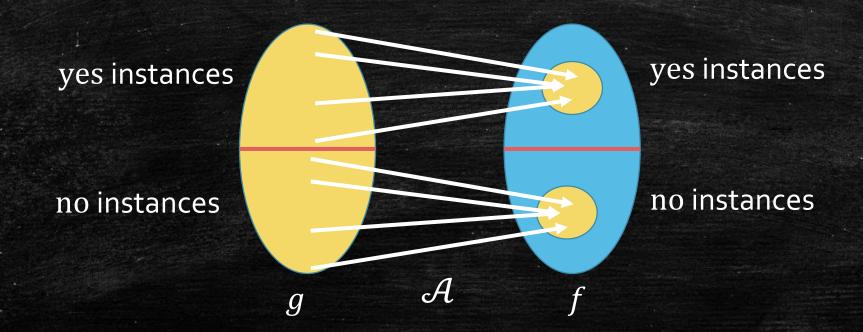
Approximation Algorithms

- 1. One more example of reduction: k-means 2. approximation algorithms

Proving f is NP-complete

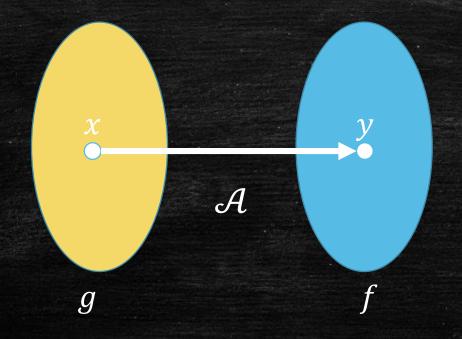
- Prove $f \in \mathbf{NP}$.
- Find an NP-complete problem g and prove $g \leq_k f$.

- $x \mapsto y$ under poly-time TM \mathcal{A}
- x is yes $\Rightarrow y$ is yes
- x is no $\Rightarrow y$ is no



- $x \mapsto y$ under poly-time TM \mathcal{A}
- x is yes $\Rightarrow y$ is yes
- x is no $\Rightarrow y$ is no

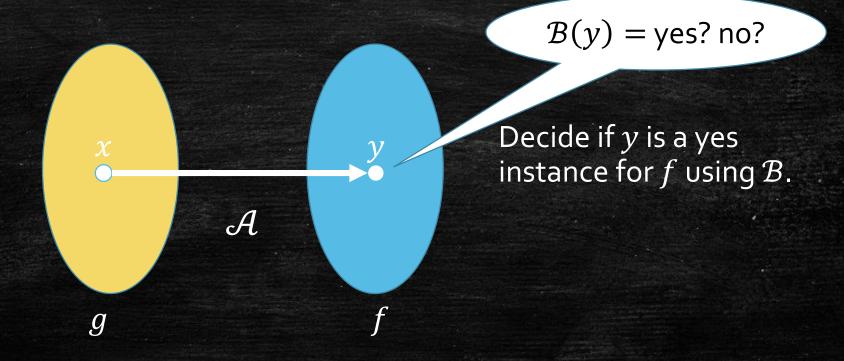
- A poly-time TM \mathcal{B} solving f
- \Rightarrow The TM $\mathcal{B} \circ \mathcal{A}$ solves g



Given any g instance x, Compute the f instance $y = \mathcal{A}(x)$.

- $x \mapsto y$ under poly-time TM \mathcal{A}
- x is yes $\Rightarrow y$ is yes
- x is no $\Rightarrow y$ is no

- A poly-time TM \mathcal{B} solving f
- \Rightarrow The TM $\mathcal{B} \circ \mathcal{A}$ solves g



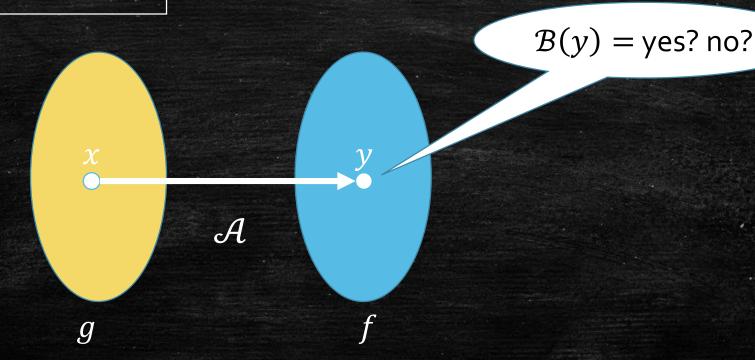
- $x \mapsto y$ under poly-time TM \mathcal{A}
- x is yes $\Rightarrow y$ is yes
- x is no $\Rightarrow y$ is no

- A poly-time TM B solving f
- \Rightarrow The TM $\mathcal{B} \circ \mathcal{A}$ solves g

This is crucial for a reduction to work!

$$y ext{ is yes} \Rightarrow x ext{ is yes}$$

 $y ext{ is no} \Rightarrow x ext{ is no}$



Four Steps for a NP-completeness Proof

- 1. Prove $f \in \mathbf{NP}$.
- 2. Construct the reduction $g \leq_k f$.
 - Fix an instance x of g. Describe the corresponding f instance y.
- 3. [Completeness] x is yes $\Rightarrow y$ is yes
- 4. [Soundness] x is no $\Rightarrow y$ is no
 - Proving the contrapositive "y is yes $\Rightarrow x$ is yes" is often easier.

NP-hardness for Optimization Problems

Optimization to Decision:

- Maximization \rightarrow decide whether OPT $\geq k$
- Minimization \rightarrow decide whether OPT $\leq k$

- A maximization problem is NP-hard if there exists $k \in \mathbb{R}$ such that deciding whether OPT $\geq k$ is NP-hard.
- A minimization problem is NP-hard if there exists $k \in \mathbb{R}$ such that deciding whether OPT $\leq k$ is NP-hard.

k-Means

- Input: $S = \{\mathbf{x} : \mathbf{x} \in \mathbb{R}^d\}$ and $k \in \mathbb{Z}^+$
- Output:
 - 1. Partition of $S = C_1 \cup C_2 \cup \cdots \cup C_k$
 - 2. A "center" $\mathbf{c}_i \in \mathbb{R}^d$ for each cluster C_i

that minimizes $\sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} ||\mathbf{x} - \mathbf{c}_i||^2$

- Only need to specify either output
 1 or output 2:
 - Given clusters, optimal centers are easy to compute...
 - Same holds for giving centers.

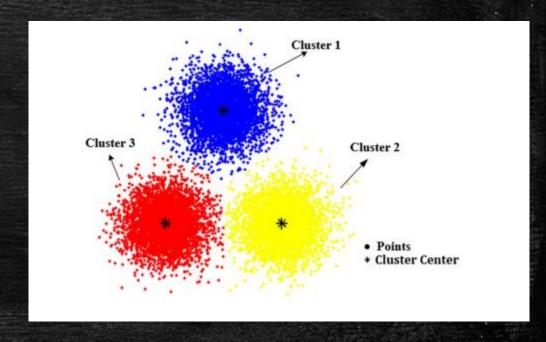


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Proving k-Means Is NP-Hard

Decision version:

• Decide if there exist
$$C_1, ..., C_k$$
 and $\mathbf{c}_1, ..., \mathbf{c}_k$ s.t.
$$\sum_{i=1}^k \sum_{\mathbf{x} \in C_i} \|\mathbf{x} - \mathbf{c}_i\|^2 \le \boldsymbol{\theta}.$$

- We will show the decision problem is NP-complete.
 - NP-hardness would be suffice, but it is NP-complete anyway...
- We will define the threshold θ later.

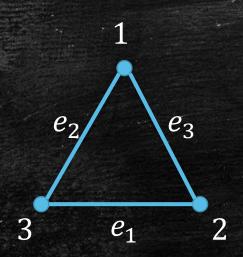
Step 1: k-Means \in **NP**

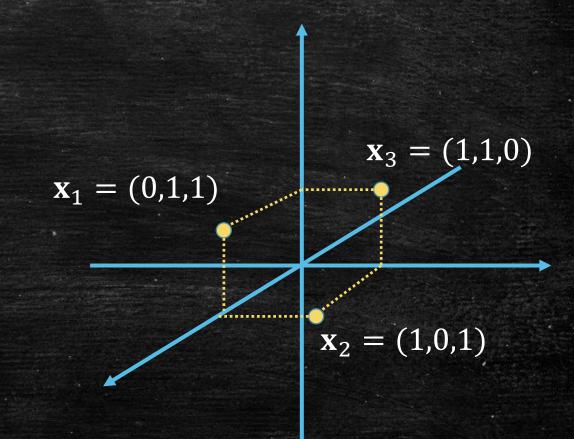
- This is obvious...
- Certificate can be
 - C_1, \ldots, C_k , or
 - $\mathbf{c}_1, \dots, \mathbf{c}_k$, or
 - both

Step 2: Define Construction

- Reduce from VertexCover
- Given any VertexCover instance (G = (V, E), k),
- construct the k-means instance $(S = \{x : x \in \mathbb{R}^d\}, k, \theta)$ as follows:
- Same parameter k in the two instances
- Threshold: $\theta = |E| k$ (you will see the reason later...)
- Dimension d = |V|
- For each $e = (i, j) \in E$, construct a data point $\mathbf{x}_e = (0, ..., 0, 1, 0, ..., 0, 1, 0, ..., 0)$ $i\text{-th} \qquad j\text{-th}$

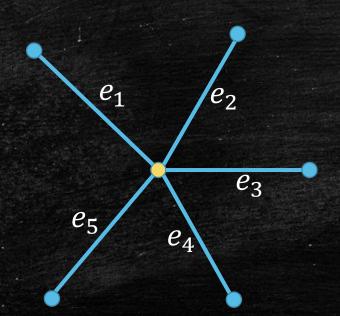
An Example





Intuition for Step 3 & 4

- edges covered by a vertex form a star
- ← corresponding data points only differ by one entry, they are "very close"



$$\mathbf{x}_1 = (1, 1, 0, 0, 0, 0)$$
 $\mathbf{x}_2 = (1, 0, 1, 0, 0, 0)$
 $\mathbf{x}_3 = (1, 0, 0, 1, 0, 0)$
 $\mathbf{x}_4 = (1, 0, 0, 0, 1, 0)$
 $\mathbf{x}_5 = (1, 0, 0, 0, 0, 1)$

Compute the Cost of a Cluster

- For Cluster C, let $G_C = (V, E_C)$ be the subgraph where E_C are the edges whose corresponding data points are in C.
- Let $d_C(i)$ be the degree of i in C.
- Lemma. The cost of a cluster C is

$$2|C| - \frac{1}{|C|} \sum_{i=1}^{|V|} (d_C(i))^2$$
.

Proving
$$cost(C) = 2|C| - \frac{1}{|C|} \sum_{i=1}^{|V|} (d_C(i))^2$$

- Let $\mu = \frac{1}{|C|} \sum_{\mathbf{x} \in C} \mathbf{x}$ be the center of C.
- By thinking about G_C , we have $\mu[i] = \frac{1}{|C|} d_C(i)$.
- $\operatorname{cost}(C) = \sum_{e \in E_C} ||\mathbf{x}_e \mu||^2 = \sum_{e \in E_C} \sum_{i=1}^{|V|} \left(\mathbf{x}_e[i] \frac{1}{|C|} d_C(i) \right)^2$

$$= \sum_{e \in E_C} \sum_{i=1}^{|V|} \left((\mathbf{x}_e[i])^2 - 2\mathbf{x}_e[i] \frac{1}{|C|} d_C(i) + \left(\frac{1}{|C|} d_C(i) \right)^2 \right)$$

$$= \sum_{e \in E_C} \sum_{i=1}^{|V|} (\mathbf{x}_e[i])^2 - \sum_{e \in E_C} \sum_{i=1}^{|V|} 2\mathbf{x}_e[i] \frac{1}{|C|} d_C(i) + \sum_{e \in E_C} \sum_{i=1}^{|V|} \left(\frac{1}{|C|} d_C(i)\right)^2$$

Proving
$$cost(C) = 2|C| - \frac{1}{|C|} \sum_{i=1}^{|V|} (d_C(i))^2$$

$$- \cot(C) = \sum_{e \in E_C} \sum_{i=1}^{|V|} (\mathbf{x}_e[i])^2 - \sum_{e \in E_C} \sum_{i=1}^{|V|} 2\mathbf{x}_e[i] \frac{1}{|C|} d_C(i) + \sum_{e \in E_C} \sum_{i=1}^{|V|} \left(\frac{1}{|C|} d_C(i)\right)^2$$

- red = $\sum_{e \in E_C} 2 = 2|C|$
- blue = $\sum_{i=1}^{|V|} \sum_{e \in E_C} 2\mathbf{x}_e[i] \frac{1}{|C|} d_C(i) = \frac{2}{|C|} \cdot \sum_{i=1}^{|V|} (d_C(i))^2$
- purple = $|C| \cdot \frac{1}{|C|^2} \cdot \sum_{i=1}^{|V|} (d_C(i))^2 = \frac{1}{|C|} \cdot \sum_{i=1}^{|V|} (d_C(i))^2$
- Putting together:

$$cost(C) = 2|C| - \frac{1}{|C|} \sum_{i=1}^{|V|} (d_C(i))^2$$

Part 3: yes to yes

- Suppose (G = (V, E), k) is a yes instance and S is a vertex cover.
- Let $S = \{1, 2, ..., k\}$ WLOG.
- Let C_i be those \mathbf{x}_e where e is covered by vertex i
 - If $i, j \in S$ for e = (i, j), include \mathbf{x}_e in any one of C_i, C_j (not both!)
- G_{C_i} is a star:
 - one vertex with degree $|C_i|$, and $|C_i|$ vertices with degree 1
- $cost(C_i) = 2|C_i| \frac{1}{|C_i|}(|C_i|^2 + 1^2 + \dots + 1^2) = |C_i| 1$
- Overall cost: $\sum_{i=1}^{k} \text{cost}(C_i) = (\sum_{i=1}^{k} |C_i|) k = |E| k = \theta$
- The k-means instance is yes!

Part 4: no to no (contrapositive)

- Suppose the k-means instance is a yes instance, and the cost of $\{C_1, \dots, C_k\}$ is at most $\theta = |E| k$.
- **Proposition**. $cost(C_i) \ge |C_i| 1$, and $cost(C_i) = |C_i| 1$ only if G_{C_i} is a star.
- Suppose G_{C_i} is not a star for some C_i . It's a contradiction:

OverallCost =
$$\sum_{i=1}^{k} cost(C_i) > \sum_{i=1}^{k} (|C_i| - 1) = |E| - k = \theta$$
.

- Thus, each G_{C_i} is a star.
- Those k "central vertex" of the k stars form a vertex cover!

Stronger Hardness Results for k-Means

- k-means is NP-hard even when k=2
 - [Aloise, Deshpande, Hansen & Popat, 2009] [Dasgupta & Freund, 2009]
- k-means is NP-hard even for \mathbb{R}^2
 - [Mahajan, Nimbhorkar & Varadarajan, 2009]
- There exists a constant $\varepsilon > 0$ such that k-means is NP-hard to approximate within factor (1ε) .
 - [Awasthi, Charikar, Krishnaswamy & Sinop, 2015]

Positive Results for *k*-Means

- There exists a poly-time $(9 + \varepsilon)$ -approximation algorithm.
 - [Kanungo, Mount, Netanyahu, Piatko, Silverman & Wu, 2003]
- Lloyd's heuristic, EM-heuristic
 - No theoretical approximation guarantee

0-1 Integer Programming

maximize
$$\mathbf{c}^{\mathsf{T}}\mathbf{x}$$

subject to $A\mathbf{x} \leq \mathbf{b}$
 $x_i \in \{0, 1\}$

- 0-1 Integer Programming is NP-hard.
- It can formulate many NP-complete problems, e.g., VertexCover

minimize
$$\sum_{v \in V} x_v$$
 subject to $x_u + x_v \ge 1$ $\forall (u, v) \in E$
$$x_v \in \{0, 1\}$$
 $\forall v \in V$

IP (Feasibility)

 Deciding whether the feasible region of an IP is non-empty is NP-complete.

VertexCover:

$$\sum_{v \in V} x_v \le k$$

$$x_u + x_v \ge 1 \qquad \forall (u, v) \in E$$

$$x_v \in \{0, 1\} \qquad \forall v \in V$$

IP: Hardness of Approximation

 Even if we only allow feasible IP as input, IP is still hard to approximate (just like TSP).

minimize
$$100000000y$$

subject to $x_u + x_v + y \ge 1$ $\forall (u,v) \in E$

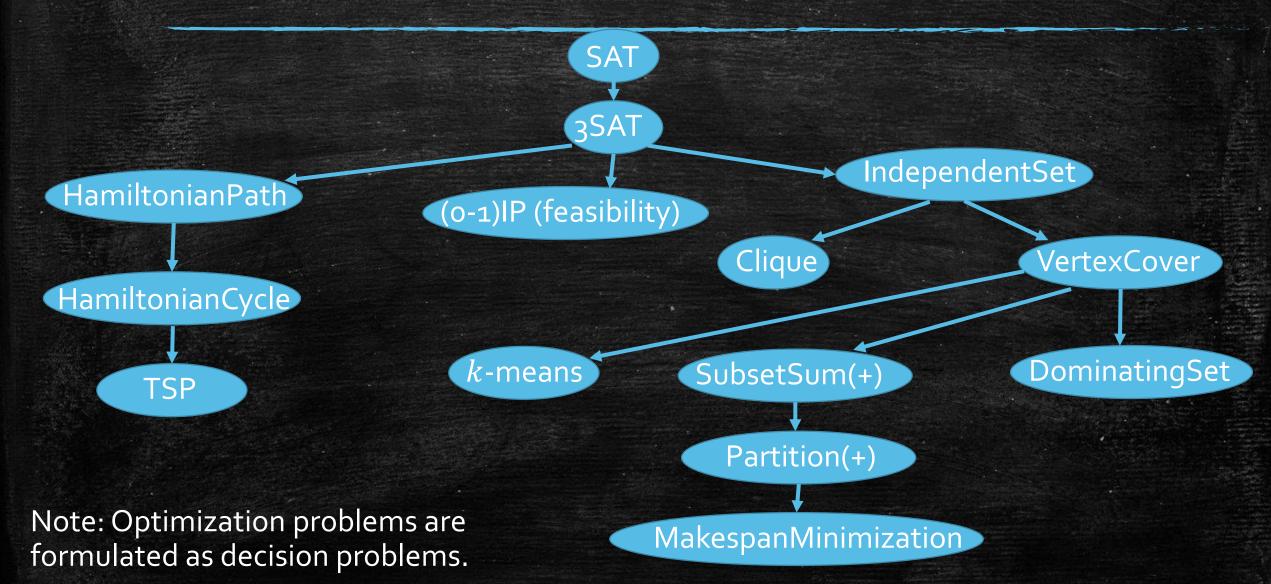
$$\sum_{v \in V} x_v \le k$$

$$x_v \in \{0,1\}$$

$$\forall v \in V$$

$$y \in \{0,1\}$$

Web of NP-Complete Problems



Deal with NP-hard Optimization Problems

Three approaches to handle NP-hard problems:

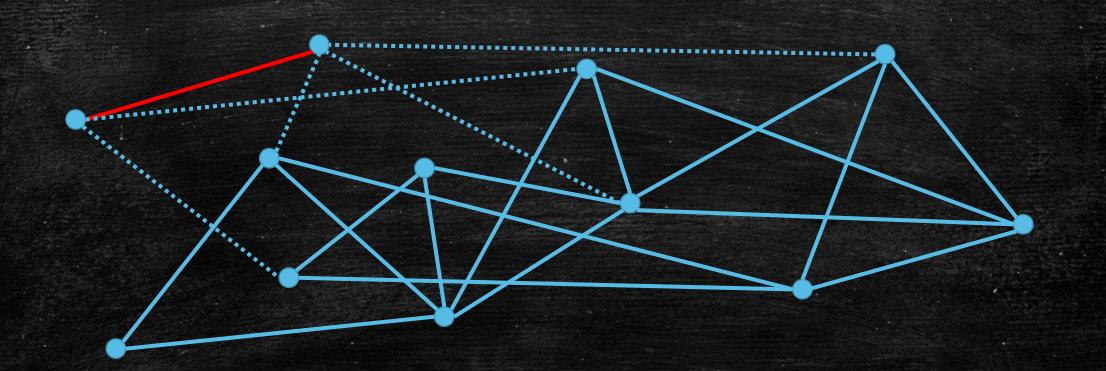
- 1. Approximation algorithms
- 2. Assumption on inputs
- 3. Heuristics
 - Heuristics: "algorithms" without theoretical support; their performances are normally justified by experiments/simulations
 - NP-hardness is about worst-case analysis. Heuristics may do well on most of the "practical instances".

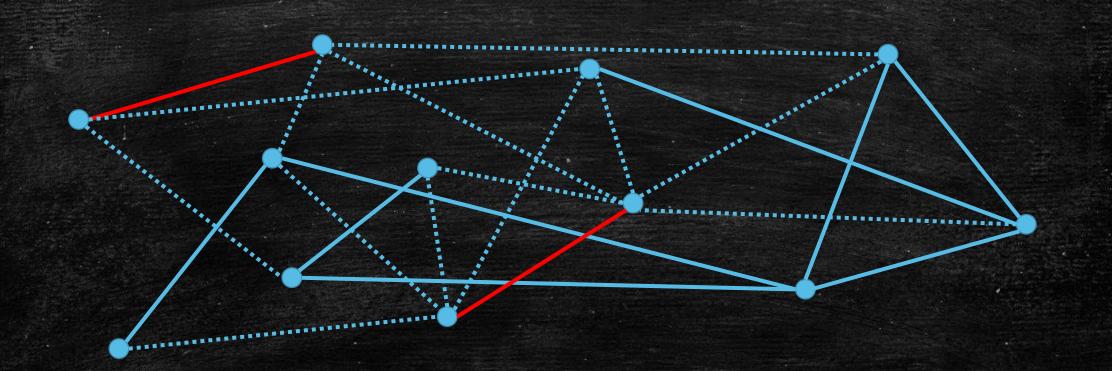
Approximation Algorithm for Min-VertexCover

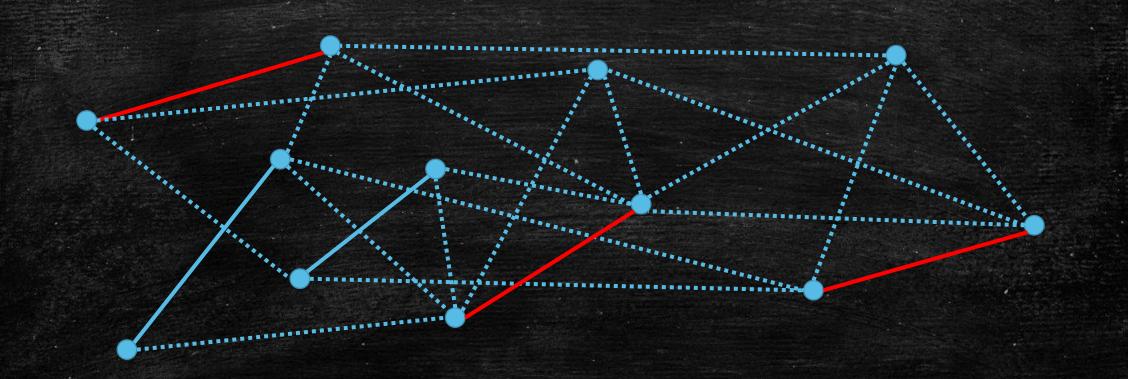
- Input: an undirected graph G = (V, E)
- Output: a vertex cover S with minimum |S|

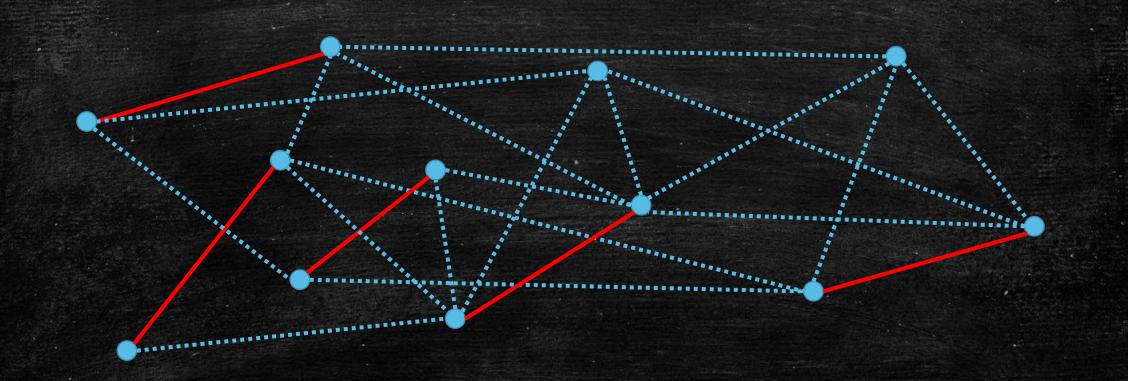
Maximal Matching

- A matching M is maximal if no more edge can be added to M while still forming a matching.
- Finding a maximal matching is simple: just iteratively add an edge until no more edges can be added!



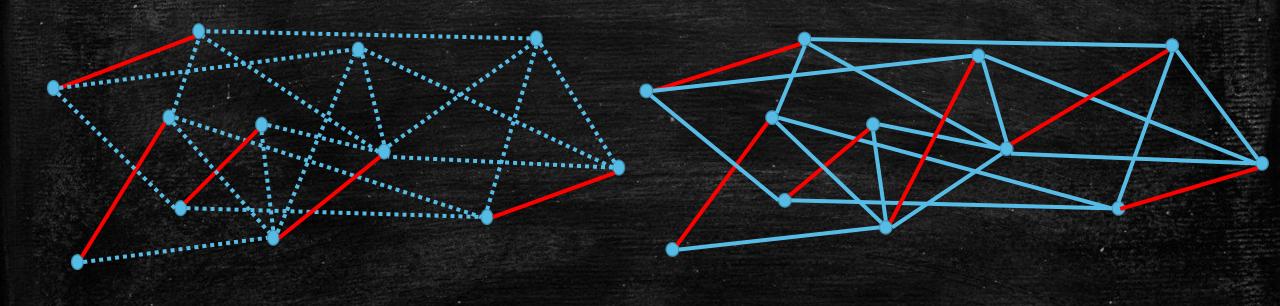




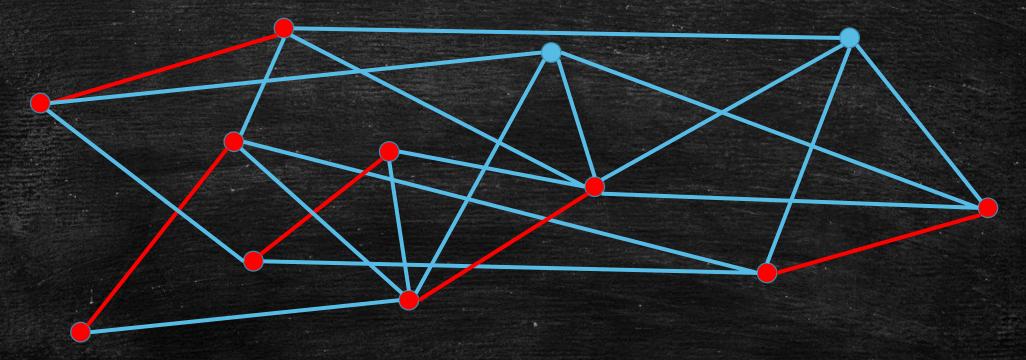


Maximal vs Maximum

A maximal matching may not be maximum!



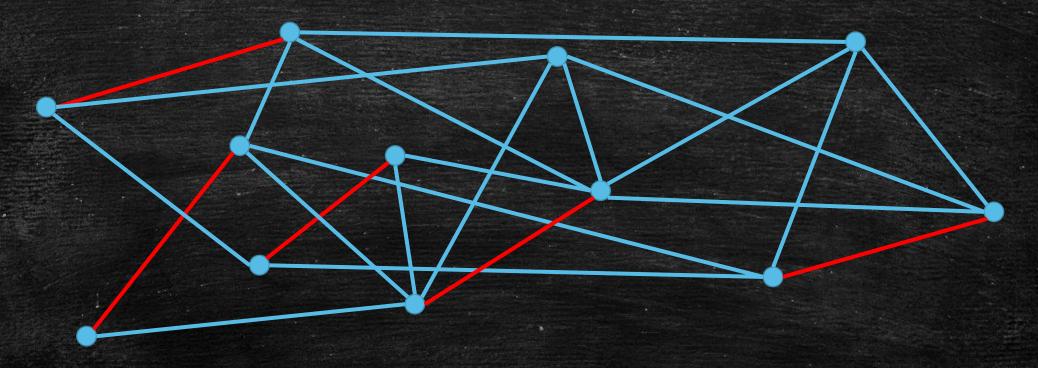
Lemma 1. The set of endpoints for all edges in a maximal matching is a vertex cover.



Proof. Let $M \subseteq E$ be a maximal matching.

- For any edge e=(u,v), one or both of u,v must be an endpoint of an edge in M. (Otherwise, M U $\{e\}$ is still a matching, and M is not maximal.)
- This already implies endpoints of M is a vertex cover!

Lemma 2. For any maximal matching M, the size of any vertex cover is at least |M|.



Proof.

- Edges in *M* must be covered
- A vertex cannot cover two edges in M
- We need |M| vertices to at least cover edges in M

A 2-approximation algorithm

Algorithm 1:

- Find a maximal matching M
- Let S be the endpoints of all edges in M
- Output S

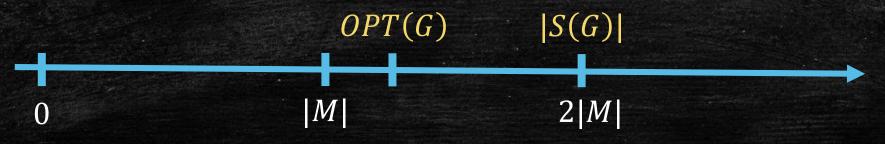
Given an undirected graph G = (V, E), let

- OPT(G) be the size of a minimum vertex cover
- S(G) be the vertex set output by Algorithm 1

Theorem: For any undirected graph G, we have $|S(G)| \leq 2 \cdot OPT(G)$

$\forall G: |S(G)| \leq 2 \cdot OPT(G)$

- Lemma 1. The set of endpoints for all edges in a maximal matching is a vertex cover.
- $\Rightarrow S(G)$ is a vertex cover
- $\bullet |S(G)| = 2|M|$
- Lemma 2: For any maximal matching M, the size of any vertex cover is at least |M|.
- $ightharpoonup
 ightharpoonup OPT(G) \geq |M|$



Approximation Algorithm

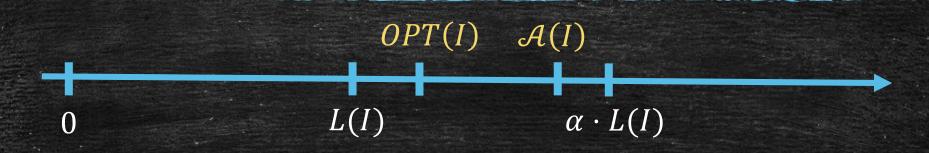
• Definition. Consider a minimization problem and an algorithm \mathcal{A} for it. Given a instance I, let $\mathcal{A}(I)$ be the value output by \mathcal{A} for input I, let OPT(I) be the optimal solution for I. \mathcal{A} is an α -approximation algorithm if

$$\forall I \colon \frac{\mathcal{A}(I)}{OPT(I)} \le \alpha$$

• Definition. For maximization problem, ${\cal A}$ is an α -approximation algorithm if

$$\forall I: \ \frac{\mathcal{A}(I)}{OPT(I)} \geq \alpha$$

General Framework for Designing Approximation Algorithms



- Find a lower bound L(I) for OPT(I) (that is easy to calculate)
- Design algorithm \mathcal{A} and find some α such that $\forall I : \mathcal{A}(I) \leq \alpha \cdot L(I)$

Revisiting our 2-approximation algorithm

Algorithm 1:

- Find a maximal matching M
- Let S be the endpoints of all edges in M
- Output S

Question: Can we do better than 2-approximation?

- Idea 1: same algorithm with a more careful analysis?
- Idea 2: another more clever algorithm?

Idea 1 doesn't work

$$G = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$
 ...

- Suppose G has 2n vertices and n edges as above.
- OPT(G) = n
- $\mathcal{A}(G) = 2n$

Idea 2 is unlikely to work

- [Khot & Regev, 2008] Assuming Unique Game Conjecture, if minimum vertex cover has a polynomial time (2ϵ) -approximation algorithm for some $\epsilon > 0$, then P = NP.
- [Khot, Minzer & Safra, 2017] If minimum vertex cover has a polynomial time $(\sqrt{2} \epsilon)$ -approximation algorithm for some $\epsilon > 0$, then $\mathbf{P} = \mathbf{NP}$.

Once we have an α -approximation algorithm...

Two natural directions for improving α :

- A more careful analysis
- A new approximation algorithm

Approximation Algorithms Based on LP-Relaxation

- Integer Programming is NP-complete, even for 0-1 case $\forall i : x_i \in \{0, 1\}.$
- Use the fact that LP is polynomial-time solvable to design approximation algorithm.
- Relax $x_i \in \{0,1\}$ to $0 \le x_i \le 1$.
- Then "round" the fractional solution to integral one: - E.g., $x_i = 0.7$ is rounded to $x_i = 1$, $x_i = 0.2$ is rounded to $x_i = 0$.
- and show that the rounded solution is feasible and achieves good approximation guarantee.

- Minimum Vertex Cover Formulation by integer program:
 - $x_u = 1$ represents $u \in V$ is selected in the cover; $x_u = 0$ otherwise.

minimize
$$\sum_{v \in V} x_v$$
 subject to $x_u + x_v \ge 1$ $\forall (u, v) \in E$
$$x_v \in \{0, 1\}$$
 $\forall v \in V$

Relax it to a linear program below:

minimize
$$\sum_{v \in V} x_v$$
 subject to $x_u + x_v \ge 1$ $\forall (u, v) \in E$
$$0 \le x_v \le 1 \qquad \forall v \in V$$

- OPT(IP) optimal objective value $\sum_{v \in V} x_v$ for IP
 - This is the objective we want for vertex cover
- OPT(LP) optimal objective value $\sum_{v \in V} x_v$ for LP
- OPT(IP) ≥ OPT(LP): because LP has a larger feasible region.

$$\begin{array}{lll} \text{minimize} & \sum_{v \in V} x_v & \text{minimize} & \sum_{v \in V} x_v \\ \text{subject to} & x_u + x_v \geq 1 & \forall (u,v) \in E & \text{subject to} & x_u + x_v \geq 1 & \forall (u,v) \in E \\ & x_v \in \{0,1\} & \forall v \in V & 0 \leq x_v \leq 1 & \forall v \in V \\ & \text{Integer Program (IP)} & \text{Linear Program (LP)} \end{array}$$

An approximation algorithm for vertex cover:

- Formulate the problem as an integer program and obtain its LPrelaxation.
- Solve the linear program and obtain its optimal solution $\{x_v^*\}_{v \in V}$.
- Return $S = \{ v \mid x_v^* \ge \frac{1}{2} \}$

Correctness

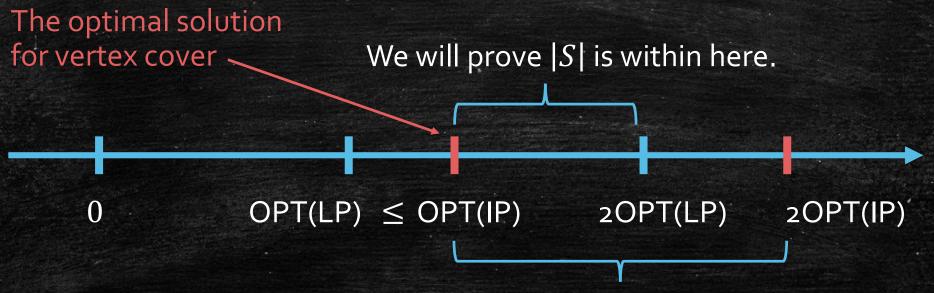
S returned by the algorithm is a vertex cover.

- Proof. Consider an arbitrary edge $(u, v) \in E$.
- We have $x_u^* + x_v^* \ge 1$ by feasibility, which implies we have either $x_u^* \ge \frac{1}{2}$ or $x_v^* \ge \frac{1}{2}$, or both.
- By our algorithm, we have either $u \in S$ or $v \in S$, or both.

The algorithm is a 2-approximation.

The algorithm is a 2-approximation algorithm: $|S| \le 2 \cdot OPT(IP)$.

■ Proof. Since we have OPT(IP) \geq OPT(LP), it suffices to prove $|S| \leq 2 \cdot \text{OPT}(\text{LP})$.



To show 2-approximation, |S| is required to be within here.

The algorithm is a 2-approximation.

The algorithm is a 2-approximation algorithm: $|S| \le 2 \cdot OPT(IP)$.

■ Proof. Since we have OPT(IP) \geq OPT(LP), it suffices to prove $|S| \leq 2 \cdot \text{OPT}(\text{LP})$.

• OPT(LP) =
$$\sum_{v \in V} x_v^* = \sum_{v: x_v^* < \frac{1}{2}} x_v^* + \sum_{v: x_v^* \ge \frac{1}{2}} x_v^*$$

$$\geq \sum_{v:x_v^* < \frac{1}{2}} 0 + \sum_{v:x_v^* \geq \frac{1}{2}} \frac{1}{2} = \frac{1}{2} \cdot |S|$$

• which implies $|S| \le 2 \cdot OPT(LP)$.

Let's Come Back to our two questions

Question: Can we do better than 2-approximation?

- Idea 1: same algorithm with a more careful analysis?
- Idea 2: another more clever algorithm?

- We know the answer to 2 is probably no...
- Let's forget about this for a moment...
- LP-Relaxation: how to analyze "it more carefully"?

Integrality Gap

- IntegralityGap = $\frac{OPT(IP)}{OPT(LP)}$
- If you analyze your approximation algorithm based on OPT(LP)...
- the best approximation ratio you can ever get is the integrality gap!

Integrality Gap for Vertex Cover

- Consider a complete graph with n vertices.
- OPT(IP) = n 1: you need n 1 vertices to cover all edges
- OPT(LP) = $\frac{n}{2}$: just assign $x_v = \frac{1}{2}$ for all $v \in V$.
- Integrality gap is 2.

Metric TSP

[TSP]

- Input: a complete weighted graph $G = (V, E = V \times V, w)$
- Output: a Hamiltonian cycle with minimum weight

[Metric TSP]

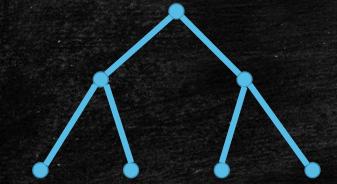
- Input: a complete weighted graph $G = (V, E = V \times V, w)$ such that $w(u, v) + w(v, w) \ge w(u, w)$ for any $u, v, w \in V$
- Output: a Hamiltonian cycle with minimum weight

Metric TSP is NP-hard

- HamiltonianCycle instance G' = (V, E')
- TSP instance $G = (V, E = V \times V, w)$ with $w(u, v) = f(x) = \begin{cases} 1, & (u, v) \in E \\ 2, & (u, v) \notin E \end{cases}$
- Yes HamiltonianCycle instance \Rightarrow OPT_{TSP} = |V|
- No HamiltonianCycle instance \Rightarrow OPT_{TSP} $\geq |V| + 1$

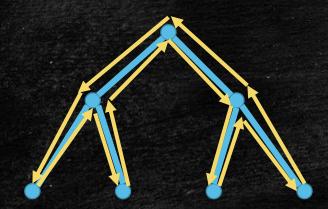
Approximation Algorithm for TSP

1. Find a minimum weight spanning tree T.



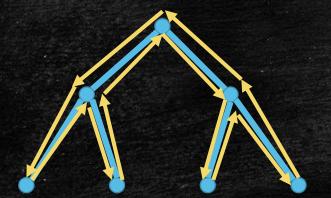
Approximation Algorithm for TSP

- 1. Find a minimum weight spanning tree T.
- 2. Find a tour C in T that visit each edge exactly twice.

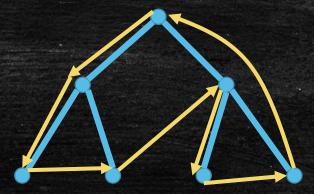


Approximation Algorithm for TSP

- 1. Find a minimum weight spanning tree T.
- 2. Find a tour C' in T that visit each edge exactly twice.
- 3. Shortcut C' to get C by skipping visited vertices.
 - So we get a valid Hamiltonian cycle...
- 4. Return C.





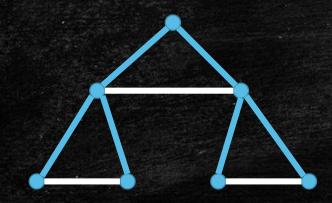


2-Approximation

- $OPT_{TSP} \ge w(T)$:
 - A Hamiltonian path is a spanning tree.
 - Min spanning tree ≤ min Hamiltonian Path ≤ min Hamiltonian Cycle
- $w(C') = 2w(T) \le 20$ PT_{TSP}
- $w(C) \leq w(C')$
 - Triangle inequality
- Putting together: $w(C) \le 20PT_{TSP}$

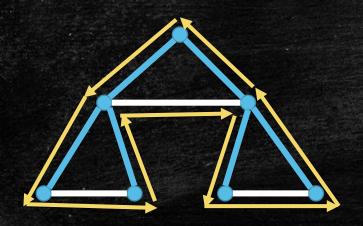
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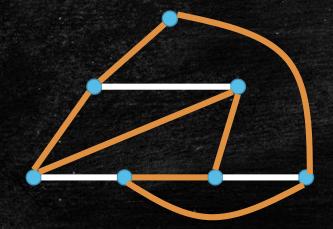
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- 2. Find a minimum weight perfect matching M on $U \subseteq V$, where U are odd-degree vertices in T.
- 3. Find a Eulerian tour C' on $T \cup M$.
- 4. Shortcut C' to C by skipping visited vertices.



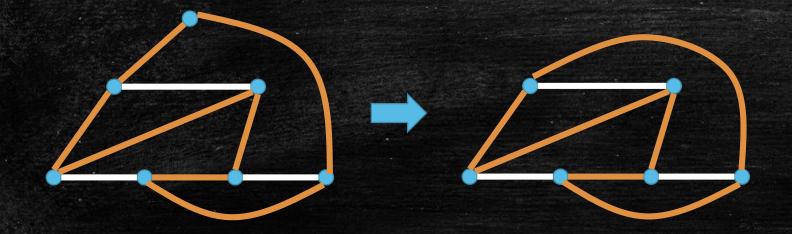
1.5-Approximation

- Same as before: $OPT_{TSP} \ge w(T)$
- $w(C) \leq w(C') = w(T) + w(M)$
- We aim to show $w(M) \le 0.5 \text{ OPT}_{TSP}$

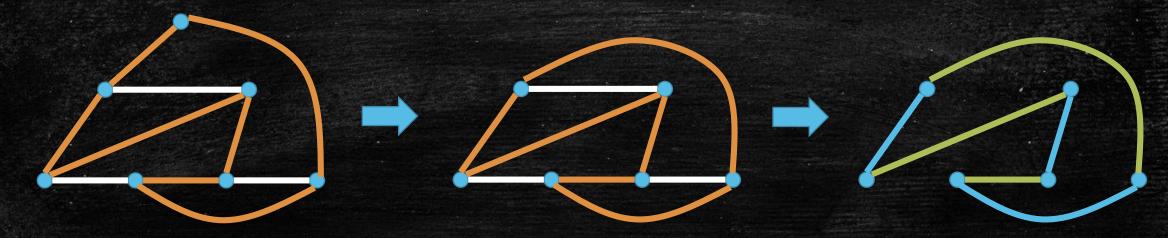
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- Let O' shortcut those vertices not in the matching.
- Two disjoint matchings M_1, M_2 in O'
- $w(M_1) + w(M_2) = w(O') \le w(O)$ (triangle inequality)
- One of M_1 or M_2 has weight at most 0.5w(0)



- Let 0 be the optimal cycle.
- Let O' shortcut those vertices not in the matching.
- Two disjoint matchings M_1, M_2 in O'
- $w(M_1) + w(M_2) = w(O') \le w(O)$ (triangle inequality)
- One of M_1 or M_2 has weight at most 0.5w(0)
- Since M has minimum weight...
- $w(M) \le 0.5w(O) = 0.50PT_{TSP}$

Metric TSP Results

- A $(1.5 10^{-36})$ -approximation algorithm
 - [Karlin, Klein, Gharan, 2020]
- NP-hard to approximate with factor $\frac{123}{122}$.
 - [Karpinski, Lampis & Schmied, 2015]

This Lecture

NP-Hardness:

• One more reduction: NP-hardness of k-means

Approximation Algorithms:

- Example:
 - VertexCover (2-approximation)
 - TSP (1.5-approximation)
- Framework:
 - find an approachable lower bound L (or upper bound in the maximization case) of OPT;
 - Show that ALG ≤ $\alpha \cdot L$
- Two techniques for designing approximation algorithms:
 - Combinatorial
 - LP-relaxation (Integrality Gap to analyze approximation ratio)