Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 3 —

http://www.ee.washington.edu/people/faculty/bilmes/classes/ee596b_spring_2016/

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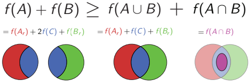

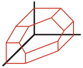

Cumulative Outstanding Reading

- Read chapter 1 from Fujishige's book.

Announcements, Assignments, and Reminders

- Homework 1 is now available at our assignment dropbox (https://canvas.uw.edu/courses/1039754/assignments), due (electronically) Friday at 5:00pm.
- Weekly Office Hours: Mondays, 3:30-4:30, or by skype or google hangout (set up meeting via our our discussion board (https://canvas.uw.edu/courses/1039754/discussion_topics)).

Class Road Map - IT-I

- L1(3/28): Motivation, Applications, & Basic Definitions
- L2(3/30): Machine Learning Apps (diversity, complexity, parameter, learning target, surrogate).
- L3(4/4): Info theory exs, more apps, definitions, graph/combinatorial examples, matrix rank example, visualization
- L4(4/6):
- L5(4/11):
- L6(4/13):
- L7(4/18):
- L8(4/20):
- L9(4/25):
- L10(4/27):
- L11(5/2):
- L12(5/4):
- L13(5/9):
- L14(5/11):
- L15(5/16):
- L16(5/18):
- L17(5/23):
- L18(5/25):
- L19(6/1):
- L20(6/6): Final Presentations maximization.

Finals Week: June 6th-10th, 2016.

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:

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{3.8}$$

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:

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \tag{3.9}$$

The incremental "value", "gain", or "cost" of v decreases (diminishes) as the context in which v is considered grows from A to B.

Two Equivalent Supermodular Definitions

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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 $f(A) = c + \sum_{a \in A} f(a)$ (often $c = 0$).

Submodularity's utility in ML

- A model of a physical process :
  - When maximizing, submodularity naturally models: diversity, coverage, span, and information.
  - When minimizing, submodularity naturally models: cooperative costs, complexity, roughness, and irregularity.
  - vice-versa for supermodularity.
- A submodular function can act as a parameter for a machine learning strategy (active/semi-supervised learning, discrete divergence, structured sparse convex norms for use in regularization).
- Itself, as an object or function to learn , based on data.
- A surrogate or relaxation strategy for optimization or analysis
  - An alternate to factorization, decomposition, or sum-product based simplification (as one typically finds in a graphical model). I.e., a means towards tractable surrogates for graphical models.
  - Also, we can "relax" a problem to a submodular one where it can be efficiently solved and offer a bounded quality solution.
  - Non-submodular problems can be analyzed via submodularity.

Ground set: E or V?

Submodular functions are functions defined on subsets of some finite set, called the ground set .

- It is common in the literature to use either E or V as the ground set — we will at different times use both (there should be no confusion).

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- It is common in the literature to use either E or V as the ground set — we will at different times use both (there should be no confusion).
- The terminology ground set comes from lattice theory, where V are the ground elements of a lattice (just above 0).

Notation $\mathbb{R}^E$

What does $x \in \mathbb{R}^E$ mean?

$\mathbb{R}^2$ $\mathbb{R}^n$

$\mathbb{R}^E \equiv \mathbb{R}^{|E|}$

$$\mathbb{R}^E = \{x = (x_j \in \mathbb{R} : j \in E)\} \tag{3.1}$$

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

$\mathbb{R}^E = \{(x_a, x_b, x_c) : x_a \in \mathbb{R}, x_b \in \mathbb{R}, x_c \in \mathbb{R}\}$

$$\mathbb{R}_+^E = \{x = (x_j : j \in E) : x \geq 0\} \tag{3.2}$$

Any vector $x \in \mathbb{R}^E$ can be treated as a normalized modular function, and vice verse. That is

$A \subseteq E$

$$x(A) = \sum_{a \in A} x_a \tag{3.3}$$

Note that x is said to be normalized since $x(\emptyset) = 0$.

characteristic vectors of sets & modular functions

- Given an $A \subseteq E$, define the vector $\mathbf{1}_A \in \mathbb{R}_+^E$ to be

$$\mathbf{1}_A(j) = \begin{cases} 1 & \text{if } j \in A; \\ 0 & \text{if } j \notin A \end{cases} \tag{3.4}$$

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- Thus, given modular function $x \in \mathbb{R}^E$, we can write $x(A)$ in a variety of ways, i.e.,

$$x(A) = x^{\intercal} \cdot \mathbf{1}_A = \sum_{i \in A} x(i) \tag{3.5}$$

Other Notation: singletons and sets

When A is a set and k is a singleton (i.e., a single item), the union is properly written as $A \cup \{k\}$, but sometimes we will write just $A + k$.

What does S^T mean when S and T are arbitrary sets?

- Let S and T be two arbitrary sets (either of which could be countable, or uncountable).

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

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- Hence, given a finite set E, $\mathbb{R}^E$ is the set of all functions that map from elements of E to the reals $\mathbb{R}$, and such functions are identical to a vector in a vector space with axes labeled as elements of E (i.e., if $m \in \mathbb{R}^E$, then for all $e \in E$, $m(e) \in \mathbb{R}$).

$m \in \mathbb{R}^E$. $\quad m : E \to \mathbb{R}$

$m \in \mathbb{R}^n \quad n \equiv \{1, 2, \ldots, n\}$

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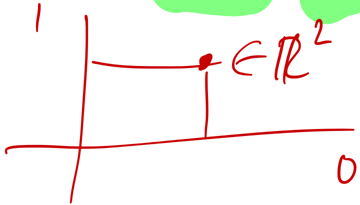

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$= \quad E \to \{0,1\}$

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- What might 3^E mean?

$\{0,1,2\}^E$

Example Submodular: Entropy from Information Theory

- Entropy is submodular. Let V be the index set of a set of random variables, then the function

$$f(A) = H(X_A) = -\sum_{x_A} p(x_A) \log p(x_A) \tag{3.6}$$

  is submodular.

- Proof: (further) conditioning reduces entropy. With $A \subseteq B$ and $v \notin B$,

$$H(X_v|X_B) = H(X_{B+v}) - H(X_B) \tag{3.7}$$
$$\leq H(X_{A+v}) - H(X_A) = H(X_v|X_A) \tag{3.8}$$

- We say "further" due to $B \setminus A$ not nec. empty.

$H(X_v) \geq H(X_v|X_A) \geq H(X_v|X_B)$

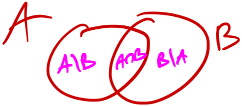
Example Submodular: Entropy from Information Theory

- Alternate Proof: Conditional mutual Information is always non-negative.
- Given $A, B \subseteq V$, consider conditional mutual information quantity:

$$I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B}) = \sum_{x_{A \cup B}} p(x_{A \cup B}) \log \frac{p(x_{A \setminus B}, x_{B \setminus A} | x_{A \cap B})}{p(x_{A \setminus B} | x_{A \cap B}) p(x_{B \setminus A} | x_{A \cap B})}$$

$$= \sum_{x_{A \cup B}} p(x_{A \cup B}) \log \frac{p(x_{A \cup B}) p(x_{A \cap B})}{p(x_A) p(x_B)} \geq 0 \qquad (3.9)$$

then



$$I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B})$$
$$= H(X_A) + H(X_B) - H(X_{A \cup B}) - H(X_{A \cap B}) \geq 0 \qquad (3.10)$$

so entropy satisfies

$$H(X_A) + H(X_B) \geq H(X_{A \cup B}) + H(X_{A \cap B}) \qquad (3.11)$$

Information Theory: Block Coding

- Given a set of random variables $\{X_i\}_{i \in V}$ indexed by set V, how do we partition them so that we can best block-code them within each block.

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- I.e., how do we form $S \subseteq V$ such that $I(X_S; X_{V \setminus S})$ is as small as possible, where $I(X_A; X_B)$ is the mutual information between random variables X_A and X_B, i.e.,

$$I(X_A; X_B) = H(X_A) + H(X_B) - H(X_A, X_B) \tag{3.12}$$

and $H(X_A) = -\sum_{x_A} p(x_A) \log p(x_A)$ is the joint entropy of the set X_A of random variables.

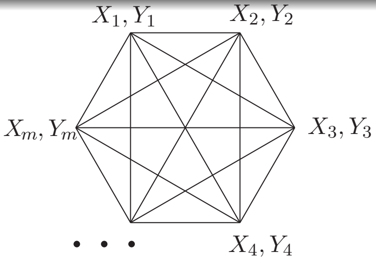
Example Submodular: Mutual Information

- Also, symmetric mutual information is submodular,

$$f(A) = I(X_A; X_{V \setminus A}) = H(X_A) + H(X_{V \setminus A}) - H(X_V) \quad (3.13)$$

Note that $f(A) = H(X_A)$ and $\bar{f}(A) = H(X_{V \setminus A})$, and adding submodular functions preserves submodularity (which we will see quite soon).

Information Theory: Network Communication



- A network of senders/receivers
- Each sender X_i is trying to communicate simultaneously with each receiver Y_i (i.e., for all i, X_i is sending to $\{Y_i\}_i$
- The X_i are not necessarily independent.

- Communication rates from i to j are $R^{(i \to j)}$ to send message $W^{(i \to j)} \in \left\{1, 2, \ldots, 2^{nR^{(i \to j)}}\right\}$.
- Goal: necessary and sufficient conditions for achievability.
- I.e., can we find functions f such that any rates must satisfy

$$\forall S \subseteq V, \quad \sum_{i \in S, j \in V \setminus S} R^{(i \to j)} \leq f(S) \tag{3.14}$$

- Special cases MAC (Multi-Access Channel) for communication over $p(y|x_1, x_2)$ and Slepian-Wolf compression (independent compression of X and Y but at joint rate $H(X, Y)$).

Monge Matrices

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

$$c_{ij} + c_{rs} \leq c_{is} + c_{rj} \tag{3.15}$$

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

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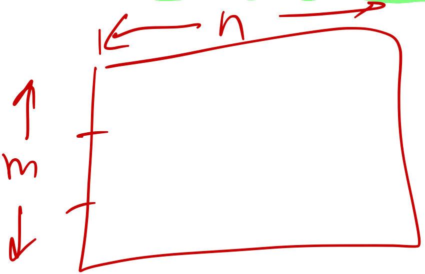
$$c_{\min(i,r),\min(j,s)} + c_{\max(i,r),\max(j,s)} \leq c_{is} + c_{rj} \tag{3.16}$$



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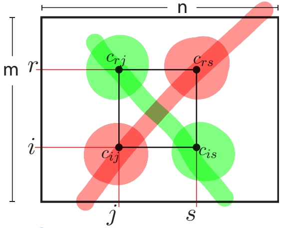
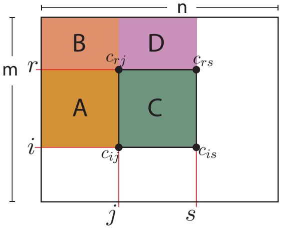
- Consider four elements of the $m \times n$ matrix:





$c_{ij} = A + B$, $c_{rj} = B$, $c_{rs} = B + D$, $c_{is} = A + B + C + D$.

Monge Matrices, where useful

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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:

$$\underset{X \in \mathbb{R}^{m \times n}}{\text{minimize}} \quad \sum_{i=1}^{m} \sum_{j=1}^{n} c_{ij} x_{ij} \tag{3.17}$$

$$\text{subject to} \quad \sum_{i=1}^{m} x_{ij} = b_j \;\; \forall j = 1, \ldots, n \tag{3.18}$$

$$\sum_{j=1}^{n} x_{ij} = a_i \;\; \forall i = 1, \ldots, m \tag{3.19}$$

$$x_{i,j} \geq 0 \;\; \forall i, j \tag{3.20}$$

Monge Matrices, Hitchcock transportation

C

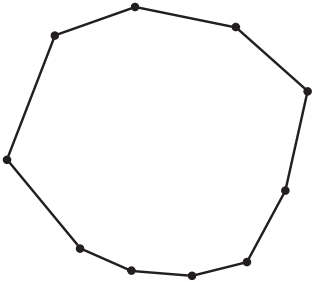
Producers, Sources, or Supply		b_1	b_2	b_3	b_4
a_1	2	0	1	3	3
a_2	1	1	4	7	10
a_3	5	0	4	9	14
		3	2	1	2

Consumers, Sinks, or Demand

- Solving the linear program can be done easily and optimally using the "North West Corner Rule" 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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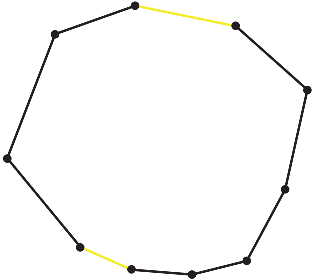

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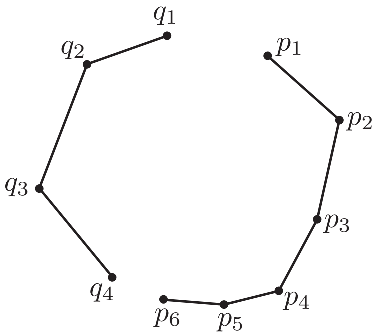

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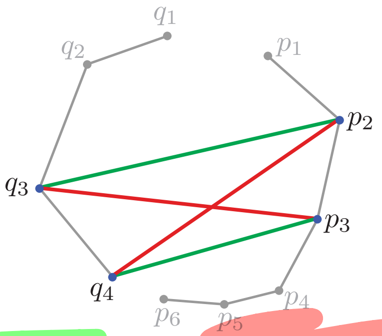

$$d(p_2, q_3) + d(p_3, q_4) \leq d(p_2, q_4) + d(p_3, q_3) \tag{3.21}$$

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- We may define submodularity as: for all $x, y \in \{0,K\}^V$, we have

$$f(x) + f(y) \geq f(x \vee y) + f(x \wedge y) \tag{3.22}$$

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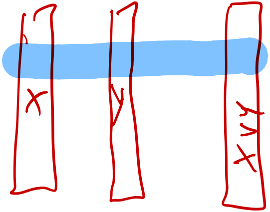
- $x \vee y$ is the (join) element-wise min of each element, that is $(x \vee y)(v) = \min(x(v), y(v))$ for $v \in V$.



Monge Matrices and Submodularity

- A submodular function has the form: $f : 2^V \to \mathbb{R}$ which can be seen as $f : \{0,1\}^V \to \mathbb{R}$
- We can generalize this to $f : \{0,K\}^V \to \mathbb{R}$ for some constant $K \in \mathbb{Z}_+$.
- We may define submodularity as: for all $x, y \in \{0,K\}^V$, we have

$$f(x) + f(y) \geq f(x \vee y) + f(x \wedge y) \tag{3.22}$$

- $x \vee y$ is the (join) element-wise min of each element, that is $(x \vee y)(v) = \min(x(v), y(v))$ for $v \in V$.
- $x \wedge y$ is the (meet) element-wise min of each element, that is, $(x \wedge y)(v) = \max(x(v), y(v))$ for $v \in V$.

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- With $K = 1$, then this is the standard definition of submodularity.
- With $|V| = 2$, and $K + 1$ the side-dimension of the matrix, we get a Monge property (on square matrices).

Two Equivalent Submodular Definitions

Definition 3.6.1 (submodular concave)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{3.8}$$

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

Definition 3.6.2 (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:

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \tag{3.9}$$

The incremental "value", "gain", or "cost" of v decreases (diminishes) as the context in which v is considered grows from A to B.

Submodular on Hypercube Verticies

- Test submodularity via values on verticies of hypercube.

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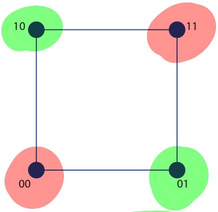
Example: with $|V| = n = 2$, this is easy:

$= V = \{u, v\}$



$f(u) + f(v)$

$\geq f(\phi) + f(\{u, v\})$

$f(v) + f(\phi) \geq f(v) + f(\phi)$

Submodular on Hypercube Verticies

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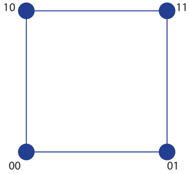
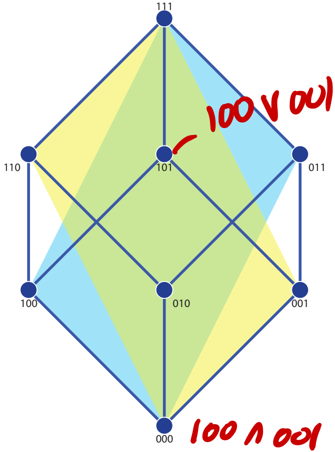


With $|V| = n = 3$, a bit harder.



How many inequalities?

Subadditive Definitions

Definition 3.6.1 (subadditive)

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

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

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

Two Equivalent Supermodular Definitions

Definition 3.6.1 (supermodular)

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

$$f(A) + f(B) \leq f(A \cup B) + f(A \cap B) \tag{3.8}$$

Definition 3.6.2 (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:

$$f(A \cup \{v\}) - f(A) \leq f(B \cup \{v\}) - f(B) \tag{3.9}$$

- 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 $f(A) = c + \sum_{a \in A} f(a)$ (often $c = 0$).

Superadditive Definitions

Definition 3.6.2 (superadditive)

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

$$f(A) + f(B) \leq f(A \cup B) \tag{3.24}$$

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

$$f(A) = \begin{cases} 1 & \text{if } |A| \leq k \\ 0 & \text{else} \end{cases} \tag{3.25}$$

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$\boxed{\text{PS.}}$

- This function is subadditive but not submodular.

Modular Definitions

Definition 3.6.3 (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

$$f(A) + f(B) = f(A \cap B) + f(A \cup B) \tag{3.26}$$

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

Proposition 3.6.4

If f is modular, it may be written as

$$f(A) = f(\emptyset) + \sum_{a \in A} \Big(f(\{a\}) - f(\emptyset) \Big) = c + \sum_{a \in A} f'(a) \tag{3.27}$$

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

Modular Definitions

Proof.

We inductively construct the value for $A = \{a_1, a_2, \dots, a_k\}$.

For $k = 2$,

$$f(a_1) + f(a_2) = f(a_1, a_2) + f(\emptyset) \tag{3.28}$$

$$\text{implies } f(a_1, a_2) = f(a_1) - f(\emptyset) + f(a_2) - f(\emptyset) + f(\emptyset) \tag{3.29}$$

then for $k = 3$,

$$f(a_1, a_2) + f(a_3) = f(a_1, a_2, a_3) + f(\emptyset) \tag{3.30}$$

$$\text{implies } f(a_1, a_2, a_3) = f(a_1, a_2) - f(\emptyset) + f(a_3) - f(\emptyset) + f(\emptyset) \tag{3.31}$$

$$= f(\emptyset) + \sum_{i=1}^{3} \big(f(a_i) - f(\emptyset) \big) \tag{3.32}$$

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 3.6.5

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

Proof.

$$\bar{f}(A) + \bar{f}(B) \geq \bar{f}(A \cup B) + \bar{f}(A \cap B) \tag{3.33}$$

follows from

$$f(V \setminus A) + f(V \setminus B) \geq f(V \setminus (A \cup B)) + f(V \setminus (A \cap B)) \tag{3.34}$$

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). $\square$

Undirected Graphs

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

Undirected Graphs

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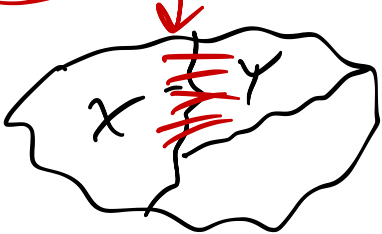
- If G is undirected, define

$$E(X, Y) = \{\{x, y\} \in E(G) : x \in X \setminus Y, y \in Y \setminus X\} \tag{3.35}$$

as the edges strictly between X and Y.



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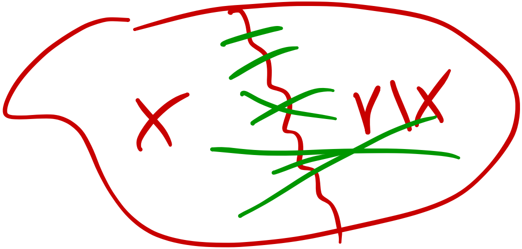
- Nodes define cuts, define the cut function $\delta(X) = E(X, V \setminus X)$.



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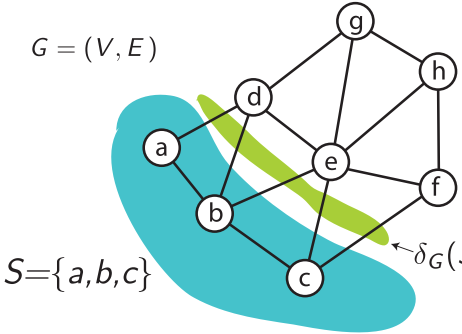

$\delta_G(S) = \{\{u, v\} \in E : u \in S, v \in V \setminus S\}.$
$= \{\{a,d\},\{b,d\},\{b,e\},\{c,e\},\{c,f\}\}$

Directed graphs, and cuts and flows

- If G is directed, define

$$E^+(X,Y) \triangleq \{(x,y) \in E(G) : x \in X \setminus Y, y \in Y \setminus X\} \tag{3.36}$$

as the edges directed strictly from X towards Y.

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and edges entering X (in-flow) as

$$\delta^-(X) \triangleq E^+(V \setminus X, X) \tag{3.38}$$

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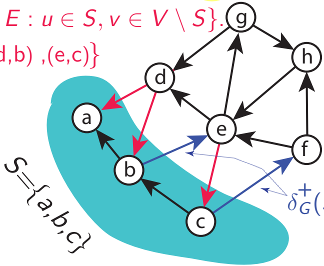
$\delta^-_G(S) = \{(v,u) \in E : u \in S, v \in V \setminus S\}.$
$= \{(d,a), (d,b), (e,c)\}$



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

The Neighbor function in undirected graphs

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

$$\Gamma(X) \triangleq \{v \in V(G) \setminus X : E(X, \{v\}) \neq \emptyset\} \tag{3.39}$$

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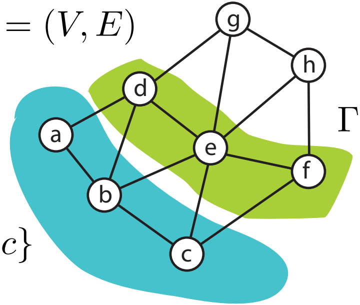
- Example:

$G = (V, E)$



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

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

Directed Cut function: property

Lemma 3.7.1

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

$$|\delta^+(X)| + |\delta^+(Y)| \\ = |\delta^+(X \cap Y)| + |\delta^+(X \cup Y)| + |E^+(X,Y)| + |E^+(Y,X)| \tag{3.40}$$

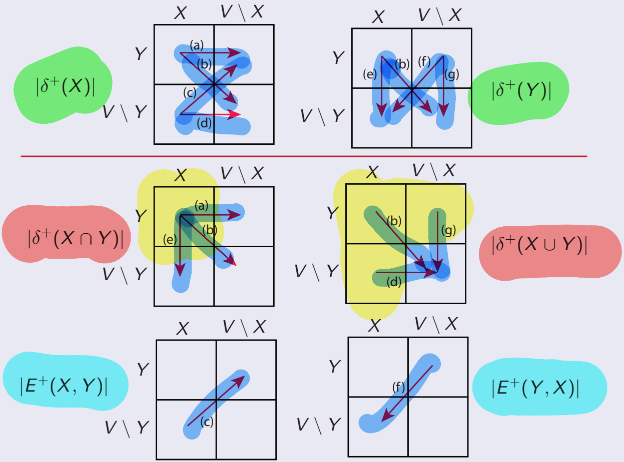
and

$$|\delta^-(X)| + |\delta^-(Y)| \\ = |\delta^-(X \cap Y)| + |\delta^-(X \cup Y)| + |E^-(X,Y)| + |E^-(Y,X)| \tag{3.41}$$

Directed Cut function: proof of property

Proof.

We can prove this using a simple geometric counting argument ($\delta^-(X)$ is similar)



Directed cut/flow functions: submodular

Lemma 3.7.2

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 case, both in-flow and out-flow are submodular on subsets of the vertices.

$$|A| = \sum_{a \in A} w(a) \qquad w(a) = 1$$

Undirected Cut/Flow & the Neighbor function: submodular

Lemma 3.7.3

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.,

$$|\delta(X)| + |\delta(Y)| = |\delta(X \cap Y)| + |\delta(X \cup Y)| + 2|E(X, Y)| \quad (3.42)$$

and

$$|\Gamma(X)| + |\Gamma(Y)| \geq |\Gamma(X \cap Y)| + |\Gamma(X \cup Y)| \quad (3.43)$$

Proof.

- Eq. (3.42) follows from Eq. (3.40): we replace each undirected edge $\{u, v\}$ with two oppositely-directed directed edges (u, v) and (v, u). Then we use same counting argument.

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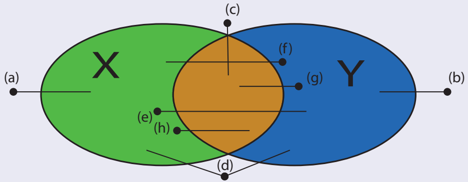
Proof.

- Eq. (3.42) follows from Eq. (3.40): we replace each undirected edge $\{u, v\}$ with two oppositely-directed directed edges (u, v) and (v, u). Then we use same counting argument.
- Eq. (3.43) follows as shown in the following page.

...

cont.



Graphically, we can count and see that

$$\Gamma(X) = (a) + (c) + (f) + (g) + (d) \tag{3.44}$$

$$\Gamma(Y) = (b) + (c) + (e) + (h) + (d) \tag{3.45}$$

$$\Gamma(X \cup Y) = (a) + (b) + (c) + (d) \tag{3.46}$$

$$\Gamma(X \cap Y) = (c) + (g) + (h) \tag{3.47}$$

so

$$\begin{aligned} |\Gamma(X)| + |\Gamma(Y)| &= (a) + (b) + 2(c) + 2(d) + (e) + (f) + (g) + (h) \\ &\geq (a) + (b) + 2(c) + (d) + (g) + (h) = |\Gamma(X \cup Y)| + |\Gamma(X \cap Y)| \end{aligned} \tag{3.48}$$

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

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- Cut weight function over those two nodes: $w(\delta_{u,v}(\cdot))$ has valuation:

$$w(\delta_{u,v}(\emptyset)) = w(\delta_{u,v}(\{u, v\})) = 0 \tag{3.49}$$

and

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

$$w(\delta_{u,v}(\{u\})) + w(\delta_{u,v}(\{v\})) \geq w(\delta_{u,v}(\{u,v\})) + w(\delta_{u,v}(\emptyset)) \tag{3.51}$$

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

$$f(X) = w(\delta(X)) = \sum_{(u,v) \in E(G)} w(\delta_{u,v}(X \cap \{u, v\})) \tag{3.52}$$

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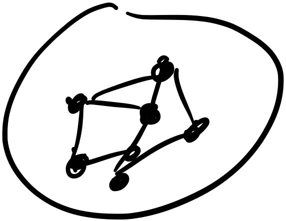
$$|E(S)| = \sum_{i,j \in S} 1$$



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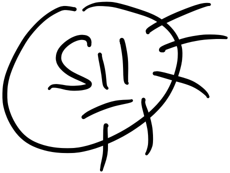

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- Consider $f(A) = |\delta^+(A)| - |\delta^+(V \setminus A)|$. Guess, submodular, supermodular, modular, or neither? Exercise: determine which one and prove it.

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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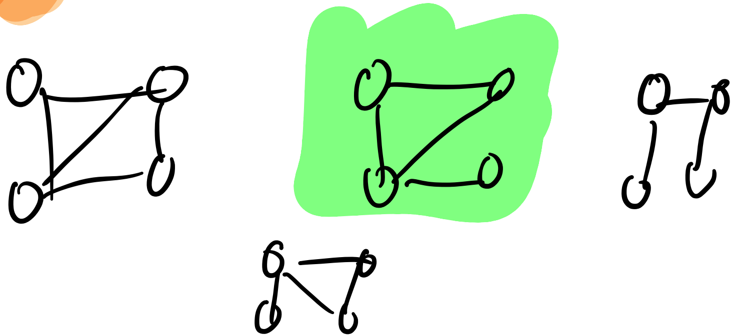

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- $\bar{c}(A) = c(E \setminus A)$ is the number of connected components in G when we remove A, so is also supermodular, but monotone non-decreasing.

Graph Strength

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- For $(u, v) = e \in E$, let $w(e)$ be a measure of the strength of the connection between vertices u and v (strength meaning the difficulty of cutting the edge e).

Graph Strength

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

$$w(A) = \sum_{e \in A} w_e \tag{3.54}$$

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.

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$$\textit{strength}(G, w) = \min_{A \subseteq E(G) : \bar{c}(A) > 1} \frac{w(A)}{\bar{c}(A) - 1} \tag{3.55}$$

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

Submodularity, Quadratic Structures, and Cuts

Lemma 3.7.4

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

$$f(X) = m^\intercal \mathbf{1}_X + \frac{1}{2}\mathbf{1}_X^\intercal \mathbf{M} \mathbf{1}_X \tag{3.56}$$

is submodular iff the off-diagonal elements of M are non-positive.

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.

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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.

Submodularity, Quadratic Structures, and Cuts

Proof of Lemma 3.7.4 cont.

- Conversely, suppose f is submodular.

$\square$

Submodularity, Quadratic Structures, and Cuts

Proof of Lemma 3.7.4 cont.

- Conversely, suppose f is submodular.
- Then $f(\{u\}) + f(\{v\}) \geq f(\{u, v\}) + f(\emptyset)$ while $f(\emptyset) = 0$.

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Submodularity, Quadratic Structures, and Cuts

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- Conversely, suppose f is submodular.
- Then $f(\{u\}) + f(\{v\}) \geq f(\{u,v\}) + f(\emptyset)$ while $f(\emptyset) = 0$.
- Then:

$$\begin{aligned}
0 &\leq f(\{u\}) + f(\{v\}) - f(\{u,v\}) && (3.57)\\
&= m(u) + \frac{1}{2}M_{u,u} + m(v) + \frac{1}{2}M_{v,v} && (3.58)\\
&\quad - \Big(m(u) + m(v) + \frac{1}{2}M_{u,u} + M_{u,v} + \frac{1}{2}M_{v,v}\Big) && (3.59)\\
&= -M_{u,v} && (3.60)
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So that $\forall u, v \in V$, $M_{u,v} \leq 0$.

□

Set Cover and Maximum Coverage

- We are given a finite set V of n elements and a set of subsets $\mathcal{V} = \{V_1, V_2, \ldots, V_m\}$ of m subsets of V, so that $V_i \subseteq V$ and $\bigcup_i V_i = V$.

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- Maximum k cover: The goal in MAXIMUM COVERAGE is, given an integer $k \leq m$, select k subsets, say $\{a_1, a_2, \ldots, a_k\}$ with $a_i \in [m]$ such that $|\bigcup_{i=1}^k V_{a_i}|$ is maximized.

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- Both SET COVER and MAXIMUM COVERAGE are well known to be NP-hard, but have a fast greedy approximation algorithm.

Other Covers

Definition 3.7.5 (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 3.7.6 (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 $|V|(F) = |V|$.

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- 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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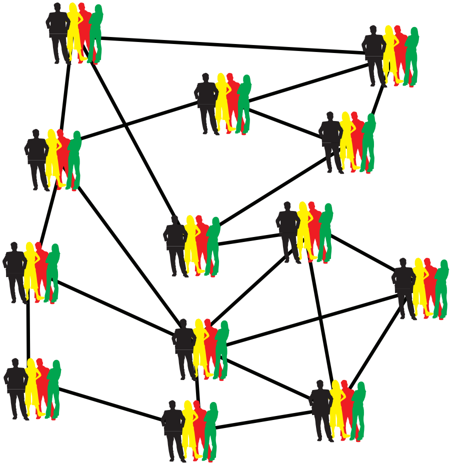
- Many examples of this, we will see more later.

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.



Facility/Plant Location (uncapacitated)

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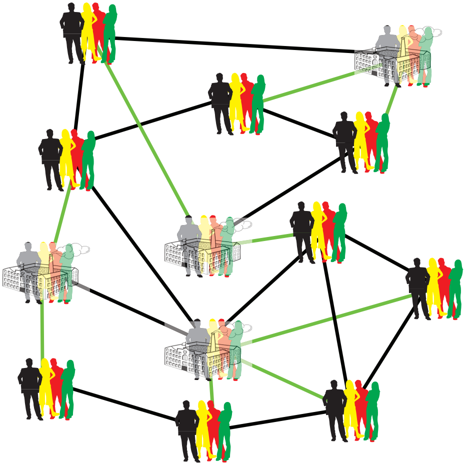

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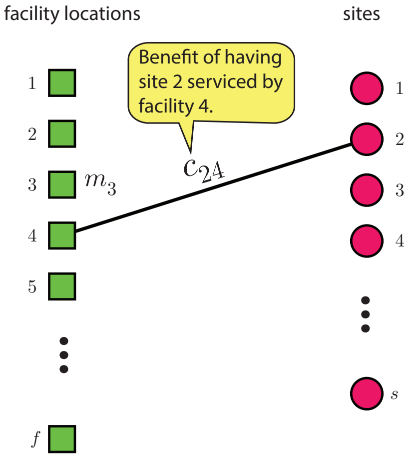
- We can model this with a weighted bipartite graph $G = (F, S, E, c)$ where F is set of possible factory/plant locations, S is set of sites needing service, E are edges indicating (factory,site) service possiblity pairs, and $c : E \to \mathbb{R}_+$ is the benefit of a given pair.
- Facility location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

$$f(A) = \sum_{i \in F} \max_{j \in A} c_{ij}. \qquad (3.61)$$



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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., $|A| \leq k$).

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- 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 $\mathbf{X}$.

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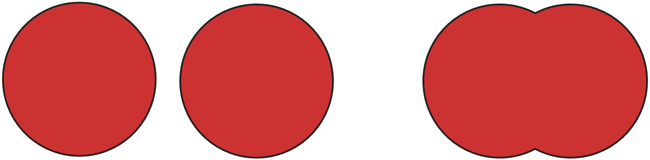

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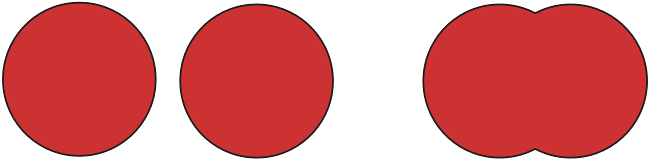

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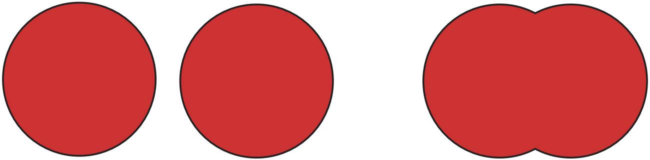

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- Any function where the above inequality is true for all $A, B \subseteq V$ is called subadditive.

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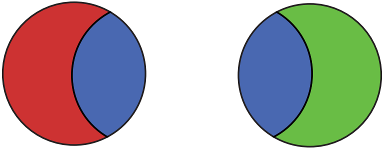

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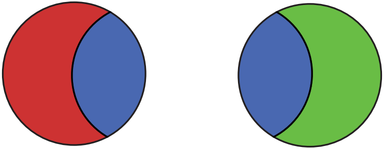

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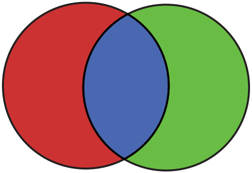

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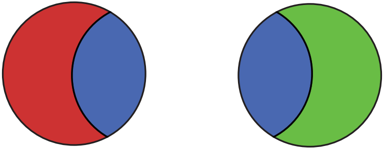

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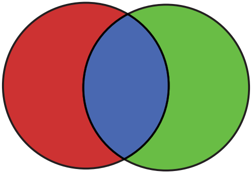

- Thus, we have subadditivity: $r(A) + r(B) \geq r(A \cup B)$. Can we add more to the r.h.s. and still have an inequality? Yes.

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- 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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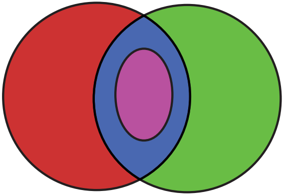

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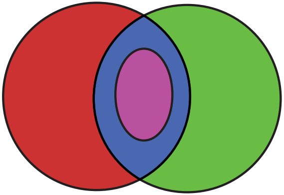

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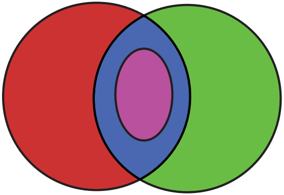

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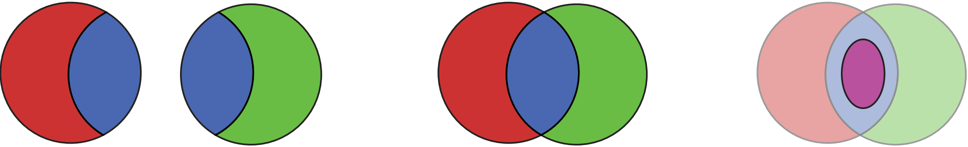
- More generally, common information (blue) is "more" (no less) than information within common index (magenta).

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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- 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 $A \subseteq B$).

Spanning trees

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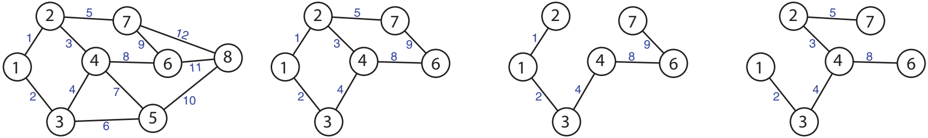
- Example: Given $G = (V, E)$, $V = \{1, 2, 3, 4, 5, 6, 7, 8\}$, $E = \{1, 2, \ldots, 12\}$. $S = \{1, 2, 3, 4, 5, 8, 9\} \subset E$. Two spanning trees have the same edge count (the rank of S).



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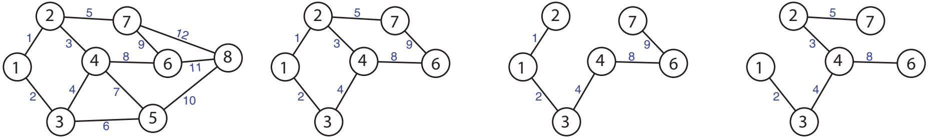

- Then $r(S)$ is submodular, and is another matrix rank function corresponding to the incidence matrix of the graph.