## **Clustering**

K-means

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Introduction to clustering

## 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

#### K-means

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

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

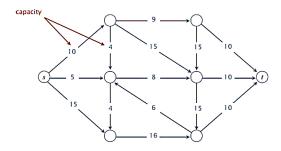
- Diagraph (V, E) with source  $s \in V$  and sink  $t \in V$ .
- Capacity c(e) > 0 for each  $e \in E$ .

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



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

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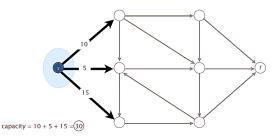
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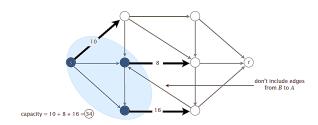
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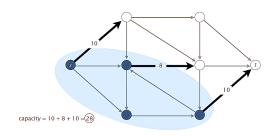
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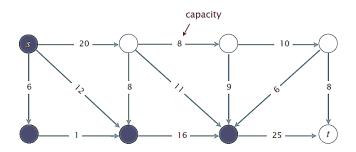
Min-cut problem. Find a cut of minimum capacity.



## Quiz 1

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)

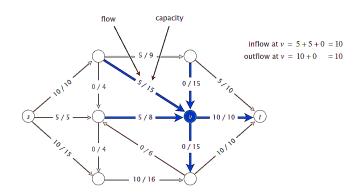


## Maximum-flow problem

## Definition

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

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



## Maximum-flow problem

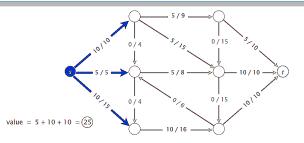
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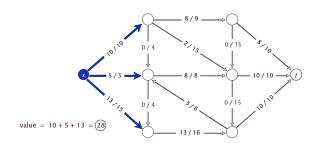
#### **Definition**

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



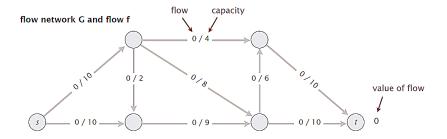
## Maximum-flow problem

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



# Ford-Fulkerson Algorithm

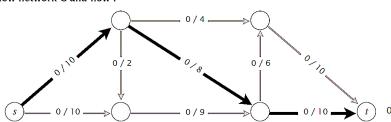
- Start with f(e) = 0 for each edge  $e \in E$ .
- Find an  $s \rightsquigarrow t$  path P where each edge has f(e) < c(e).
- Augment flow along path P.
- Repeat until you get stuck.



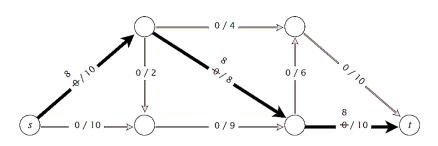
#### Greedy algorithm.

- 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).
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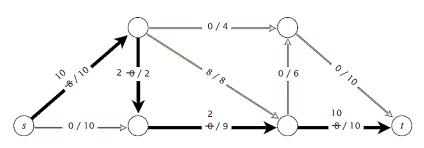
#### flow network G and flow f



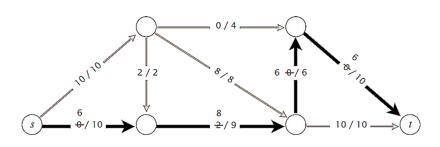
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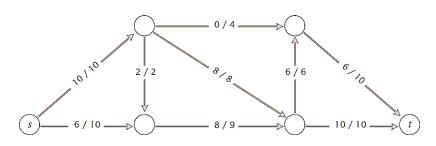
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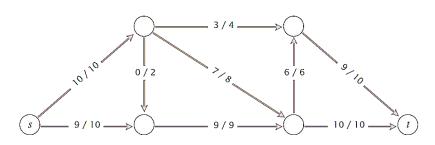
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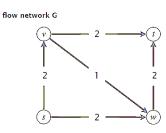
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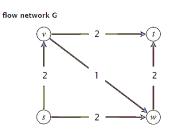
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  - Greedy algorithm could choose  $s \to v \to w \to t$  as first augmenting path.



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

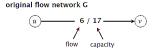
#### Residual network

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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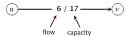
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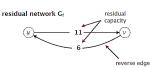
Undo flow sent.

#### Residual capacity

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

#### original flow network G





## 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  $f' \leftarrow \operatorname{Augment}(f, c, P)$ , the resulting f' is a flow and  $\operatorname{val}(f') = \operatorname{val}(f) + \operatorname{bottleneck}(G_f, P)$ .

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```
Augment(f,c,P)
\delta \leftarrow \text{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

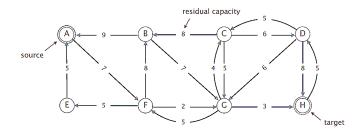
end

Return f;
```

### Network flow: quiz 2

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 algorithm

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- Start with f(e) = 0 for each edge  $e \in E$ .
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```
Ford-Fulkerson(G)
for each edge e \in E do
    f(e) \leftarrow 0
end
G_f \leftarrow \text{residual network of } G \text{ with respect to flow } f;
while there exists an s \rightsquigarrow t path P in G_f do
    f \leftarrow Augment(f,c,P);
    Update(G_f);
end
Return f:
```

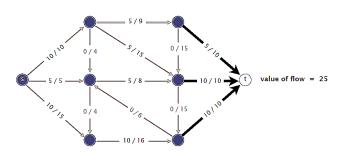
# **Max-Flow Min-Cut Theorem**

### 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).

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

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

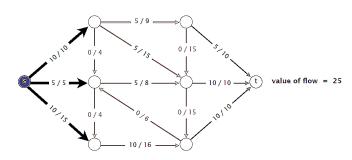


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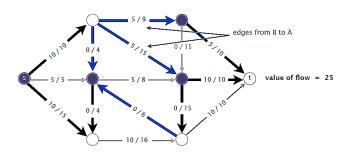


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net flow across cut = (10 + 10 + 5 + 10 + 0 + 0) - (5 + 5 + 0 + 0) = 25



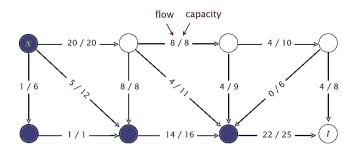
### Network flow: quiz 3

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

Proof

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

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

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

### Theorem

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

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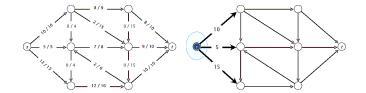
#### Proof.

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

$$\leq \sum_{e \text{ out of } A} f(e)$$

$$\leq \sum_{e \text{ out of } A} c(e)$$

$$= cap(A, B)$$



### **Certificate of optimality**

# Corollary

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

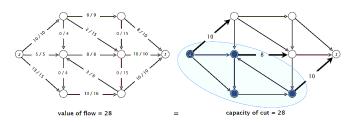
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#### Proof.

- For any flow f':  $val(f') \le cap(A, B) = val(f)$ .
- For any cut (A', B'): cap  $(A', B') \ge val(f) = cap(A, B)$



#### Max-Flow Min-Cut Theorem

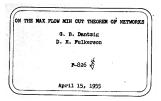
Value of a max flow = capacity of a min cut.

#### 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."



#### 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 treminal in another, through a network which constituted in summer of branches, each of which has a limited capacity. The main result is a theorem: The maximum positie flow from left to right through a notwork is equal to the minimum value samon all single 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 out-set. In the network above, some examples of cut-sets are (d, e, f), and (b, c, e, g, h),  $(d, g, h, \psi)$ . 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-set while (d, e, h, f) is now (Whose a simple cut-set isindependent of the cut-set is not considerable.

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- [i⇒ ii] This is the weak duality corollary.

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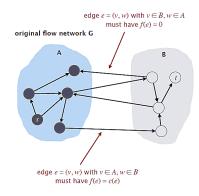
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- Suppose that there is an augmenting path with respect to f.
- Can improve flow *f* by sending flow along this path.
- Thus, f is not a max flow.

 $[iii \Rightarrow i]$ 

- 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  $f: t \notin A$ .

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



# Capacity-Scaling Algorithm

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Ford–Fulkerson terminates after at most val  $(f^*) \le nC$  augmenting paths, where  $f^*$  is a max flow.

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

# Corollary

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

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There exists an integral max flow  $f^*$ 

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

*Proof.* Can use either BFS or DFS to find an augmenting path in O(m) time.

#### **Integrality Theorem**

There exists an integral max flow  $f^*$ 

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

# Ford-Fulkerson: exponential example

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

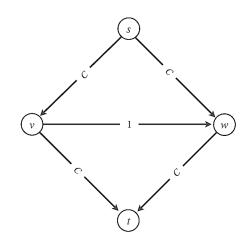
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- $s \rightarrow v \rightarrow w \rightarrow t$
- $s \rightarrow w \rightarrow v \rightarrow t$
- $s \rightarrow v \rightarrow w \rightarrow t$
- $s \rightarrow w \rightarrow v \rightarrow t$
- . . .
- $s \rightarrow v \rightarrow w \rightarrow t$
- $s \rightarrow w \rightarrow v \rightarrow t$



### Network flow: quiz 4

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.

Choose augmenting paths with:

# Choose augmenting paths with:

• Max bottleneck capacity("fattest").

## Choose augmenting paths with:

- Max bottleneck capacity ("fattest").
- Sufficiently large bottleneck capacity.

### Choose augmenting paths with:

- Max bottleneck capacity ("fattest").
- Sufficiently large bottleneck capacity.
- · 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 Colifornia, Berkeley, California

ABSTACE. This paper persents new algorithms for the maximum flow problem, the Hitcheok transportation problem, and the general minimum-next 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 stems required by earlier algorithms.

Edmonds-Karp 1972 (USA)

Dokl. Akad. Nauk SSSR Ton 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 foundation of the problem of naximal stationary flow in a network and its many applications are given in [1]. There also is given an algorithm solving the problem in the cases where the initial data are integers for what is equivalen, connecessable). In the general case this algorithm requires preliminary rounding off of the initial data, i.e. only an approximate solving of the problem is possible. In this connection the rapidity of convergence of the algorithm is inversely proportional to the shaties reserving.

Dinitz 1970 (Soviet Union)

Overview. Choosing augmented paths with large bottleneck capacity.

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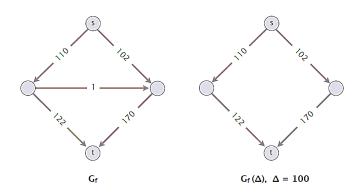
• Maintain scaling parameter  $\Delta$ .

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- Maintain scaling parameter △.
- 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  $\geq \Delta$ .



```
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 \ge 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 Augment(f, c, P);
        Update(G_{\Delta}(f));
    end
    \Delta = \Delta/2;
end
Return f:
```

Assumption. All edge capacities are integers between 1 and  ${\it C}$ .

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Invariant. The scaling parameter  $\Delta$  is a power of 2.

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Integrality invariant. Throughout the algorithm, every edge flow f(e) and residual capacity  $c_f(e)$  is an integer.

*Proof.* Same as for generic Ford–Fulkerson.

### Theorem

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If capacity-scaling algorithm terminates, then f is a max flow.

- 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  $\Delta$ -scaling phase.

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

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- Lemma 1+ Lemma 2  $\Rightarrow O(m \log C)$  augmentations.
- Finding an augmenting path takes O(m) time.

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- Let f be the flow at the beginning of a  $\Delta$ -scaling phase.
- Lemma 3  $\Rightarrow$  max-flow value  $\leq val(f) + m(2\Delta)$ .
- Each augmentation in a  $\Delta$ -phase increases val(f) by at least  $\Delta$ .

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- We show there exists a cut (A, B) such that  $cap(A, B) \leq val(f) + m\Delta$ .
- Choose A to be the set of nodes reachable from s in  $G_f(\Delta)$ .
- By definition of  $A : s \in A$ .
- By definition of flow  $f: t \notin A$ .

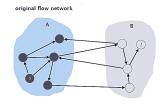
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$$\begin{aligned} val(f) &= \sum_{e \text{ out of } A} f(e) - \sum_{e \text{ in to } A} f(e) \\ &\geq \sum_{e \text{ out of } A} (c(e) - \Delta) - \sum_{e \text{ in to } A} \Delta \\ &\geq \sum_{e \text{ out of } A} c(e) - \sum_{e \text{ out of } A}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



# Shortest Augmenting Paths

# **Shortest augmenting path**

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
G_f \leftarrow \text{residual network of } G \text{ with respect to flow } f;
while there exists an s \rightsquigarrow t path in G_f do
    P \leftarrow \mathsf{BFS}((G_f));
    f \leftarrow Augment(f, c, P):
    Update(G_f);
end
Return f:
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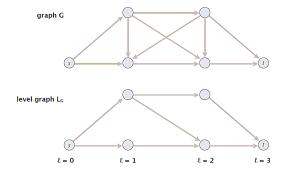
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- O(m) time to find a shortest augmenting path via BFS.
- There are  $\leq mn$  augmentations
  - at most *m* augmenting paths of length  $k \leftarrow$  Lemma 1 + Lemma 2
  - at most n-1 different lengths

### **Definition**

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

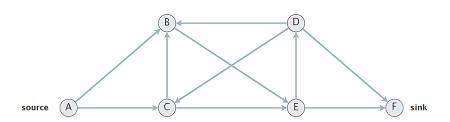
- $\ell(v)$  = number of edges in shortest  $s \rightsquigarrow v$  path.
- $L_G = (V, E_G)$  is the subgraph of G that contains only those edges  $(v, w) \in E$  with  $\ell(w) = \ell(v) + 1$ .



# Network flow: quiz 5

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

- A.  $D \rightarrow F$
- B.  $E \rightarrow F$
- C. Both A and B.
- D. Neither A nor B.

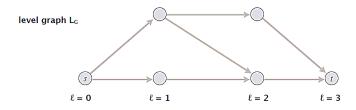


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Key property. P is a shortest  $s \rightsquigarrow v$  path in G iff P is an  $s \rightsquigarrow v$  path in  $L_G$ .



# Lemma 1

The length of a shortest augmenting path never decreases.

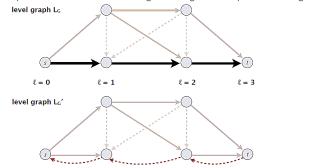
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- Let f and f' be flow before and after a shortest-path augmentation.
- Let  $L_G$  and  $L_{G'}$  be level graphs of  $G_f$  and  $G_{f'}$ .
- Only back edges added to G<sub>f'</sub>
   (any s → t path that uses a back edge is longer than previous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



# Lemma 2

After at most m shortest-path augmentations, the length of a shortest augmenting path strictly increases.

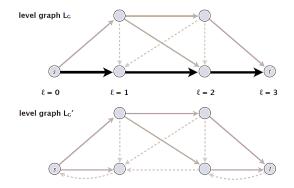
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- At least one (bottleneck) edge is deleted from  $L_G$  per augmentation.
- ullet No new edge added to  $L_G$  until shortest path length strictly increases.



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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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• Simple idea \Rightarrow O(mn^2) [Dinitz 1970]
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### Shortest augmenting path: improving the running time

Note.  $\Theta(mn)$  augmentations necessary for some flow networks.

- Try to decrease time per augmentation instead.
- Simple idea  $\Rightarrow O(mn^2)$  [Dinitz 1970]
- 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 croblems:

- (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.

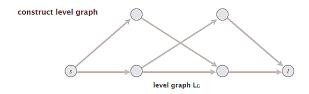
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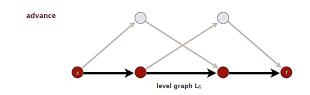
- Construct level graph  $L_G$ .
- Start at s, advance along an edge in  $L_G$  until reach t or get stuck.
- If reach t, augment flow; update  $L_G$ ; and restart from s.
- If get stuck, delete node from  $L_G$  and retreat to previous node.



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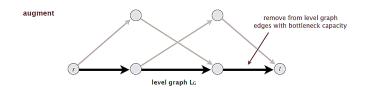
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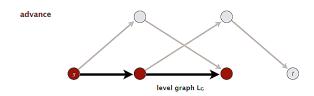
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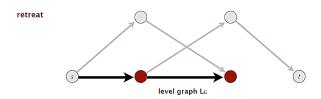
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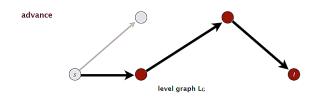
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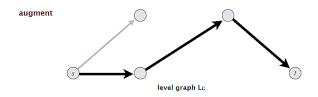
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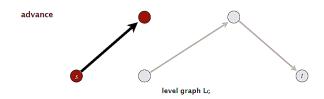
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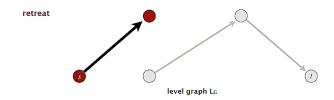
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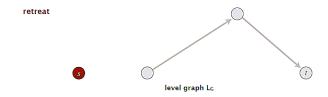
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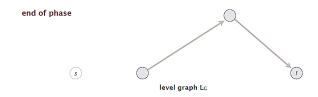
## Dinitz' algorithm

### Two types of augmentations.

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### Phase of normal augmentations.

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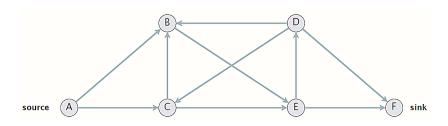
## Dinitz' algorithm (as refined by Even and Itai)

```
Initialize (G, f)
                                            Advance(v)
L_G \leftarrow level-graph of G_f
                                            if v = t then
P \leftarrow \emptyset
                                                Augment(P);
goto Advance(s);
                                                Remove saturated edges
                                                from L_G;
                                                P \leftarrow \varnothing:
                                                goto Advance(s);
Retreat(v)
                                            end
if v = s then Stop:
                                            if there exists edge (v, w) \in L_G
else
                                             then
   Delete v from L_G:
                                                Add edge (v, w) to P;
    Remove last edge (u, v)
                                                goto Advance(w);
     from P:
                                            end
end
                                            else
goto Advance(u);
                                                goto Retreat(v);
                                            end
```

## Network flow: quiz 6

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 mn advances per phase. ← O(mn) per phase (because at most n advances before retreat or augmentation)

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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	$m\log(mC)$	$O\left(m^2\log n\log(mC)\right)$
1972	capacity scaling	m log C	$O\left(m^2\log C\right)$
1985	improved capacity scaling	m log C	O(mn log C)
1970	shortest augmenting path	mn	$O\left(m^2n\right)$
1970	level graph	mn	O (mn²)
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	$O\left(mn^2C\right)$	Dantzig
1955	augmenting paths	O(mnC)	Ford-Fulkerson
1970	shortest augmenting paths	$O\left(mn^2\right)$	Edmonds–Karp, Dinitz
1974	blocking flows	$O\left(n^3\right)$	Karzanov
1983	dynamic trees	O(mn log n)	Sleator–Tarjan
1985	improved capacity scaling	O(mn log C)	Gabow
1988	push–relabel	$O\left(mn\log\left(n^2/m\right)\right)$	Goldberg-Tarjan
1998	binary blocking flows	$O\left(m^{3/2}\log\left(n^2/m\right)\log C\right)$	Goldberg-Rao
2013	compact networks	O(mn)	Orlin
2014	interior-point methods	$\tilde{O}\left(mm^{1/2}\log C\right)$	Lee-Sidford
2016	electrical flows	$\tilde{O}\left(m^{10/7}C^{1/7}\right)$	Madry
20xx		???	