0, S^{\complement}) = \infty$, then there are no paths from u_0 to any vertex in S^{\complement} , in other words, u_0 is disconnected from S^{\complement} . Suppose $d(u_0, S^{\complement})$ is a finite number, which means there exists a path $P = u_0 \cdots uv$ from u_0 to some vertex $v \in S^{\complement}$. The following are some simple observations about this path P:

- 1. P is a shortest (u_0, v) -path,
- 2. $u \in S$ and the (u_0, u) -section, $u_0 \cdots u$, is a shortest (u_0, u) -path, and
- 3. we have the equation

$$d(u_0, S^{\complement}) = d(u_0, u) + w(uv)$$
(1.4)

Equation (1.4) motivates us to state the following proposition, which is the central idea of Dijkstra's algorithm.

Proposition 1.5.1

Let G = (V, E) be a simple graph. Let $S \subseteq V$ be a subset of vertices and $u_0 \in S$ a point in it. We have

$$d(u_0, S^{\complement}) = \min_{u \in S, v \in S^{\complement}} \{ d(u_0, u) + w(uv) \}$$
(1.5)

Proof First, note that the set

$$\left\{ d(u_0, u) + w(uv) \mid u \in S, v \in S^{\complement} \right\}$$

is a finite set (possibly containing infinite numbers). Hence, it does have a minimum.

Assume there exist $u^* \in S$ and $v^* \in S^{\complement}$ such that

$$d(u_0, S^{\complement}) > d(u_0, u^*) + w(u^*v^*) \tag{1.6}$$



Note Note that (1.6) implicitly implies that u_0 and u^* are connected and u^* and v^* are connected since the right-hand side of (1.6) is a finite number.

Then there exists a (u_0, u^*) -path P such that $|P| = d(u_0, u^*)$. Note that Pv^* forms a path since all vertices in P are in S while v^* is in the complement S^* . But Pv^* is a path from u_0 to S^{\complement} with length $d(u_0, u^*) + w(u^*v^*)$, which is less than $d(u_0, S^{\complement})$ by assumption. Therefore, this leads to a contradiction. We have

$$d(u_0, S^{\complement}) \le d(u_0, u) + w(uv) \quad \forall u \in S \ \forall v \in S^{\complement}$$

And (1.5) is proved.

1.5.1 A First Attempt

Starting from an initial set $S^{(0)} = \{u_0\}$ containing just the source, we want to enlarge this set in a way that a shortest path from u_0 to any vertex within the set is known. Given $S^{(j-1)}$, in each iteration j, we find optimal vertices $u^* \in S^{(j-1)}$ and $v^* \in V \setminus S^{(j-1)}$ in the sense that equation (1.5) is satisfied. In doing so, we are guaranteed to find a shortest path from u_0 to $V \setminus S^{(j-1)}$ with the terminus v^* . Then we extend the set $S^{(j-1)}$ to $S^{(j)}$ by adding v^* .

Based on this idea, we propose our first attempt to find shortest paths in the following algorithm (Algorithm 3).

1.5.2 Dijkstra's Algorithm

Given a vertex v, its predecessor is given by $\Pi[v]$. And the predecessor of $\Pi[v]$ is $\Pi[\Pi[v]]$, and so forth. We can keep accessing the predecessors until hopefully stops at the source u_0 . In this case, we have recovered a path from u_0 to v, $u_0 \cdots \Pi[v]v$. To make our proof concise, we call this procedure recovering a (u_0, v) -path using Π .

Proof Note that there is an early return in line 22. Hence, we may not complete all n-1 iterations of the for loop (lines 7-23). Suppose we can complete k iterations.

Loop Invariants: Upon completion of the *j*-th iteration, we claim that

- 1. $D[u] = d(u_0, u) \quad \forall u \in S^{(j)},$
- 2. $D[v] = \min_{u \in S^{(j-1)}} \{ d(u_0, u) + w(uv) \} \quad \forall v \in V \setminus S^{(j)},$
- 3. we can recover a (u_0, u) -path using Π for every $u \in S^{(j)}$, and
- 4. $S^{(j)} = S^{(j-1)} \uplus u^{(j)}$.

Maintenance: Assuming all loop invariants hold for j-1. We now consider the j-th iteration. In the inner loop (lines 10-20), by referring to loop invariant 2, we note that the procedure from line 11

Algorithm 3: A First Attempt to Find the Shortest Paths

Input: A simple weighted graph G = (V, E) and a source $u_0 \in V$

Output: Dictionaries D and Π maintaining the lengths of shortest paths from u_0 and predecessors of all vertices connected to u_0 , respectively

```
1 S^{(0)} \leftarrow \{u_0\};
 D[u_0] \leftarrow 0;
 3 for j = 1, ..., |V| - 1 do
          d^* \leftarrow \infty;
          u^* \leftarrow v^* \leftarrow \text{none};
 5
          for u \in S^{(j-1)} do
 6
                for v \in V \setminus S^{(j-1)} do
 7
                     d \leftarrow D[u] + w(uv);
 8
                     if d < d^* then
 9
                           u^* \leftarrow u;
10
                          v^* \leftarrow v ;
d^* \leftarrow d ;
11
12
13
                end
14
          end
15
          if d^* = \infty then
16
                return D and \Pi;
17
18
          D[v^*] \leftarrow d^*;
19
          \Pi[v^*] \leftarrow u^*;
20
          S^{(j)} \leftarrow S^{(j-1)} \cup \{v^*\};
22 end
```

to line 15 ensures that

$$D[v] = \min \left\{ \min_{u \in S^{(j-2)}} \{ d(u_0, u) + w(uv) \}, D[u^{(j-1)}] + w(u^{(j-1)}v) \right\} \quad \forall v \in V \setminus S^{(j-1)}$$
 (1.7)

after this inner loop is completed. But invariant 1 implies that $D[u^{(j-1)}] = d(u_0, u^{(j-1)})$. Moreover, we have $S^{(j-1)} = S^{(j-2)} \uplus u^{(j-1)}$ by invariant 4. Hence, (1.7) reduces to

$$D[v] = \min \left\{ \min_{u \in S^{(j-2)}} \{ d(u_0, u) + w(uv) \}, d(u_0, u^{(j-1)}) + w(u^{(j-1)}v) \right\}$$

$$= \min_{u \in S^{(j-1)}} \{ d(u_0, u) + w(uv) \} \quad \forall v \in V \setminus S^{(j-1)} \quad (1.8)$$

Note that invariant 2 for iteration j follows directly from (1.8) because $V \setminus S^{(j)} \subseteq V \setminus S^{(j-1)}$ by line 25 if line 25 is reachable in the current iteration. If line 25 is not reachable, which means the algorithm terminates at line 22, then there is nothing to prove for this iteration.

The purpose of lines 16-19 is that upon completion of lines 10-20, we have

$$d^* = \min_{v \in V \setminus S^{(j-1)}} \min_{u \in S^{(j-1)}} \{ d(u_0, u) + w(uv) \}$$

By Proposition 1.5.1, we know d^* is the length of a shortest path from u_0 to $V \setminus S^{(j-1)}$, that is,

$$d^* = d(u_0, V \setminus S^{(j-1)})$$

Algorithm 4: Dijkstra's Algorithm

Input: A simple weighted graph G = (V, E) and a source $u_0 \in V$ **Output:** Dictionaries D and Π maintaining the lengths of shortest paths from u_0 and predecessors of all vertices connected to u_0 , respectively // initialization 1 $S^{(0)} \leftarrow \{u_0\}$; 2 for $v \in V$ do $D[v] \leftarrow \infty$; 4 end 5 $D[u_0] \leftarrow 0$; 6 $u^{(0)} \leftarrow u_0$; 7 for j = 1, ..., |V| - 1 do $d^* \leftarrow \infty$: $v^* \leftarrow \text{none}$; 9 for $v \in V \setminus S^{(j-1)}$ do 10 $d \leftarrow D[u^{(j-1)}] + w(u^{(j-1)}v)$; 11 if D[v] > d then 12 $D[v] \leftarrow d$; // update distance 13 $\Pi[v] \leftarrow u^{(j-1)}$; // update predecessor 14 end 15 if $D[v] < d^*$ then 16 $v^* \leftarrow v$; 17 $d^* \leftarrow D[v^*]$; 18 end 19 end 20 if $d^* = \infty$ then 21 **return** D and Π ; 22 23 end

We are now at the end of line 20. There are two cases.

 $u^{(j)} \leftarrow v^*$:

 $S^{(j)} \leftarrow S^{(j-1)} \cup \{u^{(j)}\};$

24

25 | 26 end

(Case 1: Early Return) If $d^* = \infty$ or equivalently $d(u_0, V \setminus S^{(j-1)}) = \infty$, then it means that u_0 is disconnected from $V \setminus S^{(j-1)}$. Since no shortest paths are to be discovered, the algorithm needs to terminate. Recall we assume we can only complete k iterations. Therefore, the current iteration must be k+1 for we are exiting the algorithm. No loop invariants need to be proved since this iteration is not completed.

(Case 2) On the other hand, we now suppose v^* is some vertex at the end of line 20. Let $u^{(j)} = v^*$ (line 24). Then invariant 4 for iteration j is proved immediately by line 25.

We now prove invariant 3 for j. Note that the predecessor of $u^{(j)}$ is $u^{(j-1)}$, i.e., $\Pi[u^{(j)}] = u^{(j-1)}$ by line 14. We then recover a $(u_0, u^{(j-1)})$ -path, say P, using Π (invariant 3 for j-1). Note that $Pu^{(j)}$ is a $(u_0, u^{(j)})$ -path, and it can be recovered using Π since $\Pi[u^{(j)}] = u^{(j-1)}$ and P itself is recovered using Π . This proves invariant 3 of iteration j.

Furthermore, by recalling $u^{(j)}=v^*$ and $d^*=d(u_0,V\setminus S^{(j-1)})$, we note that $Pu^{(j)}$ is a shortest path from u_0 to $u^{(j)}$ since its length is $d(u_0,V\setminus S^{(j-1)})$. In other words, it is also a shortest path from u_0 to $V\setminus S^{(j-1)}$. Therefore, we can write

$$d(u_0, u^{(j)}) = d^* = D[v^*]$$

where the last equality follows from line 18. Replacing v^* with $u^{(j)}$, equivalently we have

$$D[u^{(j)}] = d(u_0, u^{(j)})$$
(1.9)

This equation (1.9) along with invariant 1 for j-1 implies that invariant 1 also holds for j. Note that we have shown that all loop invariants are preserved when the current iteration (iteration j) is completed.

Termination: As the algorithm terminates, there are k+1 vertices in $S^{(k)}$. And the vertices outside $S^{(k)}$ are not reachable from the source u_0 . For each $u \in S^{(k)}$, we have $D[u] = d(u_0, u)$ (invariant 1), that is, D[u] stores the length of a shortest path from u_0 to u, as desired. And by invariant 3, we can recover a shortest (u_0, u) -path using Π . This completes the proof.

References

[1] J. A. Bondy and U. S. R. Murty. *Graph Theory with Applications*. New York: North Holland, 1976. ISBN: 978-0-444-19451-0.

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