Submodular Functions, Optimization, and Applications to Machine Learning — Fall Quarter, Lecture 3 —

http://www.ee.washington.edu/people/faculty/bilmes/classes/ee563\_spring\_2018/

#### Prof. Jeff Bilmes

University of Washington, Seattle Department of Electrical Engineering http://melodi.ee.washington.edu/~bilmes

#### Oct 7th, 2020



## • Read chapter 1 from Fujishige's book.

Logistics

# Class Road Map - EE563

- L1(9/30): Motivation, Applications, Definitions, Properties
- L2(10/5): Sums concave(modular), uses (diversity/costs, feature selection), information theory
- L3(10/7): Monge, More Definitions, Graph and Combinatorial Examples, Matrix Rank, Properties
- L4(10/12):
- L5(10/14):
- L6(10/19):
- L7(10/21):
- L8(10/26):
- L9(10/28):
- L10(11/2):

- L11(11/4):
- L12(11/9):
- L–(11/11): Veterans Day, Holiday
- L13(11/16):
- L14(11/18):
- L15(11/23):
- L16(11/25):
- L17(11/30):
- L18(12/2):
- L19(12/7):
- L20(12/9): maximization.

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

Two Equivalent Submodular Definitions

Definition 3.2.1 (submodular concave)

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

$$f(A) + f(B) \ge f(A \cup B) + f(A \cap B)$$
(3.7)

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

## Definition 3.2.2 (diminishing returns)

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

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

• Gain notation: Define  $f(v|A) \triangleq f(A+v) - f(A)$ . Then function f is submodular if  $f(v|A) \ge f(v|B)$  for all  $A \subseteq B \subseteq V \setminus \{v\}$ ,  $v \in V$ .

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## Definition 3.2.2 (supermodular (improving returns))

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

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
Mong	e Matrices			

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

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

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

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• Lined up indices

$$i < r$$
 (3.2)  
 $j < s$  (3.3)

• Equivalently, for all  $1 \le i, r \le m$ ,  $1 \le s, j \le n$ ,

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



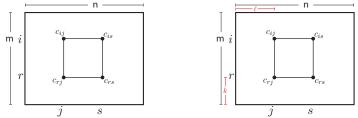
• Consider a non-negative matrix  $D = (d_{i,j})$  of order  $m \times n$  and form matrix  $C = (c_{i,j})$  with  $c_{i,j}$ th entry,  $1 \le i \le m$ ,  $1 \le j \le n$ :

$$c_{ij} = \sum_{k=i}^{m} \sum_{\ell=1}^{j} d_{k,\ell}$$
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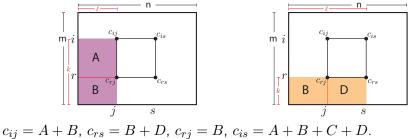
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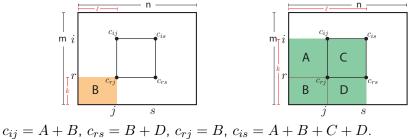
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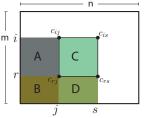


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• Consider four elements of the  $m \times n$  matrix:

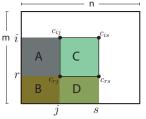


 $c_{ij} = A + B$ ,  $c_{rs} = B + D$ ,  $c_{rj} = B$ ,  $c_{is} = A + B + C + D$ .

Monge

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

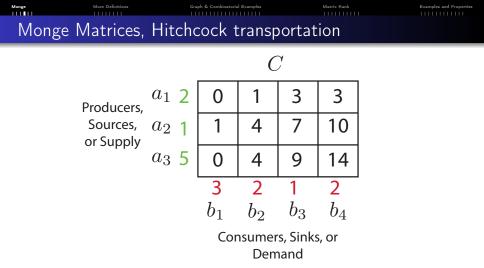


• Useful for speeding up transportation, dynamic programming, flow, search, lot-sizing and many other problems.

## Morge More Definitions Graph & Combinatorial Examples Matrix Rank Examples and Properties Monge Matrices, where useful

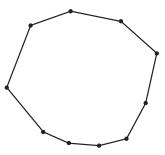
- Useful for speeding up transportation, dynamic programming, flow, search, lot-sizing and many other problems.
- Example, Hitchcock transportation problem: Given  $m \times n$  cost matrix  $C = [c_{ij}]_{ij}$ , a non-negative supply vector  $a \in \mathbb{R}^m_+$ , a non-negative demand vector  $b \in \mathbb{R}^n_+$  with  $\sum_{i=1}^m a(i) = \sum_{j=1}^n b_j$ , we wish to optimally solve the following linear program:

$$\begin{array}{ll} \underset{X \in \mathbb{R}^{m \times n}}{\text{minimize}} & \sum_{i=1}^{m} \sum_{j=1}^{n} c_{ij} x_{ij} & (3.6) \\ \text{subject to} & \sum_{i=1}^{m} x_{ij} = b_j \ \forall j = 1, \dots, n & (3.7) \\ & \sum_{j=1}^{n} x_{ij} = a_i \ \forall i = 1, \dots, m & (3.8) \\ & x_{i,j} \ge 0 \ \forall i, j & (3.9) \end{array}$$



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

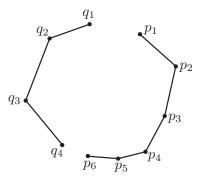
• Can generate a Monge matrix from a convex polygon - delete two segments, then separately number vertices on each chain. Distances  $c_{ij}$  satisfy Monge property (or quadrangle inequality).



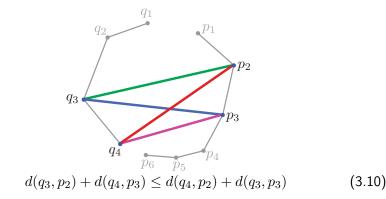
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Transport unit quantities from locations  $q_3$  and  $q_4$  to locations  $p_2$  and  $p_3$ ; to minimize total distance traveled, routes from  $q_3$  and  $q_4$  must not intersect.



• A submodular function has the form:  $f:2^V\to\mathbb{R}$  which can be seen as  $f:\{0,1\}^V\to\mathbb{R}$ 

# More More Continuous Graph & Continuous Examples Music Rank Examples and Property Monge Matrices and Submodularity

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- Non square:  $f: \{0, 1, \dots, K_1\} \times \{0, 1, \dots, K_2\} \rightarrow \mathbb{R}.$

 More Definition
 Graph & Graph & Graph & Graph & Marris Rank

 Two Equivalent Submodular Definitions

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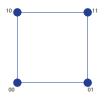
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We can test submodularity via values on vertices of hypercube.

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

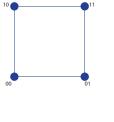
easy:

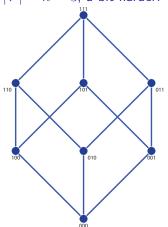




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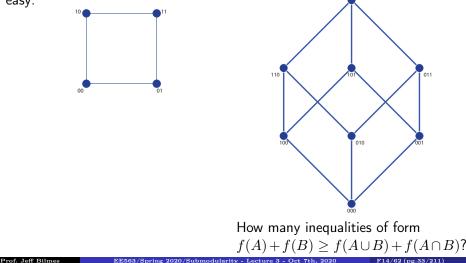






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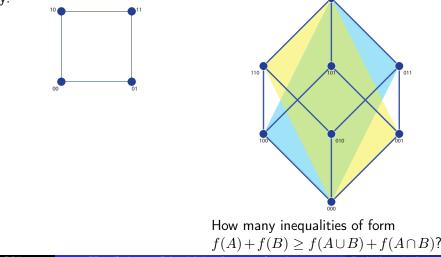
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Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
11111				
Sub	additive Definit	tions		

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



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

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

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• This function is subadditive but not submodular.

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Mod	ular Definitions			

#### Definition 3.4.3 (modular)

A function that is both submodular and supermodular is called modular

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

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

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

#### Proposition 3.4.4

If f is modular, it may be written as

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

which has only |V| + 1 parameters.

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
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#### Proof.

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

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

implies 
$$f(a_1, a_2) = f(a_1) - f(\emptyset) + f(a_2) - f(\emptyset) + f(\emptyset)$$
 (3.18)

then for k = 3,

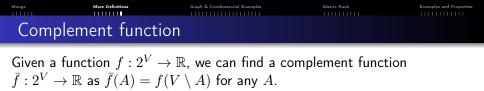
$$f(a_1, a_2) + f(a_3) = f(a_1, a_2, a_3) + f(\emptyset)$$
(3.19)

implies  $f(a_1, a_2, a_3) = f(a_1, a_2) - f(\emptyset) + f(a_3) - f(\emptyset) + f(\emptyset)$  (3.20)

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

and so on . . .

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#### Proposition 3.4.5

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

#### Proof.

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

#### follows from

$$f(V \setminus A) + f(V \setminus B) \ge f(V \setminus (A \cup B)) + f(V \setminus (A \cap B))$$
(3.23)

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

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties	
	ected Graphs				
• Let $G = (V, E)$ be a graph with vertices $V = V(G)$ and edges					

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 $E = E(G) \subseteq V \times V.$ 



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

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

as the edges strictly between X and Y.

### Undirected Graphs

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

& Combinatorial Eva

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• Nodes define cuts. Define the cut function  $\delta(X) = E(X, V \setminus X)$ , set of edges with exactly one vertex in X.

### Undirected Graphs

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& Combinatorial Exc

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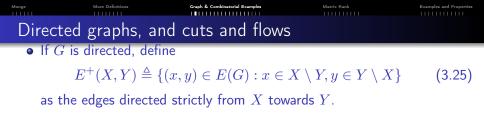
$$G = (V, E)$$

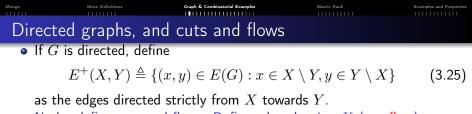
$$G = (V, E)$$

$$G = (V, E)$$

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

$$G = \{$$



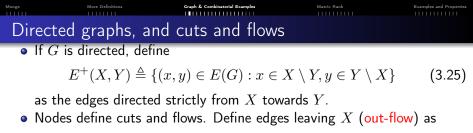


• Nodes define cuts and flows. Define edges leaving X (out-flow) as

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

and edges entering X (in-flow) as

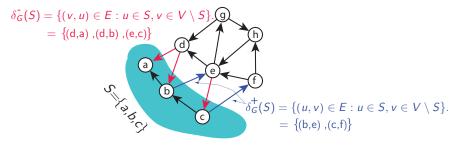
$$\delta^{-}(X) \triangleq E^{+}(V \setminus X, X)$$
(3.27)



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

and edges entering X (in-flow) as

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





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

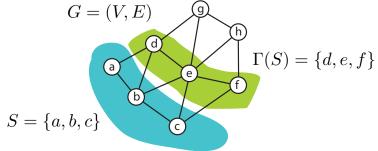
 $\Gamma(X) \triangleq \{ v \in V(G) \setminus X : E(X, \{v\}) \neq \emptyset \}$ (3.28)



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

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





Examples and Properties

## Directed Cut function: property

More Definitions

#### Lemma 3.5.1

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

$$\begin{aligned} |\delta^+(X)| + |\delta^+(Y)| \\ &= |\delta^+(X \cap Y)| + |\delta^+(X \cup Y)| + |E^+(X,Y)| + |E^+(Y,X)| \end{aligned} (3.29)$$

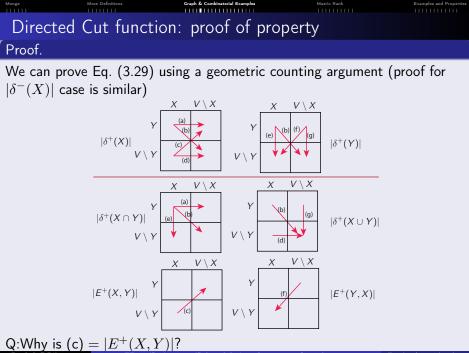
Graph & Combinatorial Examples

Matrix Rank

and

Monge

$$\begin{aligned} |\delta^{-}(X)| + |\delta^{-}(Y)| \\ &= |\delta^{-}(X \cap Y)| + |\delta^{-}(X \cup Y)| + |E^{-}(X,Y)| + |E^{-}(Y,X)| \end{aligned}$$
(3.30)



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F25/62 (pg.54/211)

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 More Definitions
 Graph & Combinatorial Examples
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 Directed
 cut/flow
 functions:
 submodular

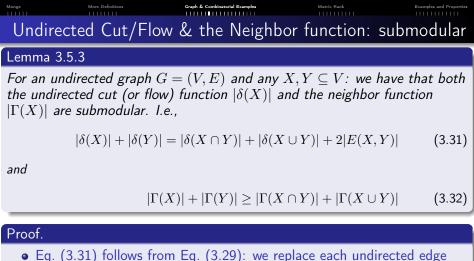
#### Lemma 3.5.2

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

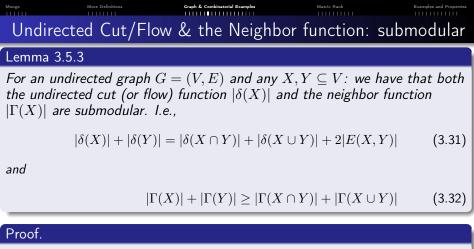
#### Proof.

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

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

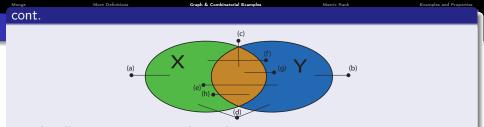


 $\{u, v\}$  with two oppositely-directed directed edges (u, v) and (v, u). Then we use same counting argument.



- Eq. (3.31) follows from Eq. (3.29): we replace each undirected edge  $\{u, v\}$  with two oppositely-directed directed edges (u, v) and (v, u). Then we use same counting argument.
- Eq. (3.32) follows as shown in the following page.

. . .



Graphically, we can count and see that

$$\Gamma(X) = (a) + (c) + (f) + (g) + (d)$$
(3.33)

$$\Gamma(Y) = (b) + (c) + (e) + (h) + (d)$$
(3.34)

$$\Gamma(X \cup Y) = (a) + (b) + (c) + (d)$$
(3.35)

$$\Gamma(X \cap Y) = (c) + (g) + (h)$$
(3.36)

SO

$$\Gamma(X)| + |\Gamma(Y)| = (a) + (b) + 2(c) + 2(d) + (e) + (f) + (g) + (h) \geq (a) + (b) + 2(c) + (d) + (g) + (h) = |\Gamma(X \cup Y)| + |\Gamma(X \cap Y)|$$
 (3.37)



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



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



- Another simple proof shows that  $|\delta(X)|$  is submodular.
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- Weighted cut function over those two nodes:  $w(\delta_{u,v}(\cdot))$  has valuation:

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

and

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• Thus,  $w(\delta_{u,v}(\cdot))$  is submodular since  $w(e) \ge 0$  and  $w(\delta_{u,v}(\{u\})) + w(\delta_{u,v}(\{v\})) \ge w(\delta_{u,v}(\{u,v\})) + w(\delta_{u,v}(\emptyset))$  (3.40)

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

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

$$f(X) = w(\delta(X)) = \sum_{(u,v) \in E(G)} w(\delta_{u,v}(X \cap \{u,v\}))$$
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 $\bullet\,$  Thus,  $w(\delta_{u,v}(\cdot))$  is submodular since  $w(e)\geq 0$  and

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



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.

# More performance Graph & Combinational Examples Match Rank Examples and Properties Other graph functions that are submodular/supermodular

- 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.

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- 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  $|I(S)| = |E(S)| + |\delta(S)|$ .

# Mage Mere Definitions Graph & Centributerial Examples Matrix Rank Examples and Properties Other graph functions that are submodular/supermodular

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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.





- Recall,  $f: 2^V \to \mathbb{R}$  is submodular, then so is  $\overline{f}: 2^V \to \mathbb{R}$  defined as  $\overline{f}(S) = f(V \setminus S)$ .
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- 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  $c(E) \ge 1$ .

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- c(A) is monotone non-increasing,  $c(A+a)-c(A)\leq 0$  .
- Then c(A) is supermodular, i.e.,

$$c(A+a) - c(A) \le c(B+a) - c(B)$$

$$a \le B \le E \setminus \{a\}.$$
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• 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.

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- 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.

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
11111	1111111			
Graph	Strength			

• So  $\bar{c}(A) = c(E \setminus A)$ , the number of connected components in G when we remove A, is supermodular.

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- An attacker wishes to choose a small number of edges (since it is cheap) to shatter the graph into as many components as possible.
- Let G = (V, E, w) with  $w : E \to \mathbb{R}+$  be a weighted graph with non-negative weights.

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Graph	n Strength			

- So  $\bar{c}(A) = c(E \setminus A)$ , the number of connected components in G when we remove A, is supermodular.
- Maximizing  $\overline{c}(A)$  would be a goal for a network attacker many connected components means that many points in the network have lost connectivity to many other points (unprotected network).
- If we can remove a small set A and shatter the graph into many connected components, then the graph is weak.
- An attacker wishes to choose a small number of edges (since it is cheap) to shatter the graph into as many components as possible.
- Let G = (V, E, w) with  $w : E \to \mathbb{R}+$  be a weighted graph with non-negative weights.
- 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).

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
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Granh	Strength			

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

$$w(A) = \sum_{e \in A} w_e \tag{3.43}$$

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

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
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Graph S	Strength			

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## More More Definitions Graph & Combinatorial Examples Matrix Bank Examples and Properties Graph Strength Interface Interface Interface Interface

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- A form of graph strength can then be defined as the following:

$$strength(G, w) = \min_{A \subseteq E(G): \bar{c}(A) > 1} \frac{w(A)}{\bar{c}(A) - 1}$$
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## More More Definitions Graph & Combinatorial Examples Matrix Rank Examples and Properties Graph Strength

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- 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.



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

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

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

#### Proof.



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

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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.



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

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#### Proof of Lemma 3.5.4 cont.

• Conversely, suppose *f* is submodular.



#### Proof of Lemma 3.5.4 cont.

- Conversely, suppose *f* is submodular.
- Then  $\forall u, v \in V$ ,  $f(\{u\}) + f(\{v\}) \ge f(\{u, v\}) + f(\emptyset)$  and  $f(\emptyset) = 0$ .



#### Proof of Lemma 3.5.4 cont.

- Conversely, suppose *f* is submodular.
- Then  $\forall u, v \in V$ ,  $f(\{u\}) + f(\{v\}) \ge f(\{u, v\}) + f(\emptyset)$  and  $f(\emptyset) = 0$ .
- This requires:

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

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

$$-\left(m(u) + m(v) + \frac{1}{2}M_{u,u} + M_{u,v} + \frac{1}{2}M_{v,v}\right)$$
(3.48)  
=  $-M_{u,v}$  (3.49)

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

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 just Special cases of Submodular Optimization
 Examples and Properties

• 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  $\{a_1, a_2, \ldots, a_k\}$  with  $a_i \in [n]$  such that  $|\bigcup_{i=1}^k U_{a_i}|$  is maximized.

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

# Manage Marco Particular Craph & Combinatoral Examples Marco Reak Examples and Properties Set Cover and Maximum Coverage just Special cases of Submodular Optimization

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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.

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
11111	1111111			
Vertex a	and Edge C	overs		

Also instances of submodular optimization

#### Definition 3.5.5 (vertex cover)

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

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

#### Definition 3.5.6 (edge cover)

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

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

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
11111	1111111			
Graph	Cut Problen	ns		
Also subi	modular optimizatio	on		

• 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  $V \setminus S$ .

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
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Graph	Cut Problem	าร		
Also sub	modular optimizatio	on		

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Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
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Graph	Cut Problem	IS		
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- Maximum cut: Given a graph G = (V, E), find a set of vertices  $S \subseteq V$  that maximize the cut (set of edges) between S and  $V \setminus S$ .
- 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.,  $\delta(x) = E(X, V \setminus X)$ .

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
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Graph	Cut Problem	IS		
Also sub	modular optimizatio	n		

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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.

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
Matrix Rank functions				

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



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

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

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



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

• Let r(S) for  $S \subseteq V$  be the rank of the set of vectors S. Then  $r(\cdot)$  is a submodular function, and in fact is called a matric matroid rank function.



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



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- Let  $V = \{1, 2, \dots, m\}$  be the set of column vector indices.



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- For any  $A \subseteq V$ , let r(A) be the rank of the column vectors indexed by A.



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- Let  $V=\{1,2,\ldots,m\}$  be the set of column vector indices.
- For any  $A \subseteq V$ , let r(A) be the rank of the column vectors indexed by A.
- r(A) is the dimensionality of the vector space spanned by the set of vectors {x<sub>a</sub>}<sub>a∈A</sub>.



- Given  $n \times m$  matrix  $\mathbf{X} = (x_1, x_2, \dots, x_m)$  with  $x_i \in \mathbb{R}^n$  for all i. There are m length-n column vectors  $\{x_i\}_i$
- Let  $V=\{1,2,\ldots,m\}$  be the set of column vector indices.
- For any  $A \subseteq V$ , let r(A) be the rank of the column vectors indexed by A.
- r(A) is the dimensionality of the vector space spanned by the set of vectors {x<sub>a</sub>}<sub>a∈A</sub>.
- Thus, r(V) is the rank of the matrix  $\mathbf{X}$ .

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

Matrix Rank

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

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• 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.•  $r(A \cup C) = 3, r(B \cup C) = 3.$ •  $r(A \cup A_r) = 3, r(B \cup B_r) = 3, r(A \cup B_r) = 4, r(B \cup A_r) = 4.$ •  $r(A \cup B) = 4, r(A \cap B) = 1 < r(C) = 2.$ 

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• Then  $r(A) = 3$ ,  $r(B) = 3$ ,  $r(C) = 2$ .  
•  $r(A \cup C) = 3$ ,  $r(B \cup C) = 3$ .  
•  $r(A \cup A_r) = 3$ ,  $r(B \cup B_r) = 3$ ,  $r(A \cup B_r) = 4$ ,  $r(B \cup A_r) = 4$ .  
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•  $6 = r(A) + r(B) = r(A \cup B) + r(C) > r(A \cup B) + r(A \cap B) = 5$ 

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
Rank	function of a	matrix		

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- If some of the dimensions spanned by A overlap some of the dimensions spanned by B (i.e., if  $\exists$  common span), then that area is counted twice in r(A) + r(B), so the inequality will be strict.
- Any function where the above inequality is true for all  $A, B \subseteq V$  is called subadditive.



• Vector sets A and B have a (possibly empty) common span and two (possibly empty) non-common residual spans.

## Marge More Definitions Graph & Combinatorial Examples Matrix Rank Examples and Properties

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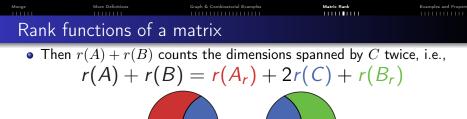
### Morge More Definitions Graph & Combinatorial Examples Matrix Rack Examples Rank functions of a matrix

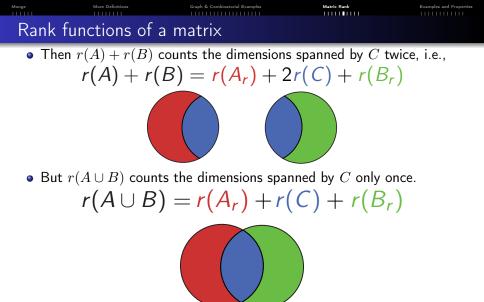
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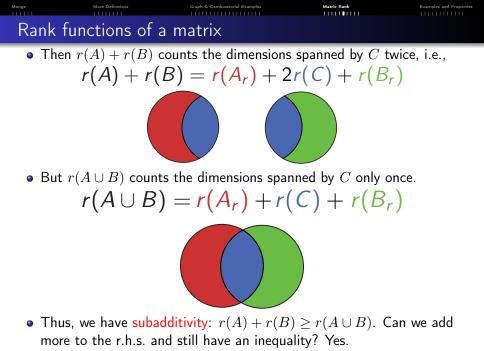
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• But  $r(A \cup B)$  counts the dimensions spanned by C only once.

$$r(A \cup B) = r(A_r) + r(C) + r(B_r)$$
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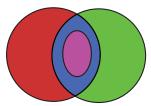




### More Perforitions Graph & Combinatorial Examples Marie Rank Examples and Properties Rank function of a matrix

Note, r(A ∩ B) ≤ r(C). Why? Vectors indexed by A ∩ 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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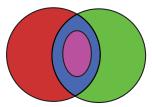


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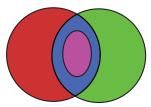
In short:

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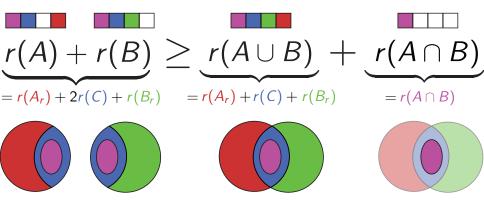


In short:

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

Monge More Definitions Graph & Combinatorial Examples Marcia Rack Examples and Properties

#### The Venn and Art of Submodularity





• Let S be a set of subspaces of a linear space (i.e., each  $s \in S$  is a subspace of dimension  $\geq 1$ ).

# More More Definitions Graph & Combinatorial Examples Marie Rank Examples and Properties Polymatroid rank function

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- Then, defining  $f: 2^S \to \mathbb{R}_+$  as follows,

$$f(X) = r(\bigcup_{s \in X} X_s) \tag{3.53}$$

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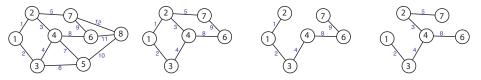
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- We use the term non-decreasing rather than increasing, the latter of which is strict (also so that a constant function isn't "increasing").

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Spanr	ning 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.

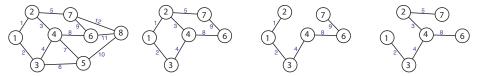
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• Then r(S) is submodular, and is another matrix rank function corresponding to the incidence matrix of the graph.



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

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

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 (3.58)

is submodular. This follows easily since

$$f(A) + f(B) = f_1(A) + f_2(A) + f_1(B) + f_2(B)$$

$$\geq f_1(A \cup B) + f_2(A \cup B) + f_1(A \cap B) + f_2(A \cap B)$$

$$= f(A \cup B) + f(A \cap B).$$
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I.e., it holds for each component of f in each term in the inequality.

# Manage Marke Definitions Graph & Combinatorial Examples Marke Definitions Examples and Properties Summing Submodular Functions Functions Functions Functions

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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  $\alpha_1, \alpha_2 \ge 0$ .



Given E, let  $f_1, m: 2^E \to \mathbb{R}$  be a submodular and a modular function.



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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

$$f': 2^E \to \mathbb{R} \text{ with } f'(A) \triangleq f(A \cap S)$$
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is submodular.

### Monge More Definitions Graph & Combinatorial Examples Matrix Rank Examples and Properties

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Proof.

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Proof. Given  $A \subseteq B \subseteq E \setminus v$ , consider  $f((A + v) \cap S) - f(A \cap S) \ge f((B + v) \cap S) - f(B \cap S)$  (3.67)

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$$f((A+v) \cap S) - f(A \cap S) \ge f((B+v) \cap S) - f(B \cap S)$$
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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

$$f(A'+v) - f(A') \ge f(B'+v) - f(B')$$
(3.68)

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

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

 $f: 2^V \to \mathbb{R}$  with  $f(A) = f_1(A \cap S_1) + f_2(A \cap S_2)$  (3.69)

is submodular. This follows easily from the preceding two results.



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

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is submodular. This follows easily from the preceding two results. Given V, let  $C = \{C_1, C_2, \ldots, C_k\}$  be a set of subsets of V, and for each  $C \in C$ , let  $f_C : 2^V \to \mathbb{R}$  be a submodular function. Then

$$f: 2^V \to \mathbb{R} \text{ with } f(A) = \sum_{C \in \mathcal{C}} f_C(A \cap C)$$
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# 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

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is submodular. This property is critical for image processing and graphical models. For example, let 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.

# More More Definitions Graph & Combinatorial Examples Matrix Rank Examples and Poperties

## Max - normalized

Given V, let  $c \in \mathbb{R}^V_+$  be a given fixed vector. Then  $f : 2^V \to \mathbb{R}_+$ , where  $f(A) = \max_{j \in A} c_j$ (3.71)

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

# Proof. Consider $\max_{j \in A} c_j + \max_{j \in B} c_j \ge \max_{j \in A \cup B} c_j + \max_{j \in A \cap B} c_j$ (3.72)which follows since we have that $\max(\max_{j \in A} c_j, \max_{j \in B} c_j) = \max_{j \in A \cup B} c_j$ (3.73)and $\min(\max_{j \in A} c_j, \max_{j \in B} c_j) \ge \max_{j \in A \cap B} c_j$ (3.74)

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
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

$$f(A) = \max_{j \in A} c_j \tag{3.75}$$

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

#### Proof.

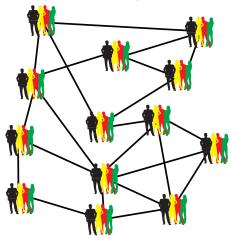
The proof is identical to the normalized case.

# Monge More Definitions Graph & Combinatorial Examples Matrix Rank

Examples and Properties

# Facility/Plant Location (uncapacitated)

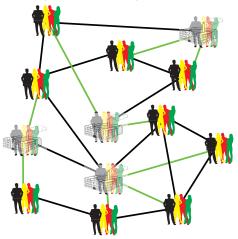
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- Goal: as efficiently as possible, place "facilities" (factories) at certain locations to satisfy sites (at all locations) having various demands.



# Mongs More Definitions Graph & Cembinatorial Examples Matrix Rank

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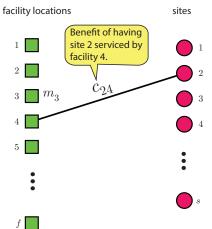


Examples and Properties

# 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.
- 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 → ℝ<sub>+</sub> is the benefit of a given pair.
- Facility location function has form:

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





• Let  $F = \{1, \ldots, f\}$  be a set of possible factory/plant locations for facilities to be built.



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# More More Definitions Graph & Combinated Examples Mattic Rank Examples and Properties Facility/Plant Location (uncapacitated) w. plant benefits

- Let  $F = \{1, \ldots, f\}$  be a set of possible factory/plant locations for facilities to be built.
- $S = \{1, \ldots, s\}$  is a set of sites (e.g., cities, clients) needing service.
- Let  $c_{ij}$  be the "benefit" or "value" (e.g.,  $1/c_{ij}$  is the cost) of servicing site i with facility location j.

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- Let  $m_j$  be the benefit (e.g., either  $1/m_j$  is the cost or  $-m_j$  is the cost) to build a plant at location j.

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- Define f(A) as the "delivery benefit" plus "construction benefit" when the locations  $A \subseteq F$  are to be constructed.



# Facility/Plant Location (uncapacitated) w. plant benefits

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- We can define the (uncapacitated) facility location function

$$f(A) = \sum_{j \in A} m_j + \sum_{i \in S} \max_{j \in A} c_{ij}.$$
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$$f(A) = \sum_{j \in A} m_j + \sum_{i \in S} \max_{j \in A} c_{ij}.$$
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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.,  $|A| \le k$ ).

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
11111				
Facilit	y Location			

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

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

#### is submodular.

#### Proof.

We can write f(A) as  $f(A) = \sum_{i \in V} f_i(A)$  where  $f_i(A) = \max_{j \in A} c_{ij}$  is submodular (max of a *i*<sup>th</sup> 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.

Examples and Properties

#### Log Determinant

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

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties

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- We have that:

 $f(A) = \log \det(\Sigma_A)$  is submodular. (3.79)

# Monge More Definitions Graph & Combinatorial Examples Matrix Rank Examples and Properties

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• The submodularity of the log determinant is crucial for determinantal point processes (DPPs) (defined later in the class).

# Monge More Definitions Graph & Combinatorial Examples Matrix Rank Examples and Properties

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• The submodularity of the log determinant is crucial for determinantal point processes (DPPs) (defined later in the class).

#### Proof of submodularity of the logdet function.

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

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

. . .

Monge	More Definitions	Graph & Combinatorial Examples	Matrix Rank	Examples and Properties
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	Determinant			
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#### ...cont.

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

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

and in particular, for a variable subset A,

$$f(A) = h(X_A) = \log \sqrt{(2\pi e)^{|A|} |\Sigma_A|}$$
 (3.82)

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

$$f(A) = h(X_A) = m(A) + \frac{1}{2}\log|\Sigma_A|$$
 (3.83)

where m(A) is a modular function.

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

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• SCCM is submodular  $f(A) = \sum_{u \in U} \phi_u(m_u(A))$  where  $m_u$  is a non-negative modular and  $\phi_u$  is concave.

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- Number of connected components in induced graph, and interior edge function, is supermodular.
- Submodular plus modular is submodular, f(A) = f'(A) + m(A).
- Complementation:  $f'(A) = f(V \setminus A)$  is submodular if f is submodular and m is modular. (supermodular) if f is submodular (supermodular).

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- Log determinant  $f(A) = \log \det(\Sigma_A)$  submodular for p.d.  $\Sigma$ .
- Matrix rank function is submodular.
- Graph cut, set cover, and incidence functions, and quadratics with non-positive off-diagonals, are all submodular.
- Number of connected components in induced graph, and interior edge function, is supermodular.
- Submodular plus modular is submodular, f(A) = f'(A) + m(A).
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- Restrictions preserve submodularity:  $f'(A) = f(A \cap S)$