Mathematical Properties of Submodularity and Applications to Machine Learning

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Get an intuitive sense for submodular functions, should be able to apply them.

Learn to recognize submodularity, or recognize when it might be useful.

Learn to realize why submodularity can be useful in machine learning. Why is it worth your time to study it.
Definition: given a finite ground set $V$, a function $f : 2^V \rightarrow \mathbb{R}$ is said to be submodular if

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V \quad (1)$$
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Goals of tutorial: will be very simple, an attempt to cover some important parts of the iceberg in 4.5 hours and in doing so give you all strong intuition and sense of applicability in ML.
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The tutorial itself is the tip of the iceberg!
Overall Outline of Tutorial

1. Part 1 (now): basics and applications
2. Part 2 (later this afternoon): Theory (from matroids to polymatroids), and other submodular properties
3. Part 3 (tomorrow): Algorithms and optimization
Outline of Part 1: Basics and Applications

1. Introduction
2. Basics
3. Submodular Applications in ML
   - Where is submodularity useful?
   - Traditional combinatorial problems
   - As a model of diversity, coverage, span, or information
   - As a model of cooperative costs, complexity, roughness, and irregularity
   - As a parameter for an ML algorithm
   - Itself, as a target for learning
   - Surrogates for optimization
   - Economic applications
Outline of Part 2: Theory

4 From Matroids to Polymatroids
- Matrix Rank
- Venn Diagrams
- Matroids

5 Submodular Definitions, Examples, and Properties
- Normalization
- Submodular Definitions
- Submodular Composition
- More Examples
Outline of Part 3: Algorithms

6 Discrete Semimodular Semigradients

7 Continuous Extensions
   • Lovász Extension
   • Concave Extension

8 Like Concave or Convex?

9 Optimization

10 Reading
Outline: Part 1

1 Introduction

2 Basics

3 Submodular Applications in ML
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Sets and set functions

We are given a finite “ground” set of objects:

$$V = \{ \text{objects} \}$$

Also given a set function $$f : 2^V \rightarrow \mathbb{R}$$ that valuates subsets $$A \subseteq V$$. Ex: $$f(V) = 6$$
Sets and set functions

Subset $A \subseteq V$ of objects:

$$A = \{ \text{sushi objects} \}$$

Also given a set function $f : 2^V \rightarrow \mathbb{R}$ that valuates subsets $A \subseteq V$.
Ex: $f(A) = 1$
Sets and set functions

Subset $B \subseteq V$ of objects:

$B = \{ \cdots \}$

Also given a set function $f : 2^V \rightarrow \mathbb{R}$ that valuates subsets $A \subseteq V$. Ex: $f(B) = 6$
# Two Equivalent Submodular Definitions

## Definition (submodular)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$$  \hspace{1cm} (2)

## Definition (submodular (diminishing returns))

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

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B)$$  \hspace{1cm} (3)

This means that the incremental “value”, “gain”, or “cost” of $v$ decreases (diminishes) as the context in which $v$ is considered grows from $A$ to $B$. 
Two Equivalent Supermodular Definitions

**Definition (submodular)**

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

$$f(A) + f(B) \leq f(A \cup B) + f(A \cap B)$$  \hspace{1cm} (4)

An alternate and equivalent definition is:

**Definition (supermodular (improving returns))**

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

$$f(A \cup \{v\}) - f(A) \leq f(B \cup \{v\}) - f(B)$$  \hspace{1cm} (5)

This means that the incremental “value”, “gain”, or “cost” of $v$ increases (improves) as the context in which $v$ is considered grows from $A$ to $B$. 

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Submodularity
Any set $A \subseteq V$ can be represented as a binary vector $x \in \{0, 1\}^V$. 
Sets and vectors

- Any set $A \subseteq V$ can be represented as a binary vector $x \in \{0, 1\}^V$.
- The characteristic vector of a set is given by $1_A \in \{0, 1\}^V$ where for all $v \in V$, we have:

$$1_A(v) = \begin{cases} 1 & \text{if } v \in A \\ 0 & \text{else} \end{cases}$$

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If $V = \{1, 2, \ldots, 20\}$ and $A = \{1, 3, 5, \ldots, 19\}$, then $1_A = (1, 0, 1, 0, \ldots)^T$. 

It is sometimes useful to go back and forth. Given $X \subseteq V$ then $x(X) \triangleq 1_X$ and $X(x) = \{v \in V : x(v) = 1\}$. 

$f(x) : \{0, 1\}^V \rightarrow \mathbb{R}$ is a pseudo-Boolean function. A submodular function is a special case.
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Any set function $m : 2^V \to \mathbb{R}$ whose valuations, for $A \subseteq V$, take form

$$m(A) = \sum_{a \in A} m(a)$$  \hspace{1cm} (7)

is called modular and normalized (meaning $m(\emptyset) = 0$).
Modular functions, and vectors in $\mathbb{R}^V$

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Hence, the characteristic vector \( \mathbf{1}_A \) of a set is modular.

Modular functions are often called additive or linear.
Modular functions, and vectors in $\mathbb{R}^V$

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If $f$ is both submodular and supermodular, then it is modular.
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Discrete Optimization

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- **Unconstrained minimization & maximization:**
  
  \[
  \min_{X \subseteq V} f(X) \quad \text{(9)} \quad \max_{X \subseteq V} f(X) \quad \text{(10)}
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- When $f$ is submodular, Eq. (9) is polytime, and Eq. (10) is constant-factor approximable.
Constrained Discrete Optimization

- Often, we are interested only in a subset of the set of possible subsets, namely $S \subseteq 2^V$. 

Examples: on only sets having bounded size $S = \{ S \subseteq V : |S| \leq k \}$ or within a budget $\{ S \subseteq V : \sum_{s \in S} w(s) \leq b \}$.

Example: the sets might need to correspond to a combinatorially feasible object (i.e., feasible $S$ might be trees, matchings, paths, vertex covers, or cuts).

Ex: $S$ might be a function of some $g$ (e.g., sub-level sets of $g$, $S = \{ S \subseteq V : g(S) \leq \alpha \}$), sup-level sets $S = \{ S \subseteq V : g(S) \geq \alpha \}$).

Constrained discrete optimization problems:

\[
\begin{align*}
\text{maximize} & \quad S \subseteq 2^V f(S) \\
\text{subject to} & \quad S \in S \\
\text{minimize} & \quad S \subseteq 2^V f(S) \\
\text{subject to} & \quad S \in S
\end{align*}
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Fortunately, when $f$ (and $g$) are submodular, solving these problems can often be done with guarantees (and often efficiently)!

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Outline: Part 1

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3. Submodular Applications in ML
   - Where is submodularity useful?
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Where is submodularity useful in ML?

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- As a **model** of a physical process:
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- As a **model** of a physical process:
  - What a submodular function is good for modeling depends on if we wish to maximize or wish to minimize it.
  - **Submodular functions naturally model aspects like:**
    - diversity,
    - coverage,
    - span, and
    - information in maximization problems,
    - cooperative costs,
    - complexity,
    - roughness, and
    - irregularity in minimization problems.

- A submodular function can act as a parameter for a machine learning strategy (active/semi-supervised learning, discrete divergence, convex norms for use in regularization).

- Itself, as an object or function to learn, based on data.

- As a surrogate or relaxation strategy for optimization
  - An alternate to factorization or decomposition based simplification (as one finds in a graphical model).
  - We can “relax” a problem to a submodular one where it can be efficiently solved and offer a bounded quality solution.
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  - Also, we can “relax” a problem to a submodular one where it can be efficiently solved and offer a bounded quality solution.
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We are given a finite set $V$ of $n$ elements and a set of subsets $\mathcal{V} = \{V_1, V_2, \ldots, V_m\}$ of $m$ subsets of $V$, so that $V_i \subseteq V$ and $\bigcup_i V_i = V$. 

Both Set Cover and Maximum Coverage are well known to be NP-hard, but have a fast greedy approximation algorithm. The set cover function $f(A) = |\bigcup_{a \in A} V_a|$ is submodular!
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The goal of minimum set cover is to choose the smallest subset $A \subseteq [m] \triangleq \{1, \ldots, m\}$ such that $\bigcup_{a \in A} V_a = V$.
**Set Cover and Maximum Coverage**

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- The goal of **minimum set cover** is to choose the smallest subset $A \subseteq [m] \triangleq \{1, \ldots, m\}$ such that $\bigcup_{a \in A} V_a = V$.

- 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.

Both set cover and maximum coverage are well known to be NP-hard, but have a fast greedy approximation algorithm. The set cover function $f(A) = |\bigcup_{a \in A} V_a|$ is submodular!
We are given a finite set $V$ of $n$ elements and a set of subsets $\mathcal{V} = \{V_1, V_2, \ldots, V_m\}$ of $m$ subsets of $V$, so that $V_i \subseteq V$ and $\bigcup_i V_i = V$.

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The set cover function $f(A) = |\bigcup_{a \in A} V_a|$ is submodular!
Let $V$ be a set of indices, and each $v \in V$ indexes a given sub-area of some region.

Let $\text{area}(v)$ be the area corresponding to item $v$.

Let $f(S) = \bigcup_{s \in S} \text{area}(s)$ be the union of the areas indexed by elements in $A$.

Then $f(S)$ is submodular.
Area of the union of areas indexed by $A$

Union of areas of elements of $A$ is given by:

$$f(A) = f(\{a_1, a_2, a_3, a_4\})$$
Area of the union of areas indexed by $A$

Area of $A$ along with with $v$:

$$f(A \cup \{v\}) = f(\{a_1, a_2, a_3, a_4\} \cup \{v\})$$
Area of the union of areas indexed by $A$

Gain (value) of $v$ in context of $A$:

$$f(A \cup \{v\}) - f(A) = f(\{v\})$$

We get full value $f(\{v\})$ in this case since the area of $v$ has no overlap with that of $A$. 
Area of the union of areas indexed by $A$

Area of $A$ once again.

$$f(A) = f(\{a_1, a_2, a_3, a_4\})$$
Area of the union of areas indexed by $A$

Union of areas of elements of $B \supset A$, where $v$ is not included:

$$f(B) \text{ where } v \notin B \text{ and where } A \subseteq B$$
Area of the union of areas indexed by $A$

Area of $B$ now also including $v$:

$$f(B \cup \{v\})$$
Area of the union of areas indexed by $A$

Incremental value of $v$ in the context of $B \supset A$.

$$f(B \cup \{v\}) - f(B) < f(\{v\}) = f(A \cup \{v\}) - f(A)$$

So benefit of $v$ in the context of $A$ is greater than the benefit of $v$ in the context of $B \supset A$. 
Consider an urn containing colored balls. Given a set $S$ of balls, $f(S)$ counts the number of distinct colors.
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- Initial value: 2 (colors in urn).
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Example Submodular: Number of Colors of Balls in Urns

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Thus, \( f \) is submodular.
Vertex and Edge Covers

Definition (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 $S$. 

Definition (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 $|V|_F = |V|$. 

$I(S)$ is submodular.
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Let $|V|_F$ be submodular.
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# Vertex and Edge Covers

## Definition (vertex cover)

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Graph Cut Problems

- Given a graph $G = (V, E)$, let $f : 2^V \rightarrow \mathbb{R}_+$ be the cut function, namely for any given set of nodes $X \subseteq V$, $f(X)$ measures the number of edges between nodes $X$ and $V \setminus X$.

$$f(X) = \left| \{(u, v) \in E : u \in X, v \in V \setminus X\} \right| \quad (13)$$
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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 $V \setminus S$. 

- Weighted versions, we have a non-negative modular function $w : 2^E \rightarrow \mathbb{R}_+$ defined on the edges that give cut costs.

$$f(X) = w\left(\{(u, v) \in E : u \in X, v \in V \setminus X\}\right)$$  \hspace{1cm} (14)

$$= \sum_{e \in \{(u, v) \in E : u \in X, v \in V \setminus X\}} w(e)$$  \hspace{1cm} (15)
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Outline

1. Introduction

2. Basics

3. Submodular Applications in ML
   - Where is submodularity useful?
   - Traditional combinatorial problems
   - As a model of diversity, coverage, span, or information
   - As a model of cooperative costs, complexity, roughness, and irregularity
   - As a parameter for an ML algorithm
   - Itself, as a target for learning
   - Surrogates for optimization
   - Economic applications
Extractive Document Summarization

- The figure below represents the sentences of a document
We extract sentences (green) as a summary of the full document.
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Extractive Document Summarization

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\[ C \]

- The summary on the left is a subset of the summary on the right.
Extractive Document Summarization

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\[ \text{diminishing returns} \leftrightarrow \text{submodularity} \]
Image collections

Many images, also that have a higher level gestalt than just a few.
The three best summaries exhibit diversity. The three worst summaries exhibit redundancy.
Let $Y$ be a random variable we wish to infer as best as possible, based on at most $n$ measurements $(X_1, X_2, \ldots, X_n) = X_V$ (or features) in a probability model $\Pr(Y, X_1, X_2, \ldots, X_n)$. 

The mutual information function $f(A) = I(Y; X_A)$ where $I(Y; X_A) = \sum_{y, x_A} \Pr(y, x_A) \log \frac{\Pr(y, x_A)}{\Pr(y) \Pr(x_A)} = H(Y) - H(Y|X_A)$ (16) $= H(X_A) - H(X_A|Y)$ (17) measures how well features $A$ are for predicting $Y$ (entropy reduction, reduction of uncertainty of $Y$).
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It is too costly to use them all, and we wish to choose a good subset $A \subseteq V$ of features to use that are within budget $|A| \leq k$. 

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$$= H(X_A) - H(X_A | Y) = H(X_A) + H(Y) - H(X_A, Y) \quad (17)$$

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Feature Selection in Pattern Classification

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- When $X_A \perp \!\!\!\!\perp X_B|Y$ for all $A, B$ (the Naïve Bayes assumption), $f(A)$ is submodular

- If not, $f(A)$ is naturally expressed as a difference of two submodular functions.
Data Subset Selection

Suppose we are given a data set $\mathcal{D} = \{x_i\}_{i=1}^n$ of $n$ data items $V = \{v_1, v_2, \ldots, v_n\}$ and we wish to choose a subset $A \subset V$ of items that is good in some way.

Example: $U$ could be a set of colors, and for an image $v \in V$, $m_u(v)$ could represent the number of pixels that are of color $u$.

Example: $U$ might be a set of textual features (e.g., ngrams), and $m_u(v)$ is the number of ngrams of type $u$ in sentence $v$. E.g., if a document consists of the sentence "Whenever I go to New York City, I visit the New York City museum.", then $m_{\text{the}}(s) = 1$ while $m_{\text{New York City}}(s) = 2$. 
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Suppose moreover each data item $v \in V$ is described by a vector of non-negative scores for a set $U$ of “features” (or properties, or characteristics, etc.) of each data item.

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J. Bilmes
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- For $X \subseteq V$, define $m_u(X) = \sum_{x \in X} m_u(x)$, so $m_u(X)$ is a modular function representing the “degree of $u$-ness” in subset $X$. 

- Consider the following class of feature functions $f: 2^V \to \mathbb{R}^+$:
  
  $$f(X) = \sum_{u \in U} \alpha_u g(m_u(X))$$

  where $g$ is a non-decreasing concave, and $\alpha_u \geq 0$ is a feature importance weight. Thus, $f$ is submodular.
Data Subset Selection

For $X \subseteq V$, define $m_u(X) = \sum_{x \in X} m_u(x)$, so $m_u(X)$ is a modular function representing the “degree of $u$-ness” in subset $X$.

Since $m_u(X)$ is modular, it does not have a diminishing returns property. I.e., as we add to $X$, the degree of $u$-ness grows additively.
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- Consider the following class of feature functions $f : 2^V \rightarrow \mathbb{R}_+$

$$f(X) = \sum_{u \in U} \alpha_u g(m_u(X))$$ \hspace{1cm} (21)

where $g$ is a non-decreasing concave, and $\alpha_u \geq 0$ is a feature importance weight. Thus, $f$ is submodular.
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$f(X)$ measures $X$’s ability to represent set of features $U$ as measured by $m_u(X)$, with diminishing returns function $g$, and importance weights $\alpha_u$. 

Let $p = \{p_u\}_{u \in U}$ (i.e., $p_u \leftarrow \alpha_u$) be a probability distribution over features (i.e., $\sum_u p_u = 1$ and $p_u \geq 0$ for all $u \in U$).

Next, normalize the modular weights for each feature:

$$\bar{m}_u(X) = \frac{m_u(X)}{\sum_{u} m_u(X)} = \frac{m_u(X)}{m(X)} \quad (22)$$

where $m(X) \triangleq \sum_{u} m_u(X)$.

Then $\bar{m}_u(X)$ can also be seen as a distribution since $\bar{m}_u(X) \geq 0$ and $\sum_u m_u(X) = 1$ for any $X \subseteq V$. Consider the KL-divergence between these two distributions:

$$D(p \parallel \{\bar{m}_u(X)\}) = \sum_{u} p_u \log p_u - \sum_{u} p_u \log(\bar{m}_u(X)) \quad (23)$$

$$= \sum_{u} p_u \log p_u - \sum_{u} p_u \log(m_u(X)) + \log(m(X))$$

$$= -H(p) + \log m(X) - \sum_{u} p_u \log(m_u(X)) \quad (24)$$
Data Subset Selection, KL-divergence

Let \( p = \{p_u\}_{u \in U} \) (i.e., \( p_u \leftarrow \alpha_u \)) be a probability distribution over features (i.e., \( \sum_u p_u = 1 \) and \( p_u \geq 0 \) for all \( u \in U \)).

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Data Subset Selection, KL-divergence

- The objective once again, treating entropy $H(p)$ as a constant,

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Hence the KL-divergence, seen as a function of $X$, i.e.,

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is quite naturally represented as a difference of submodular functions.
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- Hence the KL-divergence, seen as a function of $X$, i.e., $f(X) = D(p\|\{\bar{m}_u(X)\})$ is quite naturally represented as a difference of submodular functions.

- Alternatively, if we define

$$g(X) \triangleq \log m(X) - D(p\|\{\bar{m}_u(X)\}) = \sum_{u \in U} p_u \log (m_u(X)) \quad (26)$$

we have a submodular function $g$ that represents a combination of its quantity of $X$ via its features (i.e., $\log m(X)$) and its feature distribution closeness to some distribution $p$ (i.e., $D(p\|\{\bar{m}_u(X)\})$).
Information gain applicable not only in pattern recognition, but in the sensor coverage problem as well, where $Y$ is whatever question we wish to ask about an environment.
Sensor Placement

- Information gain applicable not only in pattern recognition, but in the sensor coverage problem as well, where $Y$ is whatever question we wish to ask about an environment.

- Given an environment, there is a set $V$ of candidate locations for placement of a sensor (e.g., temperature, gas, audio, video, bacteria or other environmental contaminant, etc.).
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- Environment could be a floor of a building, water network, monitored ecological preservation.
Sensor Placement within Buildings

- An example of a room layout. Should be possible to determine temperature at all points in the room. Sensors cannot sense beyond wall (thick black line) boundaries.
Sensor Placement within Buildings

- Example sensor placement using small range cheap sensors (located at red dots).
Sensor Placement within Buildings

- Example sensor placement using longer range expensive sensors (located at red dots).
Example sensor placement using mixed range sensors (located at red dots).
Social Networks

(from Newman, 2004). Clockwise from top left: 1) predator-prey interactions, 2) scientific collaborations, 3) sexual contact, 4) school friendships.
Let $V$ be a group of individuals. How valuable to you is a given friend $v \in V$?
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Given a group of friends $S \subseteq V$, you can valuate them with a set function $f(S)$. 
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**Submodular model:** a friend is less valuable the more friends you have.
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Which is a better model?
Information Cascades, Diffusion Networks

- How to model flow of information from source to the point it reaches users — information used in its common sense (like news events).
- How to find the most influential sources, the ones that often set off cascades, which are like large “waves” of information flow?
- Example when there is one seed source shown below:
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A model of influence in social networks

- Given a graph $G = (V, E)$, each $v \in V$ corresponds to a person, to each $v$ we have an activation function $f_v : 2^V \rightarrow [0, 1]$ dependent only on its neighbors. I.e., $f_v(A) = f_v(A \cap \Gamma(v))$. 

Goal - Viral Marketing: find a small subset $S \subseteq V$ of individuals to directly influence, and thus indirectly influence the greatest number of possible other individuals (via the social network $G$).

We define a function $f : 2^V \rightarrow \mathbb{Z}^+$ that models the ultimate influence of an initial set $S$ of nodes based on the following iterative process: At each step, a given set of nodes $S$ are activated, and we activate new nodes $v \in V \setminus S$ if $f_v(S) \geq U[0, 1]$ (where $U[0, 1]$ is a uniform random number between 0 and 1).

It can be shown that for many $f_v$ (including simple linear functions, and where $f_v$ is submodular itself) that $f$ is submodular (Kempe, Kleinberg, Tardos 1993).
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Determinantal Point Processes (DPPs)

- Sometimes we wish not only to valuate subsets $A \subseteq V$ but to induce probability distributions over all subsets.
- We may wish to prefer samples where elements of $A$ are diverse (i.e., given a sample $A$, for $a, b \in A$, we prefer $a$ and $b$ to be different).

(Kulesza & Taskar, 2011)
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A Determinantal point processes (DPPs) is a probability distribution over subsets $A$ of $V$ where the “energy” function is submodular.

More “diverse” or “complex” samples are given higher probability.

(Kulesza & Taskar, 2011)
Given binary vectors $x, y \in \{0, 1\}^V$, $y \leq x$ if $y(v) \leq x(v), \forall v \in V$. 

Given a positive-definite $n \times n$ matrix $M$ and a subset $X \subseteq V$, let $M_X$ be a submatrix (which is $|X| \times |X|$) with rows/columns specified by $X \subseteq V$.

Consider the following probability distribution on binary vectors:

$$
\Pr(X = x) = \exp\left(\log \left(\frac{|M_X(x)|}{|M + I|}\right)\right) 
$$

where $I$ is an $n \times n$ identity matrix, and $X \in \{0, 1\}^V$ is a random vector.

Equivalently,

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\sum_{x \in \{0, 1\}^V : x \geq y} \Pr(X = x) = \Pr(X \geq y) = \exp\left(\log \left(\frac{|K_Y(y)|}{|K + I|}\right)\right) 
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DPPs and log-submodular probability distributions

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\[ Pr(X = x) = \exp \left( \log |M_X|^+ |I| \right) \] (27)

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\[ \sum_{x \in \{0, 1\}^V} x \preceq y \Pr(X = x) = \Pr(X \preceq y) = \exp \left( \log |K_Y|^+ \right) \] (28)

where \(K = M(M^+ I)^{-1}\). Given a positive definite matrix $M$, function $f : 2^V \rightarrow \mathbb{R}$ with $f(A) = \log |MA|^+$ (the logdet function) is submodular.
DPPs and log-submodular probability distributions

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  \]  
  \[  (28) \]
  where $K = M(M + I)^{-1}$.
DPPs and log-submodular probability distributions

- Given binary vectors \( x, y \in \{0, 1\}^V \), \( y \leq x \) if \( y(v) \leq x(v), \forall v \in V \).
- Given a positive-definite \( n \times n \) matrix \( M \) and a subset \( X \subseteq V \), let \( M_X \) be a submatrix (which is \( |X| \times |X| \)) with rows/columns specified by \( X \subseteq V \).
- Consider the following probability distribution on binary vectors:

\[
\Pr(X = x) = \exp \left( \log \left( \frac{|M_X(x)|}{|M + I|} \right) \right) \tag{27}
\]

where \( I \) is \( n \times n \) identity matrix, and \( X \in \{0, 1\}^V \) is a random vector.

- Equivalently,

\[
\sum_{x \in \{0,1\}^V : \, x \geq y} \Pr(X = x) = \Pr(X \geq y) = \exp \left( \log \left( |K_{Y,Y}| \right) \right) \tag{28}
\]

where \( K = M(M + I)^{-1} \)

- Given positive definite matrix \( M \), function \( f : 2^V \to \mathbb{R} \) with \( f(A) = \log |M_A| \) (the logdet function) is submodular.
A probability distribution on binary vectors $p : \{0, 1\}^V \rightarrow [0, 1]$: \[ p(x) = \frac{1}{Z} \exp(-E(x)) \] where $E(x)$ is the energy function.
Graphical Model Structure Learning

- A probability distribution on binary vectors $p : \{0, 1\}^V \rightarrow [0, 1]$: 
  
  $$p(x) = \frac{1}{Z} \exp(-E(x))$$  
  
  (29)

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- A graphical model $G = (V, E)$ represents a family of probability distributions $p \in \mathcal{F}(G)$ all of which factor w.r.t. the graph.
A probability distribution on binary vectors $p : \{0, 1\}^V \rightarrow [0, 1]$: 

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I.e., if $C$ are a set of cliques of graph $G$, then we must have:

$$E(x) = \sum_{c \in C} E_c(x_c)$$  \hspace{1cm} (30)$$
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The problem of structure learning in graphical models is to find the graph \( G \) based on data.
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The problem of **structure learning in graphical models** is to find the graph $G$ based on data.

This can be viewed as a discrete optimization problem on the potential (undirected) edges of the graph $V \times V$. 


Graphical Models: Learning Tree Distributions

- Goal: find the closest distribution \( p_t \) to \( p \) subject to \( p_t \) factoring w.r.t. some tree \( T = (V, F) \), i.e., \( p_t \in \mathcal{F}(T, \mathcal{M}) \).
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- This can be expressed as a discrete optimization problem:

$$\min_{p_t \in \mathcal{F}(G, \mathcal{M})} D(p \| p_t)$$
subject to

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$T = (V, F)$ is a tree
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- Discrete problem: choose the optimal set of edges $A \subseteq E$ that constitute tree (i.e., find a spanning tree of $G$ of best quality).
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$$\begin{align*}
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\text{subject to} & \quad p_t \in \mathcal{F}(T, \mathcal{M}). \\
&T = (V, F) \text{ is a tree}
\end{align*}$$

- Discrete problem: choose the optimal set of edges $A \subseteq E$ that constitute tree (i.e., find a spanning tree of $G$ of best quality).
- Define $f : 2^E \rightarrow \mathbb{R}_+$ where $f$ is a weighted cycle matroid rank function (a type of submodular function), with weights $w(e) = w(u, v) = I(X_u; X_v)$ for $e \in E$. 
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Then finding the maximum weight base of the matroid is solved by the greedy algorithm, and also finds the optimal tree (Chow & Liu, 1968)
1 Introduction

2 Basics

3 Submodular Applications in ML
   - Where is submodularity useful?
   - Traditional combinatorial problems
   - As a model of diversity, coverage, span, or information
   - As a model of cooperative costs, complexity, roughness, and irregularity
   - As a parameter for an ML algorithm
   - Itself, as a target for learning
   - Surrogates for optimization
   - Economic applications
Given distribution \( p(x) = \frac{1}{Z} \exp(-E(x)) \)
where \( E(x) = \sum_{c \in \mathcal{C}} E_c(x_c) \) and \( \mathcal{C} \) are the cliques of a graph \( G = (V, \mathcal{E}) \).
Graphical Models and fast MAP Inference

Given distribution \( p(x) = \frac{1}{Z} \exp(-E(x)) \) where
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MAP inference problem is important in ML: compute

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x^* \in \operatorname{argmax}_{x \in \{0,1\}^V} p(x)
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Graphical Models and fast MAP Inference

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- Many approximate inference strategies utilize additional
  factorization assumptions to make inference tractable (e.g.,
  mean-field, variational inference, expectation propagation, etc).
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- Many approximate inference strategies utilize additional factorization assumptions to make inference tractable (e.g., mean-field, variational inference, expectation propagation, etc).

However, what if we could do MAP inference in polynomial time regardless of the tree-width, and without even knowing the tree-width?
Degree two (edge) graphical models

Given $G$ restrict $p \in \mathcal{F}(G, R^{(f)})$ such that we can write the global energy $E(x)$ as a sum of unary and pairwise potentials:

$$E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j)$$  \hspace{1cm} (32)
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- Since \( \log p(x) = -E(x) + \text{const.} \), the smaller \( e_v(x_v) \) or \( e_{ij}(x_i, x_j) \) become, the higher the probability becomes.
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- Since $\log p(x) = -E(x) + \text{const.}$, the smaller $e_v(x_v)$ or $e_{ij}(x_i, x_j)$ become, the higher the probability becomes.
- When $G$ is a 2D grid graph, we have
We can create auxiliary graph that involves two new terminal nodes \(s\) and \(t\) (source and sink) and connect each of \(s\) and \(t\) to all of the original nodes.

I.e., \(G_a = (V \cup \{s, t\}, E + \bigcup_{v \in V} ((s, v) \cup (v, t)))\).
Transformation from graphical model to auxiliary graph

Original Graph: \( E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \)
Transformation from graphical model to auxiliary graph

Augmented graph-cut graph.
The edge weights of graph are derived from \( \{e_v\}_{v \in V} \) and \( \{e_{ij}\}_{(i,j) \in E(G)} \).
Transformation from graphical model to auxiliary graph

Augmented graph-cut graph with indicated cut corresponding to particular vector $\bar{x} \in \{0, 1\}^n$. Each cut $\bar{x}$ has a score corresponding to $p(\bar{x})$. 
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Augmented graph-cut graph with indicated cut corresponding to particular vector $\bar{x} \in \{0, 1\}^n$. Each cut $\bar{x}$ has a score corresponding to $p(\bar{x})$. 
Setting of the weights in the auxiliary cut graph

- Any graph cut corresponds to a vector $\tilde{x} \in \{0, 1\}^n$. 

Edge weight assignments:

For $(s, v)$ with $v \in V(G)$, set edge weight $w_{s,v} = (e_v(1) - e_v(0))_{1}^{e_v(1) > e_v(0)}$.

For $(v, t)$ with $v \in V(G)$, set edge weight $w_{v,t} = (e_v(0) - e_v(1))_{1}^{e_v(0) \geq e_v(1)}$.

For original edge $(i, j) \in E$, set weight $w_{i,j} = e_{ij}(1,0) + e_{ij}(0,1) - e_{ij}(1,1) - e_{ij}(0,0)$. 
Any graph cut corresponds to a vector $\bar{x} \in \{0, 1\}^n$.

If weights are set correctly in the cut graph, and if edge functions $e_{ij}$ satisfy certain properties, then graph-cut score corresponding to $\bar{x}$ can be made equivalent to $E(x) = \log p(\bar{x}) + \text{const.}$.
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Submodular potentials

- Edge functions must be submodular (equivalently “associative”, “attractive”, “regular”, “Potts”, or “ferromagnetic”) for this to work, i.e., for all \((i, j) \in E(G)\), we must have that:

\[
e_{ij}(0, 1) + e_{ij}(1, 0) \geq e_{ij}(1, 1) + e_{ij}(0, 0)
\]

(33)

This means: on average, preservation is preferred over change. As a set function, this is the same as:

\[
f(X) = \sum_{\{i, j\} \in E(G)} f_{ij}(X \cap \{i, j\})
\]

which is submodular if each of the \(f_{ij}\)’s are submodular!

Probability form \(p(x) \propto \prod \psi_{ij}\), so \(\psi_{ij}(1, 0) \psi_{ij}(0, 1) \leq \psi_{ij}(0, 0) \psi_{ij}(1, 1)\): geometric mean of factor scores higher when neighboring pixels have the same value - a reasonable assumption about natural scenes and signals.

Weights \(w_{ij}\) in \(s, t\)-graph above are always non-negative, so graph-cut solvable.
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On log-supermodular vs. log-submodular distributions

- Log-supermodular distributions.

\[ \log Pr(x) = f(x) + \text{const.} = -E(x) + \text{const.} \quad (35) \]

where \( f \) is supermodular (\( E(x) \) is submodular). MAP (or high-probable) assignments should be “regular”, “homogeneous”, “smooth”, “simple”. E.g., attractive potentials in computer vision, ferromagnetic Potts models statistical physics.
On log-supermodular vs. log-submodular distributions

- **Log-supermodular distributions.**

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- **Log-submodular distributions:**

  \[
  \log \Pr(x) = f(x) + \text{const.}
  \]  

  where \( f \) is submodular. MAP or high-probable assignments should be “diverse”, or “complex”, or “covering”, like in determinantal point processes.
Submodular potentials in GMs: Image Segmentation

- an image needing to be segmented.
labeled data, some pixels being marked foreground (red) and others marked background (blue) to train the unaries $\{e_v(x_v)\}_{v \in V}$. 
Submodular potentials in GMs: Image Segmentation

- Set of a graph over the image, graph shows binary pixel labels.
Run graph-cut to segment the image, foreground in red, background in white.
the foreground is removed from the background.
What does graph-cut based image segmentation do with elongated structures (top) or contrast gradients (bottom)?
Shrinking bias in graph cut image segmentation

Image of a tree against a blue sky with a black and white image of a tree beside it, and a black and white image of leaves.
Shrinking bias in image segmentation

- An image needing to be segmented
- Clear high-contrast boundaries
Shrinking bias in image segmentation

- Graph-cut (MRF with submodular edge potentials) works well.
Shrinking bias in image segmentation

- Now with contrast gradient (less clear segment as we move up).
- The “elongated structure” also poses a challenge.
Shrinking bias in image segmentation

- Unary potentials \( \{ e_V(x_V) \}_{v \in V} \) prefer a different segmentation.
- Edge weights are the same regardless of where they are
  \( w_{i,j} = e_{ij}(1, 0) + e_{ij}(0, 1) - e_{ij}(1, 1) - e_{ij}(0, 0) \geq 0 \).
And the shrinking bias occurs, truncating the segmentation since it results in lower energy.
Shrinking bias in image segmentation

- With “typed” edges, we can have cut cost be sum of edge color weights, not sum of edge weights.
- Submodularity to the rescue: balls & urns.
Standard graph cut, uses a modular function \( w : 2^E \to \mathbb{R}_+ \) defined on the edges to measure cut costs. Graph cut node function is submodular.

\[
f_w(X) = w \left( \{ (u, v) \in E : u \in X, v \in V \setminus X \} \right)
\]  

(37)

Instead, we can use a submodular function \( g : 2^E \to \mathbb{R}_+ \) defined on the edges to express cooperative costs. As a node function, \( f_g : 2^V \to \mathbb{R}_+ \) is not submodular, but it uses submodularity internally to solve the shrinking bias problem. \( \Rightarrow \) cooperative cut (Jegelka & Bilmes, 2011).
Addressing shrinking bias with edge submodularity

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$\Rightarrow$ cooperative-cut (Jegelka & Bilmes, 2011).
Graph-cut vs. cooperative-cut comparisons

(Jegelka&Bilmes,’11). There are fast algorithms for solving as well (as we’ll see tomorrow).
Outline

1. Introduction

2. Basics

3. Submodular Applications in ML
   - Where is submodularity useful?
   - Traditional combinatorial problems
   - As a model of diversity, coverage, span, or information
   - As a model of cooperative costs, complexity, roughness, and irregularity
   - As a parameter for an ML algorithm
   - Itself, as a target for learning
   - Surrogates for optimization
   - Economic applications
In some cases, it may be useful to view a submodular function $f : 2^V \rightarrow \mathbb{R}$ as an input “parameter” to a machine learning algorithm.
A submodular function as a parameter

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$2^n$-dimensional since for certain $f \in \mathcal{S}$, there exists $f_\epsilon \in \mathbb{R}^{2^n}$ having no zero elements with $f + f_\epsilon \in \mathcal{S}$. 
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![Diagram of machine learning problem]

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- We next see how $f$ parameterizes problems in ML, and then address learning.
Given training data \( \mathcal{D} = \{(x_i, y_i)\}_{i=1}^m \) with \((x_i, y_i) \in \mathbb{R}^n \times \mathbb{R}\), perform the following risk minimization problem:

\[
\min_{w \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^m \ell(y_i, w^T x_i) + \lambda \Omega(w),
\]

where \( \ell(\cdot) \) is a loss function (e.g., squared error) and \( \Omega(w) \) is a norm.
Supervised And Unsupervised Machine Learning

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- When data has multiple responses $(x_i, y_i) \in \mathbb{R}^n \times \mathbb{R}^k$, learning becomes:

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\min_{w^1, \ldots, w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^j, (w^j)^\top x_i) + \lambda \Omega(w^k),
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- When data has multiple responses only that are observed, \((y_i) \in \mathbb{R}^k\) we get dictionary learning (Krause & Guestrin, Das & Kempe):

\[
\min_{x_1, \ldots, x_m} \min_{w^1, \ldots, w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^k, (w^k)^\top x_i) + \lambda \Omega(w^k),
\]

(41)
Common norms include $p$-norm $\Omega(w) = \|w\|_p = \left(\sum_{i=1}^{p} w_i^p\right)^{1/p}$

1-norm promotes sparsity (prefer solutions with zero entries).

Image denoising, **total variation** is useful, norm takes form:

$$\Omega(w) = \sum_{i=2}^{N} |w_i - w_{i-1}|$$

Points of difference should be “sparse” (frequently zero).

(Rodriguez, 2009)
Submodular parameterization of a sparse convex norm

- Prefer convex norms since they can be solved.
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- The Lovász-extension (Lovász ’82, Edmonds ’70) is easy to get via the greedy algorithm: sort $w_{\sigma_1} \geq w_{\sigma_2} \geq \cdots \geq w_{\sigma_n}$, then

\[
\tilde{f}(w) = \sum_{i=1}^{n} w_{\sigma_i} (f(\sigma_1, \ldots, \sigma_i) - f(\sigma_1, \ldots, \sigma_{i-1}))
\]  (43)

Ex: total variation is the Lovász-extension of graph cut
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Submodular Generalized Dependence

- there is a notion of “independence”, i.e., $A \perp B$:

$$f(A \cup B) = f(A) + f(B),$$

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- and a notion of “conditional independence”, i.e., \( A \perp B | C \):
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and a notion of “conditional mutual information”

$$I_f(A; B \mid C) \triangleq f(A \cup C) + f(B \cup C) - f(A \cup B \cup C) - f(C) \geq 0$$
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- and two notions of “information amongst a collection of sets”:
  \[
  I_f(S_1; S_2; \ldots; S_k) = \sum_{i=1}^{k} f(S_k) - f(S_1 \cup S_2 \cup \ldots \cup S_k)
  \]
  (47)

  \[
  I'_f(S_1; S_2; \ldots; S_k) = \sum_{A \subseteq \{1,2,\ldots,k\}} (-1)^{|A|+1} f(\bigcup_{j \in A} S_j)
  \]
  (48)
Given a submodular function $f : 2^V \rightarrow \mathbb{R}$, form the combinatorial dependence function $I_f(A; B) = f(A) + f(B) - f(A \cup B)$.
Submodular Parameterized Clustering

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- Hence, family of clustering algorithms parameterized by $f$. 

Active Transductive Semi-Supervised Learning

- Batch/Offline active learning: Given a set $V$ of unlabeled data items, learner chooses subset $L \subseteq V$ of items to be labeled.
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- Nature reveals labels $y_L \in \{0, 1\}^L$, learner predicts labels $\hat{y} \in \{0, 1\}^V$. 

J. Bilmes

Submodularity
Active Transductive Semi-Supervised Learning

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- Nature reveals labels $y_L \in \{0, 1\}^L$, learner predicts labels $\hat{y} \in \{0, 1\}^V$

- Learner suffers loss $\|\hat{y} - y\|_1$, here $\|\hat{y} - y\|_1 = 2$. 
Choosing labels: how to select $L$

- Consider the following objective

$$
\Psi(L) = \min_{T \subseteq V \setminus L: T \neq \emptyset} \frac{\Gamma(T)}{|T|} \quad (49)
$$

where $\Gamma(T) = f(T) + f(V \setminus T) - f(V)$ is an arbitrary symmetric submodular function (e.g., graph cut value between $T$ and $V \setminus T$).
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- Small $\Psi(L)$ means an adversary can separate away many ($|T|$ is big) combinatorially “independent” ($\Gamma(T)$ is small) points from $L$. 

---

$V \setminus L$ and $L$ are sets of vertices in a graph, and $T$ is a subset of $V \setminus L$. The notation $\Gamma(T)$ represents a function that quantifies the separation between $T$ and $V \setminus T$. The objective is to minimize this separation subject to the constraint that $T$ is not the empty set. This formulation is used to select a set of labels $L$ that maximizes the separation from the rest of the vertices in $V$. The choice of $L$ is guided by the minimization of the submodular function $\Gamma(T)$, which measures the cost of separating $T$ from the rest of the graph.
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![Diagram showing two scenarios: one with $\Psi(L) = 1/8$ and one with $\Psi(L) = 1$]
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This suggests choosing (bounded cost) \( L \) that maximizes \( \Psi(L) \).
Choosing labels: how to select $L$

- Given labels $L$, how to complete the labels?
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- Given labels $L$, how to complete the labels?
- We form a labeling $\hat{y} \in \{0, 1\}^V$ such that $\hat{y}_L = y_L$ (i.e., we agree with the known labels).

$$\Gamma(T)$$ measures label smoothness, how much combinatorial "information" between labels $T$ and complement $V \setminus T$ (e.g., in graph-cut case, says label change should be across small cuts). Hence, choose labels to minimize $\Gamma(\hat{y}(\hat{y}))$ such that $\hat{y}_L = y_L$.

This is submodular function minimization on function $g: 2^{V \setminus L} \rightarrow \mathbb{R}^+$ where for $A \subseteq V \setminus L$,

$$g(A) = \Gamma(A \cup \{v \in L: y_L(v) = 1\})$$

(50)

In graph cut case, this is standard min-cut (Blum & Chawla 2001) approach to semi-supervised learning.
Choosing labels: how to select \( L \)

- Given labels \( L \), how to complete the labels?
- We form a labeling \( \hat{y} \in \{0, 1\}^V \) such that \( \hat{y}_L = y_L \) (i.e., we agree with the known labels).
- \( \Gamma(T) \) measures label smoothness, how much combinatorial "information" between labels \( T \) and complement \( V \setminus T \) (e.g., in graph-cut case, says label change should be across small cuts).
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- Hence, choose labels to minimize $\Gamma(Y(\hat{y}))$ such that $\hat{y}_L = y_L$. 

This is submodular function minimization on function $g: 2^V \setminus L \to \mathbb{R}^+$ where for $A \subseteq V \setminus L$, 

$$g(A) = \Gamma(A \cup \{v \in L: y_L(v) = 1\})$$

In graph-cut case, this is standard min-cut (Blum & Chawla 2001) approach to semi-supervised learning.
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Generalized Error Bound

Theorem (Guillory & Bilmes, ’11)

For any symmetric submodular $\Gamma(S)$, assume $\hat{y}$ minimizes $\Gamma(Y(\hat{y}))$ subject to $\hat{y}_L = y_L$. Then

$$\|\hat{y} - y\|_1 \leq 2 \frac{\Gamma(Y(y))}{\Psi(L)}$$

(51)

where $y \in \{0, 1\}^V$ are the true labels.

- All is defined in terms of the symmetric submodular function $\Gamma$ (need not be graph cut), where:
  $$\Psi(S) = \min_{T \subseteq V \setminus S: T \neq \emptyset} \frac{\Gamma(T)}{|T|}$$
  (52)
  $$\Gamma(T) = f(S) + f(V \setminus S) - f(V)$$

is determined by arbitrary submodular function $f$, giving different error bound for each.

- Joint algorithm is “parameterized” by a submodular function $f$. 

A convex function parameterizes a Bregmann divergence, useful for clustering (Banerjee et al.), includes KL-divergence, squared l2, etc.
Discrete Submodular Divergences

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- Given a (not nec. differentiable) convex function $\phi$ and a sub-gradient map $\mathcal{H}_\phi$, the generalized Bregmann divergence is defined as:

$$d^{\mathcal{H}_\phi}(x, y) = \phi(x) - \phi(y) - \langle \mathcal{H}_\phi(y), x - y \rangle, \forall x, y \in \text{dom}(\phi) \quad (53)$$
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A submodular function parameterizes a discrete submodular Bregmann divergence (Iyer & Bilmes, 2012).
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- Example, lower-bound form:
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- Submodular Bregmann divergences also definable in terms of supergradients.
- General: Hamming, Recall, Precision, Cond. MI, Sq. Hamming, etc.
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Learning submodular functions is hard
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Goemans et al. (2009): “can one make only polynomial number of queries to an unknown submodular function \( f \) and constructs a \( \hat{f} \) such that \( \hat{f}(S) \leq f(S) \leq g(n)\hat{f}(S) \) where \( g : \mathbb{N} \rightarrow \mathbb{R} \)?”
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Balcan & Harvey (2011): submodular function learning problem from a learning theory perspective, given a distribution on subsets. Negative result is that can’t approximate in this setting to within a constant factor.
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But can we learn a subclass, perhaps non-negative weighted mixtures of submodular components?
Structured Prediction in Machine Learning

- Given: a finite set of training pairs \( D = \{ (x^{(i)}, y^{(i)}) \} \), where \( x^{(i)} \in \mathcal{X}, \ y^{(i)} \in \mathcal{Y} \).
- \( f: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}^M \) is a (fixed) vector of functions, and \( w \in \mathbb{R}^M \) is a vector of parameters to learn.
- Score function: \( s(x, y) = w^T f(x, y) = \sum_i w_i f_i(x, y) \).
- Decision making (inference) for a given \( \bar{x} \) is based on:

\[
\hat{y} \in h_w(\bar{x}) = \arg\max_{y \in \mathcal{Y}} s(\bar{x}, y) = \arg\max_{y \in \mathcal{Y}} w^T f(\bar{x}, y)
\] (55)

- Goal of learning: optimize \( w \) so that such decision making is “good”
- Let \( \ell: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+ \) be a loss function. I.e., \( \ell_y(\hat{y}) \) is cost of deciding \( \hat{y} \) when truth is \( y \).
- Empirical risk minimization: adjust \( w \) so that \( \sum_i \ell_y(h_w(x^{(i)})) \) is small subject to other conditions (e.g., regularization).
Structured Prediction: Approach with inference

Constraints specified in inference form:

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{T} \sum_{t} \xi_{t} + \frac{\lambda}{2} \|w\|^2 \\
\text{subject to} & \quad w^\top f_{t}(y^{(t)}) \geq \max_{y \in \mathcal{Y}_{t}} \left( w^\top f_{t}(y) + \ell_{t}(y) \right) - \xi_{t}, \forall t \\
& \quad \xi_{t} \geq 0, \forall t.
\end{align*}
\]

(56)

(57)

(58)

Exponential set of constraints reduced to an embedded optimization problem, “inference.”
Unconstrained form uses a generalized hinge-loss (Taskar 2004), which is amenable to sub-gradient descent optimization:

\[
\min_{\mathbf{w} \geq 0} \frac{1}{T} \sum_t \left[ \max_{\mathbf{y} \in \mathcal{Y}_t} \left( \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y}) \right) - \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) \right] + \frac{\lambda}{2} \|\mathbf{w}\|^2 \quad (59)
\]

Note, \( \mathbf{w} \geq 0 \) critical to preserve submodularity.

To compute a subgradient, must solve the following embedded optimization problem (“loss augmented inference”):

\[
\max_{\mathbf{y} \in \mathcal{Y}_t} \left( \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y}) \right) \quad (60)
\]

The problem is convex in \( \mathbf{w} \), and \( \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) \) is submodular (polymatroidal in fact), but what about \( \ell_t(\mathbf{y}) \)?

Often one uses Hamming loss (in general structured prediction problems) which is submodular (modular in fact).

If loss \( \ell_t(\mathbf{y}) \), more generally, is submodular, then Eq. (60) can be solved at least approximately well.
Structured Prediction: Subgradient

- Subgradient, evaluated at $w$, of the following

$$
\max_{y \in \mathcal{Y}_t} \left( w^\top f_t(y) + \ell_t(y) \right) - w^\top f_t(y^{(t)}) + \frac{\lambda}{2} \|w\|^2 
$$

(61)

can be found by computing or approximating

$$
y^* \in \arg\max_{y \in \mathcal{Y}_t} \left( w^\top f_t(y) + \ell_t(y) \right) - w^\top f_t(y^{(t)})
$$

(62)

and then finding subgradient of

$$
w^\top f_t(y^*) + \ell_t(y^*) - w^\top f_t(y^{(t)}) + \frac{\lambda}{2} \|w\|^2
$$

(63)

which has the form

$$
f_t(y^*) - f_t(y^{(t)}) + \lambda w.
$$

(64)
Structured Prediction: Subgradient Learning

Algorithm 1: Subgradient descent learning

**Input**: \( S = \{(x^{(t)}, y^{(t)})\}_{t=1}^{T} \) and a learning rate sequence \( \{\eta_t\}_{t=1}^{T} \).

\( w_0 = 0; \)

for \( t = 1, \ldots, T \) do

- Loss augmented inference: \( y^{*}_t \in \arg\max_{y \in Y_t} w_{t-1}^\top f_t(y) + \ell_t(y); \)
- Compute the subgradient: \( g_t = \lambda w_{t-1} + f_t(y^{*}) - f_t(y^{(t)}); \)
- Update the weights: \( w_t = w_{t-1} - \eta_t g_t; \)

**Return**: the averaged parameters \( \frac{1}{T} \sum_t w_t. \)
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Submodular Relaxation

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When potentials are not, we might resort to factorization (e.g., the marginal polytope in variational inference, were we optimize over a tree-constrained polytope).
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An alternative is submodular relaxation. I.e., given

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\Pr(x) = \frac{1}{Z} \exp(-E(x))
\]

(65)

where \( E(x) = E_f(x) - E_g(x) \) and both of \( E_f(x) \) and \( E_g(x) \) are submodular.
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Hence, rather than minimize $E(x)$ (hard), we can minimize $E_f(x) \geq E(x)$ (relatively easy), which is an upper bound.
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Consumer costs are very often submodular.
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$$f(\text{McDonalds}) + f(\text{hamburger}) \geq f(\text{hamburger}) + f(\text{McDonalds})$$
Ex. Submodular: Consumer Costs of Living

- Consumer costs are very often submodular. For example:

\[ f(\text{coca-cola, fries, burger}) + f(\text{fries, burger}) \geq f(\text{fries, burger}) + f(\text{coca-cola}) \]

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Consumer costs are very often submodular. For example:

\[ f(\text{Coke}) + f(\text{Fries}) \geq f(\text{Fries}) + f(\text{Coke}) \]

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- Rearranging terms, we can see this as diminishing returns:

$$f(\text{Coke and Fries}) - f(\text{Fries}) \geq f(\text{Fries and Coke}) - f(\text{Coke})$$

- This is very common: The additional cost of a coke is, say, free if you add it to fries and a hamburger, but when added just to an order of fries, the coke is not free.
Shared Fixed Costs

- Costs often interact in the real world.

\[ \text{Let } V = \{ v_1, v_2 \} \text{ be a set of actions with: } \\
\quad v_1 = \text{"buy milk at the store"}, \\
\quad v_2 = \text{"buy honey at the store"}. \\
\text{For } A \subseteq V, \text{ let } f(A) \text{ be the cost of set of items } A. \\
\]

\[ f(\{ v_1 \}) = \text{cost to drive to and from store, and cost to purchase milk, say } c_d + c_m. \\
\quad f(\{ v_2 \}) = \text{cost to drive to and from store, and cost to purchase honey, say } c_d + c_h. \\
\quad f(\{ v_1, v_2 \}) = c_d + c_m + c_h < 2(c_d + c_m + c_h) \text{ since } c_d \text{ (driving) is a shared fixed cost.} \]
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- But $f(\{v_1, v_2\}) = c_d + c_m + c_h < 2c_d + c_m + c_h$ since $c_d$ (driving) is a shared fixed cost.
- Shared fixed costs are submodular: $f(v_1) + f(v_2) \geq f(v_1, v_2) + f(\emptyset)$
What is a good model of the cost of manufacturing a set of items?
Supply Side Economies of scale

- What is a good model of the cost of manufacturing a set of items?
- Let $V$ be a set of possible items that a company might possibly wish to manufacture, and let $f(S)$ for $S \subseteq V$ be the cost to that company to manufacture subset $S$. 

Ex: $V$ might be colors of paint in a paint manufacturer: green, red, blue, yellow, white, etc. Producing green when you are already producing yellow and blue is probably cheaper than if you were only producing some other colors. 

$$f(\text{green, blue, yellow}) - f(\text{blue, yellow}) < f(\text{green, blue}) - f(\text{blue})$$ (66)

So diminishing returns (a submodular function) would be a good model.
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- consumers of a good derive positive value when size of the market increases.
- the value of a network to a user depends on the number of other users in that network. External use benefits internal use.
Demand side Economies of Scale: Network Externalities

- consumers of a good derive positive value when size of the market increases.
- the value of a network to a user depends on the number of other users in that network. External use benefits internal use.
- This is called network externalities (Katz & Shapiro 1986), and is a form of “demand” economies of scale
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- Given network externalities, a consumer in today’s market cares also about the future success of the product and competing products.
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- Given network externalities, a consumer in today’s market cares also about the future success of the product and competing products.
- If the good is durable (e.g., a car or phone) or there is human capital investment (e.g., education in a skill), the total benefits derived from a good will depend on the number of consumers who adopt compatible products in the future.
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- So supermodularity would be a good model.
Outline: Part 2

4 From Matroids to Polymatroids
- Matrix Rank
- Venn Diagrams
- Matroids

5 Submodular Definitions, Examples, and Properties
- Normalization
- Submodular Definitions
- Submodular Composition
- More Examples
Example: Rank function of a matrix

- Given an \( n \times m \) matrix, thought of as \( m \) column vectors:

\[
X = \begin{pmatrix}
1 & 2 & 3 & 4 & \cdots & m \\
x_1 & x_2 & x_3 & x_4 & \cdots & x_m
\end{pmatrix}
\]  

- Let set \( V = \{1, 2, \ldots, m\} \) be the set of column vector indices.
- For any subset of column vector indices \( A \subseteq V \), let \( r(A) \) be the rank of the column vectors indexed by \( A \).
- Hence \( r : 2^V \to \mathbb{Z}_+ \) and \( r(A) \) is the dimensionality of the vector space spanned by the set of vectors \( \{x_a\}_{a \in A} \).
- Intuitively, \( r(A) \) is the size of the largest set of independent vectors contained within the set of vectors indexed by \( A \).
Example: Rank function of a matrix

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

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

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

- Let $A = \{1, 2, 3\}$, \hspace{1cm} $B = \{3, 4, 5\}$, \hspace{1cm} $C = \{6, 7\}$, \hspace{1cm} $A_r = \{1\}$, \hspace{1cm} $B_r = \{5\}$.
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J. Bilmes
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2 & 0 & 3 & 0 & 4 & 0 & 0 & 2 & 4 \\
3 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 5 \\
4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 5
\end{pmatrix}
\]

\[
\begin{pmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
\| & \| & \| & \| & \| & \| & \| & \| & \|
\end{pmatrix}
\]

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

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

Since $r(A) + r(B) = 6 = r(A \cup B) + r(A \cap B)$, it holds that $r(A) + r(B) > 2r(A \cup B)$.
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3 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 5 \\
4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 5
\end{bmatrix}
= 
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\mid & \mid & \mid & \mid & \mid & \mid & \mid & \mid & \mid \\
\mid & \mid & \mid & \mid & \mid & \mid & \mid & \mid & \mid \\
x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8
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2 & 0 & 3 & 0 & 4 & 0 & 0 & 2 & 4 \\
3 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 5 \\
4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 5
\end{pmatrix}
= 
\begin{pmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
| | | | | | | | | \\
\times_1 & \times_2 & \times_3 & \times_4 & \times_5 & \times_6 & \times_7 & \times_8 \\
| | | | | | | | | \\
\end{pmatrix}
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2 & 0 & 3 & 4 & 0 & 0 & 2 & 4 \\
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4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 5
\end{pmatrix}
= 
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1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
\vert & \vert & \vert & \vert & \vert & \vert & \vert & \vert & \vert \\
X_1 & X_2 & X_3 & X_4 & X_5 & X_6 & X_7 & X_8
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\end{pmatrix}
= \begin{pmatrix}
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\mid & \mid & \mid & \mid & \mid & \mid & \mid & \mid \\
\times_1 & \times_2 & \times_3 & \times_4 & \times_5 & \times_6 & \times_7 & \times_8 \\
\mid & \mid & \mid & \mid & \mid & \mid & \mid & \mid
\end{pmatrix}
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\end{pmatrix}
= \begin{pmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
| & | & | & | & | & | & | & | \\
\begin{pmatrix}
x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8
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Polymatroids

Submodular Properties

Example: Rank function of a matrix

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

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

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Submodularity
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\begin{pmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
1 & 0 & 2 & 2 & 3 & 0 & 1 & 3 & 1 \\
2 & 0 & 3 & 0 & 4 & 0 & 0 & 2 & 4 \\
3 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 5 \\
4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 5
\end{pmatrix}
$$

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

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

- Let $A = \{1, 2, 3\}$, $B = \{3, 4, 5\}$, $C = \{6, 7\}$, $A_r = \{1\}$, $B_r = \{5\}$.
- Then $r(A) = 3$, $r(B) = 3$, $r(C) = 2$.
- $r(A \cup C) = 3$, $r(B \cup C) = 3$.
- $r(A \cup A_r) = 3$, $r(B \cup B_r) = 3$, $r(A \cup B_r) = 4$, $r(B \cup A_r) = 4$.
- $r(A \cup B) = 4$, $r(A \cap B) = 1 < r(C) = 2$. 
Example: Rank function of a matrix

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

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

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- Then $r(A) = 3$, $r(B) = 3$, $r(C) = 2$.
- $r(A \cup C) = 3$, $r(B \cup C) = 3$.
- $r(A \cup A_r) = 3$, $r(B \cup B_r) = 3$, $r(A \cup B_r) = 4$, $r(B \cup A_r) = 4$.
- $r(A \cup B) = 4$, $r(A \cap B) = 1 < r(C) = 2$.
- $6 = r(A) + r(B) > r(A \cup B) + r(A \cap B) = 5$
Rank function of a matrix

- Let $A, B \subseteq V$ be two subsets of column indices.
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.
Polymatroids

Submodular Properties

Rank function of a matrix

- Let $A, B \subseteq V$ be two subsets of column indices.
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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.
Vectors $A$ and $B$ have a (possibly empty) common span and two (possibly empty) non-common residual spans.
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Let $C$ index vectors spanning dimensions common to $A$ and $B$. 

Then, $r(A) = r(C) + r(A_{r})$.

Similarly, $r(B) = r(C) + r(B_{r})$.

Then $r(A) + r(B)$ counts the dimensions spanned by $C$ twice, i.e.,

$$r(A) + r(B) = r(A_{r}) + 2r(C) + r(B_{r})$$

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

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**Rank functions of a matrix**

- Then $r(A) + r(B)$ counts the dimensions spanned by $C$ twice, i.e.,
  \[ r(A) + r(B) = r(A_r) + 2r(C) + r(B_r) \]

  ![Diagram 1](image1)

- But $r(A \cup B)$ counts the dimensions spanned by $C$ only once.
  \[ r(A \cup B) = r(A_r) + r(C) + r(B_r) \]

  ![Diagram 2](image2)
Rank functions of a matrix

- Then $r(A) + r(B)$ counts the dimensions spanned by $C$ twice, i.e.,
  $$r(A) + r(B) = r(A_r) + 2r(C) + r(B_r)$$

- But $r(A \cup B)$ counts the dimensions spanned by $C$ only once.
  $$r(A \cup B) = r(A_r) + r(C) + r(B_r)$$

- Thus, we have subadditivity: $r(A) + r(B) \geq r(A \cup B)$. Can we add more to the r.h.s. and still have an inequality? Yes.
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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In short:
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In short:
- Common span (blue) is “more” (no less) than span of common index (magenta).
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\[
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\]

In short:
- Common span (blue) is “more” (no less) than span of common index (magenta).
- More generally, common information (blue) is “more” (no less) than information within common index (magenta).
The Venn and Art of Submodularity

\[ r(A) + r(B) \geq r(A \cup B) + r(A \cap B) = r(A_r) + 2r(C) + r(B_r) = r(A_r) + r(C) + r(B_r) = r(A \cap B) \]
Definition

A polymatroid function is a real-valued function $f$ defined on subsets of $V$ which is normalized, non-decreasing, and submodular. That is:

1. $f(\emptyset) = 0$ (normalized)
2. $f(A) \leq f(B)$ for any $A \subseteq B \subseteq V$ (monotone non-decreasing)
3. $f(A \cup B) + f(A \cap B) \leq f(A) + f(B)$ for any $A, B \subseteq V$ (submodular)

We can define the polyhedron $P_f^+$ associated with a polymatroid function as follows

$$P_f^+ = \left\{ y \in \mathbb{R}^V_+ : y(A) \leq f(A) \text{ for all } A \subseteq V \right\}$$ \hspace{1cm} (70)

$$= \left\{ y \in \mathbb{R}^V : y \geq 0, y(A) \leq f(A) \text{ for all } A \subseteq V \right\}$$ \hspace{1cm} (71)
Chains of sets

- Ground element $V = \{1, 2, \ldots, n\}$ set of integers w.l.o.g.
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- Given a permutation $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$ of the integers.
Chains of sets

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- Given a permutation $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$ of the integers.
- From this we can form a chain of sets $\{C_i\}_i$ with
  $\emptyset = C_0 \subseteq C_1 \subseteq \cdots \subseteq C_n = V$ formed as:

$$C_i = \{\sigma_1, \sigma_2, \ldots, \sigma_i\}, \quad \text{for } i = 1 \ldots n \quad (72)$$

\[ \text{\sigma(1) \sigma(2) \sigma(3) \sigma(4) \sigma(5) \sigma(6) \sigma(7) \sigma(8) \cdots} \]

\[ \begin{array}{c}
\sigma(1) \\
C_1 \\
\vdots \\
C_2 \\
\vdots \\
C_3 \\
\vdots \\
\end{array} \]

Can also form a chain from a vector $w \in \mathbb{R}^V$ sorted in descending order. Choose $\sigma$ so that $w(\sigma_1) \geq w(\sigma_2) \geq \cdots \geq w(\sigma_n)$. 
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\[ \sigma(1) \quad \sigma(2) \quad \sigma(3) \quad \sigma(4) \quad \sigma(5) \quad \sigma(6) \quad \sigma(7) \quad \sigma(8) \quad \cdots \]

\[ C_1 \quad C_2 \quad C_3 \]
We often wish to express the gain of an item $j \in V$ in context $A$, namely $f(A \cup \{j\}) - f(A)$. 

Submodularity's diminishing returns definition can be stated as saying that $f(A \mid \{j\})$ is a monotone non-increasing function of $A$, since $f(A \mid \{j\}) \geq f(B \mid \{j\})$ whenever $A \subseteq B$ (conditioning reduces valuation).
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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:

\[
\begin{align*}
f(A \cup \{j\}) - f(A) & \triangleq \rho_j(A) \quad (73) \\
& \triangleq \rho_A(j) \quad (74) \\
& \triangleq \nabla_j f(A) \quad (75) \\
& \triangleq f(\{j\} | A) \quad (76) \\
& \triangleq f(j | A) \quad (77)
\end{align*}
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- We’ll use \( f(j|A) \). Also, \( f(A|B) = f(A \cup B) - f(B) \).
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Polymatroidal polyhedron and greedy

Suppose we wish to solve the following linear programming problem:

\[
\begin{align*}
\text{maximize} & \quad w^T x \\
\text{subject to} & \quad x \in \{ y \in \mathbb{R}_+^V : y(A) \leq f(A) \text{ for all } A \subseteq V \} \\
\end{align*}
\] (78)

or more simply put, \( \max(wx : x \in P_f) \).
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Consider greedy solution: sort elements of \( V \) w.r.t. \( w \) so that w.l.o.g. \( V = (v_1, v_2, \ldots, v_m) \) has \( w(v_1) \geq w(v_2) \geq \cdots \geq w(v_m) \).
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Next, form chain of sets based on \( w \) sorted descended, giving:

\[
V_i \overset{\text{def}}{=} \{ v_1, v_2, \ldots, v_i \}
\]

for \( i = 0 \ldots m \). Note \( V_0 = \emptyset \), and \( f(V_0) = 0 \).
Suppose we wish to solve the following linear programming problem:

\[
\begin{align*}
\text{maximize} & \quad w^T x \\
\text{subject to} & \quad x \in \{ y \in \mathbb{R}^V_+ : y(A) \leq f(A) \text{ for all } A \subseteq V \} \quad (78)
\end{align*}
\]

or more simply put, \( \max(wx : x \in P_f) \).

Consider greedy solution: sort elements of \( V \) w.r.t. \( w \) so that \( w.l.o.g. \ V = (v_1, v_2, \ldots, v_m) \) has \( w(v_1) \geq w(v_2) \geq \cdots \geq w(v_m) \).

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\]

for \( i = 0 \ldots m \). Note \( V_0 = \emptyset \), and \( f(V_0) = 0 \).

The greedy solution is the vector \( x \in \mathbb{R}^V_+ \) with element \( x(v_i) \) for \( i = 1, \ldots, n \) defined as:

\[
x(v_i) = f(V_i) - f(V_{i-1}) = f(v_i | V_{i-1}) \quad (80)
\]
We have the following very powerful result (which generalizes a similar one that is true for matroids).

**Theorem**

Let $f : 2^V \rightarrow \mathbb{R}_+^+$ be a given set function, and $P$ is a polytope in $\mathbb{R}_+^V$ of the form $P = \{ x \in \mathbb{R}_+^V : x(A) \leq f(A), \forall A \subseteq V \}$.

Then the greedy solution to the problem $\max(wx : x \in P)$ is optimal $\forall w$ iff $f$ is monotone non-decreasing submodular (i.e., iff $P$ is a polymatroid).
Greedy does more than this. In fact, we have:

**Theorem**

For a given ordering $V = (v_1, \ldots, v_m)$ of $V$ and a given $V_i$ and $x$ generated by $V_i$ using the greedy procedure, then $x$ is an extreme point of $P_f$.

**Corollary**

If $x$ is an extreme point of $P_f$ and $B \subseteq V$ is given such that $\{v \in V : x(v) \neq 0\} \subseteq B \subseteq \bigcup (A : x(A) = f(A))$, then $x$ is generated using greedy by some ordering of $B$. 
Intuition: why greedy works with polymatroids

- Given $w$, the goal is to find $x = (x(e_1), x(e_2))$ that maximizes $x^T w = x(e_1)w(e_1) + x(e_2)w(e_2)$.
- If $w(e_2) > w(e_1)$, the upper extreme point indicated maximizes $x^T w$ over $x \in P_f^+$.
- If $w(e_2) < w(e_1)$, the lower extreme point indicated maximizes $x^T w$ over $x \in P_f^+$. 
Polymatroid with labeled edge lengths
Given these results, we can conclude that a polymatroid is really an extremely natural polyhedral generalization of a matroid. This was all realized by Jack Edmonds in the mid 1960s (and published in 1969 in his landmark paper “Submodular Functions, Matroids, and Certain Polyhedra”).

Outline: Part 2

4 From Matroids to Polymatroids
   • Matrix Rank
   • Venn Diagrams
   • Matroids

5 Submodular Definitions, Examples, and Properties
   • Normalization
   • Submodular Definitions
   • Submodular Composition
   • More Examples
Submodular (or Upper-SemiModular) Lattices

The name “Submodular” comes from lattice theory, and refers to a property of the “height” function of an upper-semimodular lattice. Ex: consider the following lattice over 7 elements.

\[
\begin{align*}
    x \lor y & : \text{height} = 3 \\
    x & : \text{height} = 2 \\
    y & : \text{height} = 1 \\
    x \land y & : \text{height} = 0
\end{align*}
\]

- Such lattices require that for all \( x, y, z \),
  \[
  h(x) + h(y) > h(x \lor y) + h(x \land y)
  \]
  \[
  2 + 2 > 3 + 0
  \]
- The lattice is upper-semimodular (submodular), height function is submodular on the lattice.
A function $f : 2^V \rightarrow \mathbb{R}$ is submodular if for any $A, B \subseteq V$, we have that:

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

General submodular function, $f$ need not be monotone, non-negative, nor normalized (i.e., $f(\emptyset)$ need not be $= 0$).
Given any submodular function $f : 2^V \rightarrow \mathbb{R}$, form a normalized variant $f' : 2^V \rightarrow \mathbb{R}$, with

$$f'(A) = f(A) - f(\emptyset)$$

(82)

Then $f'(\emptyset) = 0$.

This operation does not affect submodularity, or any minima or maxima.

It is often assumed that all submodular functions are so normalized.
Given any arbitrary submodular function $f : 2^V \rightarrow \mathbb{R}$, consider the identity

$$f(A) = f(A) - m(A) + m(A) = \bar{f}(A) + m(A)$$

(83)

for a modular function $m : 2^V \rightarrow \mathbb{R}$, where

$$m(a) = f(a | V \setminus \{a\})$$

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Given any arbitrary submodular function \( f : 2^V \to \mathbb{R} \), consider the identity

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Then \( \bar{f}(A) \) is polymatroidal since \( \bar{f}(\emptyset) = 0 \) and for any \( a \) and \( A \)

\[
\bar{f}(a|A) = f(a|A) - f(a|V \setminus \{a\}) \geq 0
\]
Totally Normalized

- $\bar{f}$ is called the totally normalized version of $f$
Totally Normalized

- $\bar{f}$ is called the totally normalized version of $f$
- polytope of $\bar{f}$ and $f$ is the same shape, just shifted.

$$P_f = \left\{ x \in \mathbb{R}^V : x(A) \leq f(A), \forall A \subseteq V \right\} \quad (86)$$

$$= \left\{ x \in \mathbb{R}^V : x(A) \leq \bar{f}(A) + m(A), \forall A \subseteq V \right\} \quad (87)$$
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\begin{align*}
P_f &= \left\{ x \in \mathbb{R}^V : x(A) \leq f(A), \forall A \subseteq V \right\} \quad (86) \\
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- $m$ is like a unary score, $\bar{f}$ is where things interact. All of the real structure is in $\bar{f}$
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- $m$ is like a unary score, $\bar{f}$ is where things interact. All of the real structure is in $\bar{f}$
- Hence, any submodular function is a sum of polymatroid and modular.
Telescoping Summation

Given a chain set of sets $A_1 \subseteq A_2 \subseteq \cdots \subseteq A_r$
Telescoping Summation

- Given a chain set of sets $A_1 \subseteq A_2 \subseteq \cdots \subseteq A_r$
- Then the telescoping summation property of the gains is as follows:

$$
\sum_{i=1}^{r-1} f(A_{i+1} | A_i) = \sum_{i=2}^{r} f(A_i) - \sum_{i=1}^{r-1} f(A_i) = f(A_r) - f(A_1) \quad (88)
$$
Submodular Definitions

**Theorem**

Given function \( f : 2^V \rightarrow \mathbb{R} \), then

\[
f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \quad \text{for all } A, B \subseteq V \tag{SC}
\]

if and only if

\[
f(v|X) \geq f(v|Y) \quad \text{for all } X \subseteq Y \subseteq V \text{ and } v \notin B \tag{DR}
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**Theorem**

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**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 $f(A) - f(A \cap B) \geq f(A \cup B) - f(B)$ implies $(DR)$.

$(DR) \Rightarrow (SC)$: Order $A \setminus B = \{v_1, v_2, \ldots, v_r\}$ arbitrarily. Then

$$f(v_i|A \cap B \cup \{v_1, v_2, \ldots, v_{i-1}\}) \geq f(v_1|B \cup \{v_1, v_2, \ldots, v_{i-1}\}), \quad i \in [r - 1]$$

Applying telescoping summation to both sides, we get:

$$f(A) - f(A \cap B) \geq f(A \cup B) - f(B)$$
Many (Equivalent) Definitions of Submodularity

\[ f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V \] 

(89)
Many (Equivalent) Definitions of Submodularity

\[ f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \ \forall A, B \subseteq V \]  \hspace{1cm} (89)

\[ f(j|S) \geq f(j|T), \ \forall S \subseteq T \subseteq V, \ \text{with } j \in V \setminus T \]  \hspace{1cm} (90)
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f(A \cup B|A \cap B) \leq f(A|A \cap B) + f(B|A \cap B), \quad \forall A, B \subseteq V \tag{93}
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\[ f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \ \forall S, T \subseteq V \quad (94) \]
Many (Equivalent) Definitions of Submodularity

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Given submodular $f_1, f_2, \ldots, f_k$ each $\in 2^V \rightarrow \mathbb{R}$, then conic combinations are submodular. I.e.,

$$f(A) = \sum_{i=1}^{k} \alpha_i f_i(A)$$

where $\alpha_i \geq 0$. 

Restrictions: $f(A) = g(A \cap C)$ is submodular whenever $g$ is, for all $C$.

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Basic ops: Sums, Restrictions, Conditioning

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The “or” of two polymatroid functions

- Given two polymatroid functions \( f \) and \( g \), suppose feasible \( A \) are defined as \( \{ A : f(A) \geq \alpha_f \text{ or } g(A) \geq \alpha_g \} \) for real \( \alpha_f, \alpha_g \).
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- Define: \( h(A) = \bar{f}(A)\bar{g}(V) + \bar{f}(V)\bar{g}(A) - \bar{f}(A)\bar{g}(A) \).
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Theorem (Guillory & Bilmes, 2011)

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$h(A) = \alpha_f\alpha_g$ if and only if $\bar{f}(A) = \alpha_f$ or $\bar{g}(A) = \alpha_g$
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**Theorem**

$h(A) = \alpha_f\alpha_g$ if and only if $\bar{f}(A) = \alpha_f$ or $\bar{g}(A) = \alpha_g$

- Therefore, $h$ can be used as a submodular surrogate for the “or” of multiple submodular functions.
Convex/Concave have many nice properties of composition (see Boyd & Vandenberghe, “Convex Optimization”)
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A submodular function $f : 2^V \to \mathbb{R}$ has a different type of input and output, so composing two submodular functions directly makes no sense.
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A submodular function $f : 2^V \rightarrow \mathbb{R}$ has a different type of input and output, so composing two submodular functions directly makes no sense.

However, we have a number of forms of composition results that preserve submodularity, which we turn to next:
Given submodular $f : 2^V \rightarrow \mathbb{R}$ and a grouping of $V = V_1 \cup V_2 \cup \cdots \cup V_k$ into $k$ possibly overlapping clusters.
Given submodular $f : 2^V \to \mathbb{R}$ and a grouping of $V = V_1 \cup V_2 \cup \cdots \cup V_k$ into $k$ possibly overlapping clusters.

Define new function $g : 2^k \to \mathbb{R}$ where $\forall D \subseteq [k] = \{1, 2, \ldots, k\}$,

$$g(D) = f\left( \bigcup_{d \in D} V_d \right) \quad \text{(99)}$$
Grouping elements, set cover, and bipartite neighborhoods

- Given submodular \( f : 2^V \to \mathbb{R} \) and a grouping of \( V = V_1 \cup V_2 \cup \cdots \cup V_k \) into \( k \) possibly overlapping clusters.
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  g(D) = f(\bigcup_{d \in D} V_d)
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- Then \( g \) is submodular if either \( f \) is monotone non-decreasing or the sets \( \{V_i\} \) are disjoint.
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Ex: Bipartite neighborhoods: Let \( \Gamma : 2^V \rightarrow \mathbb{R} \) be the neighbor function in a bipartite graph \( G = (V, U, E, w) \). \( V \) is set of “left” nodes, \( U \) is set of right nodes, \( E \subseteq V \times U \) are edges, and \( w : 2^E \rightarrow \mathbb{R} \) is a modular function on edges.
Polymatroids

Submodular Properties

Grouping elements, set cover, and bipartite neighborhoods

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- Define new function $g : 2^{[k]} \to \mathbb{R}$ where $\forall D \subseteq [k] = \{1, 2, \ldots, k\}$,
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- Ex: Bipartite neighborhoods: Let $\Gamma : 2^V \to \mathbb{R}$ be the neighbor function in a bipartite graph $G = (V, U, E, w)$. $V$ is set of “left” nodes, $U$ is set of right nodes, $E \subseteq V \times U$ are edges, and $w : 2^E \to \mathbb{R}$ is a modular function on edges.
- Neighbors defined as $\Gamma(X) = \{u \in U : |X \times \{u\} \cap E| \geq 1\}$ for $X \subseteq V$. 
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Grouping elements, set cover, and bipartite neighborhoods

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- Ex: Bipartite neighborhoods: Let $\Gamma : 2^V \to \mathbb{R}$ be the neighbor function in a bipartite graph $G = (V, U, E, w)$. $V$ is set of “left” nodes, $U$ is set of right nodes, $E \subseteq V \times U$ are edges, and $w : 2^E \to \mathbb{R}$ is a modular function on edges.
- Neighbors defined as $\Gamma(X) = \{u \in U : |X \times \{u\} \cap E| \geq 1\}$ for $X \subseteq V$. Then $f(\Gamma(X))$ is submodular. Special case: set cover.
- In fact, all integral polymatroid functions can be obtained in $g$ above for $f$ a matroid rank function and $\{V_d\}$ appropriately chosen.
We also have the following composition property with concave functions:

**Theorem**

Given functions $f : 2^V \rightarrow \mathbb{R}$ and $g : \mathbb{R} \rightarrow \mathbb{R}$, the composition $h = f \circ g : 2^V \rightarrow \mathbb{R}$ (i.e., $h(S) = g(f(S))$) is nondecreasing submodular, if $g$ is non-decreasing concave and $f$ is nondecreasing submodular.
Concave composed with non-negative modular

Theorem

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

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

2. $g : \mathbb{R}_+ \rightarrow \mathbb{R}$ is concave.

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

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- If $g$ is non-decreasing concave, then $f$ is polymatroidal.
- Sums of concave over modular functions are submodular

\[
    f(A) = \sum_{i=1}^{K} g_i(m_i(A)) \tag{100}
\]
Concave composed with non-negative modular

**Theorem**

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

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- Very large class of functions, including graph cut, bipartite neighborhoods, set cover (Stobbe & Krause).
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(100)

- Very large class of functions, including graph cut, bipartite neighborhoods, set cover (Stobbe & Krause).
- However, Vondrak showed that a graphic matroid rank function over $K_4$ can't be represented in this fashion.
Weighted Matroid Rank Functions

- We saw matroid rank is submodular. Given matroid \((V, \mathcal{I})\),

\[
  f(B) = \max \{ |A| : A \subseteq B \text{ and } A \in \mathcal{I} \} \tag{101}
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  \[
  f(B) = \max \{m(A) : A \subseteq B \text{ and } |A| \leq k\}
  \]  
  (103)

- Take a 1-partition matroid with limit 1, we get the max function:
  \[
  f(B) = \max_{b \in B} m(b)
  \]  
  (104)
Given a set of $k$ matroids $(V, \mathcal{I}_i)$ and $k$ modular weight functions $m_i$, the following is submodular:

$$f(A) = \sum_{i=1}^{k} \alpha_i \max \{ m_i(A) : A \subseteq B \text{ and } A \in \mathcal{I}_i \}$$  \hfill (105)
Facility Location

• Given a set of $k$ matroids $(V, \mathcal{I}_i)$ and $k$ modular weight functions $m_i$, the following is submodular:

$$f(A) = \sum_{i=1}^{k} \alpha_i \max \{ m_i(A) : A \subseteq B \text{ and } A \in \mathcal{I}_i \}$$  \hspace{1cm} (105)

• Take all $\alpha_i = 1$, all matroids 1-partition matroids, and set $w_{ij} = m_i(j)$, and $k = |V|$ for some weighted graph $G = (V, E, w)$, we get the uncapacitated facility location function:

$$f(A) = \sum_{i \in V} \max_{a \in A} w_{ai}$$  \hspace{1cm} (106)
Information and Complexity functions

- Given a set $V$ of items, we might wish to measure the “information” or “complexity” in a subset $A \subset V$. 
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- Matroid rank $r(A)$ can measure the “information” or “complexity” via the dimensionality spanned by vectors with indices $A$. 

Entropy of a set of random variables $\{X_v\}_{v \in V}$, where $f(A) = H(X_A) = H(\bigcup_{a \in A} X_a) = -\sum_{x \in A} \Pr(x_A) \log \Pr(x_A)$ (107)

Entropy is submodular due to non-negativity of conditional mutual information. Given $A, B, C \subseteq V$,

$$I(X_A \setminus B; X_B \setminus A | X_A \cap B) = H(X_A) + H(X_B) - H(X_A \cup B) - H(X_A \cap B) \geq 0 \quad (108)$$
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Submodular Generalized Dependence

- there is a notion of “independence”, i.e., \( A \perp B \):
  \[
  f(A \cup B) = f(A) + f(B),
  \]
  (44)

- and a notion of “conditional independence”, i.e., \( A \perp B \mid C \):
  \[
  f(A \cup B \cup C) + f(C) = f(A \cup C) + f(B \cup C)
  \]
  (45)

- and a notion of “dependence” (conditioning reduces valuation):
  \[
  f(A \mid B) \triangleq f(A \cup B) - f(B) < f(A),
  \]
  (46)

- and a notion of “conditional mutual information”
  \[
  I_f(A; B \mid C) \triangleq f(A \cup C) + f(B \cup C) - f(A \cup B \cup C) - f(C) \geq 0
  \]

- and two notions of “information amongst a collection of sets”:
  \[
  I_f(S_1; S_2; \ldots; S_k) = \sum_{i=1}^{k} f(S_k) - f(S_1 \cup S_2 \cup \cdots \cup S_k)
  \]
  (47)

  \[
  I'_f(S_1; S_2; \ldots; S_k) = \sum_{A \subseteq \{1, 2, \ldots, k\}} (-1)^{|A|+1} f(\bigcup_{j \in A} S_j)
  \]
  (48)
Gaussian entropy, and the log-determinant function

**Definition (differential entropy $h(X)$)**

\[
h(X) = -\int_{\mathbb{S}} f(x) \log f(x) \, dx
\]

(109)

When $x \sim \mathcal{N}(\mu, \Sigma)$ is multivariate Gaussian, the (differential) entropy of the r.v. $X$ is given by

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

(110)

and in particular, for a variable subset $A$ and a constant $\gamma$,

\[
f(A) = h(X_A) = \log \sqrt{(2\pi e)^{|A|}|\Sigma_A|} = \gamma |A| + \frac{1}{2} \log |\Sigma_A|
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(111)
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\]

- Application of Jensen's inequality shows that

\[
I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B}) = h(X_A) + h(X_B) - h(X_{A \cup B}) - h(X_{A \cap B}) \geq 0.
\]

Hence differential entropy is submodular, and thus so is the logdet function.
Are all polymatroid functions entropy functions?

No, entropy functions must also satisfy the following:

**Theorem (Yeung)**

For any four discrete random variables \{X, Y, Z, U\}, then

\[ I(X; Y) = I(X; Y|Z) = 0 \]  \hspace{1cm} (112)

implies that

\[ I(X; Y|Z, U) \leq I(Z; U|X, Y) + I(X; Y|U) \] \hspace{1cm} (113)

where \( I(\cdot; \cdot|\cdot) \) is the standard Shannon mutual information function.
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- This is not required for all polymatroid-based conditional mutual information functions \( I_f(\cdot; \cdot|\cdot) \).
Submodular functions ⊃ Polymatroid functions ⊃ Entropy functions ⊃ Gaussian Entropy functions = DPPs.
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DPPs (Kulesza & Taskar) are a point process where \( \Pr(Y = Y) \propto \det(L_Y) \) for some positive-definite matrix \( L \), so DPPs are log-submodular, as we saw.
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DPPs (Kulesza & Taskar) are a point process where \( \Pr(\mathbf{Y} = \mathbf{Y}) \propto \det(L_{\mathbf{Y}}) \) for some positive-definite matrix \( L \), so DPPs are log-submodular, as we saw.

Thanks to the properties of matrix algebra (e.g., determinants), DPPs are computationally extremely attractive and are now widely used in ML.
Outline: Part 3

6 Discrete Semimodular Semigradients

7 Continuous Extensions
- Lovász Extension
- Concave Extension

8 Like Concave or Convex?

9 Optimization

10 Reading
A convex function $f$ has a subgradient at any in-domain point $b$, namely there exists $f_b$ such that

$$f(x) - f(b) \geq \langle f_b, x - b \rangle, \forall x.$$  \hfill (114)
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We have that $f(x)$ is convex, $f_b(x)$ is affine, and is a tight subgradient (tight at $b$, affine lower bound on $f(x)$).
A concave $f$ has a supergradient at any in-domain point $b$, namely there exists $f^b$ such that

$$f(x) - f(b) \leq \langle f^b, x - b \rangle, \forall x.$$  

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A concave $f$ has a supergradient at any in-domain point $b$, namely there exists $f^b$ such that

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We have that $f(x)$ is concave, $f^b(x)$ is affine, and is a tight supergradient (tight at $b$, affine upper bound on $f(x)$).
Trivial additive upper/lower bounds

- Any submodular function has trivial additive upper and lower bounds. That is for all $A \subseteq V$,

$$m_f(A) \leq f(A) \leq m^f(A) \quad (116)$$

where

$$m^f(A) = \sum_{a \in A} f(a) \quad (117)$$

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$$m_f(A) = \sum_{a \in A} f(a | V \setminus \{a\}) \quad (118)$$
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- $m^f \in \mathbb{R}^V$ and $m_f \in \mathbb{R}^V$ are both modular (or additive) functions.
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A “semigradient” is customized, and at least at one point is tight.
Submodular Subgradients

For submodular function $f$, the subdifferential (all subgradients tight at $X \subseteq V$) can be defined as:

$$\partial f(X) = \{ x \in \mathbb{R}^V : \forall Y \subseteq V, x(Y) - x(X) \leq f(Y) - f(X) \}$$  (119)
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This partitions $\mathbb{R}^V$:
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- Extreme points are easy to get via Edmonds’s greedy algorithm:
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**Theorem (Fujishige 2005, Theorem 6.11)**

A point $y \in \mathbb{R}^V$ is an extreme point of $\partial f(X)$, iff there exists a maximal chain $\emptyset = S_0 \subset S_1 \subset \cdots \subset S_n$ with $X = S_j$ for some $j$, such that $y(S_i \setminus S_{i-1}) = y(S_i) - y(S_{i-1}) = f(S_i) - f(S_{i-1})$. 

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The Submodular Subgradients (Fujishige 2005)

- For an arbitrary $Y \subseteq V$
- Let $\sigma$ be a permutation of $V$ and define $S^\sigma_i = \{\sigma(1), \sigma(2), \ldots, \sigma(i)\}$ as $\sigma$’s chain where $S^\sigma_k = Y$ where $|Y| = k$.
- We can define a subgradient $h_f^Y$ corresponding to $f$ as:

$$h_{f,Y,\sigma}^f(\sigma(i)) = \begin{cases} f(S^\sigma_1) & \text{if } i = 1 \\ f(S^\sigma_i) - f(S^\sigma_{i-1}) & \text{otherwise} \end{cases}$$

- We get a tight modular lower bound of $f$ as follows:

$$h_{f,Y,\sigma}^f(X) = \sum_{x \in X} h_{f,Y,\sigma}^f(x) \leq f(X), \forall X \subseteq V.$$  

Note, tight at $Y$ means $h_{f,Y,\sigma}^f(Y) = f(Y)$. 

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Convexity and Tight Sub- and Super-gradients?

- Can there be both a tight linear upper bound and tight linear lower bound on a convex (or concave) function, where each bound is tight at the same point?
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- If a continuous function has both a sub- and super-gradient at a point, then the function must be affine.
Convexity and Tight Sub- and Super-Gradients?

- Can there be both a tight linear upper bound and tight linear lower bound on a convex (or concave) function, where each bound is tight at the same point?

If a continuous function has both a sub- and super-gradient at a point, then the function must be affine.

- What about discrete set functions?
The Submodular Supergradients

- Can a submodular function also have a supergradient? We saw that in the continuous case, simultaneous sub/super gradients meant linear.

- (Nemhauser, Wolsey, & Fisher 1978) established the following iff conditions for submodularity (if either hold, \( f \) is submodular):

\[
\begin{align*}
   f(Y) & \leq f(X) - \sum_{j \in X \setminus Y} f(j|X \setminus j) + \sum_{j \in Y \setminus X} f(j|X \cap Y), \\
   f(Y) & \leq f(X) - \sum_{j \in X \setminus Y} f(j|(X \cup Y) \setminus j) + \sum_{j \in Y \setminus X} f(j|X)
\end{align*}
\]

Recall that \( f(A|B) \triangleq f(A \cup B) - f(B) \) is the gain of adding \( A \) in the context of \( B \).
Using submodularity further, these can be relaxed to produce two tight modular upper bounds (Jegelka & Bilmes, 2011, Iyer & Bilmes 2013):

\[ f(Y) \leq m^{f}_{X,1}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j | X \setminus j) + \sum_{j \in Y \setminus X} f(j | \emptyset), \]

\[ f(Y) \leq m^{f}_{X,2}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j | X \setminus j) + \sum_{j \in Y \setminus X} f(j | X). \]

Hence, this yields three tight (at set \( X \)) modular upper bounds \( m^{f}_{X,1}, m^{f}_{X,2} \) for any submodular function \( f \).
Theorem

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

- The semi-gradients above offer a majorization/maximization framework to minimize any function that is naturally expressed as such a difference.
- E.g., to minimize $f = g - h$, starting with a candidate solution $X$, repeatedly choose a modular supergradient for $g$ and modular subgradient for $h$, and perform modular minimization (easy). (see Iyer & Bilmes, 2012).
- Similar strategy used for other combinatorial constraints (e.g., cooperative cut, submodular on edges, see Jegelka & Bilmes 2011)
- Opens the doors to first-order methods for discrete optimization.
Outline: Part 3

6. Discrete Semimodular Semigradients

7. Continuous Extensions
   - Lovász Extension
   - Concave Extension

8. Like Concave or Convex?

9. Optimization

10. Reading
Any function \( f : 2^V \rightarrow \mathbb{R} \) (equivalently \( f : \{0, 1\}^V \rightarrow \mathbb{R} \)) can be extended to a continuous function \( \tilde{f} : [0, 1]^V \rightarrow \mathbb{R} \).
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In fact, any such discrete function defined on the vertices of the $n$-D hypercube $\{0, 1\}^n$ has a variety of both convex and concave extensions tight at the vertices (Crama & Hammer). Example $n = 1$, ...
Continuous Extensions of Discrete Set Functions

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  \]

- Since there are an exponential number of vertices \( \{0, 1\}^n \), important questions regarding such extensions is:
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\[
\tilde{f} : [0, 1] \rightarrow \mathbb{R} \quad \text{Convex Extensions} \\
\tilde{f} : [0, 1] \rightarrow \mathbb{R} \quad \text{Concave Extensions} \\
f : \{0, 1\}^V \rightarrow \mathbb{R} \quad \text{Discrete Function}
\]

- Since there are an exponential number of vertices \( \{0, 1\}^n \), important questions regarding such extensions is:
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\[
\begin{align*}
\text{Concave Extensions} & \quad \tilde{f} : [0, 1] \rightarrow \mathbb{R} \\
\text{Discrete Function} & \quad f : \{0, 1\}^V \rightarrow \mathbb{R} \\
\text{Convex Extensions} & \quad \tilde{f} : [0, 1] \rightarrow \mathbb{R}
\end{align*}
\]

- Since there are an exponential number of vertices \( \{0, 1\}^n \), important questions regarding such extensions is:
  1. When are they computationally feasible to obtain or estimate?
  2. When do they have nice mathematical properties?
  3. When are they useful for something practical?
A continuous extension of $f$

Given a submodular function $f$, a $w \in \mathbb{R}^V$, define chain $V_i = \{v_1, v_2, \ldots, v_i\}$ based on $w$ sorted in decreasing order. Then Edmonds's greedy algorithm gives us:

$$\tilde{f}(w)$$
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$$\tilde{f}(w) = \max(wx : x \in P_f)$$  \hspace{1cm} (120)
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\[
\tilde{f}(w) = \max (wx : x \in P_f) \tag{120}
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\[
= \sum_{i=1}^{m} w(v_i)f(v_i|V_{i-1}) \tag{121}
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\[
= w(v_m)f(V_m) + \sum_{i=1}^{m-1} (w(v_i) - w(v_{i+1}))f(V_i) \tag{122}
\]
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- Definition of the continuous extension, once again:

$$
\tilde{f}(w) = \max(wx : x \in P_f)
$$  \hspace{1cm} (124)
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  \[ \tilde{f}(w) = \max(wx : x \in P_f) \]  
  (124)

- Therefore, if $f$ is a submodular function, we can write

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  \[
  \tilde{f}(w) = w(v_m)f(V_m) + \sum_{i=1}^{m-1} (w(v_i) - w(v_{i+1}))f(V_i) \quad (125)
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$$= \sum_{i=1}^{m} \lambda_i f(V_i)$$  \hspace{1cm} (126)
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  \] (126)

  where $\lambda_m = w(v_m)$ and otherwise $\lambda_i = w(v_i) - w(v_{i+1})$, where the elements are sorted according to $w$ as before.
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  \]  
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  \]  
  (126)

  where $\lambda_m = w(v_m)$ and otherwise $\lambda_i = w(v_i) - w(v_{i+1})$, where the elements are sorted according to $w$ as before.

- From convex analysis, we know $\tilde{f}(w) = \max(wx : x \in P)$ is always convex in $w$ for any set $P \subseteq R^V$, since it is the maximum of a set of linear functions (true even when $f$ is not submodular or $P$ is not a convex set).
An extension of $f$

- But, for any $f : 2^V \rightarrow \mathbb{R}$, even non-submodular $f$, we can define an extension in this way, with

$$\tilde{f}(w) = \sum_{i=1}^{m} \lambda_i f(V_i)$$  \hspace{1cm} (127)

with the $V_i = \{v_1, \ldots, v_i\}$’s defined based on sorted descending order of $w$ as in $w(v_1) \geq w(v_2) \geq \cdots \geq w(v_m)$, and where

$$\lambda_i = \begin{cases} w(v_i) - w(v_{i+1}) & \text{if } i < m \\ w(v_{m}) & \text{if } i = m \end{cases}$$  \hspace{1cm} (128)

so that $w = \sum_{i=1}^{m} \lambda_i 1_{V_i}$
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$$\text{for } i \in \{1, \ldots, m\}, \quad \lambda_i = \begin{cases} w(v_i) - w(v_{i+1}) & \text{if } i < m \\ w(v_m) & \text{if } i = m \end{cases} \quad (128)$$

so that $w = \sum_{i=1}^{m} \lambda_i 1_{V_i}$

- Note that $w = \sum_{i=1}^{m} \lambda_i 1_{V_i}$ is an interpolation of certain vertices of the hypercube, and that $\tilde{f}(w) = \sum_{i=1}^{m} \lambda_i f(V_i)$ is the corresponding interpolation of the values of $f$ at sets corresponding to each hypercube vertex.
Lovász proved the following important theorem.

**Theorem**

A function $f : 2^V \rightarrow \mathbb{R}$ is submodular iff its continuous extension defined above as $\tilde{f}(w) = \sum_{i=1}^{m} \lambda_i f(V_i)$ with $w = \sum_{i=1}^{m} \lambda_i 1_{V_i}$ is a convex function in $\mathbb{R}^V$. 
Minimizing $\tilde{f}$ vs. minimizing $f$

**Theorem**

Let $f$ be submodular and $\tilde{f}$ be its Lovász extension. Then

$$\min \{ f(A) | A \subseteq V \} = \min_{w \in \{0,1\}^V} \tilde{f}(w) = \min_{w \in [0,1]^V} \tilde{f}(w).$$

- Let $w^* \in \text{argmin} \left\{ \tilde{f}(w) | w \in [0,1]^V \right\}$ and let $A^* \in \text{argmin} \{ f(A) | A \subseteq V \}.$
Minimizing \( \tilde{f} \) vs. minimizing \( f \)

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\]

- Let \( w^* \in \arg\min \left\{ \tilde{f}(w) | w \in [0, 1]^V \right\} \) and let \( A^* \in \arg\min \{ f(A) | A \subseteq V \} \).
- Define chain \( \{ V_i^* \} \) based on descending sort of \( w^* \). Then by greedy evaluation of L.E. we have

\[
\tilde{f}(w^*) = \sum_i \lambda_i^* f(V_i^*) = f(A^*) = \min \{ f(A) | A \subseteq V \} \quad (129)
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- Then we can show that, for each $i$ s.t. $\lambda_i > 0$,

\[
f(V_i^*) = f(A^*) \quad (130)
\]

So such $\{ V_i^* \}$ are also minimizers.
Let $f$ be a submodular function with $\tilde{f}$ its Lovász extension. Then the following two problems are duals:

\[
\begin{align*}
\text{minimize} & \quad \tilde{f}(w) + \frac{1}{2} \|w\|_2^2 & \quad (131) \\
\text{subject to} & \quad x \in B_f
\end{align*}
\]

where $B_f = P_f \cap \{x \in \mathbb{R}^V : x(V) = f(V)\}$ is the base polytope of submodular function $f$, and $\|x\|_2^2 = \sum_{e \in V} x(e)^2$ is the squared 2-norm.


Unknown worst-case running time, although in practice it usually performs quite well.
“fast” submodular function minimization, as mentioned above.

Structured sparse-encouraging convex norms (Bach-2011), semi-supervised learning, image denoising (as mentioned yesterday).

Non-linear measures (Denneberg), non-linear aggregation functions (Grabisch et. al), and fuzzy set theory.

Note, many of the critical properties of the Lovász extension were given by Jack Edmonds in the 1960s. Choquet proposed an identical integral in 1954, and G. Vitali proposed a similar integral in 1925!

G.Vitali, Sulla definizione di integrale delle funzioni di una variabile, Annali di Matematica Serie IV, Tomo I,(1925), 111-121
Submodular Concave Extension

- Finding a concave extension (the concave envelope, smallest concave upper bound) of a submodular function is NP-hard (Vondrak).
Submodular Concave Extension

- Finding a concave extension (the concave envelope, smallest concave upper bound) of a submodular function is NP-hard (Vondrak).
- However, a useful surrogate is the multi-linear extension.
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However, a useful surrogate is the multi-linear extension.

**Definition**

For a set function $f : 2^V \to \mathbb{R}$, define its multilinear extension $F : [0, 1]^V \to \mathbb{R}$ by

$$F(x) = \sum_{S \subseteq V} f(S) \prod_{i \in S} x_i \prod_{j \in V \setminus S} (1 - x_j) \quad (133)$$

Not concave, but still provides useful approximations for many constrained maximization algorithms (e.g., multiple matroid and/or knapsack constraints) via the continuous greedy algorithm followed by rounding. Often has to be approximated.
Submodular Concave Extension

- Finding a concave extension (the concave envelope, smallest concave upper bound) of a submodular function is NP-hard (Vondrak).
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Outline: Part 3

6 Discrete Semimodular Semigradients

7 Continuous Extensions
   • Lovász Extension
   • Concave Extension

8 Like Concave or Convex?

9 Optimization

10 Reading
Are submodular functions more like convex or more like concave functions?
Submodular is like Concave

- **Convex 1:** Like convex functions, submodular functions can be minimized efficiently (polynomial time).
Submodular is like Concave

**Convex 1:** Like convex functions, submodular functions can be minimized efficiently (polynomial time).

**Convex 2:** The Lovász extension of a discrete set function is convex iff the set function is submodular.
Submodular is like Concave

- **Convex 3**: Frank’s discrete separation theorem: Let $f : 2^V \rightarrow \mathbb{R}$ be a submodular function and $g : 2^V \rightarrow \mathbb{R}$ be a supermodular function such that for all $A \subseteq V$,

$$g(A) \leq f(A)$$  \hspace{1cm} (134)

Then there exists modular function $x \in \mathbb{R}^V$ such that for all $A \subseteq V$:

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Convex 3: Frank's discrete separation theorem: Let \( f : 2^V \to \mathbb{R} \) be a submodular function and \( g : 2^V \to \mathbb{R} \) be a supermodular function such that for all \( A \subseteq V \),

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Compare to convex/concave case.
Submodular is like Concave

- **Convex 4:** Set of minimizers of a convex function is a convex set. Set of minimizers of a submodular function is a lattice. I.e., if $A, B \in \arg\min_{A \subseteq V} f(A)$ then $A \cup B \in \arg\min_{A \subseteq V} f(A)$ and $A \cap B \in \arg\min_{A \subseteq V} f(A)$.
Submodular is like Concave

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- **Convex 5:** Submodular functions have subdifferentials and subgradients tight at any point.
Submodularity and Concave

**Concave 1:** A function is submodular if for all $X \subseteq V$ and $j, k \in V$

$$f(X + j) + f(X + k) \geq f(X + j + k) + f(X) \quad (136)$$
Submodularity and Concave

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- With the gain defined as $\nabla_j f(X) = f(X + j) - f(X)$, seen as a form of discrete gradient, this trivially becomes a second-order condition, akin to concave functions: A function is submodular if for all $X \subseteq V$ and $j, k \in V$, we have:

  $$\nabla_j \nabla_k f(X) \leq 0 \quad (137)$$
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- **Concave 2:** Recall, Theorem 16: composition $h = f \circ g : 2^V \rightarrow \mathbb{R}$ (i.e., $h(S) = g(f(S)))$ is nondecreasing submodular, if $g$ is non-decreasing concave and $f$ is nondecreasing submodular.
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- **Concave 3:** Submodular functions have superdifferentials and supergradients tight at any point.

- **Concave 4:** Concave maximization solved via local gradient ascent. Submodular maximization is (approximately) solvable via greedy (coordinate-ascent-like) algorithms.
Submodularity and neither Concave nor Convex

- **Neither 1:** Submodular functions have simultaneous sub- and super-gradients, tight at any point.
Submodularity and neither Concave nor Convex

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- **Neither 4:** Convex functions can’t, in general, be efficiently or approximately maximized, while submodular functions can be.
- **Neither 5:** Convex functions have local optimality conditions of the form $\nabla_x f(x) = 0$. Analogous submodular function semi-gradient condition $m(X) = 0$ offers no such guarantee (for neither maximization nor minimization) — although there are other forms of local guarantees.
Outline: Part 3

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## Submodular Optimization Results Summary

<table>
<thead>
<tr>
<th></th>
<th>Maximization</th>
<th>Minimization</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Unconstrained</strong></td>
<td>In general, NP-hard, greedy gives $1 - 1/e$ approximation for polymatroid</td>
<td>Polynomial time but inefficient $O(n^5 \gamma + n^6)$. Special cases (graph</td>
</tr>
<tr>
<td></td>
<td>cardinality constrained, improved with curvature.</td>
<td>representable, sums of concave over modular) much faster, min-norm empirically</td>
</tr>
<tr>
<td></td>
<td></td>
<td>often works well.</td>
</tr>
<tr>
<td><strong>Constrained</strong></td>
<td>NP-hard. For some constraints (matroid, knapsack), approximable with greedy</td>
<td>In general, NP-hard even to approximate, but for many submodular functions</td>
</tr>
<tr>
<td></td>
<td>(or approximate concave relaxations). Curvature dependence for combinatorial</td>
<td>still approximable. Curvature dependence for combinatorial and submodular</td>
</tr>
<tr>
<td></td>
<td>and submodular constraints.</td>
<td>constraints.</td>
</tr>
</tbody>
</table>
## General Submodular Function Minimization

- **Semigradients**
  - Extensions
  - Concave or Convex?
  - Optimization
  - Refs

### SFM Summary (modified from S. Iwata’s slides)

**General Submodular Function Minimization**

- Wolfe (1976)/von Hohenbalken (1975)
- Ellipsoid Method
- Edmonds (1965/1970)
- Bixby, Cunningham, Topkis (1984)
- Cunningham (1985)
- Iwata, Fleischer, Fujishige (2000)
- Iwata, Orlin (2009)
- Wolfe (1976)/von Hohenbalken (1975)
- Schrijver (2000)
- Iwata (2003)
- Orlin (2007)
- Bach (2012/13)
- gen. convex methods

### Algorithms and Time Complexities

- \(O(n^5 \gamma \log M)\)
- \(O(n^7 \gamma \log n)\)
- \(O(n^7 \gamma + n^8)\)
- \(O((n^4 \gamma + n^5) \log M)\)
- \(O(n^5 \gamma + n^6)\)

**References**

- Ellipsoid Method
- Cunningham (1985)
- Bixby, Cunningham, Topkis (1984)
- Edmonds (1965/1970)
- Iwata (2002)
- Fully Combinatorial
- Iwata, Fleischer, Fujishige (2000)
- Iwata (2003)
- Orlin (2007)
- Iwata, Orlin (2009)
Theoretical Results: Constrained Submodular Min

\[
\text{minimize } f(S) : S \in \mathcal{S}
\]  

- Constraint set $\mathcal{S}$ might either be cuts, paths, matchings, cardinality constraints, etc.
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- Constraint set \( \mathcal{S} \) might either be cuts, paths, matchings, cardinality constraints, etc.
- Minimization algorithms should have multiplicative approximation guarantee, i.e., \( f(S) \leq \alpha f(S^*) \) where \( S^* \) is optimal solution, \( \alpha \geq 1 \).
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- Minimization algorithms should have multiplicative approximation guarantee, i.e., \( f(S) \leq \alpha f(S^*) \) where \( S^* \) is optimal solution, \( \alpha \geq 1 \).
- In general, how good are the algorithms? Depends on the constraint:

<table>
<thead>
<tr>
<th>Constraint:</th>
<th>MMin</th>
<th>EA</th>
<th>Lower bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>trees/matchings</td>
<td>( n )</td>
<td>( \sqrt{m} )</td>
<td>( n )</td>
</tr>
<tr>
<td>cuts</td>
<td>( m )</td>
<td>( \sqrt{m} )</td>
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</table>

Goel et al (09), Goemans et al (2009), Jegelka-Bilmes (11) ...
Theoretical Results: Constrained Submodular Min

\[
\text{minimize } f(S) : S \in \mathcal{S}
\]  

- Constraint set \( \mathcal{S} \) might either be cuts, paths, matchings, cardinality constraints, etc.
- Minimization algorithms should have multiplicative approximation guarantee, i.e., \( f(S) \leq \alpha f(S^*) \) where \( S^* \) is optimal solution, \( \alpha \geq 1 \).
- In general, how good are the algorithms? Depends on the constraint:

<table>
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</tr>
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<tbody>
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<td>trees/matchings</td>
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<td>( n )</td>
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- Worst case polynomial upper/lower bounds.
Theoretical Results: Constrained Submodular Min

\[
\text{minimize } f(S) : S \in \mathcal{S} \quad (138)
\]

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- Worst case polynomial upper/lower bounds.
- Other forms of constraints are “easy” (e.g., certain lattices, odd/even sets (see McCormick’s SFM tutorial paper).
Submodular Maximization: Unconstrained

- In general, NP-hard. Bound take form \( f(S) \geq \alpha f(S^*) \), \( \alpha \leq 1 \).
- The greedy algorithm for monotone submodular maximization:

\[\text{Algorithm 2: The Greedy Algorithm}\]

Set \( S_0 \leftarrow \emptyset \);

\[
\text{for } i \leftarrow 0 \ldots |V| - 1 \text{ do}
\]

Choose \( v_i \) as follows: \( v_i = \left\{ \arg\max_{v \in V \setminus S_i} f(S_i \cup \{v\}) \right\} \);

Set \( S_{i+1} \leftarrow S_i \cup \{v_i\} \);

- has a strong guarantee:

\[\text{Theorem}\]

Given a polymatroid function \( f \), the above greedy algorithm returns sets \( S_i \) such that for each \( i \) we have \( f(S_i) \geq (1 - 1/e) \max_{|S| \leq i} f(S) \).
### Submodular Max, Constrained

#### Monotone Maximization

<table>
<thead>
<tr>
<th>Constraint</th>
<th>Approximation</th>
<th>Hardness</th>
<th>Technique</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>S</td>
<td>\leq k$ matroid</td>
<td>$1 - 1/e$</td>
</tr>
<tr>
<td>$O(1)$ knapsacks</td>
<td>$1 - 1/e$</td>
<td>$1 - 1/e$</td>
<td>multilinear ext.</td>
</tr>
<tr>
<td>$k$ matroids</td>
<td>$k + \epsilon$</td>
<td>$k/\log k$</td>
<td>local search</td>
</tr>
<tr>
<td>$k$ matroids and $O(1)$ knapsacks</td>
<td>$O(k)$</td>
<td>$k/\log k$</td>
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#### Nonmonotone Maximization

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<th>Technique</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unconstrained</td>
<td>$1/2$</td>
<td>$1/2$</td>
<td>combinatorial</td>
</tr>
<tr>
<td>matroid</td>
<td>$1/e$</td>
<td>$0.48$</td>
<td>multilinear ext.</td>
</tr>
<tr>
<td>$O(1)$ knapsacks</td>
<td>$1/e$</td>
<td>$0.49$</td>
<td>multilinear ext.</td>
</tr>
<tr>
<td>$k$ matroids</td>
<td>$k + O(1)$</td>
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, compiled by J. Vondrak
Constrained Submodular Minimization

- Bounds can be improved if we use a function’s “curvature”
**Constrained Submodular Minimization**

- Bounds can be improved if we use a function’s “curvature”
- **Curvature of a monotone submodular function:**

  \[
  \kappa_f(X) \triangleq 1 - \min_j \frac{f(j|X\setminus j)}{f(j)}. \tag{139}
  \]

  The solutions \( \hat{X} \) then have guarantees in terms of curvature \( \kappa_f \):

  \[
  0 \leq \kappa_f \triangleq \kappa_f(V) \leq 1 \tag{140}
  \]
Constrained Submodular Minimization

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- Curvature dependent constrained maximization bounds:

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<th>Lower bound</th>
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<tr>
<td>Cardinality</td>
<td>Greedy</td>
<td>( \frac{1}{\kappa_f} (1 - e^{-\kappa_f}) )</td>
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</tr>
<tr>
<td>Matroid</td>
<td>Greedy</td>
<td>( \frac{1}{1 + \kappa_f} )</td>
<td>( \frac{1}{\kappa_f} (1 - e^{-\kappa_f}) )</td>
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<td>Knapsack</td>
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Bounds can be improved if we use a function’s “curvature”

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Curvature dependent constrained maximization bounds:

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Improve curvature independent bounds when \( \kappa_f < 1 \).
Minimization bounds take the form:

\[
f(\hat{X}) \leq \frac{|X^*|}{1 + (|X^*| - 1)(1 - \kappa_f(X^*))} f(X^*) \leq \frac{1}{1 - \kappa_f(X^*)} f(X^*)
\]
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Lower curvature \( \Rightarrow \) Better guarantees!
Minimization bounds take the form:

\[ f(\hat{X}) \leq \frac{|X^*|}{1 + (|X^*| - 1)(1 - \kappa_f(X^*))} f(X^*) \leq \frac{1}{1 - \kappa_f(X^*)} f(X^*) \]

- Lower curvature \( \Rightarrow \) Better guarantees!

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<th>Semigradient</th>
<th>Curvature-Ind.</th>
<th>Lower bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Card. LB</td>
<td>( \frac{k}{1+(k-1)(1-\kappa_f)} )</td>
<td>( \theta(n^{1/2}) )</td>
<td>( \tilde{\Omega}(\frac{\sqrt{n}}{1+(\sqrt{n}-1)(1-\kappa_f)}) )</td>
</tr>
<tr>
<td>Spanning Tree</td>
<td>( \frac{n}{1+(n-1)(1-\kappa_f)} )</td>
<td>( \theta(n) )</td>
<td>( \tilde{\Omega}(\frac{n}{1+(n-1)(1-\kappa_f)}) )</td>
</tr>
<tr>
<td>Matchings</td>
<td>( \frac{n}{2+(n-2)(1-\kappa_f)} )</td>
<td>( \theta(n) )</td>
<td>( \tilde{\Omega}(\frac{n^{n^2/3}}{1+(n^{2/3}-1)(1-\kappa_f)}) )</td>
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<tr>
<td>s-t path</td>
<td>( \frac{n}{1+(n-1)(1-\kappa_f)} )</td>
<td>( \theta(n^{2/3}) )</td>
<td>( \tilde{\Omega}(\frac{n^{2/3}}{1+(n^{2/3}-1)(1-\kappa_f)}) )</td>
</tr>
<tr>
<td>s-t cut</td>
<td>( \frac{m}{1+(m-1)(1-\kappa_f)} )</td>
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Outline: Part 3

6 Discrete Semimodular Semigradients

7 Continuous Extensions
   - Lovász Extension
   - Concave Extension

8 Like Concave or Convex?

9 Optimization

10 Reading
Classic References

Classic Books

- Fujishige, “Submodular Functions and Optimization”, 2005
- Narayanan, “Submodular Functions and Electrical Networks”, 1997
- Schrijver, “Combinatorial Optimization”, 2003
Recent online material with an ML slant

- My class, most proofs for above are given. http://j.ee.washington.edu/~bilmes/classes/ee596b_spring_2014/. All lectures being placed on youtube!
- Francis Bach’s updated 2013 text. http://hal.archives-ouvertes.fr/docs/00/87/06/09/PDF/submodular_fot_revised_hal.pdf
- Tom McCormick’s overview paper on submodular minimization http://people.commerce.ubc.ca/faculty/mccormick/sfmchap8a.pdf
- Georgia Tech’s 2012 workshop on submodularity: http://www.arc.gatech.edu/events/arc-submodularity-workshop
Learn to:
- Greedily choose your data sets with a 1 − 1/e guarantee!
- Minimize your functions in polynomial time!
- Draw beautiful polyhedra!
- Solve exponentially large linear programs in polynomial time!

Paul E. Matroid
Moniton Submodularanian
Wonmy Neuswon Overee

\[ f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \]