Submodular Functions, Optimization, and Applications to Machine Learning

— Fall Quarter, Lecture 4 —

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

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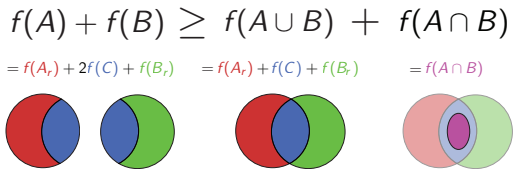
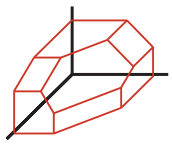
Oct 12th, 2020





Announcements, Assignments, and Reminders

- Homework 1 is out, due Friday at 11:59pm.

Class Road Map - EE563

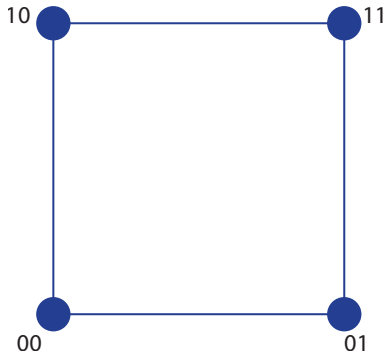
- L1(9/30): Motivation, Applications, Definitions, Properties
- L2(10/5): Sums concave(modular), uses (diversity/costs, feature selection), information theory
- L3(10/7): Monge, More Definitions, Graph and Combinatorial Examples,
- L4(10/12): Graph & Combinatorial Examples, Matrix Rank, Properties, Other Defs, Independence
- 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

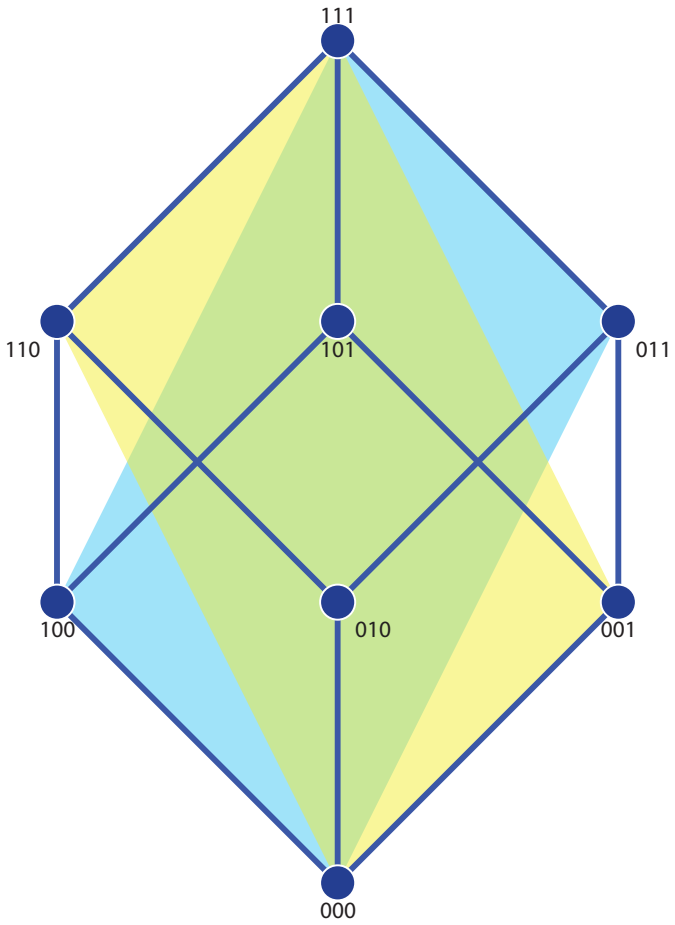
The Submodular Square, and Hypercube Vertices

We can test submodularity via values on vertices of hypercube.

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



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 4.2.1 (subadditive)

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

$$f(A) + f(B) \geq f(A \cup B) \tag{4.7}$$

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

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- This means that the "whole" is greater than the sum of the parts.
- In general, submodular and subadditive (and supermodular and superadditive) are different properties.
- Ex: Let $0 < k < |V|$, and consider $f : 2^V \to \mathbb{R}_+$ where:

$$f(A) = \begin{cases} 1 & \text{if } |A| \leq k \\ 0 & \text{else} \end{cases} \tag{4.8}$$

- This function is subadditive but not submodular.

Modular Definitions

Definition 4.2.1 (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

$$f(A) + f(B) = f(A \cap B) + f(A \cup B) \tag{4.7}$$

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

Proposition 4.2.2

If f is modular, it may be written as

$$f(A) = f(\emptyset) + \sum_{a \in A} \Big(f(\{a\}) - f(\emptyset) \Big) = c + \sum_{a \in A} f'(a) \tag{4.8}$$

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

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 4.2.1

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

Proof.

$$\bar{f}(A) + \bar{f}(B) \geq \bar{f}(A \cup B) + \bar{f}(A \cap B) \tag{4.12}$$

follows from

$$f(V \setminus A) + f(V \setminus B) \geq f(V \setminus (A \cup B)) + f(V \setminus (A \cap B)) \tag{4.13}$$

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). □

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.
- Let $E(S)$ be the edges with both vertices in $S \subseteq V(G)$. Then $|E(S)|$ (the interior edge function) is supermodular.
- Let $I(S)$ be the edges with at least one vertex in $S \subseteq V(G)$. Then $|I(S)|$ (the incidence function) is submodular.
- Recall $|\delta(S)|$, is the number of edges with exactly one vertex in $S \subseteq V(G)$ is submodular (cut function). Thus, we have $I(S) = E(S) \cup \delta(S)$ and $E(S) \cap \delta(S) = \emptyset$, and thus that $|I(S)| = |E(S)| + |\delta(S)|$. So we can get a submodular function by summing a submodular and a supermodular function. If you had to guess, is this always the case?
- 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 $\bar{f}(S) = f(V \setminus S)$.
- Hence, if $g : 2^V \to \mathbb{R}$ is supermodular, then so is $\bar{g} : 2^V \to \mathbb{R}$ defined as $\bar{g}(S) = g(V \setminus S)$.
- Given a graph $G = (V, E)$, for each $A \subseteq E(G)$, let $c(A)$ denote the number of connected components of the (spanning) subgraph $(V(G), A)$, with $c : 2^E \to \mathbb{R}_+$. Thus, $c(\emptyset) = |V|$, and $c(E) \geq 1$.
- $c(A)$ is monotone non-increasing, $c(A + a) - c(A) \leq 0$.
- Then $c(A)$ is supermodular, i.e.,
$$c(A + a) - c(A) \leq c(B + a) - c(B) \tag{4.26}$$
with $A \subseteq B \subseteq E \setminus \{a\}$.
- Intuition: an edge is "more" (no less) able to bridge separate components (and reduce the number of connected components) when edge is added in a smaller context than when added in a larger context.
- $\bar{c}(A) = c(E \setminus A)$ is number of connected components in G when we remove A; supermodular monotone non-decreasing but not normalized.

Graph Strength

- Then $w(A)$ for $A \subseteq E$ is a modular function

$$w(A) = \sum_{e \in A} w_e \tag{4.26}$$

  so that $w(E(G[S]))$ is the "internal strength" of the vertex set S.
- Suppose removing A shatters G into a graph with $\bar{c}(A) > 1$ components — then $w(A)/(\bar{c}(A) - 1)$ is like the "effort per achieved/additional component" for a network attacker.
- A form of graph strength can then be defined as the following:

$$\textit{strength}(G, w) \triangleq \min_{A \subseteq E(G): \bar{c}(A) > 1} \frac{w(A)}{\bar{c}(A) - 1} \tag{4.27}$$

- Graph strength is like the minimum effort per component. An attacker would use the argument of the min to choose which edges to attack. A network designer would maximize, over G and/or w, the graph strength, *strength*(G, w).
- Since submodularity, problems have strongly-poly-time solutions.

Quadratic forms

- Consider $\phi : \mathbb{R}^n \to R$ with

$$\phi(x) = \langle m, x \rangle + \frac{1}{2} x^\intercal M x \tag{4.1}$$

M is an nxn matrix

Quadratic forms

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Quadratic forms

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$$\phi(x) = \langle m, x \rangle + \frac{1}{2} x^\intercal M x \tag{4.1}$$

- $\phi(x)$ is convex iff M is symmetric positive semidefinite (requiring all diagonal entries to be non-negative).
- $\phi(x)$ is concave iff M is symmetric negative semidefinite (requiring all diagonal entries to be non-positive)
- A matrix M with the requirement only of having non-positive off-diagonal entries could lead to a function that is either convex, concave, or neither. Exercise.

Submodularity, Quadratic Structures, and Cuts

Lemma 4.3.1

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*

$$f(X) = \overbrace{m^\intercal \mathbf{1}_X}^{m(X)} + \frac{1}{2}\mathbf{1}_X^\intercal \mathbf{M}\mathbf{1}_X \tag{4.2}$$

is submodular <u>*iff*</u> *the off-diagonal elements of* M *are non-positive.*

Proof.

1) diff. requirement on m then concave or convex.

2) latter, see how this is related to lattice theory & DR submodularity.

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Proof.

- Given a complete graph $G = (V, E)$, recall that $E(X)$ is the edge set with both vertices in $X \subseteq V(G)$, and that $|E(X)|$ is supermodular.

$$|E(X)| = \sum_{i,j \in X} 1$$

...

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- Given a complete graph $G = (V, E)$, recall that $E(X)$ is the edge set with both vertices in $X \subseteq V(G)$, and that $|E(X)|$ is supermodular.
- Non-negative modular weights $w^+ : E \to \mathbb{R}_+$, $w(E(X))$ is also supermodular, so $-w(E(X))$ is submodular.

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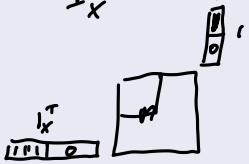
$1_X^T \cdot M \cdot 1_X = \sum_{i,j \in X} m_{ij}$

$$f(X) = m^\intercal \mathbf{1}_X + \frac{1}{2}\mathbf{1}_X^\intercal \mathbf{M} \mathbf{1}_X \tag{4.2}$$

$\| \quad \sum_{i,j \in X} m_{ij} = \sum_{\substack{i,j \in X \\ i \neq j}} m_{ij} + \sum_{i \in X} m_{ii}$



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- Non-negative modular weights $w^+ : E \to \mathbb{R}_+$, $w(E(X))$ is also supermodular, so $-w(E(X))$ is submodular.
- f is a modular function $m^\intercal \mathbf{1}_A = m(A)$ added to a weighted submodular function, hence f is submodular.

...

Submodularity, Quadratic Structures, and Cuts

Proof of Lemma 4.3.1 cont.

- Conversely, suppose f is submodular. Consider $u, v \in V$ with $u \neq v$.

$\square$

Submodularity, Quadratic Structures, and Cuts

Proof of Lemma 4.3.1 cont.

- Conversely, suppose f is submodular. Consider $u, v \in V$ with $u \neq v$.
- Then $f(\{u\}) + f(\{v\}) \geq f(\{u, v\}) + f(\emptyset)$ and $f(\emptyset) = 0$

$\square$

Submodularity, Quadratic Structures, and Cuts

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- Then $f(\{u\}) + f(\{v\}) \geq f(\{u, v\}) + f(\emptyset)$ and $f(\emptyset) = 0$ (note that $u = v$ would lead to a vacuous statement).
- This requires:

$$
\begin{aligned}
0 &\leq f(\{u\}) + f(\{v\}) - f(\{u, v\}) && (4.3)\\
&= m(u) + \frac{1}{2}M_{u,u} + m(v) + \frac{1}{2}M_{v,v} && (4.4)\\
&\quad - \left(m(u) + m(v) + \frac{1}{2}M_{u,u} + M_{u,v} + \frac{1}{2}M_{v,v}\right) && (4.5)\\
&= -M_{u,v} && (4.6)
\end{aligned}
$$

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

□

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 $\bigcup_i U_i = U$.

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- 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.

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- $f : 2^{[n]} \to \mathbb{Z}_+$ where for $A \subseteq [n]$, $f(A) = |\bigcup_{a \in A} U_a|$ is the set cover function and is submodular.

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$[n] = \{1, 2, 3, \ldots, n\}$

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- Weighted set cover: $f(A) = w(\bigcup_{a \in A} U_a)$ where $w : U \to \mathbb{R}_+$.

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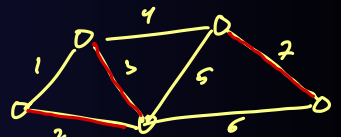
- Weighted set cover: $f(A) = w(\bigcup_{a \in A} U_a)$ where $w : U \to \mathbb{R}_+$.
- Both Set cover and maximum coverage are well known to be NP-hard, but have a fast greedy approximation algorithm, and hence are instances of submodular optimization.

Vertex and Edge Covers

Also instances of submodular optimization

$S = \{a, c, d\}$ is a vertex cover.



$A = \{4, 3, 7\}$ is an edge cover.

plastic cover, the plastic is doing the covering.

Definition 4.3.2 (vertex cover), the vertices are doing the covering.

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 4.3.3 (edge cover), the edge are doing the covering

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.

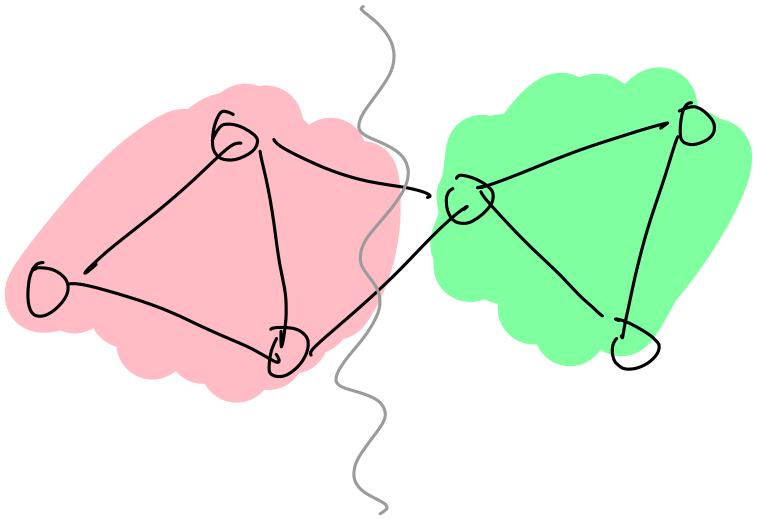
$|V(F)|$

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

Matrix Rank functions

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

x_{v_i}

$$x_v = \sum_{i=1}^{k} \alpha_i x_{v_i} \tag{4.7}$$

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

Matrix Rank functions

- Let V, with $|V| = n$ be an index set of a set of vectors in $\mathbb{R}^m$ for some m (unrelated to n). Thus, $\forall v \in V$, $\exists x_v \in \mathbb{R}^m$.
- For a given set $\{v, v_1, v_2, \dots, v_k\}$, it might or might not be possible to find $(\alpha_i)_i$ such that:

$$x_v = \sum_{i=1}^{k} \alpha_i x_{v_i} \tag{4.7}$$

  If not, then x_v is linearly independent of $x_{v_1}, \dots, x_{v_k}$.
- 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 $m \times n$ matrix $\mathbf{X} = (x_1, x_2, \ldots, x_n)$ with $x_i \in \mathbb{R}^m$ for all i. There are n length-m column vectors $\{x_i\}_i$

$$X = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & & | \end{bmatrix} \quad m$$

Skip matrix rank example

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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 $V = \{1, 2, 3, 4, 5, 6, 7, 8\}$. $m=4$ $n=8$

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

- Let $A = \{1, 2, 3\}$, $B = \{3, 4, 5\}$, $C = \{6, 7\}$, $A_r = \{1\}$, $B_r = \{5\}$.
- Then $r(A) = 3$, $r(B) = 3$, $r(C) = 2$.
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  C ~~is~~ spans the common spanned dimension of A & B.
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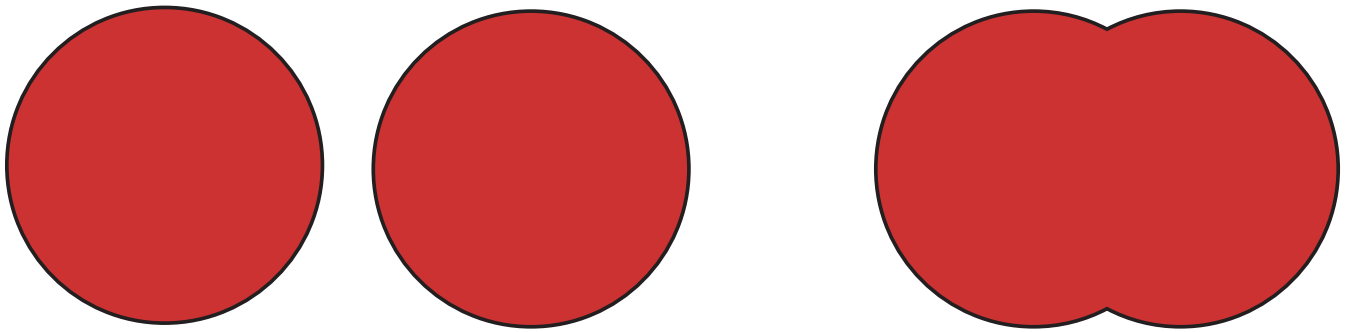

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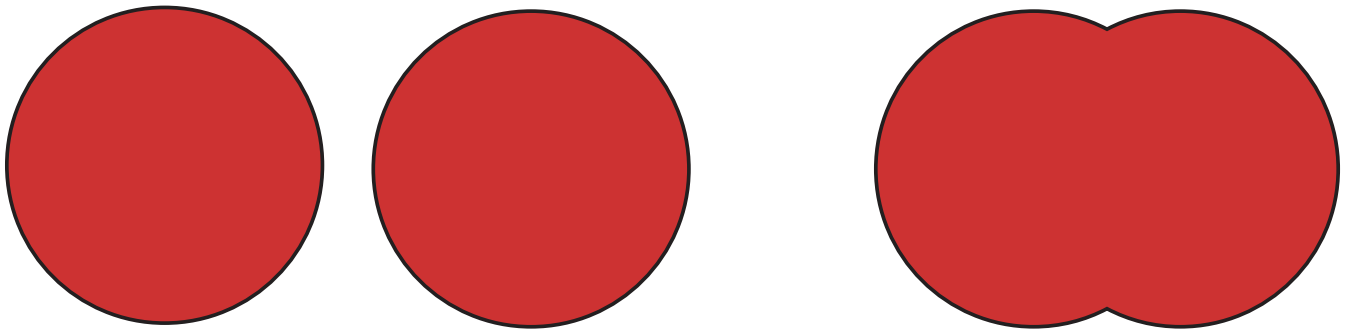

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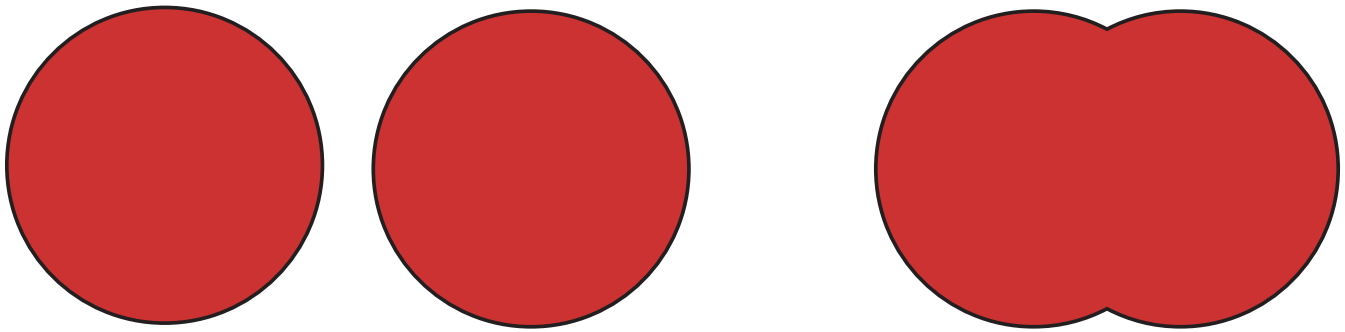

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- Any function where the above inequality is true for all $A, B \subseteq V$ is called subadditive.

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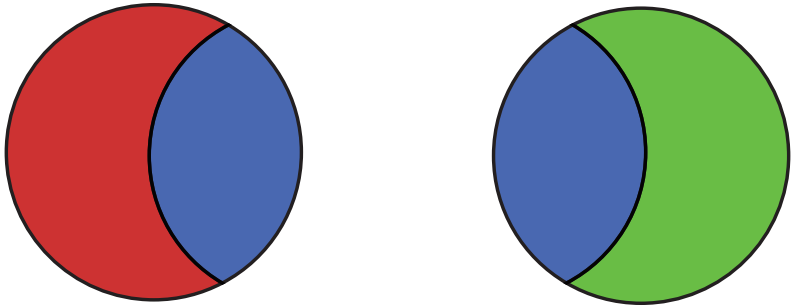

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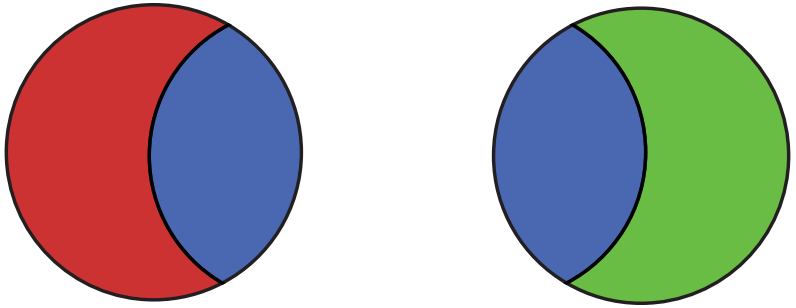

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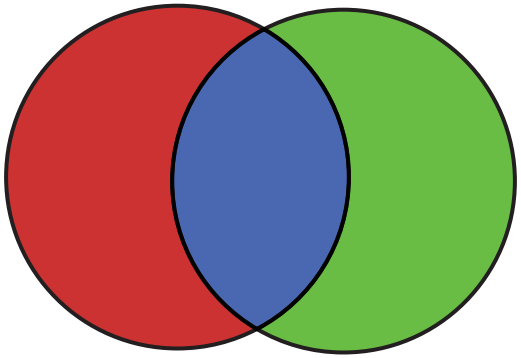

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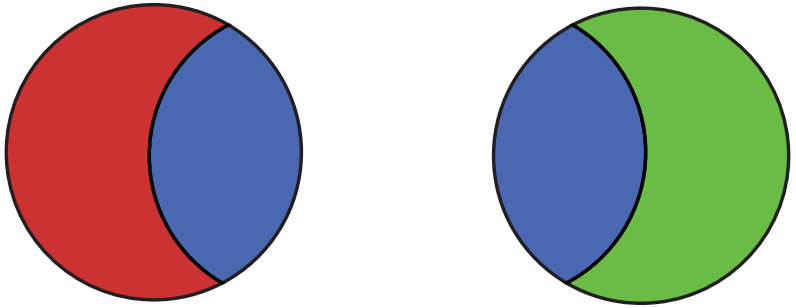

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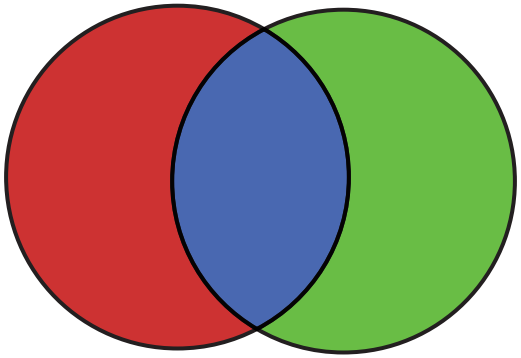

- Thus, we have subadditivity: $r(A) + r(B) \geq r(A \cup B)$. Can we add more to the r.h.s. and still have an inequality? Yes.

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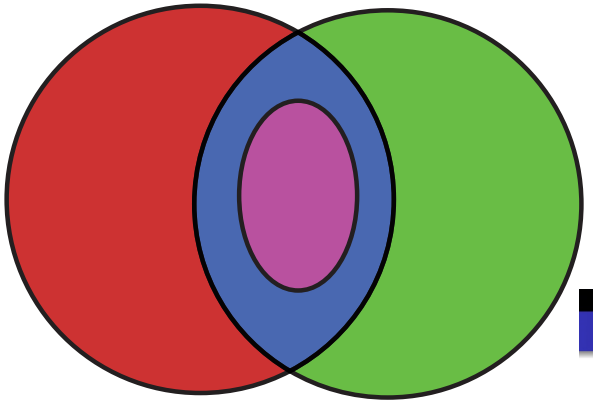

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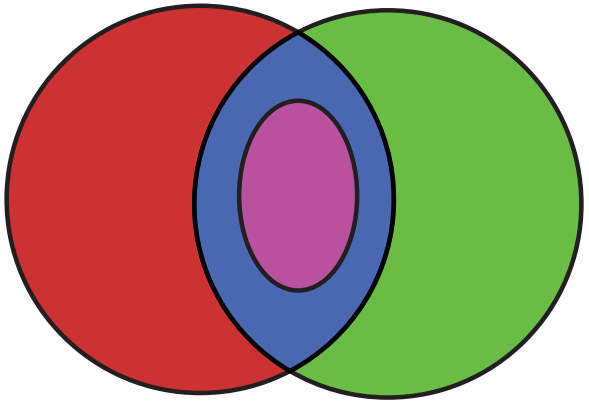

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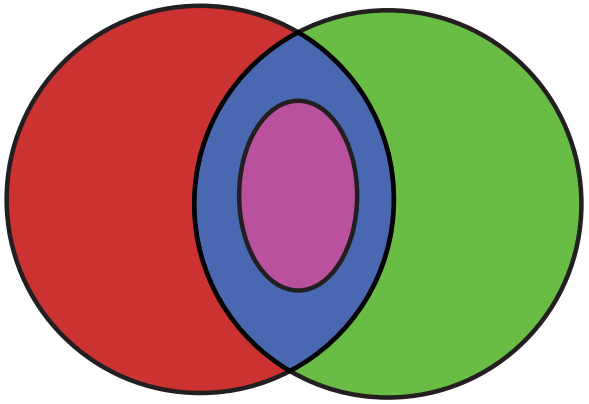

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The Venn and Art of Submodularity




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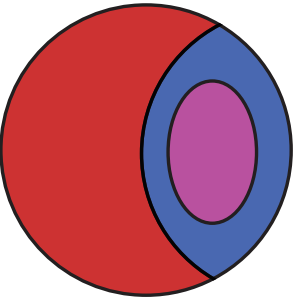
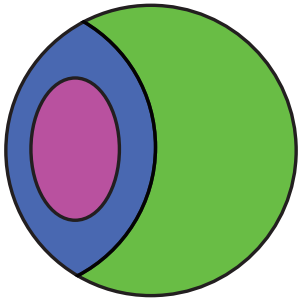
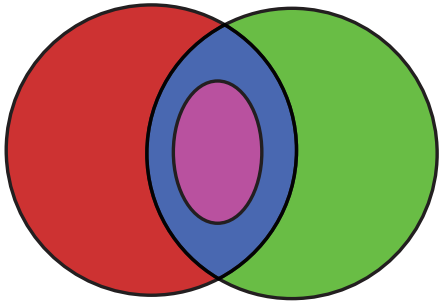
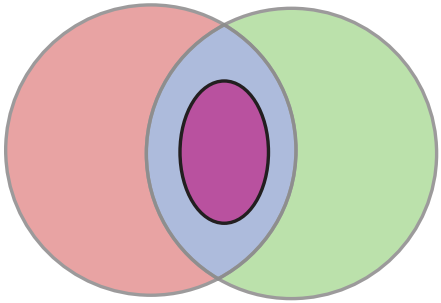

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$X \subseteq S$ $\quad X = \{ s_1, s_3 \}$

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- We use the term non-decreasing rather than increasing, the latter of which is strict (also so that a constant function isn't "increasing").

Spanning trees

- 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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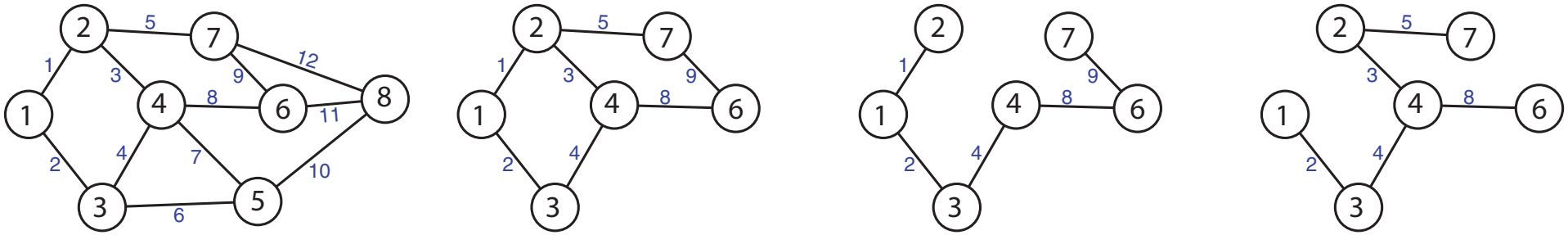

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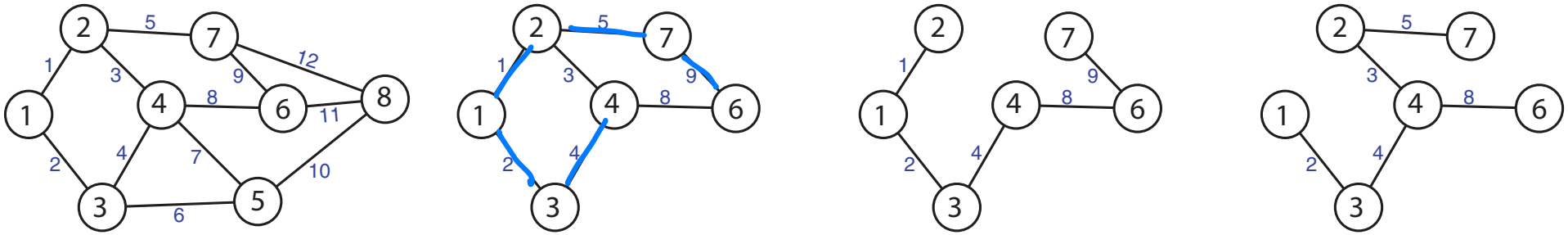

- Then $r(S)$ is submodular, and is another matrix rank function corresponding to the incidence matrix of the graph.

Summing Submodular Functions

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

$$f : 2^E \to \mathbb{R} \text{ with } f(A) = f_1(A) + f_2(A) \tag{4.15}$$

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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 $\alpha_1, \alpha_2 \geq 0$.

$$\sum_i \alpha_i f_i(A) = f(A)$$

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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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Given $A \subseteq B \subseteq E \setminus v$, consider

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If $v \notin S$, then both differences on each size are zero. If $v \in S$, then we can consider this

$$f(A' + v) - f(A') \geq f(B' + v) - f(B') \tag{4.25}$$

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

Summing Restricted Submodular Functions

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

$$f : 2^V \to \mathbb{R} \text{ with } f(A) = f_1(A \cap S_1) + f_2(A \cap S_2) \tag{4.26}$$

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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 $f_C : \cancel{2^V \to \mathbb{R}}$ be a submodular function. Then

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$$f(A) = \sum_{e=(u,v) \in E(G)} f_e(A \cap \{u,v\})$$

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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

$$f(A) = \max_{j \in A} c_j \tag{4.28}$$

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

Proof.

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

$$\max_{j \in A} c_j + \max_{j \in B} c_j \geq \max_{j \in A \cup B} c_j + \max_{j \in A \cap B} c_j \tag{4.29}$$

which follows since we have that

$$\max(\max_{j \in A} c_j, \max_{j \in B} c_j) = \max_{j \in A \cup B} c_j \tag{4.30}$$

and

$$\min(\max_{j \in A} c_j, \max_{j \in B} c_j) \geq \max_{j \in A \cap B} c_j \tag{4.31}$$

□

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

$$f(A) = \max_{j \in A} c_j \tag{4.32}$$

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)

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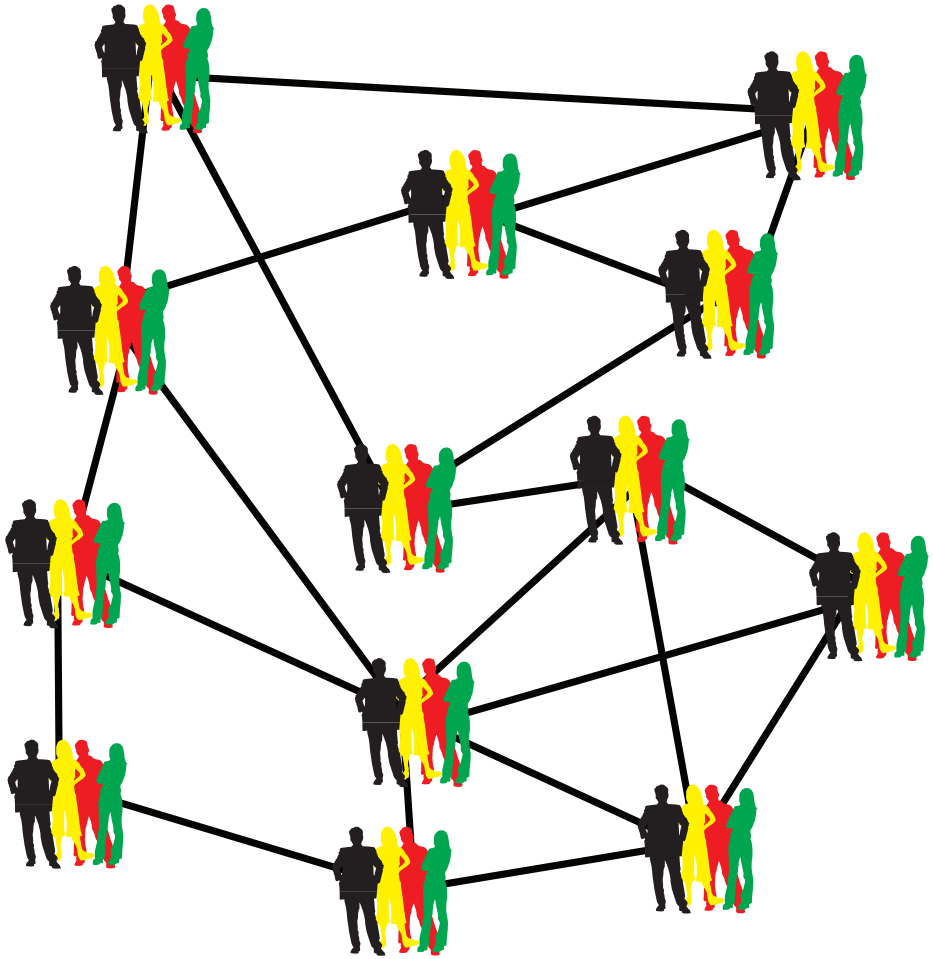
- Goal: as efficiently as possible, place "facilities" (factories) at certain locations to satisfy sites (at all locations) having various demands.



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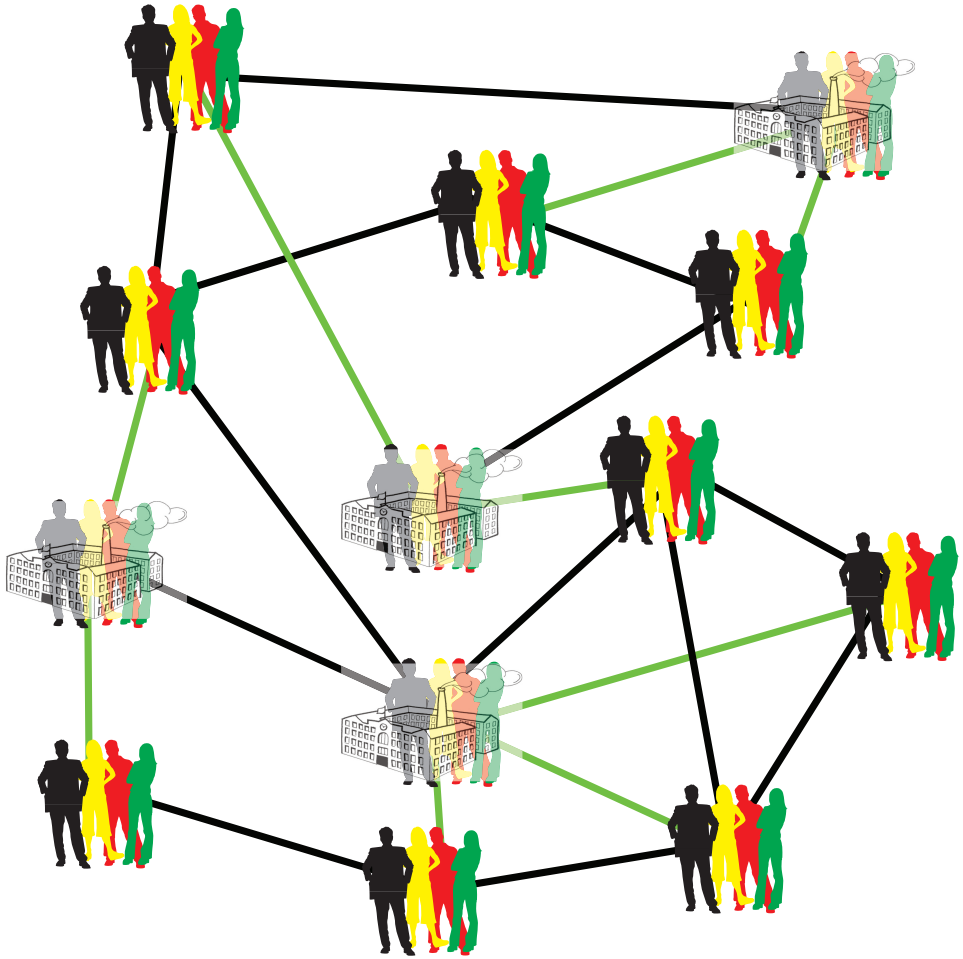

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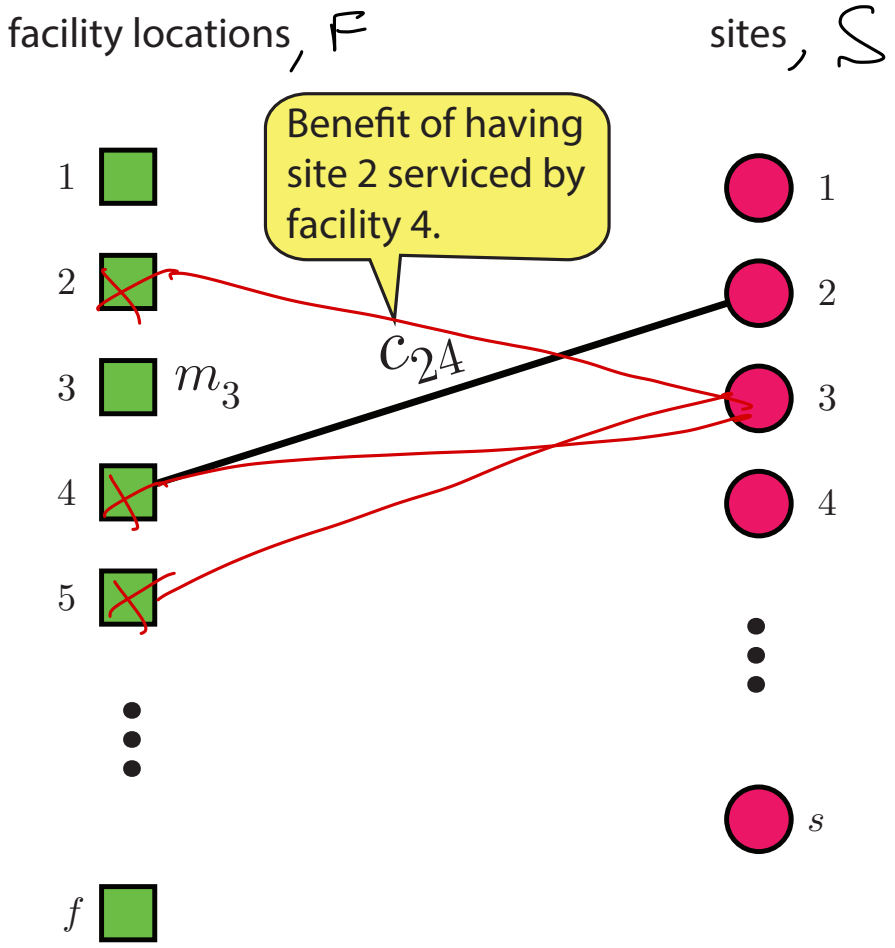
- We can model this with a weighted bipartite graph $G = (F, S, E, c)$ where F is set of possible factory/plant locations, S is set of sites needing service, E are edges indicating (factory,site) service possibility pairs, and $c : E \to \mathbb{R}_+$ is the benefit of a given pair.
- Facility location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

$A \subseteq F$,

$$f(A) = \sum_{i \in S} \max_{j \in A} c_{ij}. \qquad (4.33)$$



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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

$$f : 2^E \to \mathbb{R}, \text{ where } f(A) = \sum_{i \in V} \max_{j \in A} c_{ij} \tag{4.35}$$

is submodular.

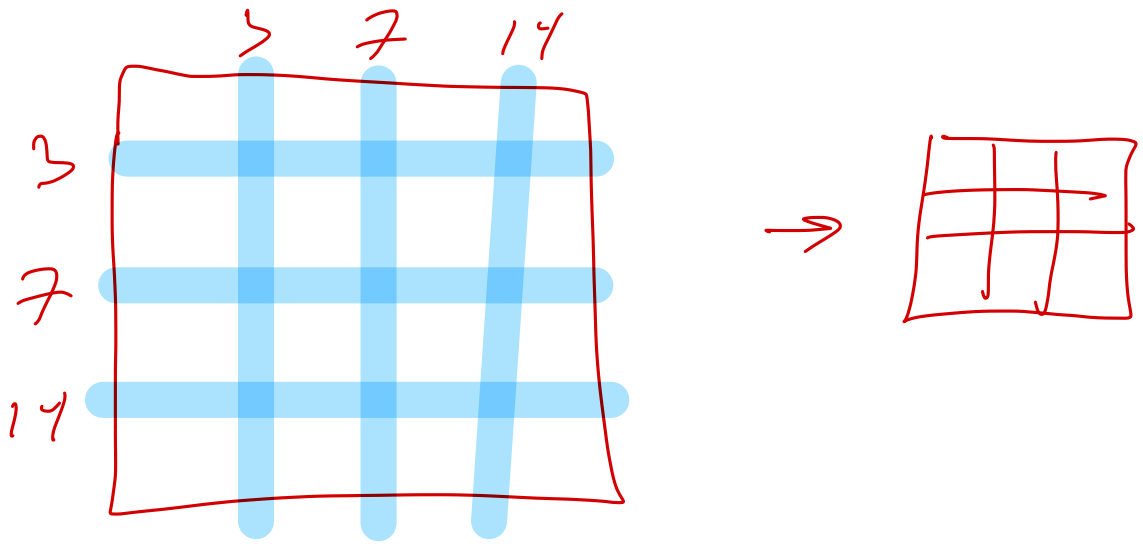
Proof.

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

$$x \in p(x) = \frac{1}{\sqrt{|2\pi\mathbf{\Sigma}|}} \exp\left(-\frac{1}{2}(x-\mu)^T \mathbf{\Sigma}^{-1}(x-\mu)\right) \tag{4.37}$$

...

Log Determinant

$I(X_A; X_B \mid X_C) \geq 0$

...cont.

$H(X_A, X_C) + H(X_B, X_C) - H(X_A, X_B, X_C) - H(X_C) \geq 0$

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

$$h(X) = \log \sqrt{|2\pi e \mathbf{\Sigma}|} = \log \sqrt{(2\pi e)^n |\mathbf{\Sigma}|} \tag{4.38}$$

and in particular, for a variable subset A,

$$f(A) = h(X_A) = \log \sqrt{(2\pi e)^{|A|} |\mathbf{\Sigma}_A|} \tag{4.39}$$

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

$$f(A) = h(X_A) = m(A) + \frac{1}{2} \log |\mathbf{\Sigma}_A| \tag{4.40}$$

where $m(A)$ is a modular function. □

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

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- Log determinant $f(A) = \log \det(\mathbf{\Sigma}_A)$ submodular for p.d. Σ.

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- Conix mixture: $\alpha_i \geq 0$, $f_i : 2^V \to \mathbb{R}$ submodular, then so is $\sum_i \alpha_i f_i$.
- Restrictions preserve submodularity: $f'(A) = f(A \cap S)$

Concave over non-negative modular

Let $m \in \mathbb{R}_+^E$ be a non-negative modular function, and ϕ a concave function over $\mathbb{R}$. Define $f : 2^E \to \mathbb{R}$ as

$$f(A) = \phi(m(A)) \tag{4.41}$$

then f is submodular.

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Proof.

Given $A \subseteq B \subseteq E \setminus v$, we have $0 \leq a = m(A) \leq b = m(B)$, and $0 \leq c = m(v)$. For g concave, we have $\phi(a + c) - \phi(a) \geq \phi(b + c) - \phi(b)$, and thus

$$\phi(m(A) + m(v)) - \phi(m(A)) \geq \phi(m(B) + m(v)) - \phi(m(B)) \tag{4.42}$$

□

A form of converse is true as well.

Concave composed with non-negative modular

Theorem 4.5.1

Given a ground set V. The following two are equivalent:

1. *For all modular functions $m : 2^V \to \mathbb{R}_+$, then $f : 2^V \to \mathbb{R}$ defined as $f(A) = \phi(m(A))$ is submodular*
2. $\phi : \mathbb{R}_+ \to \mathbb{R}$ *is concave.*

- If ϕ is non-decreasing concave w. $\phi(0) = 0$, then f is polymatroidal.

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- Very large class of functions, including graph cut, bipartite neighborhoods, set cover (Stobbe & Krause 2011), and "feature-based submodular functions" (Wei, Iyer, & Bilmes 2014).
- However, Vondrak showed that a graphic matroid rank function over K_4 (we'll define this after we define matroids) are not members.

Monotonicity

Definition 4.5.2

A function $f : 2^V \to \mathbb{R}$ is monotone nondecreasing (resp. monotone increasing) if for all $A \subset B$, we have $f(A) \leq f(B)$ (resp. $f(A) < f(B)$).

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Definition 4.5.3

A function $f : 2^V \to \mathbb{R}$ is monotone nonincreasing (resp. monotone decreasing) if for all $A \subset B$, we have $f(A) \geq f(B)$ (resp. $f(A) > f(B)$).

Composition of non-decreasing submodular and non-decreasing concave

Theorem 4.5.4

Given two functions, one defined on sets

$$f : 2^V \to \mathbb{R} \tag{4.44}$$

and another continuous valued one:

$$\phi : \mathbb{R} \to \mathbb{R} \tag{4.45}$$

the composition formed as $h = \phi \circ f : 2^V \to \mathbb{R}$ *(defined as* $h(S) = \phi(f(S))$*) is nondecreasing submodular, if* ϕ *is non-decreasing concave and* f *is nondecreasing submodular.*

Monotone difference of two functions

Let f and g both be submodular functions on subsets of V and let $(f-g)(\cdot)$ be either monotone non-decreasing or monotone non-increasing Then $h : 2^V \to R$ defined by

$$h(A) = \min(f(A), g(A)) \tag{4.46}$$

is submodular.

Proof.

If h agrees with f on both X and Y (or g on both X and Y), and since

$$h(X) + h(Y) = f(X) + f(Y) \geq f(X \cup Y) + f(X \cap Y) \tag{4.47}$$

or

$$h(X) + h(Y) = g(X) + g(Y) \geq g(X \cup Y) + g(X \cap Y), \tag{4.48}$$

the result (Equation 4.46 being submodular) follows since

$$\begin{matrix} f(X) + f(Y) \\ g(X) + g(Y) \end{matrix} \geq \min(f(X \cup Y), g(X \cup Y)) + \min(f(X \cap Y), g(X \cap Y)) \tag{4.49}$$

...

Monotone difference of two functions

...cont.

Otherwise, w.l.o.g., $h(X) = f(X)$ and $h(Y) = g(Y)$, giving

$$h(X) + h(Y) = f(X) + g(Y) \geq f(X \cup Y) + f(X \cap Y) + g(Y) - f(Y) \tag{4.50}$$

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Assume the case where $f - g$ is monotone non-decreasing. Hence, $f(X \cup Y) + g(Y) - f(Y) \geq g(X \cup Y)$ giving

$$h(X) + h(Y) \geq g(X \cup Y) + f(X \cap Y) \geq h(X \cup Y) + h(X \cap Y) \tag{4.51}$$

□

What is an easy way to prove the case where $f - g$ is monotone non-increasing?

Saturation via the $\min(\cdot)$ function

Let $f : 2^V \to \mathbb{R}$ be a monotone non-decreqasing or non-increasing submodular function and let α be a constant. Then the function $h : 2^V \to \mathbb{R}$ defined by

$$h(A) = \min(\alpha, f(A)) \tag{4.52}$$

is submodular.

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For constant k, we have that $(f - k)$ is non-decreasing (or non-increasing) so this follows from the previous result. □

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Note also, $g(a) = \min(k, a)$ for constant k is a non-decreasing concave function, so when f is monotone nondecreasing submodular, we can use the earlier result about composing a monotone concave function with a monotone submodular function to get a version of this.

More on Min - the saturate trick

- minimax facility location is similar to the following maximin function (a form of "robust facility location"): $h(A) = \min_{v \in V} \max_{a \in A} s(i, a)$ and the goal is to maximize this $\max_{A \subseteq V : |A| \leq k} h(A)$. h therefore is the min of a set of submodular functions.

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- However, when wishing to maximize two monotone non-decreasing submodular functions f, g, we can define function $h_\alpha : 2^V \to \mathbb{R}$ as

$$h_\alpha(A) = \frac{1}{2}\Big(\min(\alpha, f(A)) + \min(\alpha, g(A))\Big) \tag{4.53}$$

then h_α is submodular, and $h_\alpha(A) \geq \alpha$ if and only if both $f(A) \geq \alpha$ and $g(A) \geq \alpha$, for constant $\alpha \in \mathbb{R}$.

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  then h_α is submodular, and $h_\alpha(A) \geq \alpha$ if and only if both $f(A) \geq \alpha$ and $g(A) \geq \alpha$, for constant $\alpha \in \mathbb{R}$.
- Useful in applications. Like DS functions, another instance of a submodular surrogate (where we take a non-submodular problem and find a submodular one that can tell us something about it).

Arbitrary functions: difference between submodular funcs.

Theorem 4.5.5

Given an arbitrary set function h, it can be expressed as a difference between two submodular functions (i.e., $\forall h \in 2^V \to \mathbb{R}$, $\exists f, g$ s.t. $\forall A, h(A) = f(A) - g(A)$ where both f and g are submodular).

Proof.

Let h be given and arbitrary, and define:

$$\alpha \triangleq \min_{X,Y:X \not\subseteq Y, Y \not\subseteq X} \Big(h(X) + h(Y) - h(X \cup Y) - h(X \cap Y) \Big) \tag{4.54}$$

If $\alpha \geq 0$ then h is submodular, so by assumption $\alpha < 0$.

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If $\alpha \geq 0$ then h is submodular, so by assumption $\alpha < 0$. Now let f be an arbitrary strict submodular function and define

$$\beta \triangleq \min_{X,Y:X \not\subseteq Y, Y \not\subseteq X} \Big(f(X) + f(Y) - f(X \cup Y) - f(X \cap Y) \Big). \tag{4.55}$$

Strict means that $\beta > 0$. ...

Arbitrary functions as difference between submodular funcs.

...cont.

Define $h' : 2^V \to \mathbb{R}$ as

$$h'(A) = h(A) + \frac{|\alpha|}{\beta} f(A) \tag{4.56}$$

Then h' is submodular (why?), and $h = h'(A) - \frac{|\alpha|}{\beta} f(A)$, a difference between two submodular functions as desired.

□

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- This is called the gain and is used so often, there are equally as many ways to notate this. I.e., you might see:

$$f(A \cup \{j\}) - f(A) \triangleq \rho_j(A) \tag{4.57}$$

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- We'll use $f(j|A)$.
- diminishing returns can be stated as saying that $f(j|A)$ is a monotone non-increasing function of A, since $f(j|A) \geq f(j|B)$ whenever $A \subseteq B$ (i.e., further conditioning reduces valuation).

Gain Notation

It will also be useful to extend this to sets.
Let A, B be any two sets. Then

$$f(A|B) \triangleq f(A \cup B) - f(B) \tag{4.62}$$

So when j is any singleton

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Inspired from information theory notation and the notation used for conditional entropy $H(X_A|X_B) = H(X_A, X_B) - H(X_B)$.

Totally normalized functions

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- E.g., $g(A) = [g(A) + \alpha|A|] - \alpha|A|$, $\alpha \geq |\min_{v, A \subseteq V \setminus v} f(v|A)|$.
- Given arbitrary normalized submodular $g : 2^V \to \mathbb{R}$, construct a function $\bar{g} : 2^V \to \mathbb{R}$ as follows:

$$\bar{g}(A) = g(A) - \sum_{a \in A} g(a|V \setminus \{a\}) = g(A) - m_g(A) \tag{4.64}$$

where $m_g(A) \triangleq \sum_{a \in A} g(a|V \setminus \{a\})$ is a modular function.

Totally normalized functions

- Any normalized submodular function g (even non-monotone) can be represented as a sum of a polymatroid (normalized monotone non-decreasing submodular) function $\bar{g}$ and a modular function m_g.
- E.g., $g(A) = [g(A) + \alpha|A|] - \alpha|A|$, $\alpha \geq |\min_{v, A \subseteq V \setminus v} f(v|A)|$.
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- $\bar{g}$ is called the totally normalized version of g.
- Then $g(A) = \bar{g}(A) + m_g(A)$.

Arbitrary function as difference between two polymatroids

- Any normalized function h (i.e., $h(\emptyset) = 0$) can be represented as a difference not only between submodular, but between polymatroid (normalized monotone non-decreasing submodular) functions.

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- Given arbitrary $h = f - g$ where f and g are normalized submodular,

$$h = f - g = \bar{f} + m_f - (\bar{g} + m_g) \tag{4.66}$$
$$= \bar{f} - \bar{g} + (m_f - m_g) \tag{4.67}$$
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where m^+ is the positive part of modular function m. That is, $m^+(A) = \sum_{a \in A} m(a)\mathbf{1}(m(a) > 0)$.

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- Both $\bar{f} + m^+_{f-g}$ and $\bar{g} + (-m_{f-g})^+$ are polymatroid functions!
- Thus, any function can be expressed as a difference between two, not only submodular (DS), but polymatroid functions.

Two Equivalent Submodular Definitions

Definition 4.6.1 (submodular concave)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{4.7}$$

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

Definition 4.6.2 (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:

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \tag{4.8}$$

• 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 $A \subseteq B \subseteq V \setminus \{v\}$, $v \in V$.

Submodular Definition: Group Diminishing Returns

An alternate and equivalent definition is:

Definition 4.6.1 (group diminishing returns)

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

$$f(A \cup C) - f(A) \geq f(B \cup C) - f(B) \tag{4.70}$$

This means that the incremental "value" or "gain" of set C decreases as the context in which C is considered grows from A to B (diminishing returns)

Submodular Definition Basic Equivalencies

We want to show that Submodular Concave (Definition 4.6.1), Diminishing Returns (Definition 4.6.2), and Group Diminishing Returns (Definition 4.6.1) are identical.

Submodular Definition Basic Equivalencies

We want to show that Submodular Concave (Definition 4.6.1), Diminishing Returns (Definition 4.6.2), and Group Diminishing Returns (Definition 4.6.1) are identical. We will show that:

- Submodular Concave $\Rightarrow$ Diminishing Returns
- Diminishing Returns $\Rightarrow$ Group Diminishing Returns
- Group Diminishing Returns $\Rightarrow$ Submodular Concave

Submodular Concave $\Rightarrow$ Diminishing Returns

$f(S) + f(T) \geq f(S \cup T) + f(S \cap T) \Rightarrow f(v|A) \geq f(v|B), A \subseteq B \subseteq V \setminus v.$

- Assume Submodular concave, so $\forall S, T$ we have $f(S) + f(T) \geq f(S \cup T) + f(S \cap T)$.

$\square$

Submodular Concave $\Rightarrow$ Diminishing Returns

$f(S) + f(T) \geq f(S \cup T) + f(S \cap T) \Rightarrow f(v|A) \geq f(v|B), A \subseteq B \subseteq V \setminus v.$

- Assume Submodular concave, so $\forall S, T$ we have $f(S) + f(T) \geq f(S \cup T) + f(S \cap T)$.
- Given A, B and $v \in V$ such that: $A \subseteq B \subseteq V \setminus \{v\}$, we have from submodular concave that:

$$f(A + v) + f(B) \geq f(B + v) + f(A) \tag{4.71}$$

$\square$

Submodular Concave $\Rightarrow$ Diminishing Returns

$f(S) + f(T) \geq f(S \cup T) + f(S \cap T) \Rightarrow f(v|A) \geq f(v|B), A \subseteq B \subseteq V \setminus v.$

- Assume Submodular concave, so $\forall S, T$ we have $f(S) + f(T) \geq f(S \cup T) + f(S \cap T)$.
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- Rearranging, we have

$$f(A + v) - f(A) \geq f(B + v) - f(B) \tag{4.72}$$

$\square$

Diminishing Returns $\Rightarrow$ Group Diminishing Returns

$f(v|S) \geq f(v|T), S \subseteq T \subseteq V \setminus v \Rightarrow f(C|A) \geq f(C|B), A \subseteq B \subseteq V \setminus C.$

Let $C = \{c_1, c_2, \dots, c_k\}$. Then diminishing returns implies

$$f(A \cup C) - f(A) \tag{4.73}$$

$$= f(A \cup C) - \sum_{i=1}^{k-1} \Big(f(A \cup \{c_1, \dots, c_i\}) - f(A \cup \{c_1, \dots, c_i\}) \Big) - f(A) \tag{4.74}$$

$$= \sum_{i=1}^{k} \Big(f(A \cup \{c_1 \dots c_i\}) - f(A \cup \{c_1 \dots c_{i-1}\}) \Big) = \sum_{i=1}^{k} f(c_i | A \cup \{c_1 \dots c_{i-1}\}) \tag{4.75}$$

$$\geq \sum_{i=1}^{k} f(c_i | B \cup \{c_1 \dots c_{i-1}\}) = \sum_{i=1}^{k} \Big(f(B \cup \{c_1 \dots c_i\}) - f(B \cup \{c_1 \dots c_{i-1}\}) \Big) \tag{4.76}$$

$$= f(B \cup C) - \sum_{i=1}^{k-1} \Big(f(B \cup \{c_1, \dots, c_i\}) - f(B \cup \{c_1, \dots, c_i\}) \Big) - f(B) \tag{4.77}$$

$$= f(B \cup C) - f(B) \tag{4.78}$$

$\square$

Group Diminishing Returns $\Rightarrow$ Submodular Concave

$f(U|S) \geq f(U|T), S \subseteq T \subseteq V \setminus U \Rightarrow f(A) + f(B) \geq f(A \cup B) + f(A \cap B).$

Assume group diminishing returns. Assume $A \neq B$ otherwise trivial. Define $A' = A \cap B$, $C = A \setminus B$, and $B' = B$. Then since $A' \subseteq B'$,

$$f(A' + C) - f(A') \geq f(B' + C) - f(B') \tag{4.79}$$

giving

$$f(A' + C) + f(B') \geq f(B' + C) + f(A') \tag{4.80}$$

or

$$f(A \cap B + A \setminus B) + f(B) \geq f(B + A \setminus B) + f(A \cap B) \tag{4.81}$$

which is the same as the submodular concave condition

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{4.82}$$

Submodular Definition: Four Points

Definition 4.6.2 ("singleton", or "four points")

A function $f : 2^V \to \mathbb{R}$ is submodular iff for any $A \subset V$, and any $a, b \in V \setminus A$, we have that:

$$f(A \cup \{a\}) + f(A \cup \{b\}) \geq f(A \cup \{a, b\}) + f(A) \tag{4.83}$$

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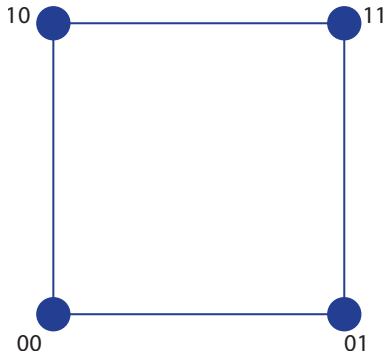
This follows immediately from diminishing returns. To achieve diminishing returns, assume $A \subset B$ with $B \setminus A = \{b_1, b_2, \dots, b_k\}$. Then

$$\begin{aligned}
f(A + a) - f(A) &\geq f(A + b_1 + a) - f(A + b_1) && (4.84)\\
&\geq f(A + b_1 + b_2 + a) - f(A + b_1 + b_2) && (4.85)\\
&\geq \dots && (4.86)\\
&\geq f(A + b_1 + \dots + b_k + a) - f(A + b_1 + \dots + b_k) && (4.87)\\
&= f(B + a) - f(B) && (4.88)
\end{aligned}$$

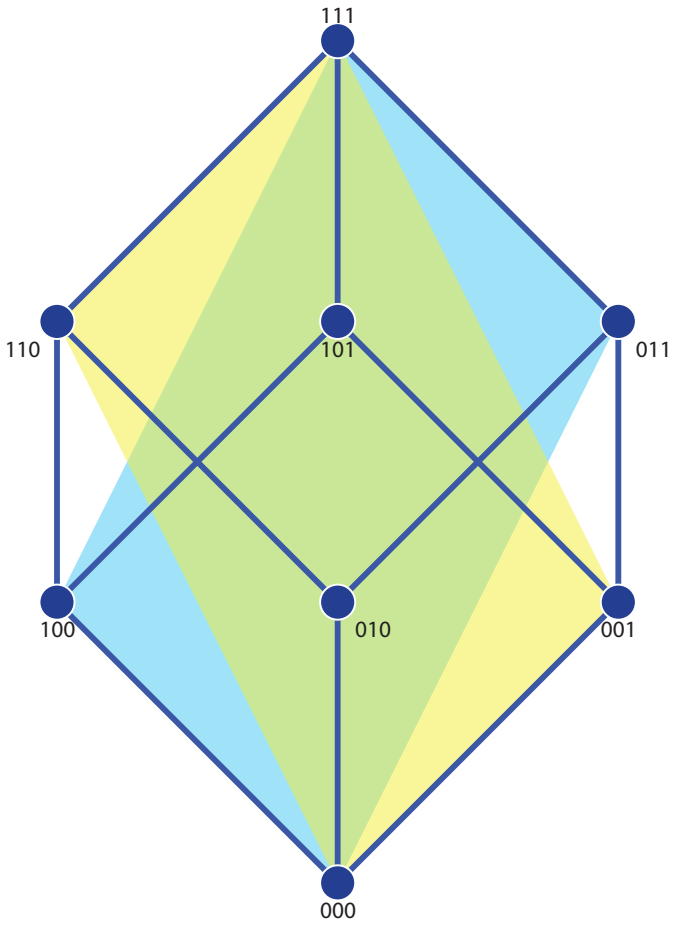
The Submodular Square, and Hypercube Vertices

We can test submodularity via values on vertices of hypercube.

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



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



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

Submodular Concave $\equiv$ Diminishing Returns, in one slide.

Theorem 4.6.3

Given function $f : 2^V \to \mathbb{R}$, *then*

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \text{ for all } A, B \subseteq V \qquad \text{(SC)}$$

if and only if

$$f(v|X) \geq f(v|Y) \text{ for all } X \subseteq Y \subseteq V \text{ and } v \notin Y \qquad \text{(DR)}$$

Proof.

(SC)$\Rightarrow$(DR): Set $A \leftarrow X \cup \{v\}$, $B \leftarrow Y$. Then $A \cup B = Y \cup \{v\}$ and $A \cap B = X$ and $f(A) - f(A \cap B) \geq f(A \cup B) - f(B)$ implies (DR).

(DR)$\Rightarrow$(SC): Order $A \setminus B = \{v_1, v_2, \ldots, v_r\}$ arbitrarily. For $i \in 1 : r$,

$$f(v_i|(A \cap B) \cup \{v_1, v_2, \ldots, v_{i-1}\}) \geq f(v_i|B \cup \{v_1, v_2, \ldots, v_{i-1}\}).$$

Applying telescoping summation to both sides, we get:

$$\sum_{i=1}^{r} f(v_i|(A \cap B) \cup \{v_1, v_2, \ldots, v_{i-1}\}) \geq \sum_{i=1}^{r} f(v_i|B \cup \{v_1, v_2, \ldots, v_{i-1}\})$$

$$\Rightarrow \qquad f(A) - f(A \cap B) \geq f(A \cup B) - f(B)$$

$\square$

Many (Equivalent) Definitions of Submodularity

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V \tag{4.94}$$

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$$f(A \cup B|A \cap B) \leq f(A|A \cap B) + f(B|A \cap B), \ \ \forall A, B \subseteq V \tag{4.98}$$

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$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \ \forall S, T \subseteq V \tag{4.99}$$

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$$f(j|S) \geq f(j|S \cup \{k\}), \ \forall S \subseteq V \text{ with } j \in V \setminus (S \cup \{k\}) \tag{4.97}$$

$$f(A \cup B|A \cap B) \leq f(A|A \cap B) + f(B|A \cap B), \quad \forall A, B \subseteq V \tag{4.98}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \ \forall S, T \subseteq V \tag{4.99}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S), \ \forall S \subseteq T \subseteq V \tag{4.100}$$

$$f(T) \leq f(S) - \sum_{j \in S \setminus T} f(j|S \setminus \{j\}) + \sum_{j \in T \setminus S} f(j|S \cap T) \ \forall S, T \subseteq V \tag{4.101}$$

$$f(T) \leq f(S) - \sum_{j \in S \setminus T} f(j|S \setminus \{j\}), \ \forall T \subseteq S \subseteq V \tag{4.102}$$

Equivalent Definitions of Submodularity

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We next show that Eq. 4.97 $\Rightarrow$ Eq. 4.99 $\Rightarrow$ Eq. 4.100 $\Rightarrow$ Eq. 4.97.

Approach

To show these next results, we essentially first use:

$$f(S \cup T) = f(S) + f(T|S) \leq f(S) + \text{upper-bound} \tag{4.103}$$

and

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leading to

$$f(T) + \text{lower-bound} \leq f(S) + \text{upper-bound} \tag{4.105}$$

or

$$f(T) \leq f(S) + \text{upper-bound} - \text{lower-bound} \tag{4.106}$$

Eq. 4.97 $\Rightarrow$ Eq. 4.99

Let $T \setminus S = \{j_1, \dots, j_r\}$ and $S \setminus T = \{k_1, \dots, k_q\}$.
First, we upper bound the gain of T in the context of S:

$$f(S \cup T) - f(S) = \sum_{t=1}^{r} \Big(f(S \cup \{j_1, \dots, j_t\}) - f(S \cup \{j_1, \dots, j_{t-1}\}) \Big) \tag{4.107}$$

$$= \sum_{t=1}^{r} f(j_t | S \cup \{j_1, \dots, j_{t-1}\}) \leq \sum_{t=1}^{r} f(j_t | S) \tag{4.108}$$

$$= \sum_{j \in T \setminus S} f(j|S) \tag{4.109}$$

or

$$f(T|S) \leq \sum_{j \in T \setminus S} f(j|S) \tag{4.110}$$

Eq. 4.97 $\Rightarrow$ Eq. 4.99

Let $T \setminus S = \{j_1, \ldots, j_r\}$ and $S \setminus T = \{k_1, \ldots, k_q\}$.
Next, lower bound S in the context of T:

$$f(S \cup T) - f(T) = \sum_{t=1}^{q} [f(T \cup \{k_1, \ldots, k_t\}) - f(T \cup \{k_1, \ldots, k_{t-1}\})] \tag{4.111}$$

$$= \sum_{t=1}^{q} f(k_t | T \cup \{k_1, \ldots, k_t\} \setminus \{k_t\}) \geq \sum_{t=1}^{q} f(k_t | T \cup S \setminus \{k_t\}) \tag{4.112}$$

$$= \sum_{j \in S \setminus T} f(j | S \cup T \setminus \{j\}) \tag{4.113}$$

Eq. 4.97 $\Rightarrow$ Eq. 4.99

Let $T \setminus S = \{j_1, \dots, j_r\}$ and $S \setminus T = \{k_1, \dots, k_q\}$.
So we have the upper bound

$$f(T|S) = f(S \cup T) - f(S) \leq \sum_{j \in T \setminus S} f(j|S) \tag{4.114}$$

and the lower bound

$$f(S|T) = f(S \cup T) - f(T) \geq \sum_{j \in S \setminus T} f(j|S \cup T \setminus \{j\}) \tag{4.115}$$

This gives upper and lower bounds of the form

$$f(T) + \text{lower bound} \leq f(S \cup T) \leq f(S) + \text{upper bound}, \tag{4.116}$$

and combining directly the left and right hand side gives the desired inequality.

Eq. 4.99 $\Rightarrow$ Eq. 4.100

This follows immediately since if $S \subseteq T$, then $S \setminus T = \emptyset$, and the last term of Eq. 4.99 vanishes.

Many (Equivalent) Definitions of Submodularity

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V \tag{4.94}$$

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$$f(T) \leq f(S) - \sum_{j \in S \setminus T} f(j|S \setminus \{j\}), \ \forall T \subseteq S \subseteq V \tag{4.102}$$

Eq. 4.100 $\Rightarrow$ Eq. 4.97

Here, we set $T = S \cup \{j, k\}$, $j \notin S \cup \{k\}$ into Eq. 4.100 to obtain

$$
\begin{aligned}
f(S \cup \{j,k\}) &\leq f(S) + f(j|S) + f(k|S) && (4.117)\\
&= f(S) + f(S + \{j\}) - f(S) + f(S + \{k\}) - f(S) && (4.118)\\
&= f(S + \{j\}) + f(S + \{k\}) - f(S) && (4.119)\\
&= f(j|S) + f(S + \{k\}) && (4.120)
\end{aligned}
$$

giving

$$
\begin{aligned}
f(j|S \cup \{k\}) &= f(S \cup \{j,k\}) - f(S \cup \{k\}) && (4.121)\\
&\leq f(j|S) && (4.122)
\end{aligned}
$$

Submodular Concave

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- A continuous twice differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ is concave iff $\nabla^2 f \preceq 0$ (the Hessian matrix is nonpositive definite).
- Define a "discrete derivative" or difference operator defined on discrete functions $f : 2^V \to \mathbb{R}$ as follows:

$$(\nabla_B f)(A) \triangleq f(A \cup B) - f(A \setminus B) = f\big(B|(A \setminus B)\big) \tag{4.123}$$

read as: the derivative of f at A in the direction B.

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  read as: the derivative of f at A in the direction B.
- Hence, if $A \cap B = \emptyset$, then $(\nabla_B f)(A) = f(B|A)$.
- Consider a form of second derivative or 2nd difference:

$$(\nabla_B \nabla_C f)(A) = \nabla_B [\overbrace{f(A \cup C) - f(A \setminus C)}^{(\nabla_C f)(A)}] \tag{4.124}$$

$$= (\nabla_B f)(A \cup C) - (\nabla_B f)(A \setminus C) \tag{4.125}$$

$$= f(A \cup B \cup C) - f((A \cup C) \setminus B) - f((A \setminus C) \cup B) + f((A \setminus C) \setminus B) \tag{4.126}$$

Submodular Concave

- If the second difference operator everywhere nonpositive:

$$f(A \cup B \cup C) - f((A \cup C) \setminus B) \\ - f((A \setminus C) \cup B) + f(A \setminus C \setminus B) \leq 0 \qquad (4.127)$$

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- Define $A' = (A \cup C) \setminus B$ and $B' = (A \setminus C) \cup B$. Then the above implies:

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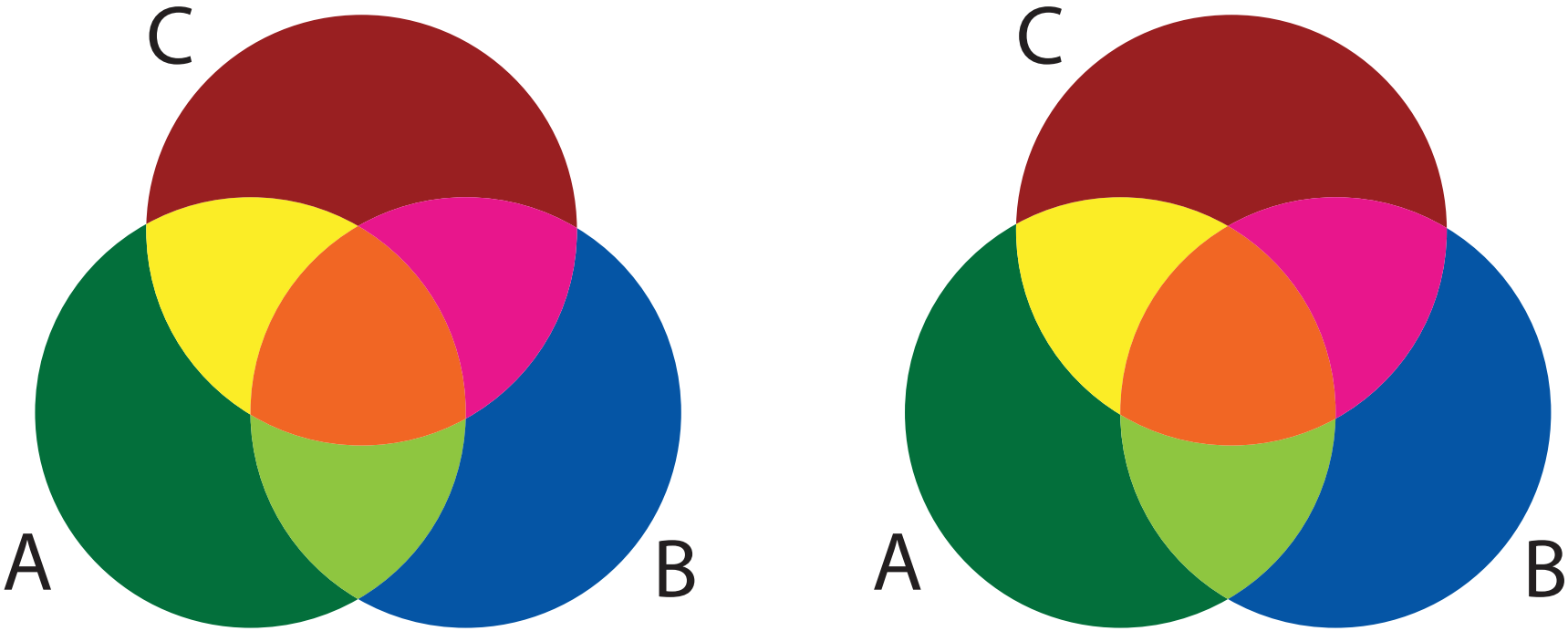
- One sense in which submodular functions are like concave functions.

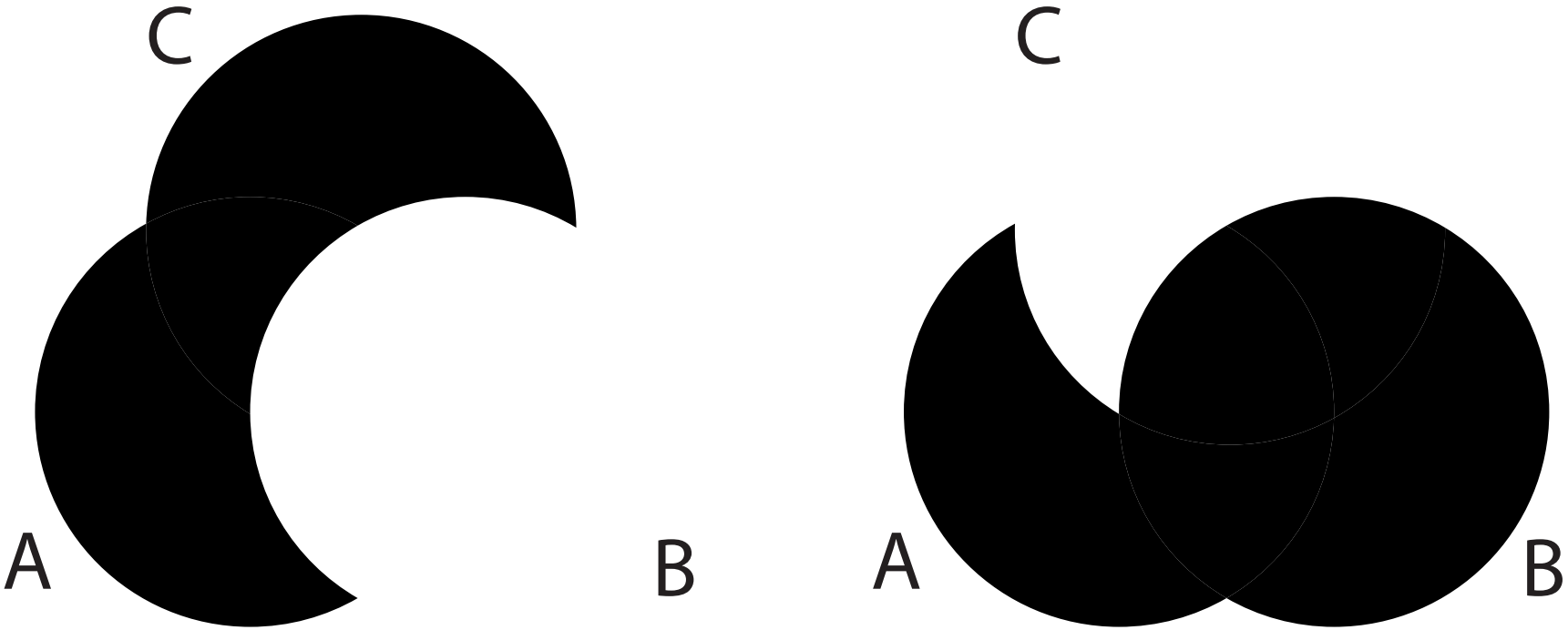
Submodular Concave



(a) $A' = (A \cup C) \setminus B$ (b) $B' = (A \setminus C) \cup B$

Figure: A figure showing $A' \cup B' = A \cup B \cup C$ and $A' \cap B' = A \setminus C \setminus B$.

Submodular Concave



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- This gives us a simpler notion corresponding to concavity.
- Define gain as $\nabla_j(X) = f(X + j) - f(X)$, a form of discrete gradient.
- Trivially becomes a second-order condition, akin to concave functions: A function is submodular if for all $X \subseteq V$ and $j, k \in V$, we have:

$$\nabla_j \nabla_k f(X) \leq 0 \tag{4.131}$$

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 $A = \{1, 2, 3\}$, $B = \{3, 4, 5\}$, $C = \{6, 7\}$, $A_r = \{1\}$, $B_r = \{5\}$.
- Then $r(A) = 3$, $r(B) = 3$, $r(C) = 2$.
- $r(A \cup C) = 3$, $r(B \cup C) = 3$.
- $r(A \cup A_r) = 3$, $r(B \cup B_r) = 3$, $r(A \cup B_r) = 4$, $r(B \cup A_r) = 4$.
- $r(A \cup B) = 4$, $r(A \cap B) = 1 < r(C) = 2$.
- $6 = r(A) + r(B) = r(A \cup B) + r(C) > r(A \cup B) + r(A \cap B) = 5$

On Rank

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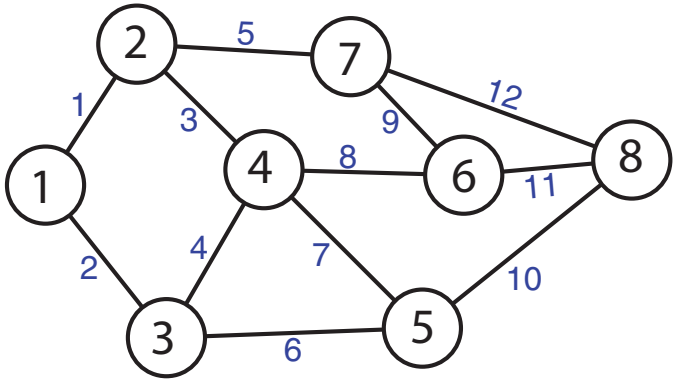
- To stress this point, note that the above condition is $|A| < |B|$, **not** $A \subseteq B$ which is sufficient (to be able to find an independent vector) but not required.
- In other words, given A, B with rank$(A) = |A|$ & rank$(B) = |B|$, then $|A| < |B| \Leftrightarrow \exists$ an $b \in B$ such that rank$(A \cup \{b\}) = |A| + 1$.

Spanning trees/forests

- We are given a graph $G = (V, E)$, and consider the edges $E = E(G)$ as an index set.
- Consider the $|V| \times |E|$ incidence matrix of undirected graph G, which is the matrix $\mathbf{X}_G = (x_{v,e})_{v \in V(G), e \in E(G)}$ where

$$x_{v,e} = \begin{cases} 1 & \text{if } v \in e \\ 0 & \text{if } v \notin e \end{cases} \tag{4.132}$$



$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \begin{array}{c} \begin{array}{cccccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \end{array} \\ \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix} \end{array} \tag{4.133}$$

Spanning trees/forests & incidence matrices

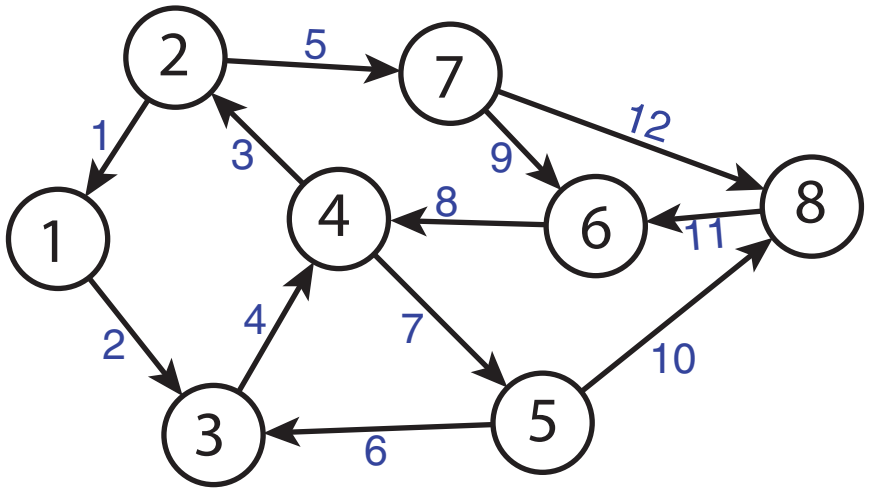
- We are given a graph $G = (V, E)$, we can arbitrarily orient the graph (make it directed) consider again the edges $E = E(G)$ as an index set.
- Consider instead the $|V| \times |E|$ incidence matrix of undirected graph G, which is the matrix $\mathbf{X}_G = (x_{v,e})_{v \in V(G), e \in E(G)}$ where

$$x_{v,e} = \begin{cases} 1 & \text{if } v \in e^+ \\ -1 & \text{if } v \in e^- \\ 0 & \text{if } v \notin e \end{cases} \tag{4.134}$$

and where e^+ is the tail and e^- is the head of (now) directed edge e.

Spanning trees/forests & incidence matrices

- A directed version of the graph (right) and its adjacency matrix (below).
- Orientation can be arbitrary.
- Note, rank of this matrix is 7.



$$
\begin{array}{c}
 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8
\end{array}
\begin{array}{c}
\begin{array}{cccccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \end{array} \\
\begin{pmatrix}
-1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
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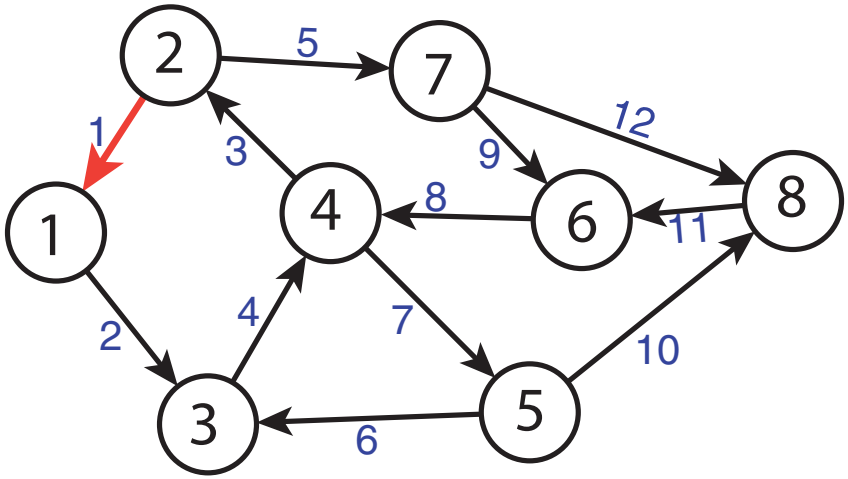
0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1
\end{pmatrix}
\end{array}
$$

Spanning trees

- We can consider edge-induced subgraphs and the corresponding matrix columns.



$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \begin{array}{c} 1 \\ \begin{pmatrix} -1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \end{array} \tag{4.135}$$

Here, $\text{rank}(\{x_1\}) = 1$.

Spanning trees

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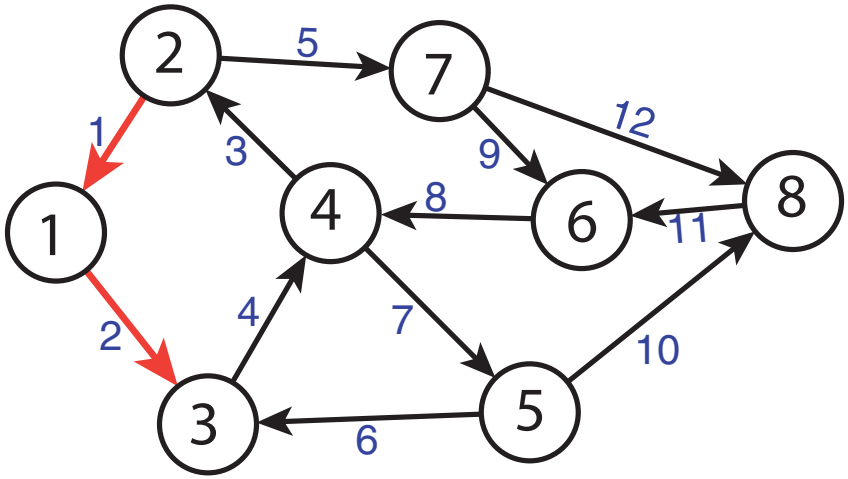
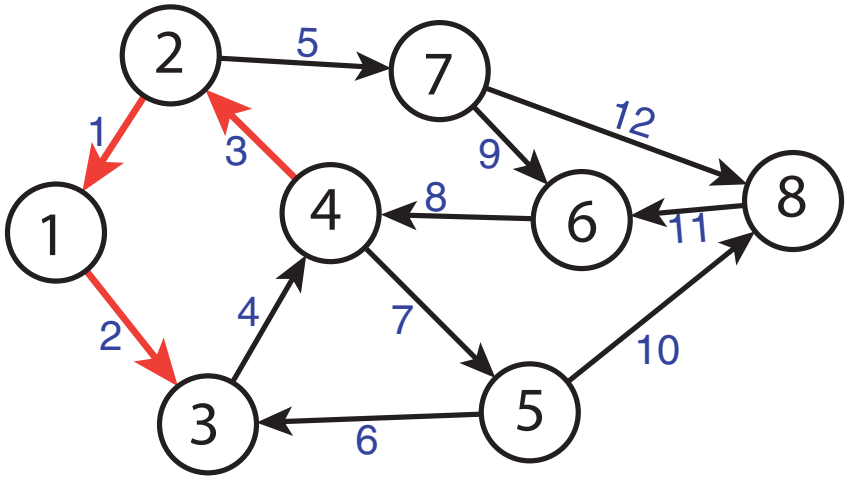


$$\begin{array}{c c} & \begin{array}{cc} 1 & 2 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} & \begin{pmatrix} -1 & 1 \\ 1 & 0 \\ 0 & -1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \end{array} \tag{4.135}$$

Here, rank$(\{x_1, x_2\}) = 2$.

Spanning trees

- We can consider edge-induced subgraphs and the corresponding matrix columns.



$$\begin{array}{c c} & \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} & \begin{pmatrix} -1 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{array} \tag{4.135}$$

Here, $\text{rank}(\{x_1, x_2, x_3\}) = 3$.

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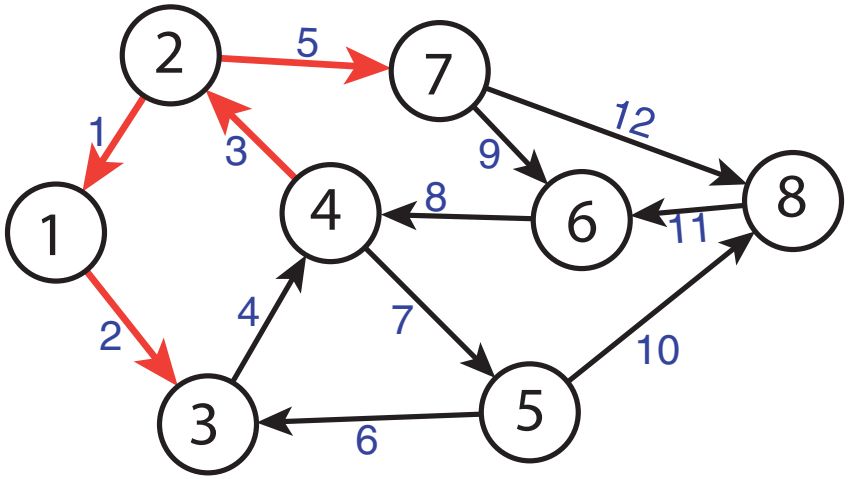

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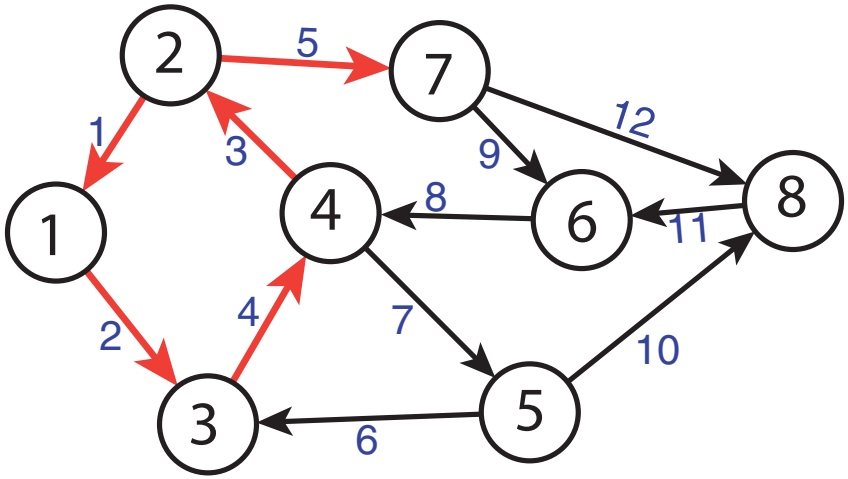

$$
\begin{array}{c}
 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8
\end{array}
\begin{array}{c}
\begin{array}{ccccc} 1 & 2 & 3 & 4 & 5 \end{array} \\
\begin{pmatrix}
-1 & 1 & 0 & 0 & 0 \\
1 & 0 & -1 & 0 & 1 \\
0 & -1 & 0 & 1 & 0 \\
0 & 0 & 1 & -1 & 0 \\
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\end{pmatrix}
\end{array}
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$$

Here, rank$(\{x_1, x_2, x_3, x_4, x_5\}) = 4$.

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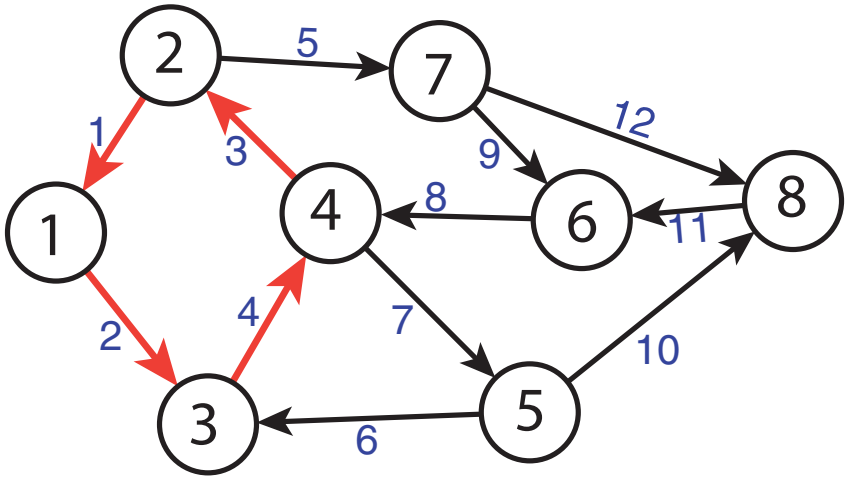

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- We have rank$(A) = |V(G)| - k_G(A)$.

Spanning Tree Algorithms

- We are now given a positive edge-weighted connected graph $G = (V, E, w)$ where $w : E \to \mathbb{R}_+$ is a modular function the edges of the graph. The goal is to find the minimum spanning tree (MST) of the graph.
- Given a tree T, the cost of the tree is $\text{cost}(T) = \sum_{e \in T} w(e)$, the sum of the weights of the edges.
- There are several algorithms for MST:

Algorithm 1: Kruskal's Algorithm

```
Sort the edges so that w(e_1) ≤ w(e_2) ≤ ··· ≤ w(e_m) ;
T ← (V(G), ∅) = (V, ∅) ;
for i = 1 to m do
    if E(T) ∪ {e_i} does not create a cycle in T then
        E(T) ← E(T) ∪ {e_i} ;
```

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Algorithm 2: Jarník/Prim/Dijkstra Algorithm

$T \leftarrow \emptyset$;
while T *is not a spanning tree* **do**
  $T \leftarrow T \cup \{e\}$ for $e =$ the minimum weight edge extending the tree T to a not-yet connected vertex ;

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Algorithm 3: Borůvka's Algorithm

```
F ← ∅ /* We build up the edges of a forest in F */
while G(V, F) is disconnected do
    forall components C_i of F do
        F ← F ∪ {e_i} for e_i = the min-weight edge out of C_i;
```

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- The above are all examples of a matroid, which is the fundamental reason why the greedy algorithms work.