

Clustering

K-means

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Introduction to clustering

Definition

A cluster is a collection of objects which are “similar” between them and are “dissimilar” to the objects belonging to other clusters.

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Clustering is the algorithm that recognizes clusters from a given data set.

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Part of common application domains in which the clustering problem arises are as follows:

- Multimedia Data Analysis
- Responding to public health crises
- Intermediate Step for other fundamental data mining problems
- Intelligent Transportation

K-means Algorithm

The **k-means clustering** problem is one of the oldest and most important questions in all of computational geometry.

Given an integer k and a set of n data points in \mathbb{R}^d , the goal of this problem is to choose **k centers** so as to **minimize the total squared distance between each point and its closest center**.

The most common K-means algorithm was first proposed by **Stuart Lloyd** of Bell Labs in 1957.

Max-Flow and Min-Cut Problems

A **flow network** is a tuple $G = (V, E, s, t, c)$.

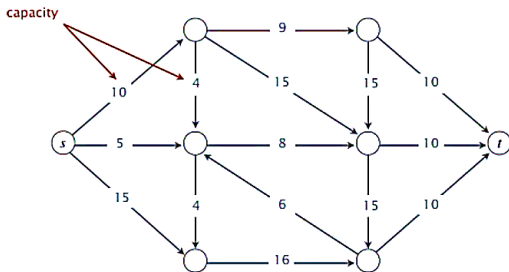
- Diagraph (V, E) with **source** $s \in V$ and **sink** $t \in V$.
- Capacity $c(e) > 0$ for each $e \in E$.

A Flow network

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Intuition. Material flowing through a transportation network, which originates at source and is sent to sink.



Definition

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Its **capacity** is the sum of the capacities of the edges from A to B .

$$\text{cap}(A, B) = \sum_{e \text{ out of } A} c(e)$$

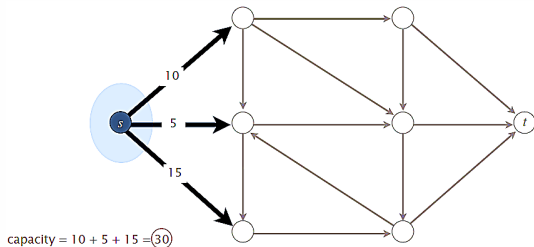
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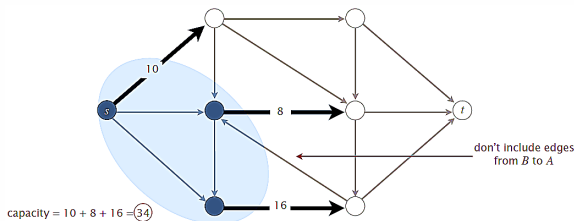
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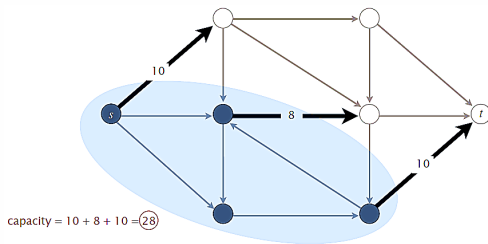
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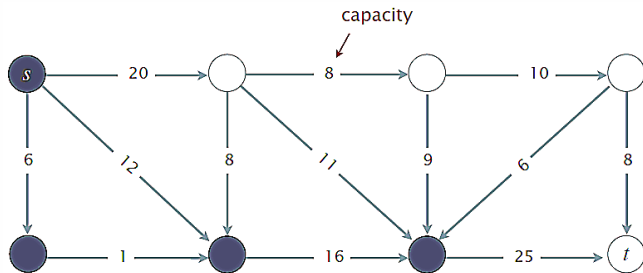


Min-cut problem. Find a cut of minimum capacity.



Which is the capacity of the given st-cut?

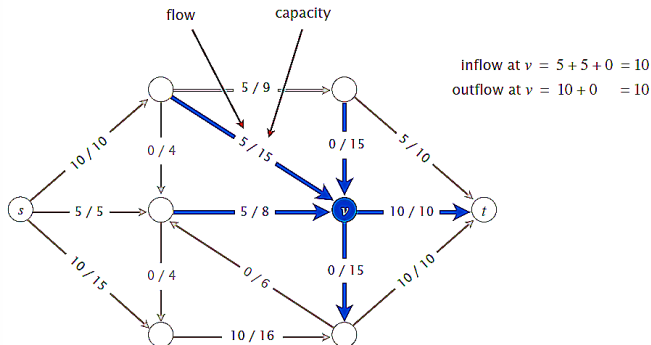
- A. 11 ($20 + 25 - 8 - 11 - 9 - 6$)
- B. 34 ($8 + 11 + 9 + 6$)
- C. 45 ($20 + 25$)
- D. 79 ($20 + 25 + 8 + 11 + 9 + 6$)



Definition

An **st-flow**(flow) f is a function that satisfies:

- For each $e \in E$: $0 \leq f(e) \leq c(e)$
- For each $v \in V - \{s, t\}$: $\sum_{e \text{ in to } v} f(e) = \sum_{e \text{ out of } v} f(e)$



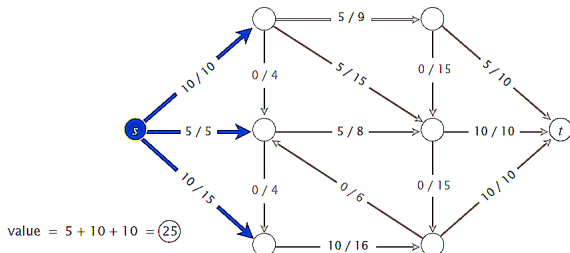
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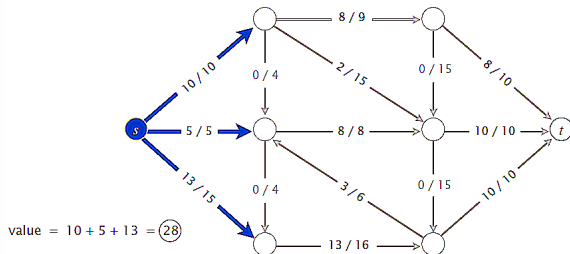
- For each $e \in E$: $0 \leq f(e) \leq c(e)$
- For each $v \in V - \{s, t\}$: $\sum_{e \text{ in to } v} f(e) = \sum_{e \text{ out of } v} f(e)$

Definition

The **value** of a flow f is: $\text{val}(f) = \sum_{e \text{ out of } s} f(e) - \sum_{e \text{ in to } s} f(e)$



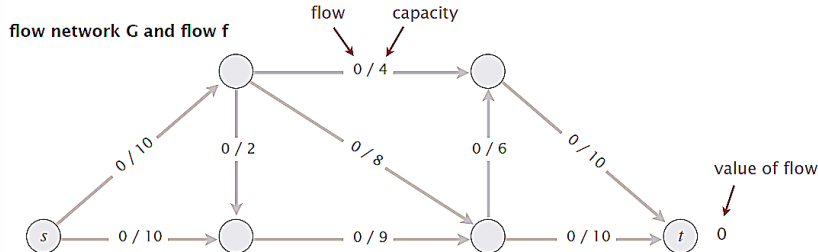
Max-flow problem. Find a flow of maximum value.



Ford-Fulkerson Algorithm

Greedy algorithm.

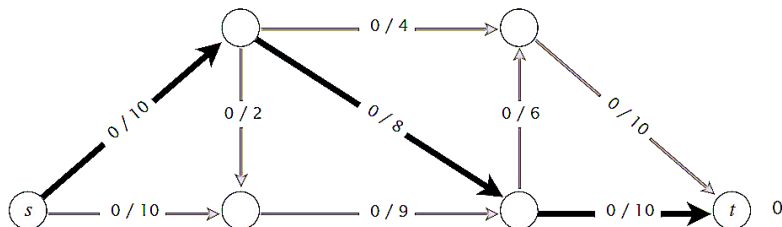
- Start with $f(e) = 0$ for each edge $e \in E$.
- Find an $s \rightsquigarrow t$ path P where each edge has $f(e) < c(e)$.
- Augment flow along path P .
- Repeat until you get stuck.



Greedy algorithm.

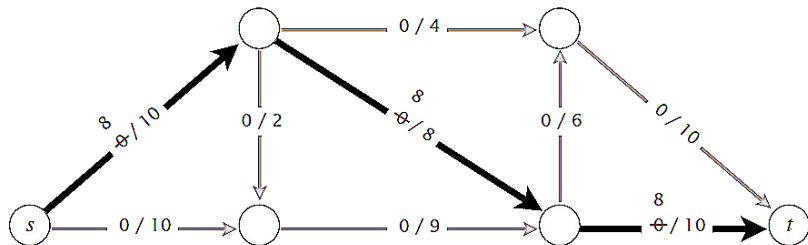
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flow network G and flow f



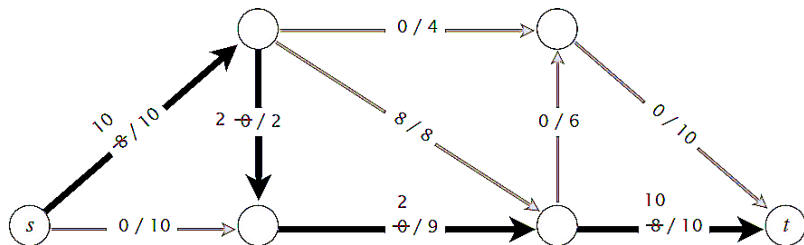
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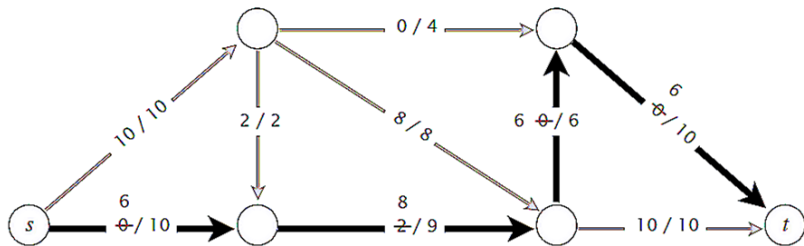
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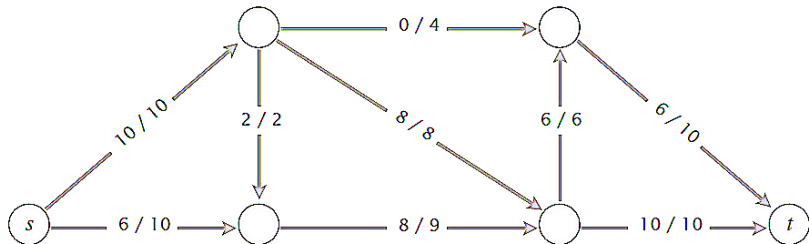
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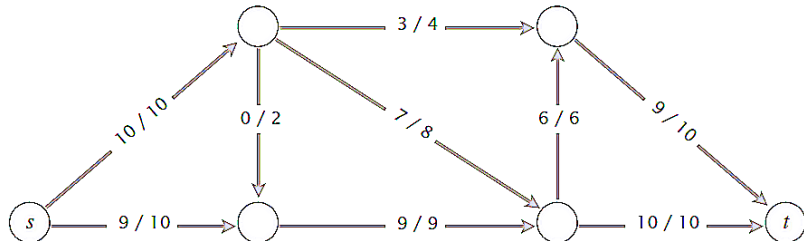
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Why the greedy algorithm fails

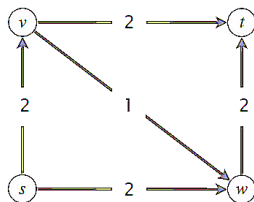
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Ex. Consider flow network G .

- The unique max flow has $f^*(v, w) = 0$.
- Greedy algorithm could choose $s \rightarrow v \rightarrow w \rightarrow t$ as first augmenting path.

flow network G



Why the greedy algorithm fails

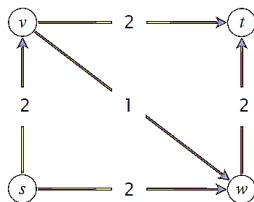
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Bottom line. Need some mechanism to **undo** a bad decision.

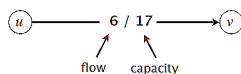
Original edge $e = (u, v) \in E$.

- Flow $f(e)$.
- Capacity $c(e)$

Reverse edge $e^{\text{reverse}} = (v, u)$

- Undo flow sent.

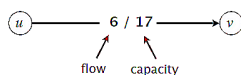
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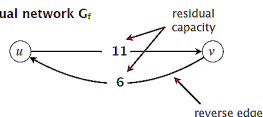
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Residual capacity

$$c_f(e) = \begin{cases} c(e) - f(e) & \text{if } e \in E \\ f(e) & \text{if } e^{\text{reverse}} \in E \end{cases}$$

residual network G_f



Residual network $G_f = (V, E_f, s, t, c_f)$

- $E_f = \{e : f(e) < c(e)\} \cup \{e^{\text{reverse}} : f(e) > 0\}$.
- Key property: f' is a flow in G_f iff $f + f'$ is a flow in G

Definition

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Definition

The **bottleneck capacity** of an augmenting path P is the minimum residual capacity of any edge in P .

Key Property. Let f be a flow and let P be an augmenting path in G_f . After calling $f' \leftarrow \text{Augment}(f, c, P)$, the resulting f' is a flow and $\text{val}(f') = \text{val}(f) + \text{bottleneck}(G_f, P)$.

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```
Augment(f,c,P)
```

```
   $\delta \leftarrow$  bottleneck capacity of augmenting path  $P$ ;
```

```
  for each edge  $e \in P$  do
```

```
    if  $(e \in E)$  then  $f(e) \leftarrow f(e) + \delta$ ;
```

```
    else
```

```
      |  $f(e^{\text{reverse}}) \leftarrow f(e^{\text{reverse}}) - \delta$ 
```

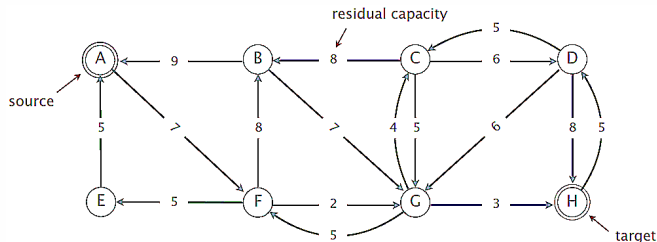
```
    end
```

```
  end
```

```
  Return  $f$ ;
```

Which is the augmenting path of highest bottleneck capacity?

1. $A \rightarrow F \rightarrow G \rightarrow H$
2. $A \rightarrow B \rightarrow C \rightarrow D \rightarrow H$
3. $A \rightarrow F \rightarrow B \rightarrow G \rightarrow H$
4. $A \rightarrow F \rightarrow B \rightarrow G \rightarrow C \rightarrow D \rightarrow H$



Ford–Fulkerson augmenting path algorithm.

- Start with $f(e) = 0$ for each edge $e \in E$.
- Find an $s \rightsquigarrow t$ path P in the residual network G_f .
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```
Ford–Fulkerson( $G$ )
```

```
  for each edge  $e \in E$  do
```

```
    |  $f(e) \leftarrow 0$ 
```

```
  end
```

```
   $G_f \leftarrow$  residual network of  $G$  with respect to flow  $f$ ;
```

```
  while there exists an  $s \rightsquigarrow t$  path  $P$  in  $G_f$  do
```

```
    |  $f \leftarrow \text{Augment}(f, c, P)$ ;
```

```
    |  $\text{Update}(G_f)$ ;
```

```
  end
```

```
  Return  $f$ ;
```

Max-Flow Min-Cut Theorem

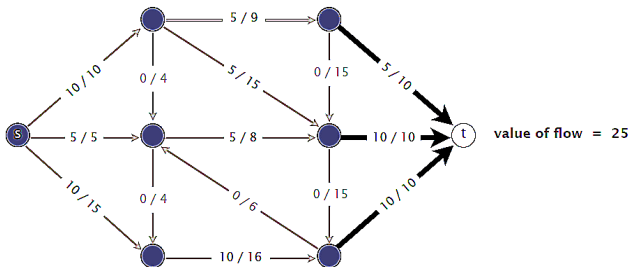
Relationship between flows and cuts

Lemma

Let f be any flow and let (A, B) be any cut. Then, the value of the flow f equals the net flow across the cut (A, B) .

$$\text{val}(f) = \sum_{\text{out of } A} f(e) - \sum_{\text{e in to } A} f(e)$$

net flow across cut = $5 + 10 + 10 = 25$



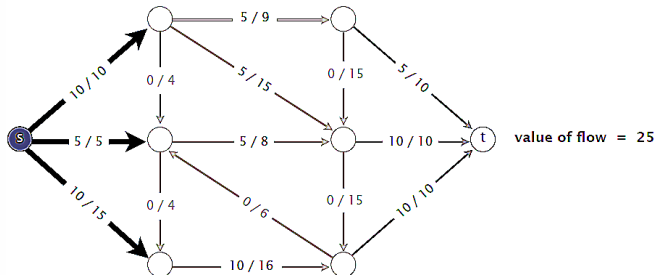
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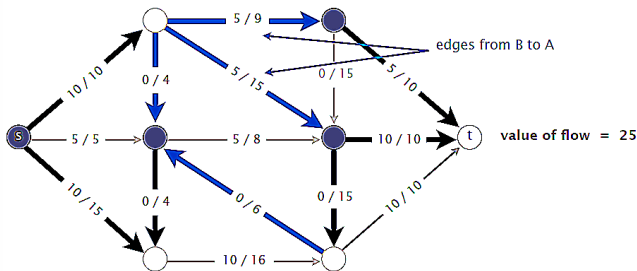
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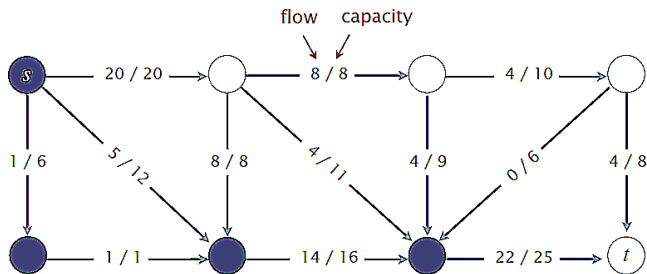
$$\text{val}(f) = \sum_{\text{out of } A} f(e) - \sum_{\text{e in to } A} f(e)$$

$$\text{net flow across cut} = (10 + 10 + 5 + 10 + 0 + 0) - (5 + 5 + 0 + 0) = 25$$



Which is the net flow across the given cut?

1. 11 ($20 + 25 - 8 - 11 - 9 - 6$)
2. 26 ($20 + 22 - 8 - 4 - 4$)
3. 42 ($20 + 22$)
4. 45 ($20 + 25$)



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Let f be any flow and let (A, B) be any cut. Then, the value of the flow f equals the net flow across the cut (A, B) .

$$\text{val}(f) = \sum_{\text{out of } A} f(e) - \sum_{\text{e in to } A} f(e)$$

Proof.

$$\begin{aligned} \text{val}(f) &= \sum_{\text{e out of } s} f(e) - \sum_{\text{e in to } s} f(e) \\ &= \sum_{v \in A} \left(\sum_{\text{e out of } v} f(e) - \sum_{\text{e in to } v} f(e) \right) \\ &= \sum_{\text{e out of } A} f(e) - \sum_{\text{e in to } A} f(e). \end{aligned}$$

Theorem

Weak Duality Let f be any flow and (A, B) be any cut. Then, $\text{val}(f) \leq \text{cap}(A, B)$.

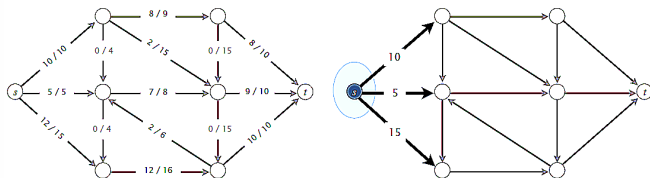
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Proof.

$$\begin{aligned}\text{val}(f) &= \sum_{e \text{ out of } A} f(e) - \sum_{e \text{ in to } A} f(e) \\ &\leq \sum_{e \text{ out of } A} f(e) \\ &\leq \sum_{e \text{ out of } A} c(e) \\ &= \text{cap}(A, B)\end{aligned}$$



Corollary

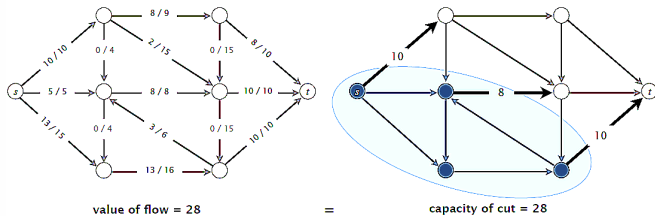
Let f be a flow and let (A, B) be any cut. If $\text{val}(f) = \text{cap}(A, B)$, then f is a max flow and (A, B) is a min cut.

Corollary

Let f be a flow and let (A, B) be any cut. If $\text{val}(f) = \text{cap}(A, B)$, then f is a max flow and (A, B) is a min cut.

Proof.

- For any flow f' : $\text{val}(f') \leq \text{cap}(A, B) = \text{val}(f)$.
- For any cut (A', B') : $\text{cap}(A', B') \geq \text{val}(f) = \text{cap}(A, B)$



Max-Flow Min-Cut Theorem

Value of a max flow = capacity of a min cut.

MAXIMAL FLOW THROUGH A NETWORK

L. R. FORD, JR. AND D. R. FULKERSON

Introduction. The problem discussed in this paper was formulated by T. Harris as follows:

"Consider a rail network connecting two cities by way of a number of intermediate cities, where each link of the network has a number assigned to it representing its capacity. Assuming a steady state condition, find a maximal flow from one given city to the other."

ON THE MAX FLOW MIN CUT THEOREM OF NETWORKS

G. B. Dantzig
D. R. Fulkerson

P-826

April 15, 1955

A Note on the Maximum Flow Through a Network*

P. ELIAS†, A. FEINSTEIN‡, AND C. E. SHANNON§

Summary—This note discusses the problem of maximizing the rate of flow from one terminal to another, through a network which consists of a number of branches, each of which has a limited capacity. The main result is a theorem: The maximum possible flow from left to right through a network is equal to the minimum value among all simple cut-sets. This theorem is applied to solve a more general problem, in which a number of input nodes and a number of output nodes are used.

from one terminal to the other in the original network passes through at least one branch in the cut-set. In the network above, some examples of cut-sets are (d, e, f) , and (b, c, e, g, h) , (d, g, h, i) . By a *simple cut-set* we will mean a cut-set such that if any branch is omitted it is no longer a cut-set. Thus (d, e, f) and (b, c, e, g, h) are simple cut-sets while (d, e, h, i) is not. When a simple cut set is

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- i. There exists a cut (A, B) such that $\text{cap}(A, B) = \text{val}(f)$.
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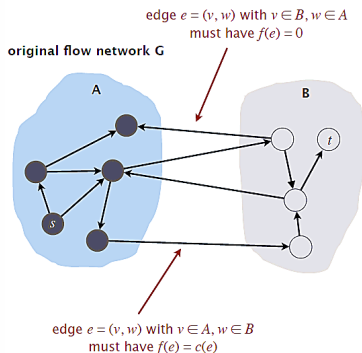
[ii \Rightarrow iii] We prove contrapositive: $\neg \text{iii} \Rightarrow \neg \text{ii}$.

- Suppose that there is an augmenting path with respect to f .
- Can improve flow f by sending flow along this path.
- Thus, f is not a max flow.

[iii \Rightarrow i]

- Let f be a flow with no augmenting paths.
- Let A be set of nodes reachable from s in residual network G_f .
- By definition of A : $s \in A$.
- By definition of flow f : $t \notin A$.

$$\begin{aligned}\text{val}(f) &= \sum_{e \text{ out of } A} f(e) - \sum_{e \text{ in to } A} f(e) \\ &= \sum_{e \text{ out of } A} c(e) - 0 \\ &= \text{cap}(A, B)\end{aligned}$$



Capacity-Scaling Algorithm

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Proof. Each augmentation increases the value of the flow by at least 1.

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The running time of Ford–Fulkerson is $O(mnC)$.

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Proof. Since Ford–Fulkerson terminates, theorem follows from integrality invariant.

Q. Is generic Ford–Fulkerson algorithm poly-time in input size?

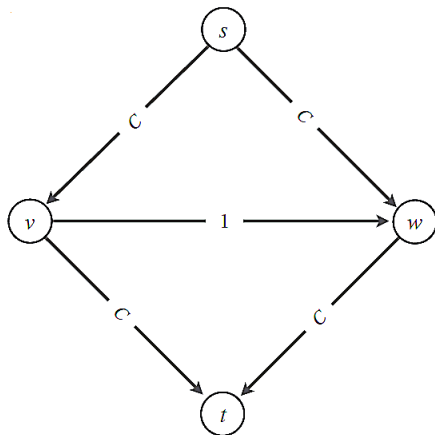
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The Ford–Fulkerson algorithm is guaranteed to terminate if the edge capacities are . . .

- A. Rational numbers.
- B. Real numbers.
- C. Both A and B.
- D. Neither A nor B.

Use care when selecting augmenting paths.

- Some choices lead to exponential algorithms.
- Clever choices lead to polynomial algorithms.

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Pathology. When edge capacities can be irrational, no guarantee that Ford–Fulkerson terminates (or converges to a maximum flow)!

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Pathology. When edge capacities can be irrational, no guarantee that Ford–Fulkerson terminates (or converges to a maximum flow)!

Goal. Choose augmenting paths so that:

- Can find augmenting paths efficiently.
- Few iterations.

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Choose augmenting paths with:

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- Fewest edges.

Theoretical Improvements in Algorithmic Efficiency for Network Flow Problems

JACK EDMONDS

University of Waterloo, Waterloo, Ontario, Canada

AND

RICHARD M. KARP

University of California, Berkeley, California

ABSTRACT. This paper presents new algorithms for the maximum flow problem, the Hitchcock transportation problem, and the general minimum-cost flow problem. Upper bounds on the numbers of steps in these algorithms are derived, and are shown to compare favorably with upper bounds on the numbers of steps required by earlier algorithms.

Edmonds-Karp 1972 (USA)

Dokl. Akad. Nauk SSSR
Tom 194 (1970), No. 4

Soviet Math. Dokl.
Vol. 11 (1970), No. 5

ALGORITHM FOR SOLUTION OF A PROBLEM OF MAXIMUM FLOW IN A NETWORK WITH POWER ESTIMATION

UDC 518.5

E. A. DINIC

Different variants of the formulation of the problem of maximal stationary flow in a network and its many applications are given in [1]. There also is given an algorithm solving the problem in the case where the initial data are integers (or, what is equivalent, commensurable). In the general case this algorithm requires preliminary rounding off of the initial data, i.e. only an approximate solution of the problem is possible. In this connection the rapidity of convergence of the algorithm is inversely proportional to the relative precision.

Dinitz 1970 (Soviet Union)

Overview. Choosing augmented paths with **large** bottleneck capacity.

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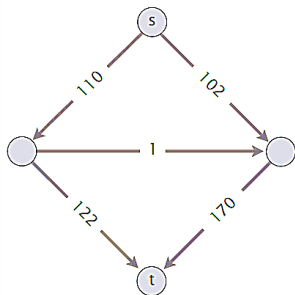
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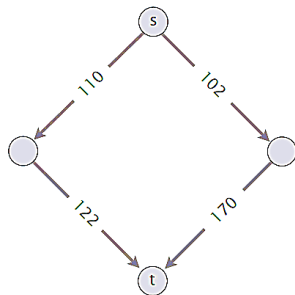
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- Maintain scaling parameter Δ .
- Let $G_f(\Delta)$ be the part of the residual network containing only those edges with capacity $\geq \Delta$.
- Any augmenting path in $G_f(\Delta)$ has bottleneck capacity $\geq \Delta$.



G_f



$G_f(\Delta), \Delta = 100$

Capacity-Scaling(G)

for each edge $e \in E$ do

$f(e) \leftarrow 0$

end

$\Delta \leftarrow$ largest power of 2 $\leq C$;

while $\Delta \geq 1$ do

$G_f(\Delta) \leftarrow \Delta$ -residual network of G with respect to flow f ;

 while there exists an $s \rightsquigarrow t$ path P in $G_f(\Delta)$ do

$f \leftarrow \text{Augment}(f, c, P)$;

$\text{Update}(G_\Delta(f))$;

 end

$\Delta = \Delta/2$;

end

Return f ;

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Proof. Same as for generic Ford–Fulkerson.

Theorem

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Proof.

- By integrality invariant, when $\Delta = 1 \Rightarrow G_f(\Delta) = G_f$
- Upon termination of $\Delta = 1$ phase, there are no augmenting paths.
- Result follows augmenting path theorem.

Lemma 1

There are $1 + \lfloor \log_2 C \rfloor$ scaling phases.

Lemma 2

There are $\leq 2m$ augmentations per scaling phase.

Lemma 3

Let f be the flow at the end of a Δ -scaling phase.

Then, the max-flow value $\leq \text{val}(f) + m\Delta$.

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The capacity-scaling algorithm takes $O(m^2 \log C)$ time.

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- Lemma 1 + Lemma 2 $\Rightarrow O(m \log C)$ augmentations.
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- Let f be the flow at the beginning of a Δ -scaling phase.
- Lemma 3 \Rightarrow max-flow value $\leq \text{val}(f) + m(2\Delta)$.
- Each augmentation in a Δ -phase increases $\text{val}(f)$ by at least Δ .

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- Choose A to be the set of nodes reachable from s in $G_f(\Delta)$.
- By definition of $A : s \in A$.
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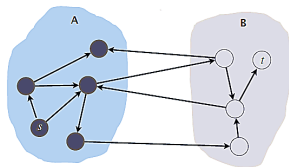
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$$\begin{aligned}\text{val}(f) &= \sum_{e \text{ out of } A} f(e) - \sum_{e \text{ in to } A} f(e) \\ &\geq \sum_{e \text{ out of } A} (c(e) - \Delta) - \sum_{e \text{ in to } A} \Delta \\ &\geq \sum_{e \text{ out of } A} c(e) - \sum_{e \text{ out of } A} \Delta - \sum_{e \text{ in to } A} \Delta \\ &\geq \text{cap}(A, B) - m\Delta\end{aligned}$$

original flow network



Shortest Augmenting Paths

Q. How to choose next augmenting path in Ford–Fulkerson?

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```
Shortest-Augmenting-Path( $G$ )
```

```
  for each edge  $e \in E$  do
```

```
     $f(e) \leftarrow 0$ 
```

```
  end
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```
   $G_f \leftarrow$  residual network of  $G$  with respect to flow  $f$ ;
```

```
  while there exists an  $s \rightsquigarrow t$  path in  $G_f$  do
```

```
     $P \leftarrow \text{BFS}((G_f));$ 
```

```
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```
     $\text{Update}(G_f);$ 
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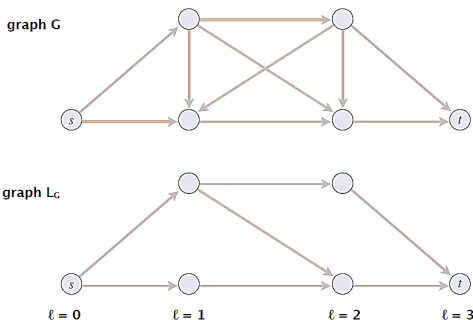
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- $O(m)$ time to find a shortest augmenting path via BFS.
- There are $\leq mn$ augmentations
 - at most m augmenting paths of length $k \leftarrow \text{Lemma 1} + \text{Lemma 2}$
 - at most $n - 1$ different lengths

Definition

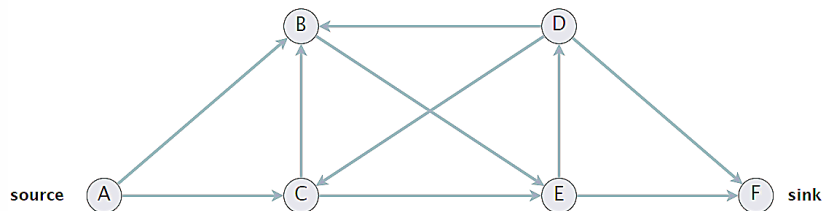
Given a **digraph** $G = (V, E)$ with source s , its **level graph** is defined by:

- $\ell(v)$ = number of edges in shortest $s \rightsquigarrow v$ path.
- $L_G = (V, E_G)$ is the subgraph of G that contains only those edges $(v, w) \in E$ with $\ell(w) = \ell(v) + 1$.



Which edges are in the level graph of the following digraph?

- A. $D \rightarrow F$
- B. $E \rightarrow F$
- C. Both A and B.
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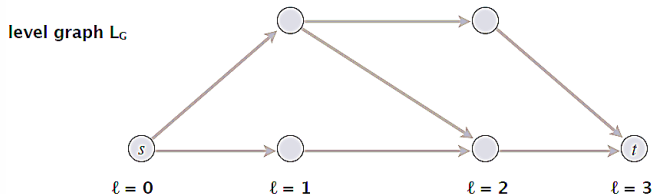


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Key property. P is a shortest $s \rightsquigarrow v$ path in G iff P is an $s \rightsquigarrow v$ path in L_G .



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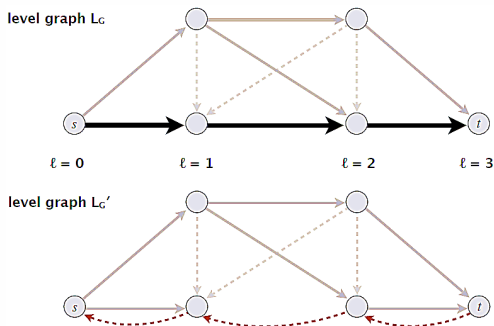
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Proof.

- Let f and f' be flow before and after a shortest-path augmentation.
- Let L_G and $L_{G'}$ be level graphs of G_f and $G_{f'}$.
- Only back edges added to $G_{f'}$
(any $s \rightsquigarrow t$ path that uses a back edge is longer than previous length)



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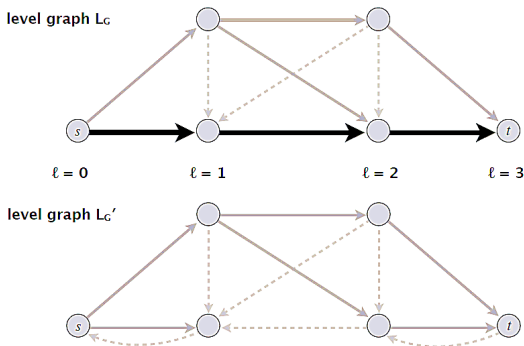
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Proof.

- At least one (bottleneck) edge is deleted from L_G per augmentation.
- No new edge added to L_G until shortest path length strictly increases.



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The shortest-augmenting-path algorithm takes $O(m^2n)$ time.

Shortest augmenting path: improving the running time

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- Dynamic trees $\Rightarrow O(mn \log n)$ [Sleator–Tarjan 1983]

A Data Structure for Dynamic Trees

DANIEL D. SLEATOR AND ROBERT ENDRE TARJAN

Bell Laboratories, Murray Hill, New Jersey 07974

Received May 8, 1982; revised October 18, 1982

A data structure is proposed to maintain a collection of vertex-disjoint trees under a sequence of two kinds of operations: a *link* operation that combines two trees into one by adding an edge, and a *cut* operation that divides one tree into two by deleting an edge. Each operation requires $O(\log n)$ time. Using this data structure, new fast algorithms are obtained for the following problems:

- (1) Computing nearest common ancestors.
- (2) Solving various network flow problems including finding maximum flows, blocking flows, and acyclic flows.
- (3) Computing certain kinds of constrained minimum spanning trees.
- (4) Implementing the network simplex algorithm for minimum-cost flows.

The most significant application is (2); an $O(mn \log n)$ -time algorithm is obtained to find a maximum flow in a network of n vertices and m edges, beating by a factor of $\log n$ the fastest algorithm previously known for sparse graphs.

Dinitz' Algorithm

Two types of augmentations.

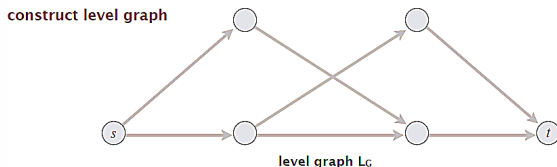
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Phase of normal augmentations.

- Construct level graph L_G .
- Start at s , advance along an edge in L_G until reach t or get stuck.
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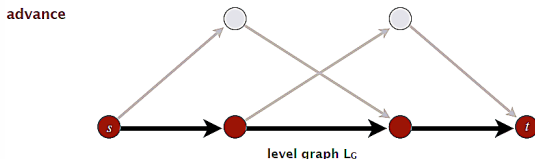


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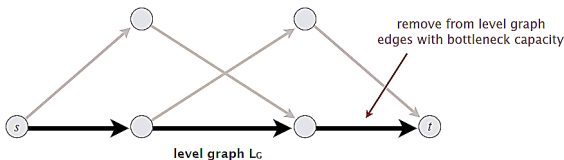
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augment

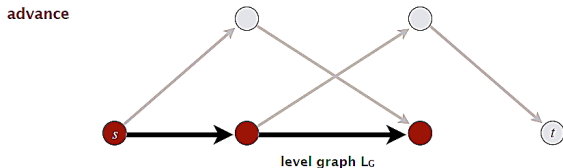


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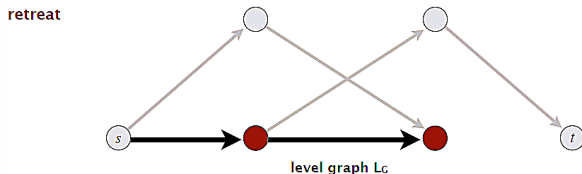


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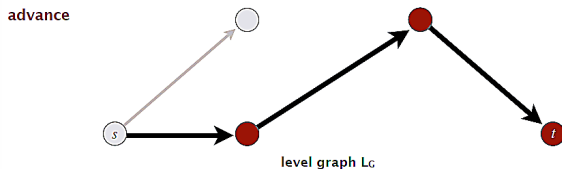


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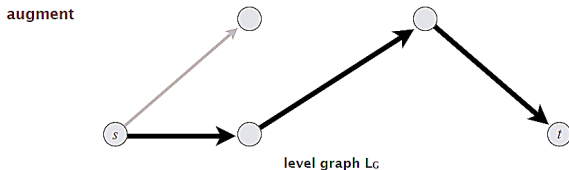


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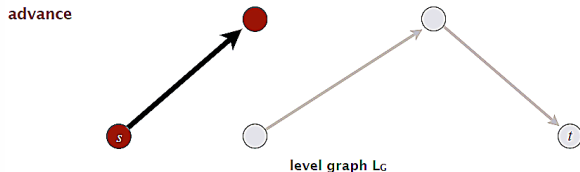


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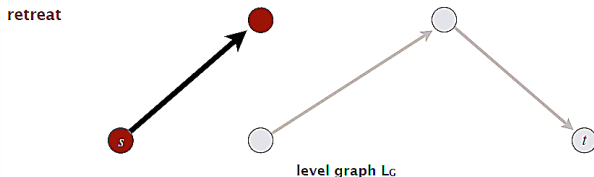


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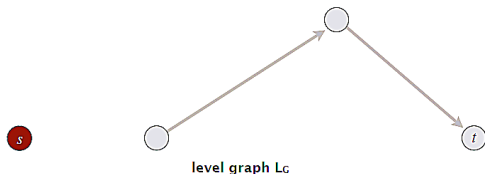
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retreat



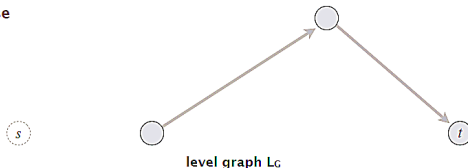
Two types of augmentations.

- **Normal**: length of shortest path does not change.
- **Special**: length of shortest path strictly increases.

Phase of normal augmentations.

- Construct level graph L_G .
- Start at s , advance along an edge in L_G until reach t or get stuck.
- If reach t , augment flow; update L_G ; and restart from s .
- If get stuck, delete node from L_G and retreat to previous node.

end of phase



Dinitz' algorithm (as refined by Even and Itai)

Initialize(G, f)

$L_G \leftarrow$ level-graph of G_f

$P \leftarrow \emptyset$

goto Advance(s);

Retreat(v)

if $v = s$ then Stop;

else

 Delete v from L_G ;
 Remove last edge (u, v)
 from P ;

end

goto Advance(u);

Advance(v)

if $v = t$ then

 Augment(P);
 Remove saturated edges
 from L_G ;
 $P \leftarrow \emptyset$;
 goto Advance(s);

end

if there exists edge $(v, w) \in L_G$

then

 Add edge (v, w) to P ;
 goto Advance(w);

end

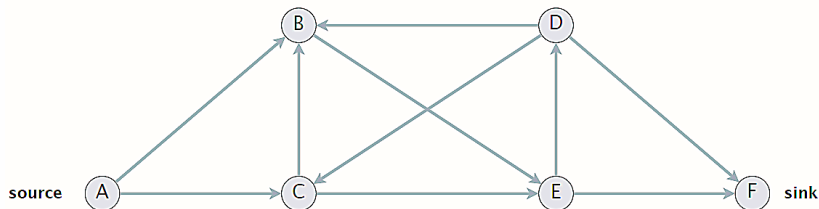
else

 goto Retreat(v);

end

How to compute the level graph L_G efficiently?

1. Depth-first search.
2. Breadth-first search.
3. Both A and B.
4. Neither A nor B.



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- At most n retreats per phase. $\leftarrow O(m + n)$ per phase
(because a retreat deletes one node from L_G)
- At most mn advances per phase. $\leftarrow O(mn)$ per phase
(because at most n advances before retreat or augmentation)

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Dinitz' algorithm runs in $O(mn^2)$ time.

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- By Lemma, $O(mn)$ time per phase.
- At most $n - 1$ phases (as in shortest-augmenting-path analysis).

Augmenting-path algorithms: summary

year	method	# augmentations	running time
1955	augmenting path	nC	$O(mnC)$
1972	fattest path	$m \log(mC)$	$O(m^2 \log n \log(mC))$
1972	capacity scaling	$m \log C$	$O(m^2 \log C)$
1985	improved capacity scaling	$m \log C$	$O(mn \log C)$
1970	shortest augmenting path	mn	$O(m^2 n)$
1970	level graph	mn	$O(mn^2)$
1983	dynamic trees	mn	$O(mn \log n)$

augmenting-path algorithms with m edges, n nodes, and integer capacities between 1 and C

Maximum-flow algorithms: theory highlights

year	method	worst case	discovered by
1951	simplex	$O(mn^2C)$	Dantzig
1955	augmenting paths	$O(mnC)$	Ford–Fulkerson
1970	shortest augmenting paths	$O(mn^2)$	Edmonds–Karp, Dinitz
1974	blocking flows	$O(n^3)$	Karzanov
1983	dynamic trees	$O(mn \log n)$	Sleator–Tarjan
1985	improved capacity scaling	$O(mn \log C)$	Gabow
1988	push–relabel	$O(mn \log(n^2/m))$	Goldberg–Tarjan
1998	binary blocking flows	$O(m^{3/2} \log(n^2/m) \log C)$	Goldberg–Rao
2013	compact networks	$O(mn)$	Orlin
2014	interior-point methods	$\tilde{O}(mn^{1/2} \log C)$	Lee–Sidford
2016	electrical flows	$\tilde{O}(m^{10/7} C^{1/7})$	Madry
20xx		???	

augmenting-path algorithms with m edges, n nodes, and integer capacities between 1 and C