Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 4 —

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

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

 $-f(A_i) + 2f(C) + f(B_i) - f(A_i) + f(C) + f(B_i) - f(A \cap B)$









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 11:55pm.
- 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)).

Logistics

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): Graph and Combinatorial Examples, matrix rank, Venn diagrams, examples of proofs of submodularity, some useful properties
- 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.

Monge Matrices

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

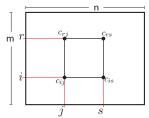
$$c_{ij} + c_{rs} \le c_{is} + c_{rj} \tag{4.15}$$

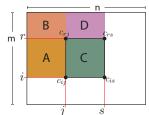
for all $1 \le i < r \le m$ and $1 \le j < s \le n$.

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

$$c_{\min(i,r),\min(j,s)} + c_{\max(i,r),\max(j,s)} \le c_{is} + c_{rj}$$
 (4.16)

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





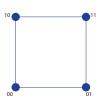
$$c_{ij} = A + B$$
, $c_{rj} = B$, $c_{rs} = B + D$, $c_{is} = A + B + C + D$.

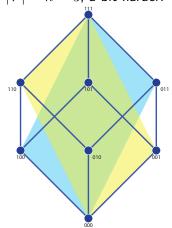
Submodular on Hypercube Vertices

Test submodularity via values on verticies of hypercube.

Example: with |V| = n = 2, this is With |V| = n = 3, a bit harder.

easy:





How many inequalities?

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:

$$f(A) + f(B) \ge f(A \cup B) \tag{4.21}$$

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:

$$f(A) = \begin{cases} 1 & \text{if } |A| \le k \\ 0 & \text{else} \end{cases} \tag{4.22}$$

This function is subadditive but not submodular.

Logistics

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

$$f(A) + f(B) = f(A \cap B) + f(A \cup B)$$
 (4.21)

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

$$f(A) = f(\emptyset) + \sum_{a \in A} (f(\{a\}) - f(\emptyset)) = c + \sum_{a \in A} f'(a)$$
 (4.22)

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.

$$\bar{f}(A) + \bar{f}(B) \ge \bar{f}(A \cup B) + \bar{f}(A \cap B) \tag{4.26}$$

follows from

$$f(V \setminus A) + f(V \setminus B) \ge f(V \setminus (A \cup B)) + f(V \setminus (A \cap B)) \tag{4.27}$$

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 set size of edges with exactly one vertex in $S\subseteq V(G)$ is submodular (cut size 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 $f: 2^V \to \mathbb{R}$ is supermodular, then so is $\bar{f}: 2^V \to \mathbb{R}$ defined as $\bar{f}(S) = f(V \setminus S)$.
- 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 $c:2^E\to\mathbb{R}_+$.
- ullet c(A) is monotone non-increasing, $c(A+a)-c(A)\leq 0$.
- ullet Then c(A) is supermodular, i.e.,

$$c(A+a)-c(A) \leq c(B+a)-c(B) \tag{4.40}$$
 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 conected components) when edge is added in a smaller context than when added in a larger context.
- $\bar{c}(A) = c(E \setminus A)$ is the number of connected components in G when we remove A, so is also supermodular, but monotone non-decreasing.

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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.
- 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).

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

$$w(A) = \sum_{e \in A} w_e \tag{4.1}$$

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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- 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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Examples and Properties

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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.

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

$$f(X) = m^{\mathsf{T}} \mathbf{1}_X + \frac{1}{2} \mathbf{1}_X^{\mathsf{T}} \mathbf{M} \mathbf{1}_X \tag{4.3}$$

is submodular \underline{iff} the off-diagonal elements of M are non-positive.

Proof.

Submodularity, Quadratic Structures, and Cuts

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

Proof of Lemma 4.3.1 cont.

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



Submodularity, Quadratic Structures, and Cuts

Proof of Lemma 4.3.1 cont.

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

$$0 \le f(\{u\}) + f(\{v\}) - f(\{u, v\}) \tag{4.4}$$

$$= m(u) + \frac{1}{2}M_{u,u} + m(v) + \frac{1}{2}M_{v,v}$$
(4.5)

$$-\left(m(u) + m(v) + \frac{1}{2}M_{u,u} + M_{u,v} + \frac{1}{2}M_{v,v}\right) \tag{4.6}$$

$$= -M_{u,v} \tag{4.7}$$

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



• We are given a finite set V of n elements and a set of subsets $\mathcal{V} = \{V_1, V_2, \dots, V_m\}$ 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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just Special cases of Submodular Optimization

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- $f: 2^{[m]} \to \mathbb{Z}_+$ where for $A \subseteq [m]$, $f(A) = |\bigcup_{a \in A} V_a|$ is the set cover function and is submodular.
- Both SET COVER and MAXIMUM COVERAGE are well known to be NP-hard, but have a fast greedy approximation algorithm, and hence are instances of submodular optimization.

Vertex and Edge Covers

Also instances of submodular optimization

Definition 4.3.2 (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 4.3.3 (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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- 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 $V \setminus X$, or $\delta(x) = E(X, V \setminus X)$.

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

Matrix Rank functions

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

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).
- 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:

$$x_v = \sum_{i=1}^k \alpha_i x_{v_i} \tag{4.8}$$

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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- Thus, r(V) is the rank of the matrix X.

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Rank function of a matrix

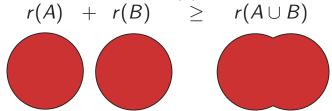
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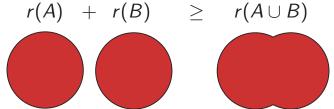
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Graph & Combinatorial Examples

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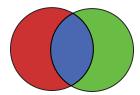
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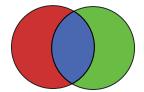
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• Thus, we have subadditivity: $r(A) + r(B) \ge r(A \cup B)$. Can we add more to the r.h.s. and still have an inequality? Yes.

Graph & Combinatorial Examples

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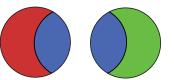
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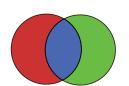
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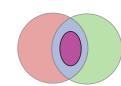
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- More generally, common information (blue) is "more" (no less) than information within common index (magenta).

The Venn and Art of Submodularity

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







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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

Graph & Combinatorial Examples

• 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 vertex-induced graph, induced by vertices incident to edges S.

Examples and Properties

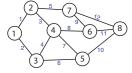
Spanning trees

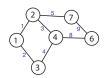
Graph & Combinatorial Examples

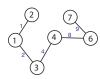
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Examples and Properties

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





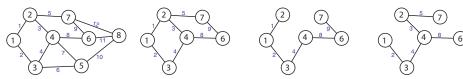




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• Then r(S) is submodular, and is another matrix rank function corresponding to the incidence matrix of the graph.

Summing Submodular Functions

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

$$f: 2^E \to \mathbb{R} \text{ with } f(A) = f_1(A) + f_2(A)$$
 (4.16)

Examples and Properties

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is submodular. This follows easily since

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

$$\geq f_1(A \cup B) + f_2(A \cup B) + f_1(A \cap B) + f_2(A \cap B)$$
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$$= f(A \cup B) + f(A \cap B). \tag{4.19}$$

I.e., it holds for each component of f in each term in the inequality.

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$$= f(A \cup B) + f(A \cap B). \tag{4.19}$$

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 $\alpha_1, \alpha_2 \geq 0$.

Summing Submodular and Modular Functions

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

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$$= f(A \cup B) + f(A \cap B). \tag{4.23}$$

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

$$f': 2^E \to \mathbb{R} \text{ with } f'(A) = f(A \cap S)$$
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Graph & Combinatorial Examples

Proof.

Other Submodular Defs

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Proof.

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

$$f(A'+v) - f(A') \ge f(B'+v) - f(B') \tag{4.26}$$

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

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

$$f: 2^V \to \mathbb{R} \text{ with } f(A) = f_1(A \cap S_1) + f_2(A \cap S_2)$$
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is submodular. This follows easily from the preceding two results. Given V, let $\mathcal{C} = \{C_1, C_2, \dots, C_k\}$ be a set of subsets of V, and for each $C \in \mathcal{C}$, let $f_C : 2^V \to \mathbb{R}$ be a submodular function. Then

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

Max - normalized

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

$$f(A) = \max_{i \in A} c_i \tag{4.29}$$

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

Proof.

Consider

$$\max_{j \in A} c_j + \max_{j \in B} c_j \ge \max_{j \in A \cup B} c_j + \max_{j \in A \cap B} c_j \tag{4.30}$$

which follows since we have that

$$\max(\max_{j \in A} c_j, \max_{j \in B} c_j) = \max_{j \in A \cup B} c_j \tag{4.31}$$

and

$$\min(\max_{j \in A} c_j, \max_{j \in B} c_j) \ge \max_{j \in A \cap B} c_j \tag{4.32}$$

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

$$f(A) = \max_{j \in A} c_j \tag{4.33}$$

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

Proof.

The proof is identical to the normalized case.



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- Each site should be serviced by only one plant but no less than one.
- Define f(A) as the "delivery benefit" plus "construction benefit" when the locations $A \subseteq F$ are to be constructed.
- We can define the (uncapacitated) facility location function

$$f(A) = \sum_{j \in A} m_j + \sum_{i \in F} \max_{j \in A} c_{ij}.$$
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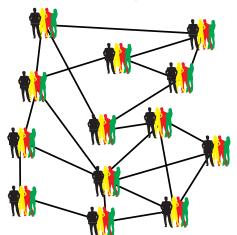
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• Goal is to find a set A that maximizes f(A) (the benefit) placing a bound on the number of plants A (e.g., $|A| \le k$).

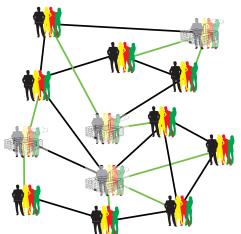
Facility/Plant Location (uncapacitated)

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



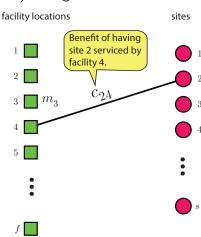
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- We can model this with a weighted bipartite graph G = (F, S, E, c)where F is set of possible factory/plant locations, S is set of sites needing service, E are edges indicating (factory, site) service possiblity pairs, and $c: E \to \mathbb{R}_+$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

$$f(A) = \sum_{i \in F} \max_{j \in A} c_{ij}.$$
 (4.35)



Graph & Combinatorial Examples

Facility Location

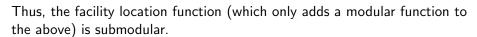
Given V, E, let $c \in \mathbb{R}^{V \times E}$ be a given $|V| \times |E|$ matrix. Then

$$f: 2^E \to \mathbb{R}, \text{ where } f(A) = \sum_{i \in V} \max_{j \in A} c_{ij}$$
 (4.36)

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^{th} row vector), so f can be written as a sum of submodular functions.



• Let Σ be an $n \times n$ positive definite matrix. Let $V = \{1, 2, \dots, n\} \equiv [n]$ be an index set, and for $A \subseteq V$, let Σ_A be the (square) submatrix of Σ 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

$$x \in p(x) = \frac{1}{\sqrt{|2\pi\Sigma|}} \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\right)$$
(4.38)

...cont.

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

$$h(X) = \log \sqrt{|2\pi e \Sigma|} = \log \sqrt{(2\pi e)^n |\Sigma|}$$
 (4.39)

and in particular, for a variable subset A,

$$f(A) = h(X_A) = \log \sqrt{(2\pi e)^{|A|} |\Sigma_A|}$$
 (4.40)

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

$$f(A) = h(X_A) = m(A) + \frac{1}{2}\log|\Sigma_A|$$
 (4.41)

where m(A) is a modular function.

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

Summary so far

• Summing: if $\alpha_i \geq 0$ and $f_i: 2^V \to \mathbb{R}$ is submodular, then so is $\sum_i \alpha_i f_i$.

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Graph & Combinatorial Examples

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Examples and Properties

- Restrictions: $f'(A) = f(A \cap S)$
- max: $f(A) = \max_{i \in A} c_i$ and facility location.
- Log determinant $f(A) = \log \det(\Sigma_A)$

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

$$f(A) = g(m(A)) \tag{4.42}$$

then f is submodular.

Proof.

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

$$g(m(A) + m(v)) - g(m(A)) \ge g(m(B) + m(v)) - g(m(B))$$
 (4.43)



Concave composed with non-negative modular

Theorem 4.5.1

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

- For all modular functions $m: 2^V \to \mathbb{R}_+$, then $f: 2^V \to \mathbb{R}$ defined as f(A) = g(m(A)) is submodular
- $g: \mathbb{R}_+ \to \mathbb{R}$ is concave.
 - If g is non-decreasing concave, 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.

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)).

Monotonicity

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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) > f(B) (resp. f(A) > f(B)).

Composition of non-decreasting submodular and non-decreasing concave

Theorem 4.5.4

Given two functions, one defined on sets

$$f: 2^V \to \mathbb{R} \tag{4.45}$$

and another continuous valued one:

$$g: \mathbb{R} \to \mathbb{R} \tag{4.46}$$

the composition formed as $h=g\circ f:2^V\to\mathbb{R}$ (defined as h(S)=g(f(S))) is nondecreasing submodular, if g 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 increasing or monotone decreasing. Then $h: 2^V \to R$ defined by

$$h(A) = \min(f(A), g(A)) \tag{4.47}$$

is submodular.

Proof.

If h(A) agrees with f on both X and Y (or g on both X and Y), and since $f(X) + f(Y) \ge f(X \cup Y) + f(X \cap Y)$ (4.48) (4.48)

$$g(X) + g(Y) \ge g(X \cup Y) + g(X \cap Y), \tag{4.49}$$

the result (Equation 4.47 being submodular) follows since

$$\frac{f(X) + f(Y)}{g(X) + g(Y)} \ge \min(f(X \cup Y), g(X \cup Y)) + \min(f(X \cap Y), g(X \cap Y))$$
(4.50)

Monotone difference of two functions

...cont.

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

$$h(X) + h(Y) = f(X) + g(Y) \ge f(X \cup Y) + f(X \cap Y) + g(Y) - f(Y)$$
(4.51)

Monotone difference of two functions

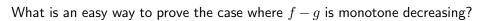
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$$h(X) + h(Y) = f(X) + g(Y) \ge f(X \cup Y) + f(X \cap Y) + g(Y) - f(Y) \tag{4.51}$$

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

$$h(X) + h(Y) \ge g(X \cup Y) + f(X \cap Y) \ge h(X \cup Y) + h(X \cap Y)$$
 (4.52)



Saturation via the $min(\cdot)$ function

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

$$h(A) = \min(k, f(A)) \tag{4.53}$$

is submodular.

Saturation via the $min(\cdot)$ function

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Proof.

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

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Proof.

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

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

• In general, the minimum of two submodular functions is not submodular (unlike concave functions, closed under min).

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- In general, the minimum of two submodular functions is not submodular (unlike concave functions, closed under min).
- However, when wishing to maximize two monotone non-decreasing submodular functions f,g, we can define function $h:2^V\to\mathbb{R}$ as

$$h_{\alpha}(A) = \min(\alpha, f(A)) + \min(\alpha, g(A)) \tag{4.54}$$

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

More on Min - the saturate trick

- In general, the minimum of two submodular functions is not submodular (unlike concave functions, closed under min).
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 This can be useful in many applications. An instance of a submodular surrogate (where we take a non-submodular problem and find a submodular one that can tell us something).

Arbitrary functions as difference between submodular funcs.

Given an arbitrary set function f, it can be expressed as a difference between two submodular functions: f = g - h where both g and h are submodular.

Proof.

Let f be given and arbitrary, and define:

$$\alpha \stackrel{\Delta}{=} \min_{X,Y} \Big(f(X) + f(Y) - f(X \cup Y) - f(X \cap Y) \Big)$$
 (4.55)

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

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 (4.55)

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

$$\beta \stackrel{\Delta}{=} \min_{X,Y:X \not\subseteq Y,Y \not\subseteq X} \Big(h(X) + h(Y) - h(X \cup Y) - h(X \cap Y) \Big). \tag{4.56}$$

Strict means that $\beta > 0$.

Arbitrary functions as difference between submodular funcs.

...cont.

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

$$f'(A) = f(A) + \frac{|\alpha|}{\beta}h(A) \tag{4.57}$$

Then f' is submodular (why?), and $f = f'(A) - \frac{|\alpha|}{\beta}h(A)$, 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:

$$f(A \cup \{j\}) - f(A) \stackrel{\Delta}{=} \rho_j(A) \tag{4.58}$$

$$\stackrel{\Delta}{=} \rho_A(j) \tag{4.59}$$

$$\stackrel{\Delta}{=} \nabla_j f(A) \tag{4.60}$$

$$\stackrel{\triangle}{=} f(\{j\}|A) \tag{4.61}$$

$$\stackrel{\Delta}{=} f(j|A) \tag{4.62}$$

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

It will also be useful to extend this to sets.

Let A, B be any two sets. Then

$$f(A|B) \triangleq f(A \cup B) - f(B) \tag{4.63}$$

So when j is any singleton

$$f(j|B) = f(\{j\}|B) = f(\{j\} \cup B) - f(B)$$
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Note that this is inspired from information theory and the notation used for conditional entropy $H(X_A|X_B)=H(X_A,X_B)-H(X_B)$.

Arbitrary function as difference between two polymatroids

 Any normalized submodular function g can be represented as a sum of a polymatroid (normalized monotone non-decreasing submodular) function \bar{g} and a modular function m_q .

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- Then, given arbitrary f = g h where g and h are normalized submodular,

$$f = g - h = \bar{g} + m_g - (\bar{h} + m_h) \tag{4.65}$$

$$= \bar{g} - \bar{h} + (m_g - m_h) \tag{4.66}$$

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 (4.68)

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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- Then, given arbitrary f=g-h where g and h are normalized submodular,

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- \bullet Then, given arbitrary f=g-h where g and h are normalized submodular,

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- But both $g+m_{g-h}^+$ and $\bar{h}+(-m_{g-h})^+$ are polymatroid functions.
- Thus, any function can be expressed as a difference between two not Prof. Jeff Bilmes

 EE596b/Spring 2016/Submodularity Lecture 4 Apr 6th, 2016

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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:

$$f(A) + f(B) \ge f(A \cup B) + f(A \cap B) \tag{4.8}$$

Examples and Properties

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:

$$f(A \cup \{v\}) - f(A) \ge f(B \cup \{v\}) - f(B) \tag{4.9}$$

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

Submodular 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:

$$f(A \cup C) - f(A) \ge f(B \cup C) - f(B) \tag{4.69}$$

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.

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 ⇒ Diminishing Returns
- Diminishing Returns ⇒ Group Diminishing Returns
- Group Diminishing Returns ⇒ Submodular Concave

Submodular Concave \Rightarrow Diminishing Returns

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

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



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

- 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:

$$f(A+v) + f(B) \ge f(B+v) + f(A)$$
 (4.70)



Submodular Concave \Rightarrow Diminishing Returns

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

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

$$f(A+v) + f(B) \ge f(B+v) + f(A)$$
 (4.70)

Rearranging, we have

$$f(A+v) - f(A) \ge f(B+v) - f(B)$$
 (4.71)



Diminishing Returns ⇒ Group Diminishing Returns

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

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

$$f(A \cup C) - f(A) \tag{4.72}$$

$$= f(A \cup C) - \sum_{i=1}^{k-1} \left(f(A \cup \{c_1, \dots, c_i\}) - f(A \cup \{c_1, \dots, c_i\}) \right) - f(A)$$
 (4.73)

$$= \sum_{i=1}^{\kappa} \left(f(A \cup \{c_1 \dots c_i\}) - f(A \cup \{c_1 \dots c_{i-1}\}) \right)$$
(4.74)

$$\geq \sum_{i=1}^{\kappa} \Big(f(B \cup \{c_1 \dots c_i\}) - f(B \cup \{c_1 \dots c_{i-1}\}) \Big)$$
(4.75)

$$= f(B \cup C) - \sum_{i=1}^{k-1} \left(f(B \cup \{c_1, \dots, c_i\}) - f(B \cup \{c_1, \dots, c_i\}) \right) - f(B)$$
 (4.76)

$$= f(B \cup C) - f(B) \tag{4.77}$$



Group Diminishing Returns ⇒ Submodular Concave

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

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

$$f(A'+C) - f(A') \ge f(B'+C) - f(B') \tag{4.78}$$

giving

$$f(A'+C) + f(B') \ge f(B'+C) + f(A')$$
 (4.79)

or

$$f(A \cap B + A \setminus B) + f(B) \ge f(B + A \setminus B) + f(A \cap B) \tag{4.80}$$

which is the same as the submodular concave condition

$$f(A) + f(B) \ge f(A \cup B) + f(A \cap B) \tag{4.81}$$

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:

$$f(A \cup \{a\}) + f(A \cup \{b\}) \ge f(A \cup \{a,b\}) + f(A)$$
 (4.82)

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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

$$f(A+a) - f(A) \ge f(A+b_1+a) - f(A+b_1)$$
(4.83)

$$\geq f(A+b_1+b_2+a) - f(A+b_1+b_2) \tag{4.84}$$

$$\geq \dots$$
 (4.85)

$$\geq f(A+b_1+\cdots+b_k+a)-f(A+b_1+\cdots+b_k)$$

$$(4.86)$$

$$= f(B+a) - f(B) (4.87)$$

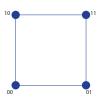
Submodular on Hypercube Vertices

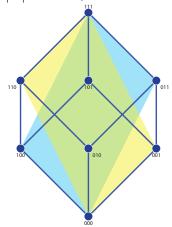
Test submodularity via values on verticies of hypercube.

Example: with |V| = n = 2, this is With |V| = n = 3, a bit harder.

easy:

Graph & Combinatorial Examples





How many inequalities?

Submodular Definitions

Theorem 4.6.3

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

$$f(A) + f(B) \ge f(A \cup B) + f(A \cap B)$$
 for all $A, B \subseteq V$ (SC)

if and only if

$$\int_{-}^{-} f(v|X) \ge f(v|Y) \text{ for all } X \subseteq Y \subseteq V \text{ and } v \notin Y$$
 (DR)

Proof.

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

(DR)
$$\Rightarrow$$
(SC): Order $A \setminus B = \{v_1, v_2, \dots, v_r\}$ arbitrarily. For $i \in 1 : r$, $f(v_i | (A \cap B) \cup \{v_1, v_2, \dots, v_{i-1}\}) \ge f(v_i | B \cup \{v_1, v_2, \dots, v_{i-1}\})$.

Applying telescoping summation to both sides, we get:

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

$$\Rightarrow$$
 $f(A) - f(A \cap B) \ge f(A \cup B) - f(B)$

• Given submodular f, and given you have $C, D \subseteq E$ with either $D \supseteq C$ or $D \subseteq C$, and have an expression of the form:

$$f(C) - f(D) \tag{4.88}$$

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ullet If $D\supseteq C$, then for any X with $D=C\cup X$ then

$$f(C) - f(D) = f(C) - f(C \cup X) \ge f(C \cap X) - f(X)$$

(4.90)

• Given submodular f, and given you have $C, D \subseteq E$ with either $D \supseteq C$ or $D \subseteq C$, and have an expression of the form:

$$f(C) - f(D) \tag{4.88}$$

• If $D \supseteq C$, then for any X with $D = C \cup X$ then

$$f(C) - f(D) = f(C) - f(C \cup X) \ge f(C \cap X) - f(X)$$
 (4.89)

or

$$f(C \cup X|C) \le f(X|C \cap X) \tag{4.90}$$

• Given submodular f, and given you have $C, D \subseteq E$ with either $D \supseteq C$ or $D \subseteq C$, and have an expression of the form:

$$f(C) - f(D) \tag{4.88}$$

• If $D \supseteq C$, then for any X with $D = C \cup X$ then

$$f(C) - f(D) = f(C) - f(C \cup X) \ge f(C \cap X) - f(X)$$
 (4.89)

or

$$f(C \cup X|C) \le f(X|C \cap X) \tag{4.90}$$

• Alternatively, if $D \subseteq C$, given any Y such that $D = C \cap Y$ then

$$f(C) - f(D) = f(C) - f(C \cap Y) \ge f(C \cup Y) - f(Y)$$

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• Equations (4.90) and (4.92) have same form.

$$f(A) + f(B) \ge f(A \cup B) + f(A \cap B), \ \forall A, B \subseteq V$$
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(4.93)

$$f(j|S) \ge f(j|T), \ \forall S \subseteq T \subseteq V, \ \text{with} \ j \in V \setminus T$$

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Many (Equivalent) Definitions of Submodularity

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$$(4.93)$$

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

(4.100)

Many (Equivalent) Definitions of Submodularity

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We next show that Eq. $4.96 \Rightarrow$ Eq. $4.98 \Rightarrow$ Eq. $4.99 \Rightarrow$ Eq. 4.96.

Approach

To show these next results, we essentially first use:

$$f(S \cup T) = f(S) + f(T|S) \le f(S) + \text{upper-bound}$$
 (4.102)

and

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

leading to

$$f(T) + \text{lower-bound} \le f(S) + \text{upper-bound}$$
 (4.104)

or

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

Eq. $4.96 \Rightarrow Eq. 4.98$

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:

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

(4.106)

$$=\sum_{t=1}^{r}f(j_{t}|S\cup\{j_{1},\ldots,j_{t-1}\})\leq\sum_{t=1}^{r}f(j_{t}|S) \quad (4.107)$$

$$= \sum_{j \in T \setminus S} f(j|S) \tag{4.108}$$

or

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

Let $T \setminus S = \{j_1, \dots, j_r\}$ and $S \setminus T = \{k_1, \dots, k_q\}$.

Next, lower bound S in the context of T:

$$f(S \cup T) - f(T) = \sum_{t=1}^{q} \left[f(T \cup \{k_1, \dots, k_t\}) - f(T \cup \{k_1, \dots, k_{t-1}\}) \right]$$

$$= \sum_{t=1}^{q} f(k_t | T \cup \{k_1, \dots, k_t\} \setminus \{k_t\}) \ge \sum_{t=1}^{q} f(k_t | T \cup S \setminus \{k_t\})$$

 $= \sum_{j \in S \setminus T} f(j|S \cup T \setminus \{j\}) \tag{4.112}$

(4.111)

Let $T \setminus S = \{j_1, \ldots, j_r\}$ and $S \setminus T = \{k_1, \ldots, k_q\}$.

So we have the upper bound

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

and the lower bound

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

This gives upper and lower bounds of the form

$$f(T) + \text{lower bound} \le f(S \cup T) \le f(S) + \text{upper bound},$$
 (4.115)

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

This follows immediately since if $S \subseteq T$, then $S \setminus T = \emptyset$, and the last term of Eq. 4.98 vanishes.

Eq. $4.99 \Rightarrow Eq. 4.96$

Here, we set $T = S \cup \{j, k\}, j \notin S \cup \{k\}$ into Eq. 4.99 to obtain

$$f(S \cup \{j, k\}) \le f(S) + f(j|S) + f(k|S)$$

$$= f(S) + f(S + \{j\}) - f(S) + f(S + \{k\}) - f(S)$$
(4.116)

$$= f(S + \{j\}) + f(S + \{k\}) - f(S)$$
(4.118)

$$= f(i|S) + f(S + \{k\}) \tag{4.119}$$

$$= f(j|S) + f(S + \{k\})$$
(4.119)

giving

$$f(j|S \cup \{k\}) = f(S \cup \{j,k\}) - f(S \cup \{k\})$$
 (4.120)

$$\leq f(j|S) \tag{4.121}$$

• Why do we call the $f(A) + f(B) \ge f(A \cup B) + f(A \cap B)$ definition of submodularity, submodular concave?

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- A continuous twice differentiable function $f: \mathbb{R}^n \to \mathbb{R}$ is concave iff $\nabla^2 f \leq 0$ (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:

$$(\nabla_B f)(A) \triangleq f(A \cup B) - f(A \setminus B) = f(B|(A \setminus B))$$
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• Hence, if $A \cap B = \emptyset$, then $(\nabla_B f)(A) = f(B|A)$.

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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:

$$(\nabla_{C}\nabla_{B}f)(A) = \nabla_{C}[\overbrace{f(A \cup B) - f(A \setminus B)}]$$

$$= (\nabla_{B}f)(A \cup C) - (\nabla_{B}f)(A \setminus C)$$

$$= f(A \cup B \cup C) - f((A \cup C) \setminus B)$$

$$- f((A \setminus C) \cup B) + f((A \setminus C) \setminus B)$$

$$(4.123)$$

• If the second difference operator everywhere nonpositive:

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

$$f(A') + f(B') \ge f(A' \cup B') + f(A' \cap B') \tag{4.128}$$

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One sense in which submodular functions are like concave functions.

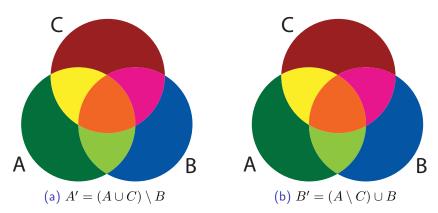


Figure: A figure showing $A' \cup B' = A \cup B \cup C$ and $A' \cap B' = A \setminus C \setminus B$.

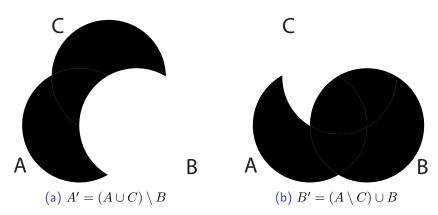


Figure: A figure showing $A' \cup B' = A \cup B \cup C$ and $A' \cap B' = A \setminus C \setminus B$.

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- 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:

$$\nabla_j \nabla_k f(X) \le 0 \tag{4.130}$$