Submodular Functions, Optimization, and Applications to Machine Learning

— Fall Quarter, Lecture 3 —

http://www.ee.washington.edu/people/faculty/bilmes/classes/ee563_spring_2018/

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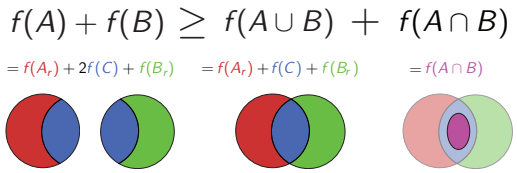
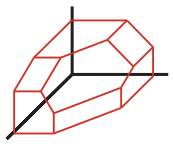
Oct 7th, 2020





Cumulative Outstanding Reading

- Read chapter 1 from Fujishige's book.

Class Road Map - EE563

- L1(9/30): Motivation, Applications, Definitions, Properties
- L2(10/5): Sums concave(modular), uses (diversity/costs, feature selection), information theory
- L3(10/7): Monge, More Definitions, Graph and Combinatorial Examples, Matrix Rank, Properties
- L4(10/12):
- L5(10/14):
- L6(10/19):
- L7(10/21):
- L8(10/26):
- L9(10/28):
- L10(11/2):
- L11(11/4):
- L12(11/9):
- L–(11/11): Veterans Day, Holiday
- L13(11/16):
- L14(11/18):
- L15(11/23):
- L16(11/25):
- L17(11/30):
- L18(12/2):
- L19(12/7):
- L20(12/9): maximization.

Last day of instruction, Fri. Dec 11th. Finals Week: Dec 12-18, 2020

Two Equivalent Submodular Definitions

Definition 3.2.1 (submodular concave)

A function $f : 2^V \to \mathbb{R}$ is submodular if for any $A, B \subseteq V$, we have that:

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{3.7}$$

An alternate and (as we will soon see) equivalent definition is:

Definition 3.2.2 (diminishing returns)

A function $f : 2^V \to \mathbb{R}$ is submodular if for any $A \subseteq B \subset V$, and $v \in V \setminus B$, we have that:

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- The incremental "value", "gain", or "cost" of v decreases (diminishes) as the context in which v is considered grows from A to B.
- Gain notation: Define $f(v|A) \triangleq f(A + v) - f(A)$. Then function f is submodular if $f(v|A) \geq f(v|B)$ for all $A \subseteq B \subseteq V \setminus \{v\}$, $v \in V$.

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Definition 3.2.2 (supermodular (improving returns))

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- Incremental "value", "gain", or "cost" of v increases (improves) as the context in which v is considered grows from A to B.
- A function f is submodular iff $-f$ is supermodular.
- If f both submodular and supermodular, then f is said to be **modular**, and $f(A) = c + \sum_{a \in A} \bar{f}(a)$ for some $\bar{f}$ (often $c = 0$).

Monge Matrices

- $m \times n$ matrices $C = [c_{ij}]_{ij}$ are called Monge matrices if they satisfy the Monge property, namely:

$$c_{ij} + c_{rs} \leq c_{is} + c_{rj} \tag{3.1}$$

for all $1 \leq i < r \leq m$ and $1 \leq j < s \leq n$.

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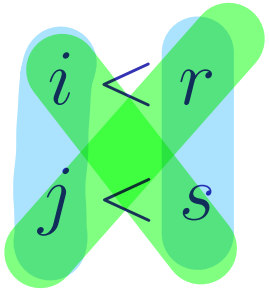

(3.2)

(3.3)

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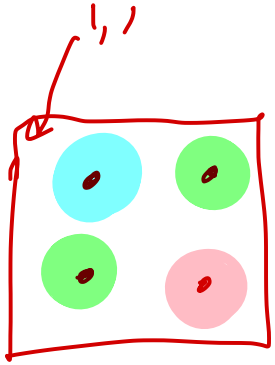
$$i < r \tag{3.2}$$

$$j < s \tag{3.3}$$



- Equivalently, for all $1 \leq i, r \leq m$, $1 \leq s, j \leq n$,

$$c_{\min(i,r),\min(s,j)} + c_{\max(i,r),\max(s,j)} \leq c_{is} + c_{rj} \tag{3.4}$$

Monge Matrices Visuals

- Consider a non-negative matrix $D = (d_{i,j})$ of order $m \times n$ and form matrix $C = (c_{i,j})$ with $c_{i,j}$th entry, $1 \leq i \leq m$, $1 \leq j \leq n$:

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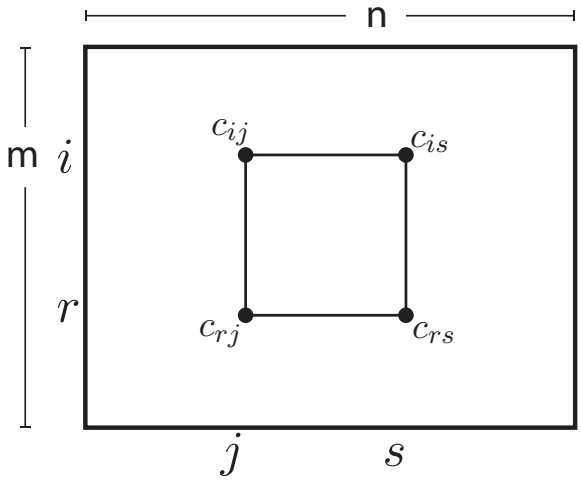

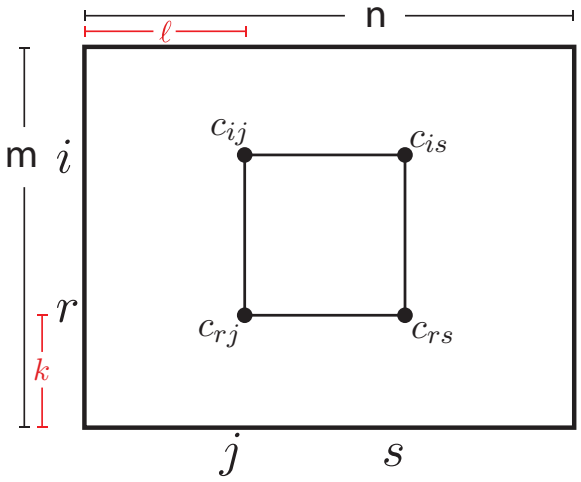

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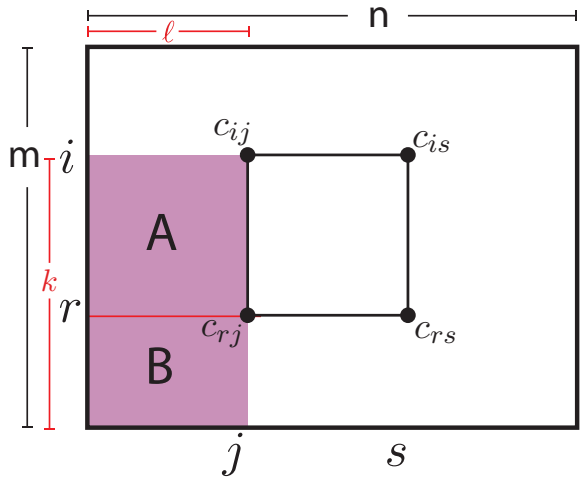

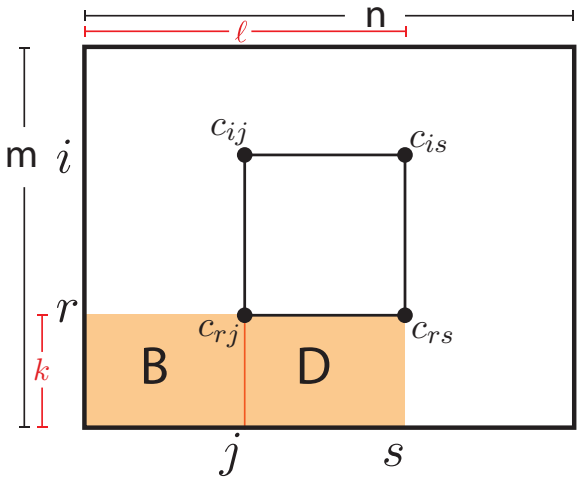

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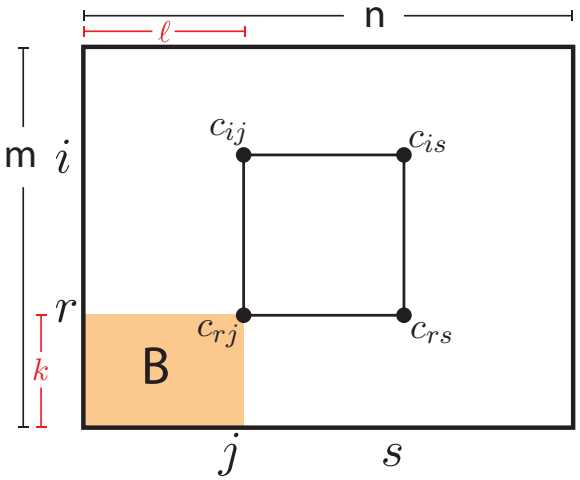

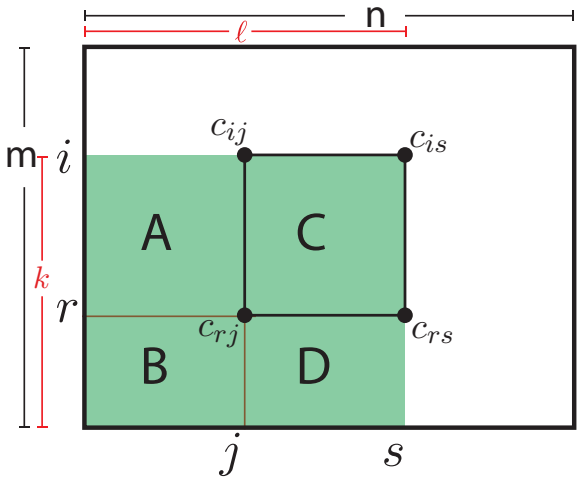

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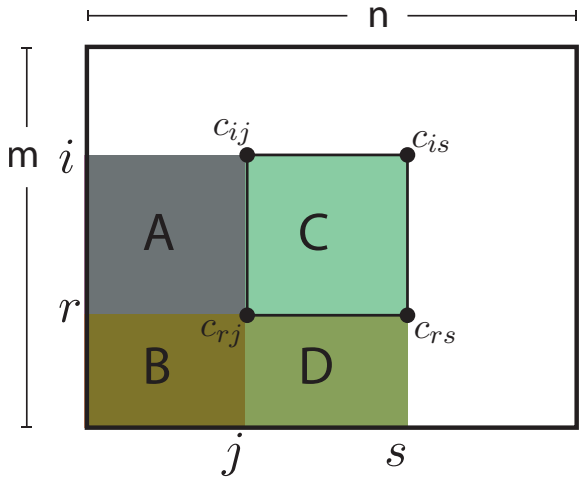

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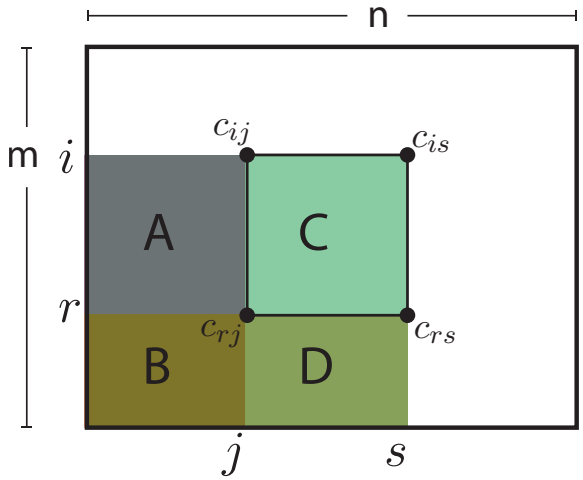

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- Then, $c_{ij} + c_{rs} < c_{is} + c_{rj}$. if $C > 0$.

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- Example, Hitchcock transportation problem: Given $m \times n$ cost matrix $C = [c_{ij}]_{ij}$, a non-negative supply vector $a \in \mathbb{R}_+^m$, a non-negative demand vector $b \in \mathbb{R}_+^n$ with $\sum_{i=1}^m a(i) = \sum_{j=1}^n b_j$, we wish to optimally solve the following linear program:

$$\underset{X \in \mathbb{R}^{m \times n}}{\text{minimize}} \quad \sum_{i=1}^{m} \sum_{j=1}^{n} c_{ij} x_{ij} \tag{3.6}$$

$$\text{subject to} \quad \sum_{i=1}^{m} x_{ij} = b_j \;\; \forall j = 1, \ldots, n \tag{3.7}$$

$$\sum_{j=1}^{n} x_{ij} = a_i \;\; \forall i = 1, \ldots, m \tag{3.8}$$

$$x_{i,j} \geq 0 \;\; \forall i, j \tag{3.9}$$

Monge Matrices, Hitchcock transportation

C

Producers, Sources, or Supply

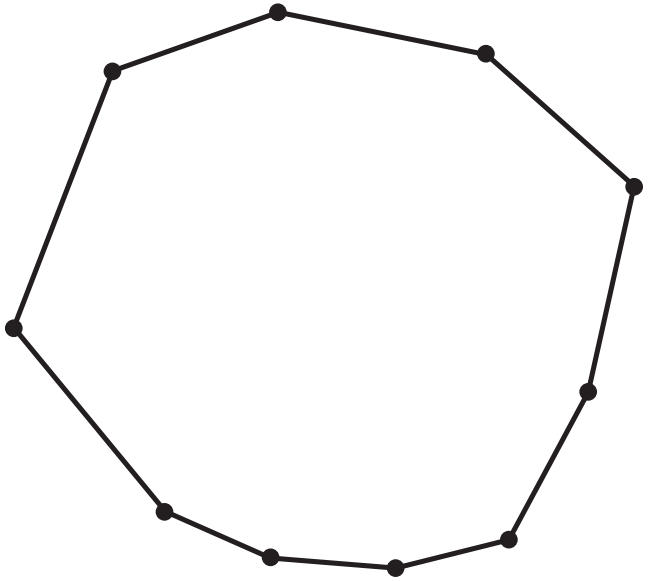
a_1	2	0	1	3	3
a_2	1	1	4	7	10
a_3	5	0	4	9	14
		3	2	1	2
		b_1	b_2	b_3	b_4

Consumers, Sinks, or Demand

- Solving the linear program can be done easily and optimally using the "North-West Corner Rule" (a 2D greedy-like approach starting at top-left and moving down or right) in only $O(m+n)$ if the matrix C is Monge!

Monge Matrices and Convex Polygons

- Can generate a Monge matrix from a convex polygon - delete two segments, then separately number vertices on each chain. Distances c_{ij} satisfy Monge property (or quadrangle inequality).



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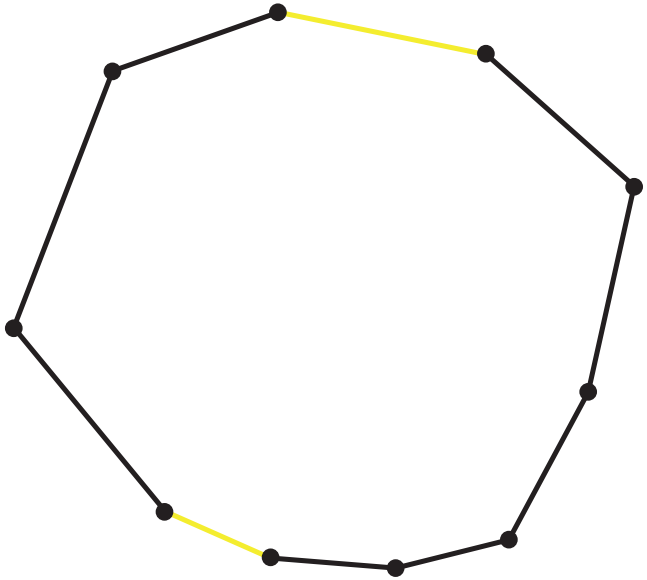

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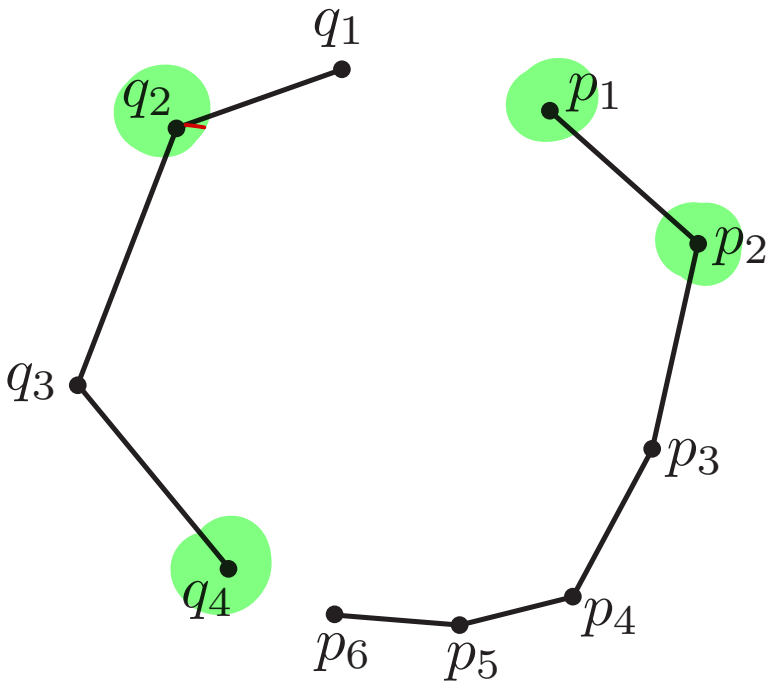

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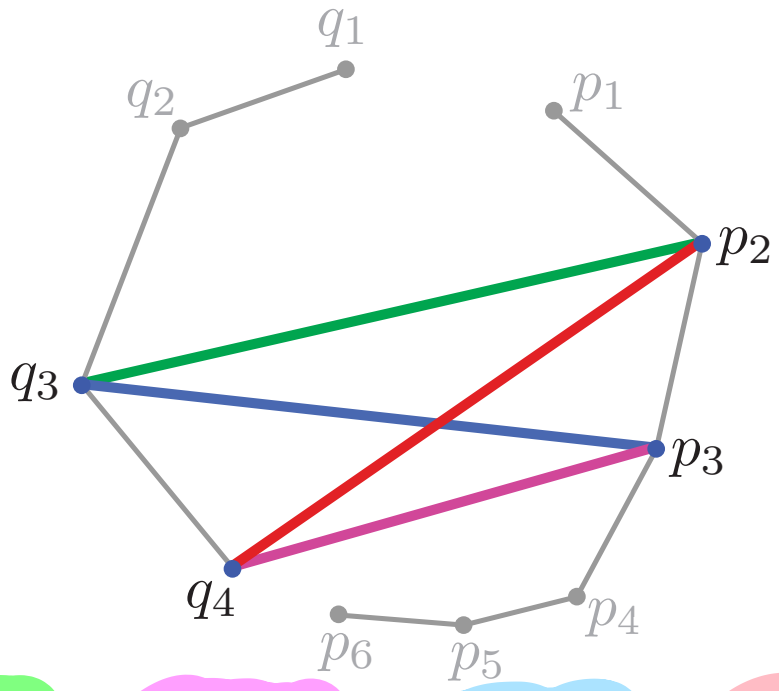

$$d(q_3, p_2) + d(q_4, p_3) \leq d(q_4, p_2) + d(q_3, p_3) \tag{3.10}$$

Transport unit quantities from locations q_3 and q_4 to locations p_2 and p_3; to minimize total distance traveled, routes from q_3 and q_4 must not intersect.

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  $f(A) = f(1_A) = f((0001110010001))$

  A

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$m \times n$ matrix

$m = n = 2$

$V = \{v_1, v_2\}$

$c_{12} + c_{21} \geq c_{11} + c_{22}$

$K = 1$

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$f(\emptyset) = c_{11}$ $f(v) = c_{22}$ $f(\{v_1\}) = c_{21}$ $f(\{v_2\}) = c_{12}$ $f(v_1) + f(v_2) \geq f(v_1 + v_2) + f(\emptyset)$

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- With $|V| = 2$, and $K + 1$ the side-dimension of the matrix, we get a Monge property (on square matrices).
- Non square: $f : \{0,1,\ldots,K_1\} \times \{0,1,\ldots,K_2\} \to \mathbb{R}$. $\Rightarrow c_{ij}$

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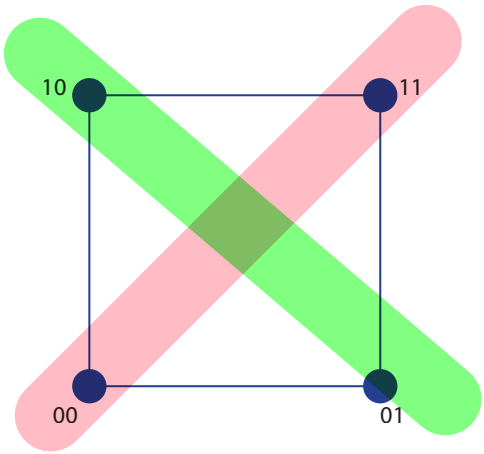
The Submodular Square, and Hypercube Vertices

We can test submodularity via values on vertices of hypercube.

Example: with $|V| = n = 2$, this is easy:

$K=2$



2D hypercube

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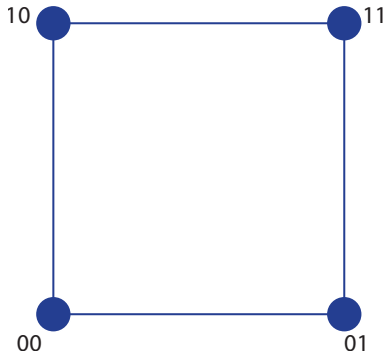
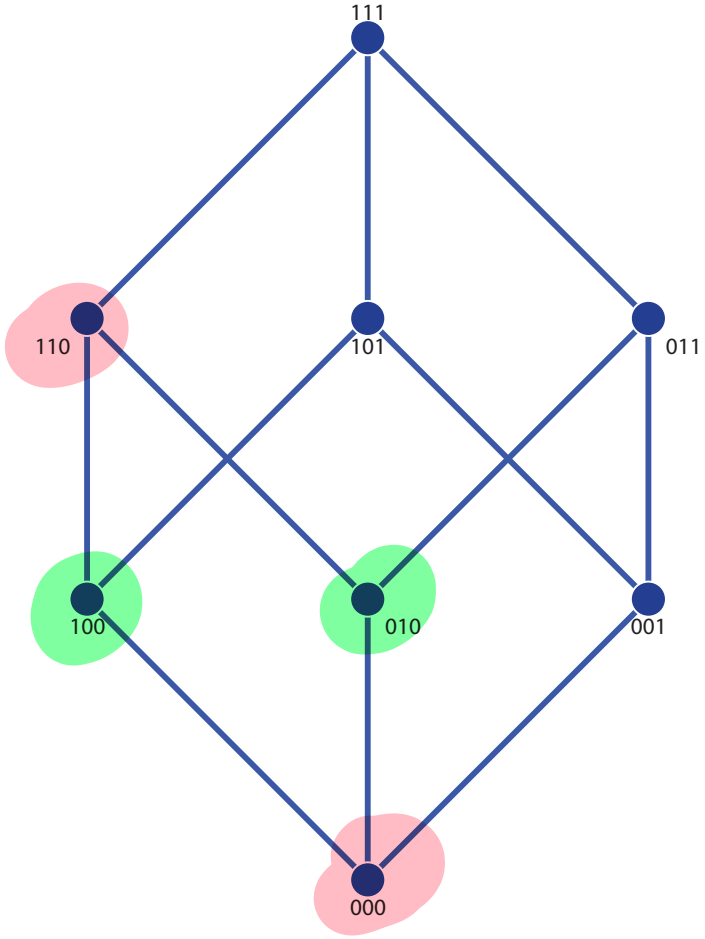


With $|V| = n = 3$, a bit harder.

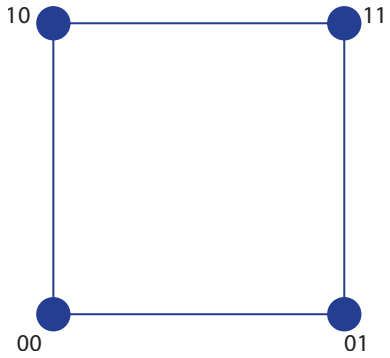


$$f(100) + f(010)$$
$$\geq f((100) \vee (010)) + f((100) \wedge (010))$$
$$= f(110) + f(000)$$

The Submodular Square, and Hypercube Vertices

We can test submodularity via values on vertices of hypercube.

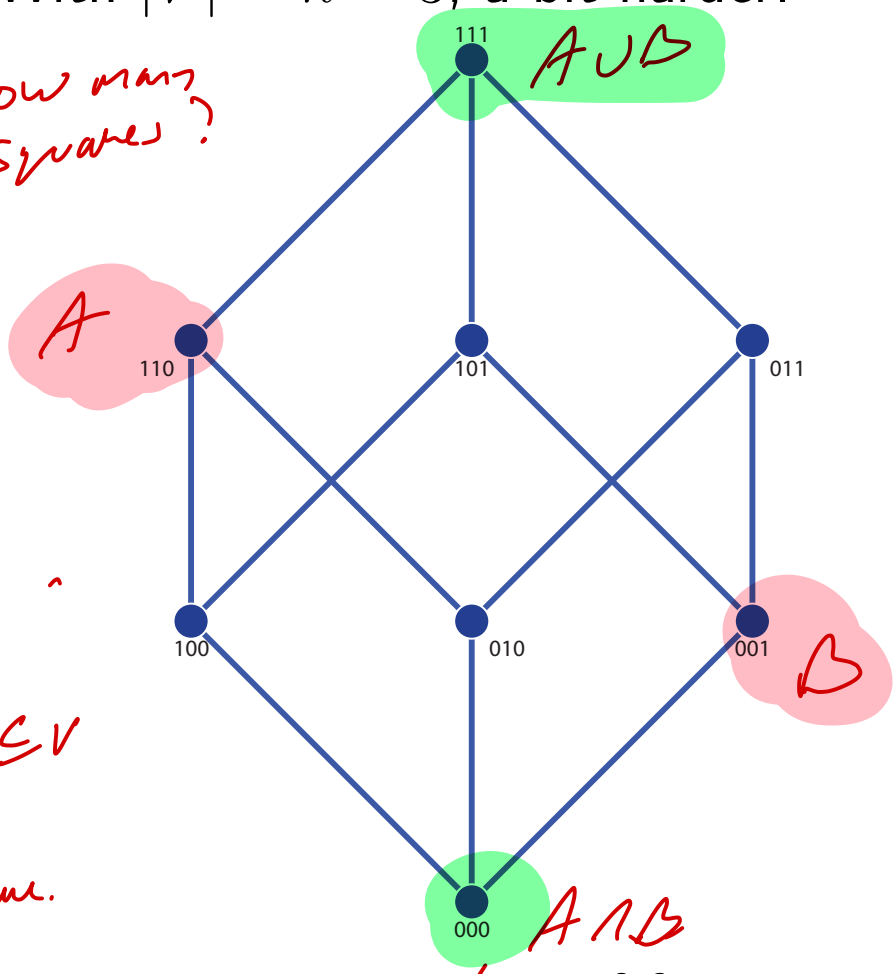
Example: with $|V| = n = 2$, this is easy:



$100 \cup 011 = 111$

With $|V| = n = 3$, a bit harder.

How many squares?



For each $A, B \subseteq V$

Each inequality is a square.

How many inequalities of form $f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$?

The Submodular Square, and Hypercube Vertices

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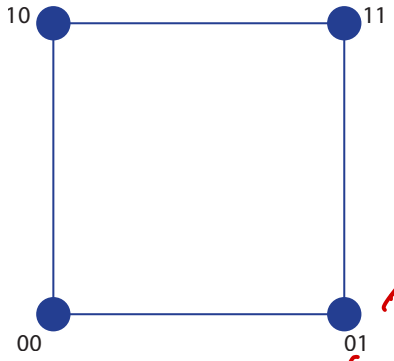


$A \cup B$ $\quad$ $A \cap B$

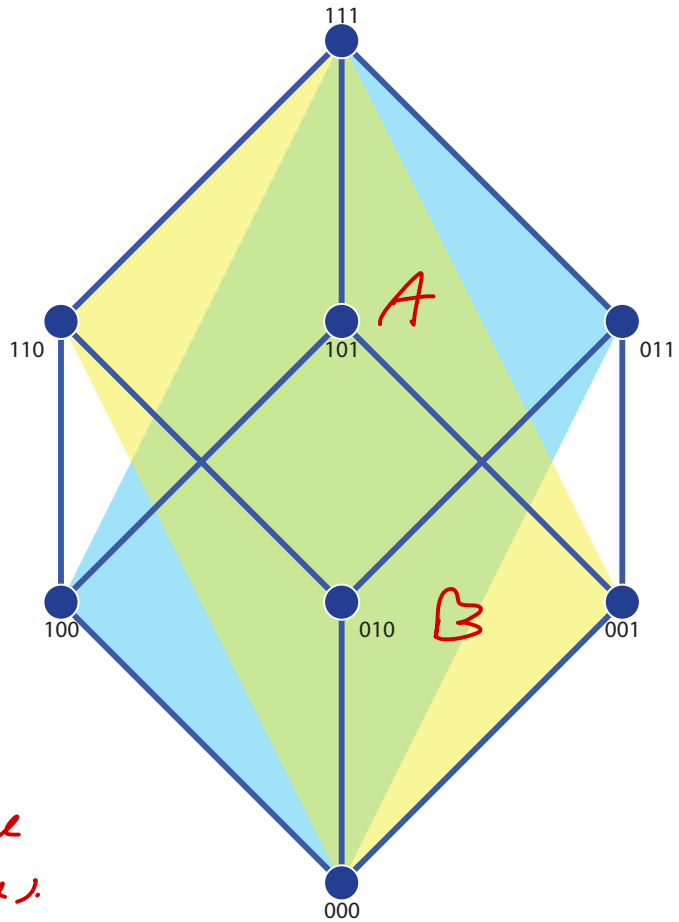
$$\underset{A}{f(X+i)} + \underset{B}{f(X+j)} \geq \underset{A \cap B}{f(X+i+j)} + f(X)$$

$\therefore$ to verify submodularity when $|V| = 3$, need to check <u>at most</u> 9 inequalities

9 unique squares.

<u>claim:</u> need only check 6 inequalities, the 6 cube faces.

With $|V| = n = 3$, a bit harder.



How many inequalities of form $f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$?

Subadditive Definitions

Definition 3.4.1 (subadditive)

A function $f : 2^V \to \mathbb{R}$ is subadditive if for any $A, B \subseteq V$, we have that:

$$f(A) + f(B) \geq f(A \cup B) \tag{3.12}$$

This means that the "whole" is less than the sum of the parts.

Two Equivalent Supermodular Definitions

Definition 3.4.1 (supermodular)

A function $f : 2^V \to \mathbb{R}$ is supermodular if for any $A, B \subseteq V$, we have that:

$$f(A) + f(B) \leq f(A \cup B) + f(A \cap B) \tag{3.7}$$

Definition 3.4.2 (supermodular (improving returns))

A function $f : 2^V \to \mathbb{R}$ is supermodular if for any $A \subseteq B \subset V$, and $v \in V \setminus B$, we have that:

$$f(A \cup \{v\}) - f(A) \leq f(B \cup \{v\}) - f(B) \tag{3.8}$$

- Incremental "value", "gain", or "cost" of v increases (improves) as the context in which v is considered grows from A to B.
- A function f is submodular iff $-f$ is supermodular.
- If f both submodular and supermodular, then f is said to be **modular**, and $f(A) = c + \sum_{a \in A} \bar{f}(a)$ for some $\bar{f}$ (often $c = 0$).

Superadditive Definitions

Definition 3.4.2 (superadditive)

A function $f : 2^V \to \mathbb{R}$ is superadditive if for any $A, B \subseteq V$, we have that:

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- Ex: Let $0 < k < |V|$, and consider $f : 2^V \to \mathbb{R}_+$ where:

$$f(A) = \begin{cases} 1 & \text{if } |A| \leq k \\ 0 & \text{else} \end{cases} \tag{3.14}$$

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$$f(A) = \begin{cases} 1 & \text{if } |A| \leq k \\ 0 & \text{else} \end{cases} \tag{3.14}$$

- This function is subadditive but not submodular.

$f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$

Modular Definitions

Definition 3.4.3 (modular)

A function that is both submodular and supermodular is called **modular**

If f is a modular function, than for any $A, B \subseteq V$, we have

$$f(A) + f(B) = f(A \cap B) + f(A \cup B) \tag{3.15}$$

In modular functions, elements do not interact (or cooperate, or compete, or influence each other), and have value based only on singleton values.

Proposition 3.4.4

If f is modular, it may be written as

$$f(A) = f(\emptyset) + \sum_{a \in A} \Big(f(\{a\}) - f(\emptyset) \Big) = c + \sum_{a \in A} f'(a) \tag{3.16}$$

which has only $|V| + 1$ parameters.

normalized $\Rightarrow$ $c = 0$

$\therefore$ modular function vector $\in \mathbb{R}^V$

Modular Definitions

Proof.

We inductively construct the value for $A = \{a_1, a_2, \ldots, a_k\}$.
For $k = 2$,

$$f(a_1) + f(a_2) = f(a_1, a_2) + f(\emptyset) \tag{3.17}$$

$$\text{implies } f(a_1, a_2) = f(a_1) - f(\emptyset) + f(a_2) - f(\emptyset) + f(\emptyset) \tag{3.18}$$

then for $k = 3$,

$$f(a_1, a_2) + f(a_3) = f(a_1, a_2, a_3) + f(\emptyset) \tag{3.19}$$

$$\text{implies } f(a_1, a_2, a_3) = f(a_1, a_2) - f(\emptyset) + f(a_3) - f(\emptyset) + f(\emptyset) \tag{3.20}$$

$$= f(\emptyset) + \sum_{i=1}^{3} \big(f(a_i) - f(\emptyset)\big) \tag{3.21}$$

and so on ... □

Complement function

Given a function $f : 2^V \to \mathbb{R}$, we can find a complement function $\bar{f} : 2^V \to \mathbb{R}$ as $\bar{f}(A) = f(V \setminus A)$ for any A.

Proposition 3.4.5

$\bar{f}$ is submodular iff f is submodular.

Proof.

$$\bar{f}(A) + \bar{f}(B) \geq \bar{f}(A \cup B) + \bar{f}(A \cap B) \tag{3.22}$$

follows from

$$f(V \setminus A) + f(V \setminus B) \geq f(V \setminus (A \cup B)) + f(V \setminus (A \cap B)) \tag{3.23}$$

which is true because $V \setminus (A \cup B) = (V \setminus A) \cap (V \setminus B)$ and $V \setminus (A \cap B) = (V \setminus A) \cup (V \setminus B)$ (De Morgan's laws for sets). □

Undirected Graphs

- Let $G = (V, E)$ be a graph with vertices $V = V(G)$ and edges $E = E(G) \subseteq V \times V$.

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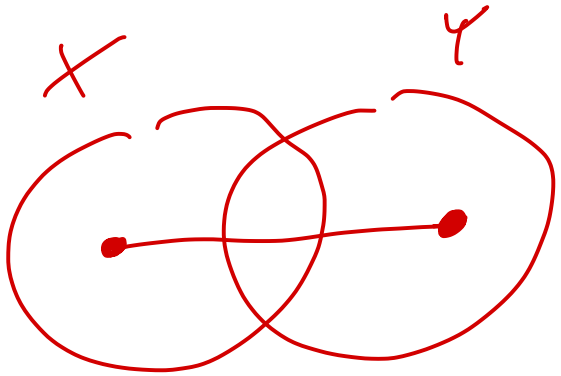
- If G is undirected, define

$$E(X, Y) \triangleq \{\{x, y\} \in E(G) : x \in X \setminus Y, y \in Y \setminus X\} \tag{3.24}$$

as the edges strictly between X and Y.



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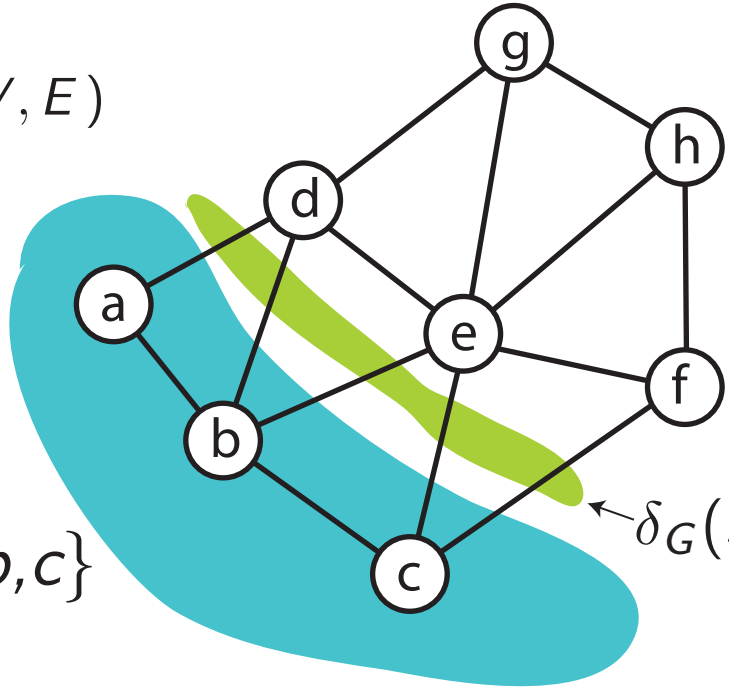
$G = (V, E)$



$S = \{a, b, c\}$

$\delta_G(S) = \{\{u, v\} \in E : u \in S, v \in V \setminus S\}.$
$= \{\{a,d\},\{b,d\},\{b,e\},\{c,e\},\{c,f\}\}$

Directed graphs, and cuts and flows

- If G is directed, define

$$E^+(X,Y) \triangleq \{(x,y) \in E(G) : x \in X \setminus Y, y \in Y \setminus X\} \tag{3.25}$$

as the edges directed strictly from X towards Y.

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- Nodes define cuts and flows. Define edges leaving X (out-flow) as

$$\delta^+(X) \triangleq E^+(X, V \setminus X) \tag{3.26}$$

and edges entering X (in-flow) as

$$\delta^-(X) \triangleq E^+(V \setminus X, X) \tag{3.27}$$

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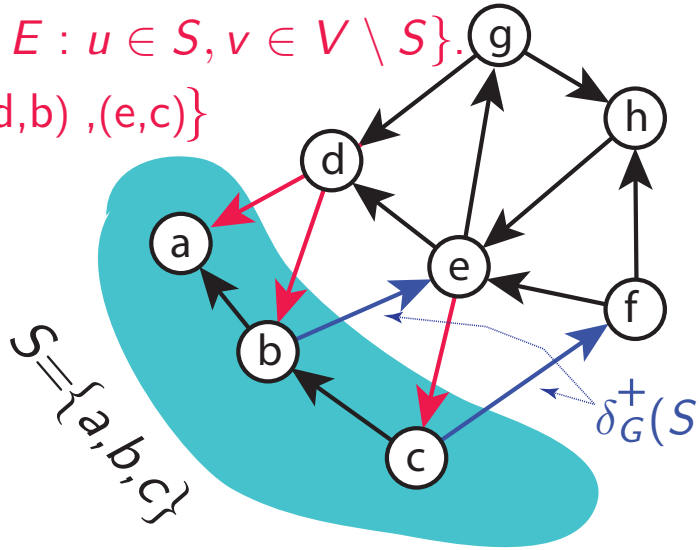
$$\delta^-(X) \triangleq E^+(V \setminus X, X) \tag{3.27}$$

$\delta_G^-(S) = \{(v,u) \in E : u \in S, v \in V \setminus S\}.$
$= \{(d,a), (d,b), (e,c)\}$



$\delta_G^+(S) = \{(u,v) \in E : u \in S, v \in V \setminus S\}.$
$= \{(b,e), (c,f)\}$

The Neighbor function in undirected graphs

- Given a set $X \subseteq V$, the neighbor function of X is defined as

$$\Gamma(X) \triangleq \{v \in V(G) \setminus X : E(X, \{v\}) \neq \emptyset\} \tag{3.28}$$

The Neighbor function in undirected graphs

- Given a set $X \subseteq V$, the neighbor function of X is defined as

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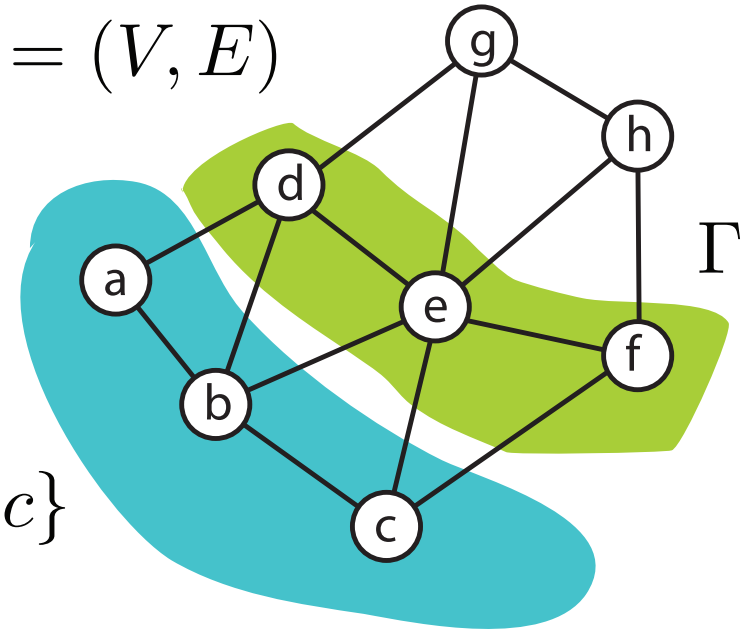
- Example:

$$G = (V, E)$$



$$\Gamma(S) = \{d, e, f\}$$

$$S = \{a, b, c\}$$

Directed Cut function: property

Lemma 3.5.1

For a digraph $G = (V, E)$ and any $X, Y \subseteq V$: we have

$$|\delta^+(X)| + |\delta^+(Y)| = |\delta^+(X \cap Y)| + |\delta^+(X \cup Y)| + |E^+(X, Y)| + |E^+(Y, X)| \tag{3.29}$$

and

$$|\delta^-(X)| + |\delta^-(Y)| = |\delta^-(X \cap Y)| + |\delta^-(X \cup Y)| + |E^-(X, Y)| + |E^-(Y, X)| \tag{3.30}$$

$\therefore$ $f^+(X) = |\delta^+(X)|$ is submodular

$f^-(X) = |\delta^-(X)|$ is submodular.

Directed Cut function: proof of property

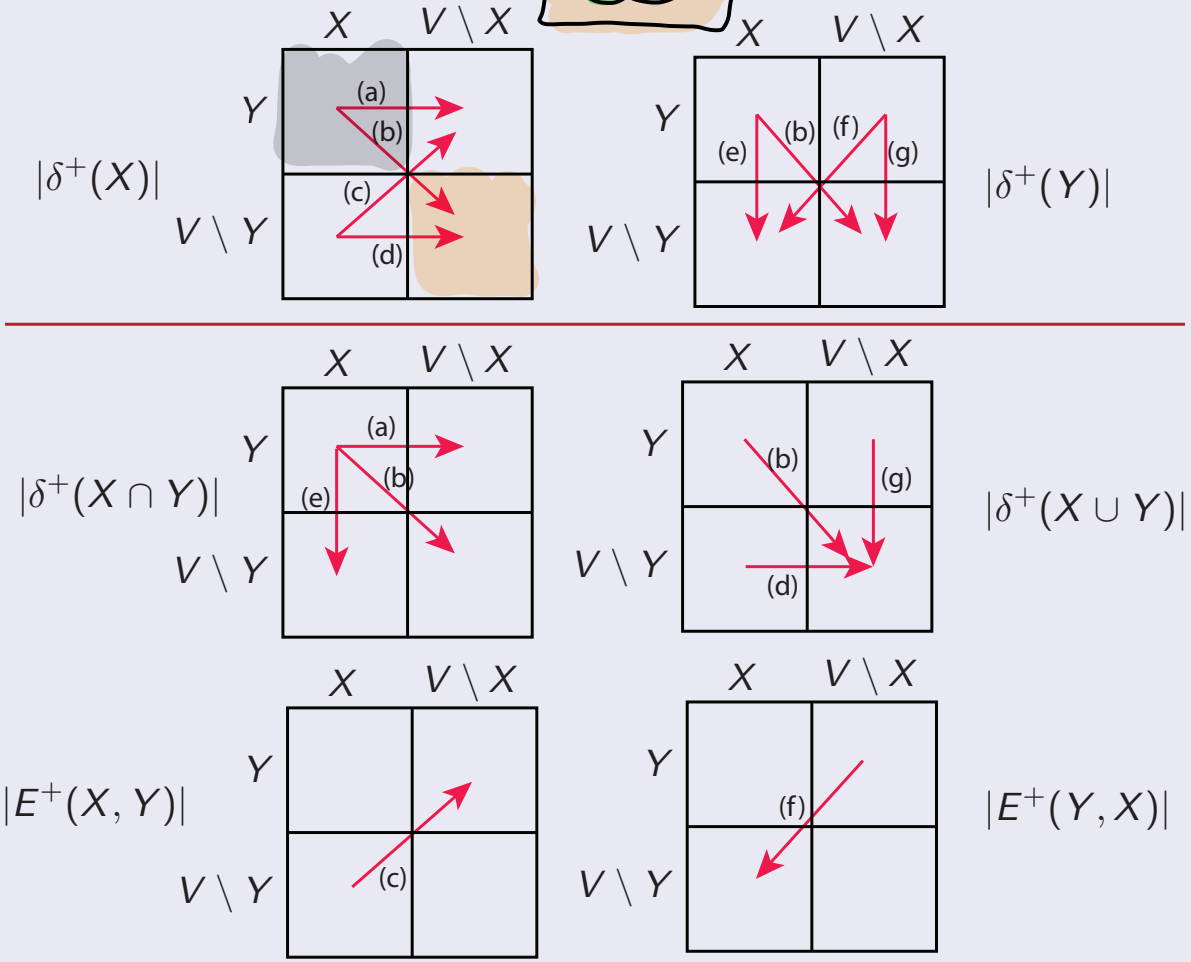
Proof.

We can prove Eq. (3.29) using a geometric counting argument (proof for $|\delta^-(X)|$ case is similar)

$w(\delta^+(X)) = f(X)$

$h(X) = f(\delta^+(X))$

$|A| = m(A)$



Q:Why is (c) $= |E^+(X,Y)|$?

Directed cut/flow functions: submodular

Lemma 3.5.2

For a digraph $G = (V, E)$ and any $X, Y \subseteq V$: both functions $|\delta^+(X)|$ and $|\delta^-(X)|$ are submodular.

Proof.

$|E^+(X, Y)| \geq 0$ and $|E^-(X, Y)| \geq 0$. □

More generally, in the non-negative weighted edge case, both in-flow and out-flow are submodular on subsets of the vertices.

Undirected Cut/Flow & the Neighbor function: submodular

Lemma 3.5.3

For an undirected graph $G = (V, E)$ and any $X, Y \subseteq V$: we have that both the undirected cut (or flow) function $|\delta(X)|$ and the neighbor function $|\Gamma(X)|$ are submodular. I.e.,

$$|\delta(X)| + |\delta(Y)| = |\delta(X \cap Y)| + |\delta(X \cup Y)| + 2|E(X, Y)| \tag{3.31}$$

and

$$|\Gamma(X)| + |\Gamma(Y)| \geq |\Gamma(X \cap Y)| + |\Gamma(X \cup Y)| \tag{3.32}$$

Proof.

- Eq. (3.31) follows from Eq. (3.29): we replace each undirected edge $\{u, v\}$ with two oppositely-directed directed edges (u, v) and (v, u). Then we use same counting argument.

$$|\delta(X)| = \frac{|\delta^+(X)| + |\delta^-(X)|}{2}$$

...

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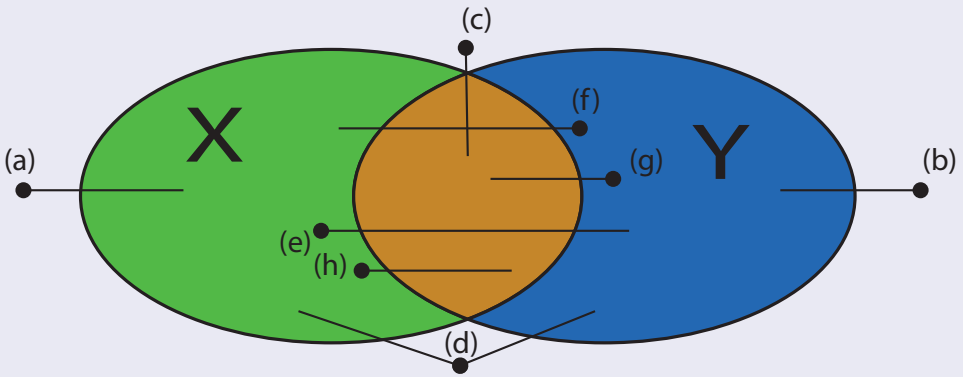
- Eq. (3.32) follows as shown in the following page.

...

cont.



Graphically, we can count and see that

$$\Gamma(X) = (a) + (c) + (f) + (g) + (d) \tag{3.33}$$
$$\Gamma(Y) = (b) + (c) + (e) + (h) + (d) \tag{3.34}$$
$$\Gamma(X \cup Y) = (a) + (b) + (c) + (d) \tag{3.35}$$
$$\Gamma(X \cap Y) = (c) + (g) + (h) \tag{3.36}$$

so

$$\begin{aligned} |\Gamma(X)| + |\Gamma(Y)| &= (a) + (b) + 2(c) + 2(d) + (e) + (f) + (g) + (h) \\ &\geq (a) + (b) + 2(c) + (d) + (g) + (h) = |\Gamma(X \cup Y)| + |\Gamma(X \cap Y)| \end{aligned} \tag{3.37}$$

Undirected Neighbor functions

Therefore, the undirected cut function $|\delta(A)|$ and the neighbor function $|\Gamma(A)|$ of a graph G are both submodular.

Undirected cut/flow is submodular: alternate proof

- Another simple proof shows that $|\delta(X)|$ is submodular.

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- Define a graph $G_{uv} = (\{u, v\}, \{e\}, w)$ with two nodes u, v and one edge $e = \{u, v\}$ with non-negative weight $w(e) \in \mathbb{R}_+$.

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- Define a graph $G_{uv} = (\{u, v\}, \{e\}, w)$ with two nodes u, v and one edge $e = \{u, v\}$ with non-negative weight $w(e) \in \mathbb{R}_+$.
- Weighted cut function over those two nodes: $w(\delta_{u,v}(\cdot))$ has valuation:

$$w(\delta_{u,v}(\emptyset)) = w(\delta_{u,v}(\{u, v\})) = 0 \tag{3.38}$$

and

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- Thus, $w(\delta_{u,v}(\cdot))$ is submodular since $w(e) \geq 0$ and

$$w(\delta_{u,v}(\{u\})) + w(\delta_{u,v}(\{v\})) \geq w(\delta_{u,v}(\{u, v\})) + w(\delta_{u,v}(\emptyset)) \tag{3.40}$$

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- General non-negative weighted graph $G = (V, E, w)$, define $w(\delta(\cdot))$:

$$f(X) = w(\delta(X)) = \sum_{(u,v) \in E(G)} w(\delta_{u,v}(X \cap \{u, v\})) \tag{3.41}$$

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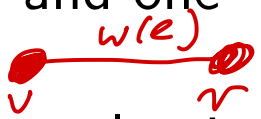

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and

$f(x) = g(x \cap S)$

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- This is easily shown to be submodular using properties we will soon see (namely, submodularity closed under summation and restriction).

Other graph functions that are submodular/supermodular

These come from Narayanan's book 1997. Let G be an undirected graph.

- Let $V(X)$ be the vertices adjacent to some edge in $X \subseteq E(G)$, then $|V(X)|$ (the vertex function) is submodular.

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- Let $E(S)$ be the edges with both vertices in $S \subseteq V(G)$. Then $|E(S)|$ (the interior edge function) is supermodular.

$$g(S) = \sum_{i,j \in S} w_{ij}$$

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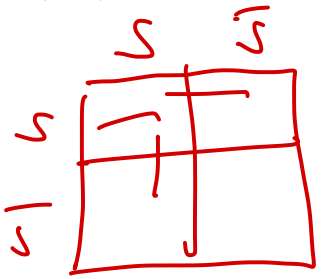

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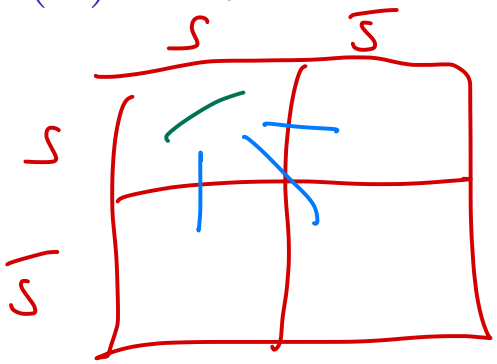

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- Consider $f(A) = |\delta^+(A)| - |\delta^+(V \setminus A)|$. Guess, submodular, supermodular, modular, or neither? Exercise: determine which one and prove it.

Number of connected components in a graph via edges

- Recall, $f : 2^V \to \mathbb{R}$ is submodular, then so is $\bar{f} : 2^V \to \mathbb{R}$ defined as $\bar{f}(S) = f(V \setminus S)$.

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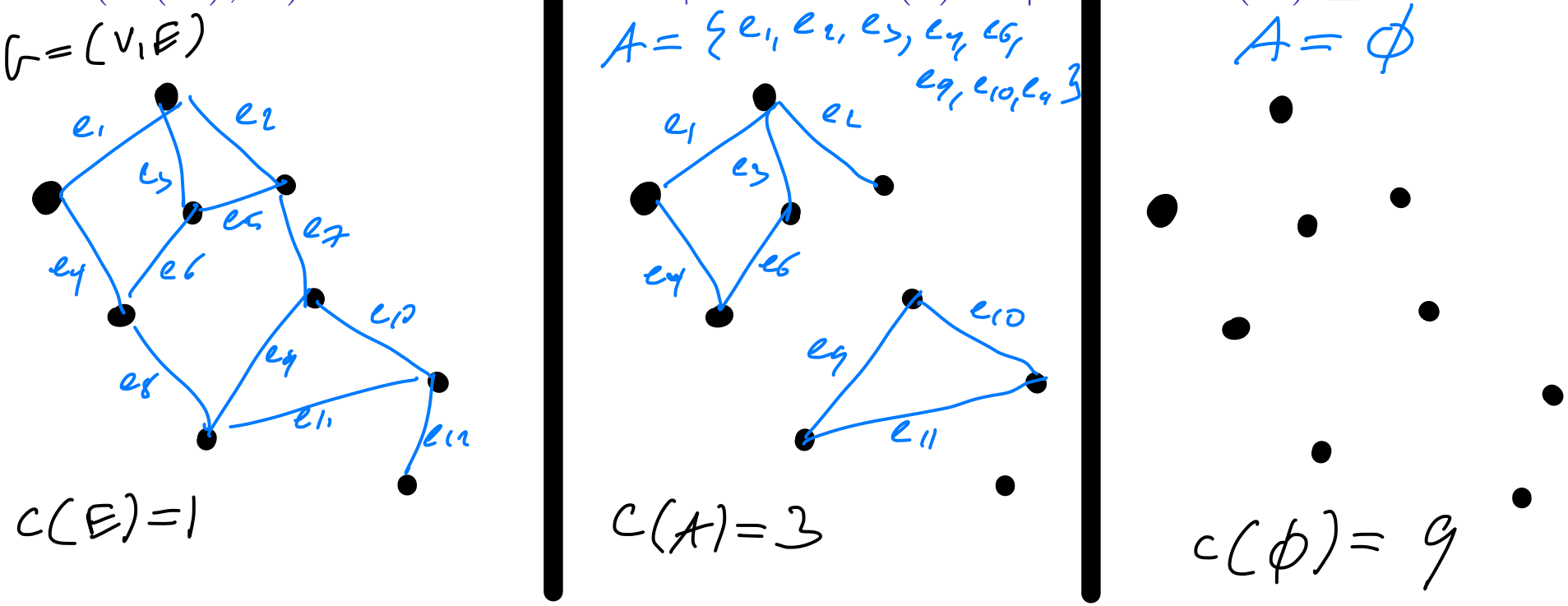

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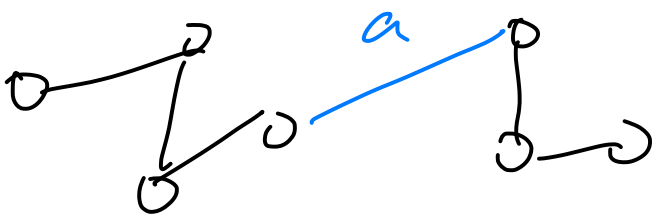

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- $\bar{c}(A) = c(E \setminus A)$ is number of connected components in G when we remove A; supermodular monotone non-decreasing but not normalized.

$c(\phi) \geq 1$

Graph Strength

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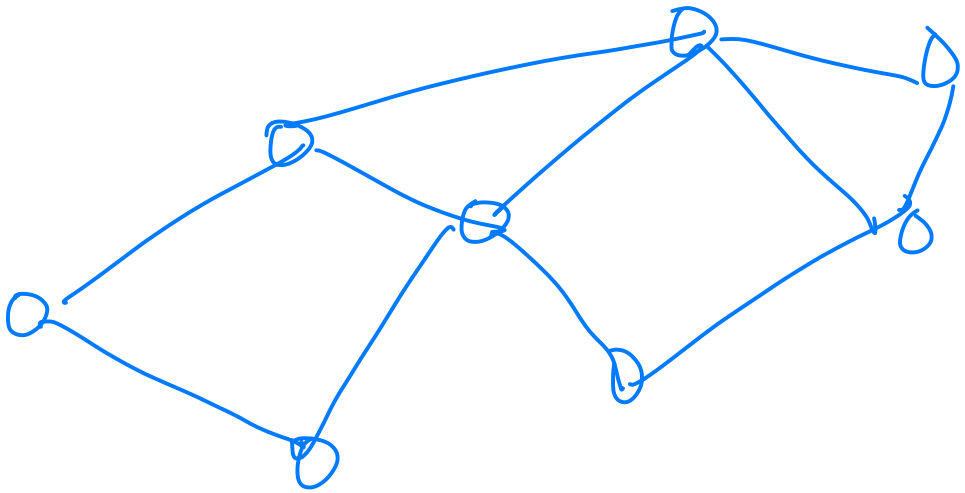

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so that $w(E(G[S]))$ is the "internal strength" of the vertex set S.
Notation: S is a set of nodes, $G[S]$ is the vertex-induced subgraph of G induced by vertices S, $E(G[S])$ are the edges contained within this induced subgraph, and $w(E(G[S]))$ is the weight of these edges. $w(E(G[S])) = \sum_{i,j \in S} w(i,j)$.

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$\forall \lambda \geq 0$

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- Since submodularity, problems have strongly-poly-time solutions.

Submodularity, Quadratic Structures, and Cuts

Lemma 3.5.4

Let $\mathbf{M} \in \mathbb{R}^{n \times n}$ *be a symmetric matrix and* $m \in \mathbb{R}^n$ *be a vector. Then* $f : 2^V \to \mathbb{R}$ *defined as*

$$f(X) = m^\intercal \mathbf{1}_X + \frac{1}{2}\mathbf{1}_X^\intercal \mathbf{M}\mathbf{1}_X \tag{3.45}$$

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- f is a modular function $m^\intercal \mathbf{1}_A = m(A)$ added to a weighted submodular function, hence f is submodular.

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Proof of Lemma 3.5.4 cont.

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- This requires:

$$0 \leq f(\{u\}) + f(\{v\}) - f(\{u, v\}) \tag{3.46}$$

$$= m(u) + \frac{1}{2}M_{u,u} + m(v) + \frac{1}{2}M_{v,v} \tag{3.47}$$

$$- \left(m(u) + m(v) + \frac{1}{2}M_{u,u} + M_{u,v} + \frac{1}{2}M_{v,v}\right) \tag{3.48}$$

$$= -M_{u,v} \tag{3.49}$$

So that $\forall u, v \in V$, $M_{u,v} \leq 0$.

□

Set Cover and Maximum Coverage

just Special cases of Submodular Optimization

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Set Cover and Maximum Coverage

just Special cases of Submodular Optimization

- We are given a finite set U of m elements and a set of subsets $\mathcal{U} = \{U_1, U_2, \dots, U_n\}$ of n subsets of U, so that $U_i \subseteq U$ and $\bigcup_i U_i = U$.
- The goal of minimum set cover is to choose the smallest subset $A \subseteq [n] \triangleq \{1, \dots, n\}$ such that $\bigcup_{a \in A} U_a = U$.
- Maximum k cover: The goal in maximum coverage is, given an integer $k \leq n$, select k subsets, say $\{a_1, a_2, \dots, a_k\}$ with $a_i \in [n]$ such that $|\bigcup_{i=1}^k U_{a_i}|$ is maximized.
- $f : 2^{[n]} \to \mathbb{Z}_+$ where for $A \subseteq [n]$, $f(A) = |\bigcup_{a \in A} U_a|$ is the set cover function and is submodular.
- Weighted set cover: $f(A) = w(\bigcup_{a \in A} U_a)$ where $w : U \to \mathbb{R}_+$.
- Both Set cover and maximum coverage are well known to be NP-hard, but have a fast greedy approximation algorithm, and hence are instances of submodular optimization.

Vertex and Edge Covers

Also instances of submodular optimization

Definition 3.5.5 (vertex cover)

A *vertex cover* (a "vertex-based cover of edges") in graph $G = (V, E)$ is a set $S \subseteq V(G)$ of vertices such that every edge in G is incident to at least one vertex in S.

- Let $I(S)$ be the number of edges incident to vertex set S. Then we wish to find the smallest set $S \subseteq V$ subject to $I(S) = |E|$.

Definition 3.5.6 (edge cover)

A *edge cover* (an "edge-based cover of vertices") in graph $G = (V, E)$ is a set $F \subseteq E(G)$ of edges such that every vertex in G is incident to at least one edge in F.

- Let $|V|(F)$ be the number of vertices incident to edge set F. Then we wish to find the smallest set $F \subseteq E$ subject to $|V|(F) = |V|$.

Graph Cut Problems

Also submodular optimization

- Minimum cut: Given a graph $G = (V, E)$, find a set of vertices $S \subseteq V$ that minimize the cut (set of edges) between S and $V \setminus S$.

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- Let $\delta : 2^V \to \mathbb{R}_+$ be the cut function, namely for any given set of nodes $X \subseteq V$, $|\delta(X)|$ measures the number of edges between nodes X and $V \setminus X$ — i.e., $\delta(x) = E(X, V \setminus X)$.

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- Weighted versions, where rather than count, we sum the (non-negative) weights of the edges of a cut, $f(X) = w(\delta(X))$.
- Hence, Minimum cut and Maximum cut are also special cases of submodular optimization.

Matrix Rank functions

- Let V, with $|V| = m$ be an index set of a set of vectors in $\mathbb{R}^n$ for some n (unrelated to m). Thus, $\forall v \in V$, $\exists x_v \in \mathbb{R}^n$.

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- For a given set $\{v, v_1, v_2, \ldots, v_k\}$, it might or might not be possible to find $(\alpha_i)_i$ such that:

$$x_v = \sum_{i=1}^{k} \alpha_i x_{v_i} \tag{3.50}$$

If not, then x_v is linearly independent of $x_{v_1}, \ldots, x_{v_k}$.

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  If not, then x_v is linearly independent of $x_{v_1}, \ldots, x_{v_k}$.
- Let $r(S)$ for $S \subseteq V$ be the rank of the set of vectors S. Then $r(\cdot)$ is a submodular function, and in fact is called a matric matroid rank function.

Example: Rank function of a matrix

- Given $n \times m$ matrix $\mathbf{X} = (x_1, x_2, \ldots, x_m)$ with $x_i \in \mathbb{R}^n$ for all i. There are m length-n column vectors $\{x_i\}_i$

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- $r(A)$ is the dimensionality of the vector space spanned by the set of vectors $\{x_a\}_{a \in A}$.
- Thus, $r(V)$ is the rank of the matrix $\mathbf{X}$.

Skip matrix rank example

Example: Rank function of a matrix

Consider the following 4×8 matrix, so $V = \{1, 2, 3, 4, 5, 6, 7, 8\}$.

$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} \\ \begin{pmatrix} 0 & 2 & 2 & 3 & 0 & 1 & 3 & 1 \\ 0 & 3 & 0 & 4 & 0 & 0 & 2 & 4 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & 5 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 & 5 \end{pmatrix} \end{array} = \begin{array}{c} \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} \\ \begin{pmatrix} | & | & | & | & | & | & | & | \\ x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \\ | & | & | & | & | & | & | & | \end{pmatrix} \end{array}$$

- Let $A = \{1, 2, 3\}$, $B = \{3, 4, 5\}$, $C = \{6, 7\}$, $A_r = \{1\}$, $B_r = \{5\}$.
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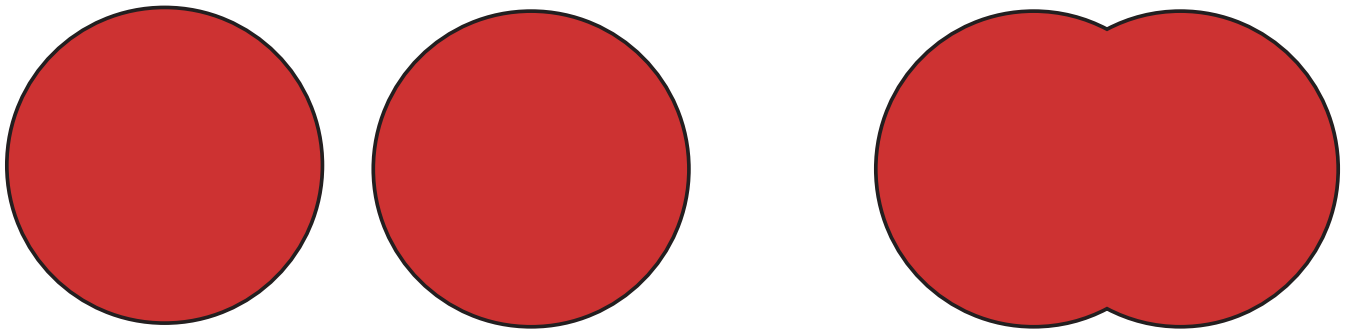

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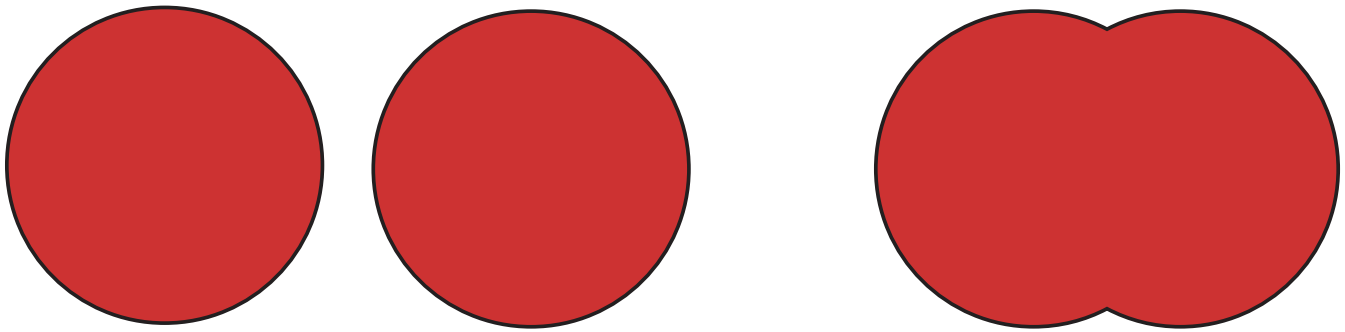

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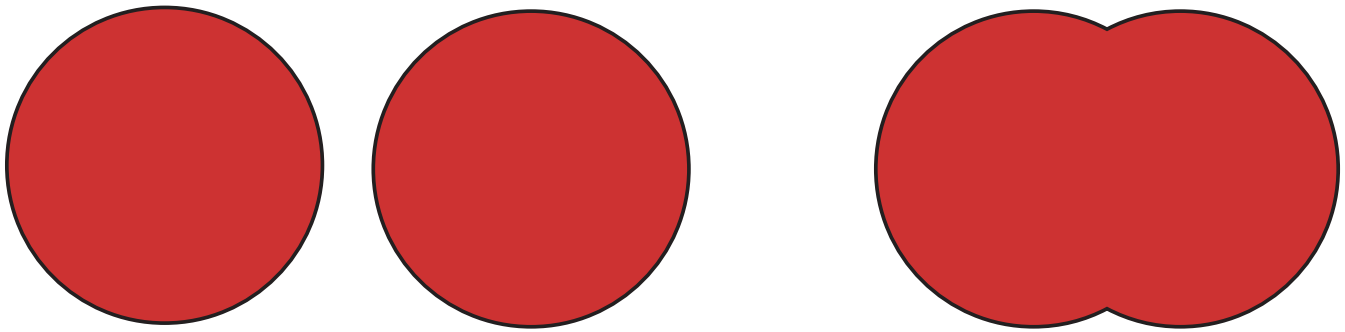

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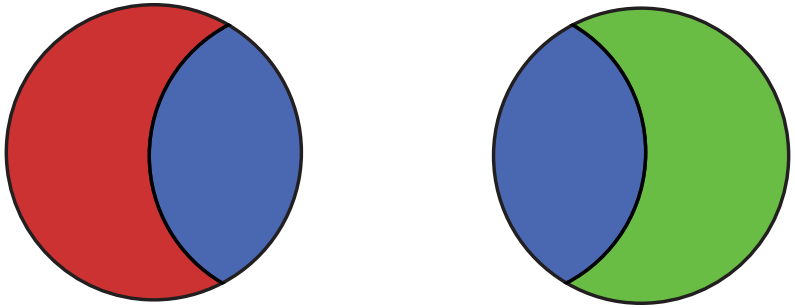

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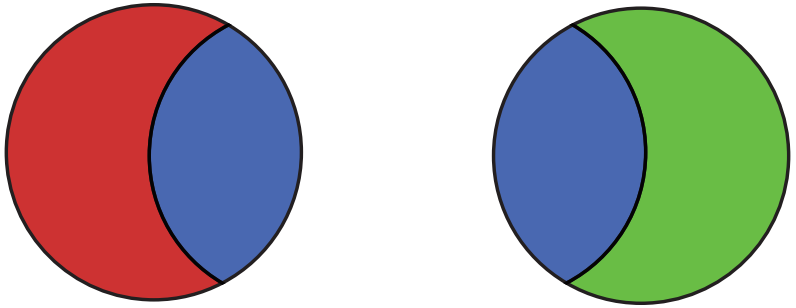

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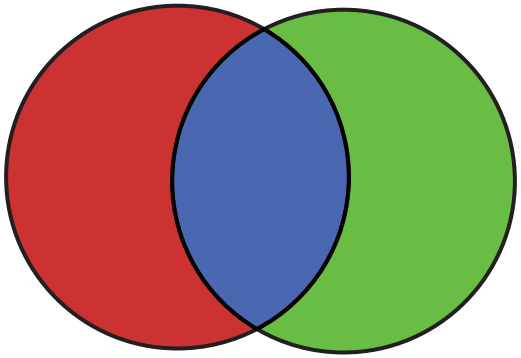

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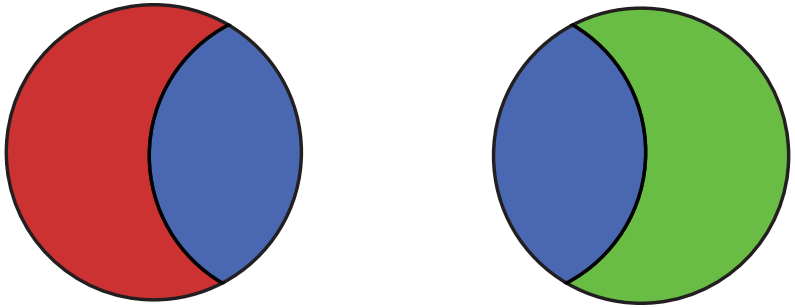

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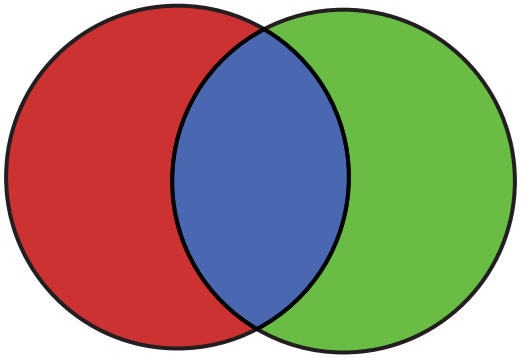

- Thus, we have subadditivity: $r(A) + r(B) \geq r(A \cup B)$. Can we add more to the r.h.s. and still have an inequality? Yes.

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- Note, $r(A \cap B) \leq r(C)$. Why? Vectors indexed by $A \cap B$ (i.e., the common index set) span no more than the dimensions commonly spanned by A and B (namely, those spanned by the professed C).

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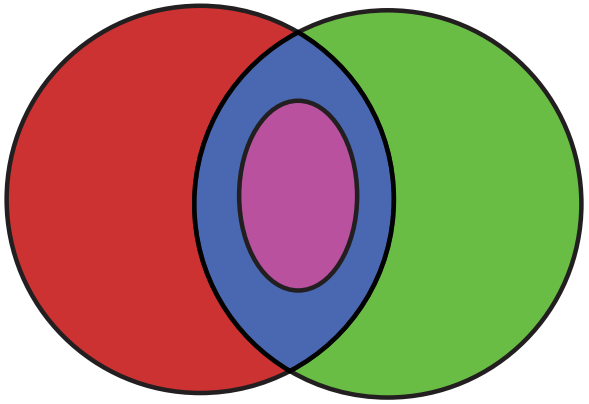

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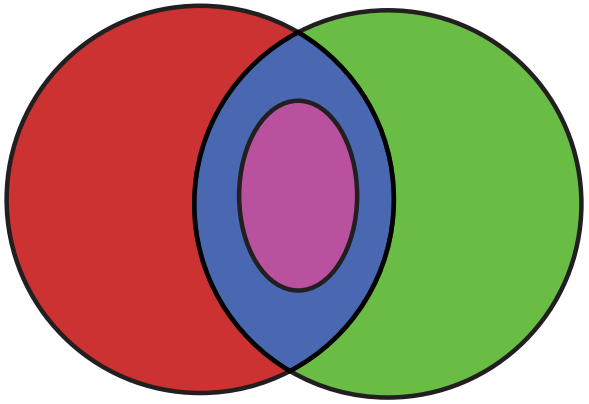

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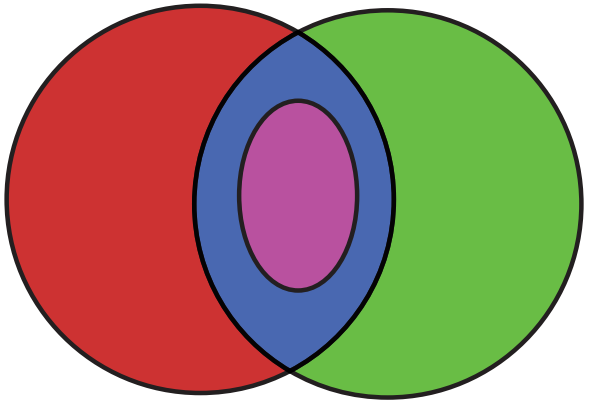

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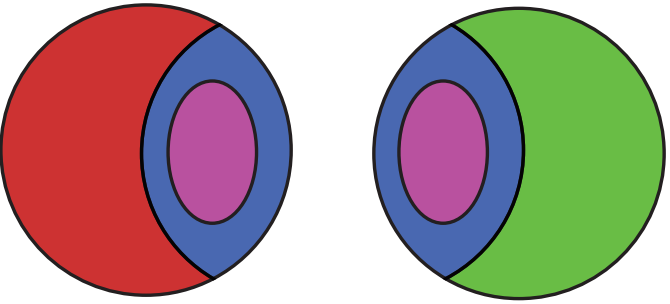
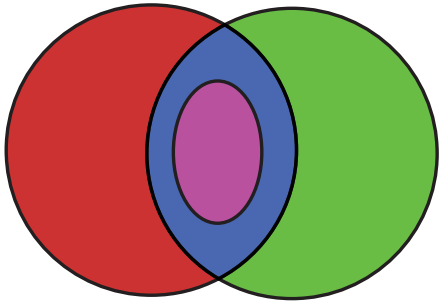
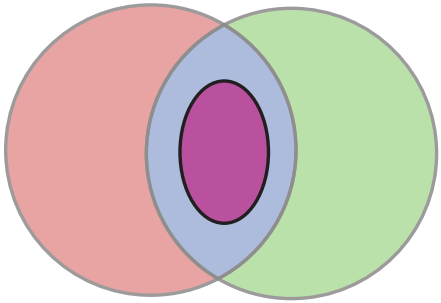
- More generally, common information (blue) is "more" (no less) than information within common index (magenta).

The Venn and Art of Submodularity

$$\underbrace{r(A) + r(B)}_{= r(A_r) + 2r(C) + r(B_r)} \geq \underbrace{r(A \cup B)}_{= r(A_r) + r(C) + r(B_r)} + \underbrace{r(A \cap B)}_{= r(A \cap B)}$$







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- We can think of S as a set of sets of vectors from the matrix rank example, and for each $s \in S$, let X_s being a set of vector indices.

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- Let S be a set of subspaces of a linear space (i.e., each $s \in S$ is a subspace of dimension ≥ 1).
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- In general (as we will see) polymatroid rank functions are submodular, normalized $f(\emptyset) = 0$, and monotone non-decreasing ($f(A) \leq f(B)$ whenever $A \subseteq B$).
- We use the term non-decreasing rather than increasing, the latter of which is strict (also so that a constant function isn't "increasing").

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- Let E be a set of edges of some graph $G = (V, E)$, and let $r(S)$ for $S \subseteq E$ be the maximum size (in terms of number of **edges**) spanning forest in the graph induced by edges S.

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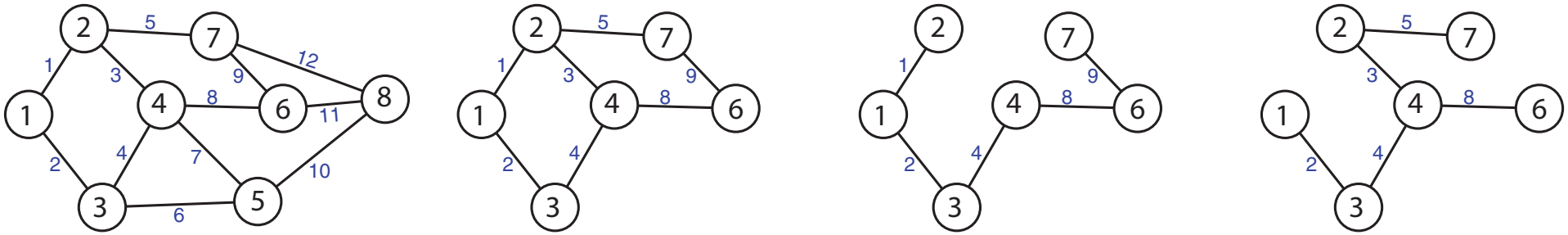

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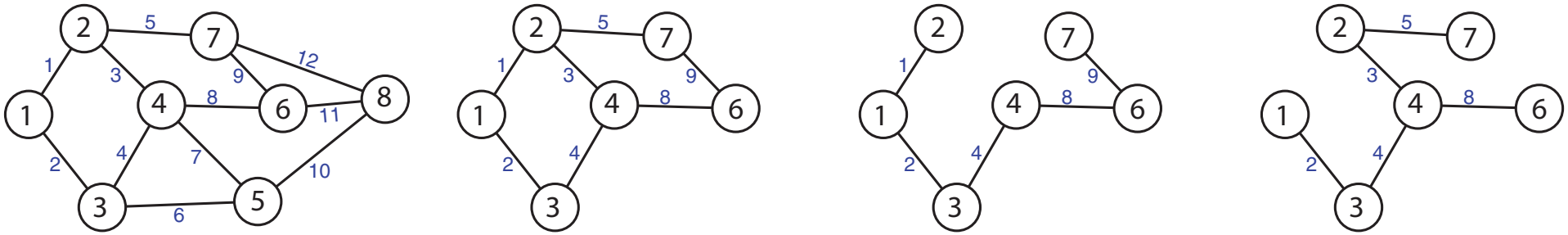

- Then $r(S)$ is submodular, and is another matrix rank function corresponding to the incidence matrix of the graph.

Summing Submodular Functions

Given E, let $f_1, f_2 : 2^E \to \mathbb{R}$ be two submodular functions. Then

$$f : 2^E \to \mathbb{R} \text{ with } f(A) = f_1(A) + f_2(A) \tag{3.58}$$

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I.e., it holds for each component of f in each term in the inequality. In fact, any conic combination (i.e., non-negative linear combination) of submodular functions is submodular, as in $f(A) = \alpha_1 f_1(A) + \alpha_2 f_2(A)$ for $\alpha_1, \alpha_2 \geq 0$.

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That is, the modular component with $m(A) + m(B) = m(A \cup B) + m(A \cap B)$ never destroys the inequality. Note of course that if m is modular than so is $-m$.

Restricting Submodular functions

Given E, let $f : 2^E \to \mathbb{R}$ be a submodular functions. And let $S \subseteq E$ be an arbitrary fixed set. Then

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$$f(A' + v) - f(A') \geq f(B' + v) - f(B') \tag{3.68}$$

with $A' = A \cap S$ and $B' = B \cap S$. Since $A' \subseteq B'$, this holds due to submodularity of f. □

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Given V, let $f_1, f_2 : 2^V \to \mathbb{R}$ be two submodular functions and let $S_1, S_2 \subseteq V$ be two arbitrary fixed sets. Then

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Given V, let $\mathcal{C} = \{C_1, C_2, \ldots, C_k\}$ be a set of subsets of V, and for each $C \in \mathcal{C}$, let $f_C : 2^V \to \mathbb{R}$ be a submodular function. Then

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is submodular. This property is critical for image processing and graphical models. For example, let $\mathcal{C}$ be all pairs of the form $\{\{u, v\} : u, v \in V\}$, or let it be all pairs corresponding to the edges of some undirected graphical model.

Max - normalized

Given V, let $c \in \mathbb{R}_+^V$ be a given fixed vector. Then $f : 2^V \to \mathbb{R}_+$, where

$$f(A) = \max_{j \in A} c_j \tag{3.71}$$

is submodular and normalized (we take $f(\emptyset) = 0$).

Proof.

Consider

$$\max_{j \in A} c_j + \max_{j \in B} c_j \geq \max_{j \in A \cup B} c_j + \max_{j \in A \cap B} c_j \tag{3.72}$$

which follows since we have that

$$\max(\max_{j \in A} c_j, \max_{j \in B} c_j) = \max_{j \in A \cup B} c_j \tag{3.73}$$

and

$$\min(\max_{j \in A} c_j, \max_{j \in B} c_j) \geq \max_{j \in A \cap B} c_j \tag{3.74}$$

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Max

Given V, let $c \in \mathbb{R}^V$ be a given fixed vector (not necessarily non-negative). Then $f : 2^V \to \mathbb{R}$, where

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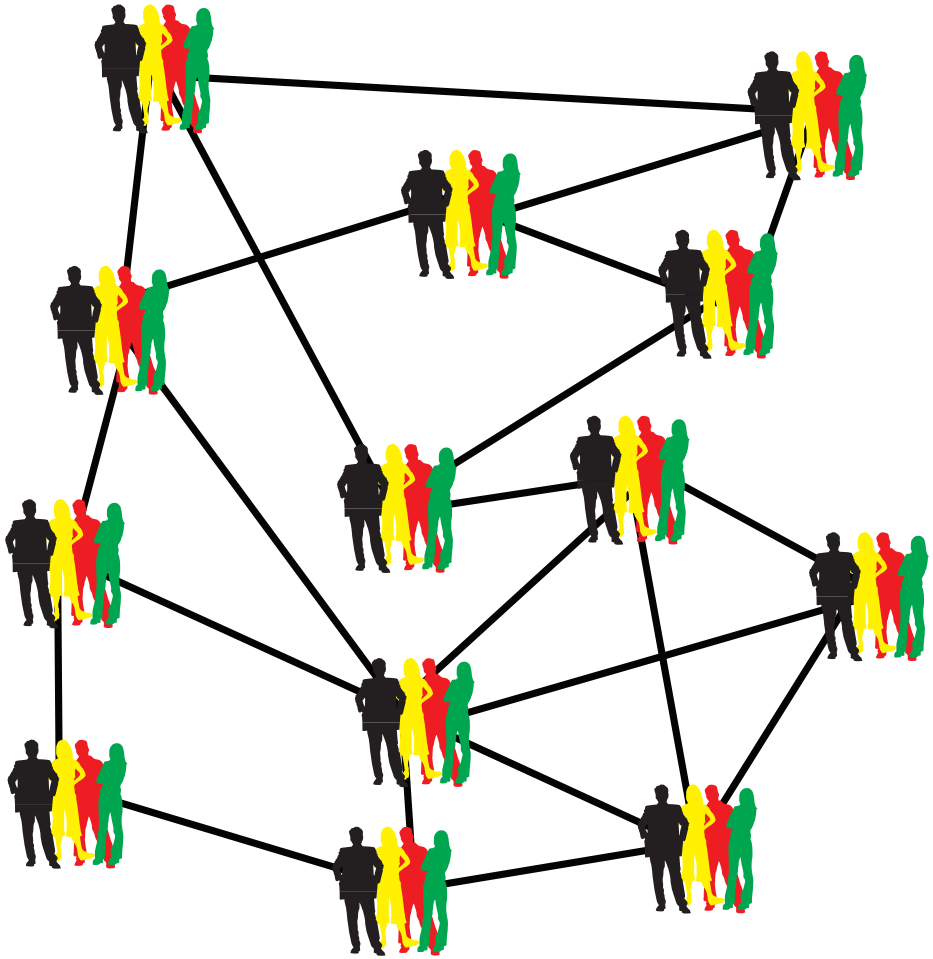
is submodular, where we take $f(\emptyset) \leq \min_j c_j$ (so the function need not be normalized).

Proof.

The proof is identical to the normalized case. □

Facility/Plant Location (uncapacitated)

- Core problem in operations research, early motivation for submodularity.
- Goal: as efficiently as possible, place "facilities" (factories) at certain locations to satisfy sites (at all locations) having various demands.



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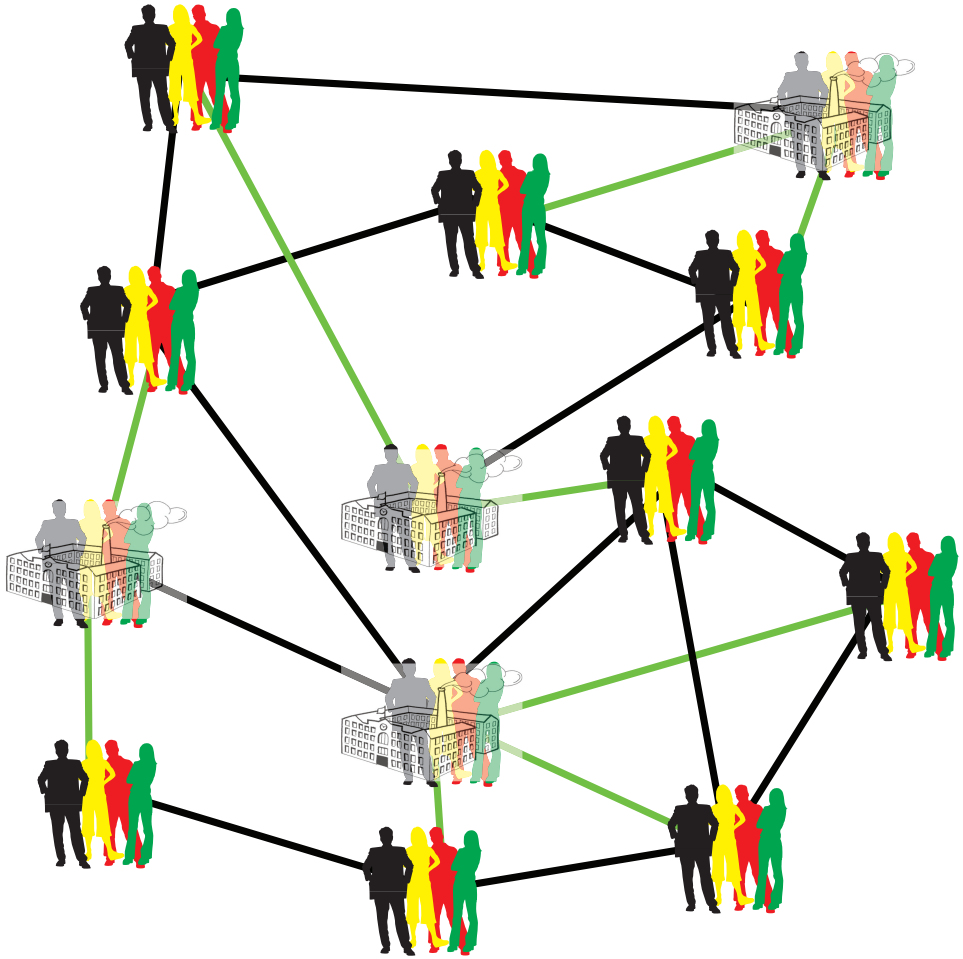

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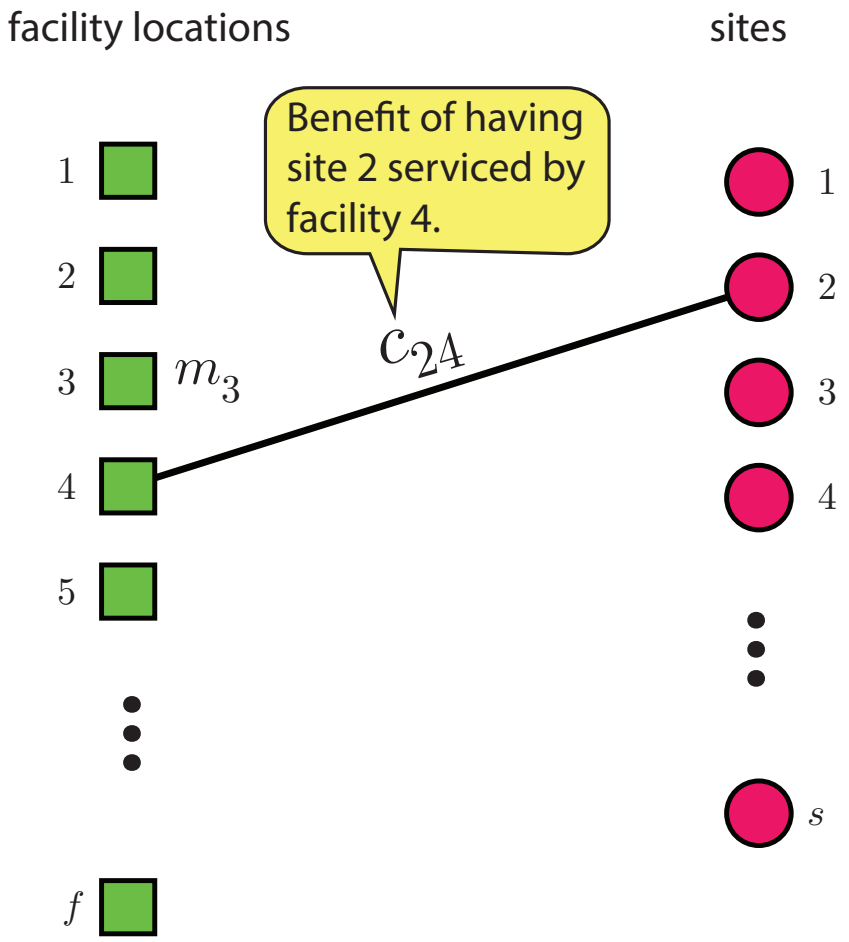
- We can model this with a weighted bipartite graph $G = (F, S, E, c)$ where F is set of possible factory/plant locations, S is set of sites needing service, E are edges indicating (factory,site) service possibility pairs, and $c : E \to \mathbb{R}_+$ is the benefit of a given pair.
- Facility location function has form:

$$f(A) = \sum_{i \in S} \max_{j \in A} c_{ij}. \qquad (3.76)$$



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- Goal is to find a set A that maximizes $f(A)$ (the benefit) placing a bound on the number of plants A (e.g., $|A| \leq k$).

Facility Location

Given V, E, let $c \in \mathbb{R}^{V \times E}$ be a given $|V| \times |E|$ matrix. Then

$$f : 2^E \to \mathbb{R}, \text{ where } f(A) = \sum_{i \in V} \max_{j \in A} c_{ij} \tag{3.78}$$

is submodular.

Proof.

We can write $f(A)$ as $f(A) = \sum_{i \in V} f_i(A)$ where $f_i(A) = \max_{j \in A} c_{ij}$ is submodular (max of a ith row vector), so f can be written as a sum of submodular functions. □

Thus, the facility location function (which only adds a modular function to the above) is submodular.

Log Determinant

- Let $\mathbf{\Sigma}$ be an $n \times n$ positive definite matrix. Let $V = \{1, 2, \ldots, n\} \equiv [n]$ be an index set, and for $A \subseteq V$, let $\mathbf{\Sigma}_A$ be the (square) submatrix of $\mathbf{\Sigma}$ obtained by including only entries in the rows/columns given by A.

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Proof of submodularity of the logdet function.

Suppose $X \in \mathbf{R}^n$ is multivariate Gaussian random variable, that is

$$x \in p(x) = \frac{1}{\sqrt{|2\pi\mathbf{\Sigma}|}} \exp\left(-\frac{1}{2}(x-\mu)^T \mathbf{\Sigma}^{-1}(x-\mu)\right) \tag{3.80}$$

...

Log Determinant

...cont.

Then the (differential) entropy of the r.v. X is given by

$$h(X) = \log \sqrt{|2\pi e \mathbf{\Sigma}|} = \log \sqrt{(2\pi e)^n |\mathbf{\Sigma}|} \tag{3.81}$$

and in particular, for a variable subset A,

$$f(A) = h(X_A) = \log \sqrt{(2\pi e)^{|A|} |\mathbf{\Sigma}_A|} \tag{3.82}$$

Entropy is submodular (further conditioning reduces entropy), and moreover

$$f(A) = h(X_A) = m(A) + \frac{1}{2} \log |\mathbf{\Sigma}_A| \tag{3.83}$$

where $m(A)$ is a modular function. □

Note: still submodular in the semi-definite case as well.

Summary: Properties so far

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- max is submodular $f(A) = \max_{j \in A} c_j$, as is facility location $f(A) = \sum_{u \in U} \max_{a \in A} s_{a,u}$.

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