## Submodular Functions, Optimization, and Applications to Machine Learning

- Spring Quarter, Lecture 1 -
http://j.ee.washington.edu/~bilmes/classes/ee596b_spring_2014/


## Prof. Jeff Bilmes

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Department of Electrical Engineering http://melodi.ee.washington.edu/~bilmes

Mar 31st, 2014


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

$=r\left(A_{)}\right)+2\left((C)+r(B)=r(A)+r(C)+r\left(B_{n}\right) \quad=r(A \cap B)\right.$



## Announcements

- Welcome to the class!
- Submodular Functions, Optimization, and Applications to Machine Learning, EE596B.
- Paccar 492.
- Weekly Office Hours: Wednesdays, 3:30-4:30, 10 minutes after class ends on Wednesdays.
- Class web page is at our web page (http://j.ee.washington. edu/~bilmes/classes/ee596b_spring_2014/)


## Directions to Paccar Hall from the EECS building

- Suggested routes

King Ln
$0.4 \mathrm{mi}, 10 \mathrm{mins}$

Spokane Ln
Pierce Ln $0.5 \mathrm{mi}, 10 \mathrm{mins}$

## Walking directions to Unknown road

## Benton Ln

1. Head northwest on Benton Ln/Grant Ln

- http://goo.gl/ maps/5P3dQ


This course will serve as an introduction to submodular functions including methods for their optimization, and how they have been (and can be) applied in many application domains.

## Rough Outline

- Introduction to submodular functions, including definitions, real-world and contrived examples of submodular functions, properties, operations that preserve submodularity, submodular variants and special submodular functions, and computational properties.
- Background on submodular functions, including a brief overview of the theory of matroids and lattices.
- Polyhedral properties of submodular functions
- The Lovász extension of submodular functions. The Choquet integral.
- Submodular maximization algorithms under simple constraints, submodular cover problems, greedy algorithms, approximation guarantees


## Rough Outline (cont. II)

- Submodular minimization algorithms, a history of submodular minimization, including both numerical and combinatorial algorithms, computational properties of these algorithms, and descriptions of both known results and currently open problems in this area.
- Submodular flow problems, the principle partition of a submodular function and its variants.
- Constrained optimization problems with submodular functions, including maximization and minimization problems with various constraints. An overview of recent problems addressed in the community.
- Applications of submodularity in computer vision, constraint satisfaction, game theory, information theory, norms, natural language processing, graphical models, and machine learning


## Classic References

- Jack Edmonds's paper "Submodular Functions, Matroids, and Certain Polyhedra" from 1970.
- Nemhauser, Wolsey, Fisher, "A Analysis of Approximations for Maximizing Submodular Set Functions-l", 1978
- Lovász's paper, "Submodular functions and convexity", from 1983.


## Useful Books

- Fujishige, "Submodular Functions and Optimization", 2005
- Narayanan, "Submodular Functions and Electrical Networks", 1997
- Welsh, "Matroid Theory", 1975.
- Oxley, "Matroid Theory", 1992 (and 2011).
- Lawler, "Combinatorial Optimization: Networks and Matroids", 1976.
- Schrijver, "Combinatorial Optimization", 2003
- Gruenbaum, "Convex Polytopes, 2nd Ed", 2003.
- Additional readings that will be announced here.


## Recent online material (some with an ML slant)

- Previous version of this class http: //j.ee.washington.edu/~bilmes/classes/ee596a_fall_2012/.
- Stefanie Jegelka \& Andreas Krause's 2013 ICML tutorial http://techtalks.tv/talks/
submodularity-in-machine-learning-new-directions-part-i/ 58125/
- NIPS, 2013 tutorial on submodularity http://melodi.ee.washington.edu/~bilmes/pgs/
b2hd-bilmes2013-nips-tutorial.html and http://youtu.be/c4rBof38nKQ
- Andreas Krause's web page http://submodularity.org.
- 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


## Facts about the class

- Prerequisites: ideally knowledge in probability, statistics, convex optimization, and combinatorial optimization these will be reviewed as necessary. The course is open to students in all UW departments. Any questions, please contact me.
- Text: We will be drawing from the book by Satoru Fujishige entitled "Submodular Functions and Optimization" 2nd Edition, 2005, but we will also be reading research papers that will be posted here on this web page, especially for some of the application areas.
- Grades and Assignments: Grades will be based on a combination of a final project ( $45 \%$ ), homeworks ( $55 \%$ ). There will be between 3-6 homeworks during the quarter.
- Final project: The final project will consist of a 4-page paper (conference style) and a final project presentation. The project must involve using/dealing mathematically with submodularity in some way or another.


## Facts about the class

- Homework/n must be submitted electronically using our assignment dropbox (https://canvas.uw.edu/courses/895956/assignments). PDF submissions only please. Photos of neatly hand written solutions, combined into one PDF, are fine
- Lecture slides - are being prepared as we speak. I will try to have them up on the web page the night before each class. I will not only draw from the book but other sources which will be listed at the end of each set of slides.
- Slides from previous version of this class are at http://j.ee. washington.edu/~bilmes/classes/ee596a_fall_2012/.


## Other logistics

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\begin{equation*}
f(A)=f(V \backslash A) \tag{1.1}
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By the way $V \backslash A \equiv\{v \in V: v \notin A\}$ is set subtraction, sometimes written as $V-A$.

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- Exception to these rules is in the review sections, where theorems, equation, etc. (even if repeated) will have new reference numbers.


## Cumulative Outstanding Reading

- Read chapter 1 from Fujishige book.


## Announcements, Assignments, and Reminders

- Please do use our discussion board (https:
//canvas.uw.edu/courses/895956/discussion_topics) for all questions, comments, so that all will benefit from them being answered.


## Class Road Map - IT-I

- L1 (3/31): Motivation, Applications, \&
- L11: Basic Definitions
- L12:
- L2:
- L13:
- L3:
- L14:
- L4:
- L15:
- L5:
- L16:
- L17:
- L7:
- L8:
- L9:
- L18:
- L19:
- L20:
- L10:

Finals Week: June 9th-13th, 2014.

## Review

- This is where each day we will be reviewing previous lecture material.


## Submodular Definitions

## Definition 1.3.1 (submodular concave)

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

$$
\begin{equation*}
f(A)+f(B) \geq f(A \cup B)+f(A \cap B) \tag{1.2}
\end{equation*}
$$

An alternate and (as we see in lecture 3) equivalent definition is:

## Definition 1.3.2 (diminishing returns)

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

$$
\begin{equation*}
f(A \cup\{v\})-f(A) \geq f(B \cup\{v\})-f(B) \tag{1.3}
\end{equation*}
$$

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 $B$.

## Sets and set functions

We are given a finite "ground" set of objects:


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

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Subset $A \subseteq V$ of objects:



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## Sets and set functions

Subset $B \subseteq V$ of objects:


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

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- We may be interested only in a subset of the set of possible subsets, namely $\mathcal{S} \subseteq 2^{V}$. E.g., $\mathcal{S}=\{S \subseteq V:|S| \leq k\}$. The set of sets $\mathcal{S}$ might or might not itself be a function of $f$ (e.g.,
$\mathcal{S}=\{S \subseteq V: f(S) \leq \alpha\}$.


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- A general discrete optimization problem we consider here is:

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\begin{array}{ll}
\underset{S \subseteq 2^{V}}{\operatorname{maximize}} & f(S) \\
\text { subject to } & S \in \mathcal{S} \tag{1.4}
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- Alternatively, we may minimize rather than maximize.


## Set functions are pseudo-Boolean functions

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- The characteristic vector of a set is given by $\mathbf{1}_{A} \in\{0,1\}^{V}$ where for all $v \in V$, we have:

$$
\mathbf{1}_{A}(v)=\left\{\begin{array}{ll}
1 & \text { if } v \in A  \tag{1.5}\\
0 & \text { else }
\end{array}\right\}
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$$
X(x) \subseteq V
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- It is sometimes useful to go back and forth between $X$ and $x(X) \triangleq \mathbf{1}_{X}$.
- $f(x):\{0,1\}^{V} \rightarrow \mathbb{R}$ is a pseudo-Boolean function, and submodular functions are a special case.


## Discrete Optimization Problems

- Ignoring how complex and general this problem can be for the moment, lets consider some possible applications.
- In the rest of this section of slides, we will see many seemingly different applications that, ultimately, you will all hopefully see are strongly related to submodularity.
- We'll see, submodularity is as common and natural for discrete problems as is convexity for continuous problems.


## Example Discrete Optimization Problems

- Combinatorial Problems: e.g., set cover, max $k$ coverage, vertex cover, edge cover, graph cut problems.
- Operations Research: facility location (uncapacited)
- Sensor placement
- Information: Information gain and feature selection, information theory
- Mathematics: e.g., monge matrices
- Networks: Social networks, influence, viral marketing, information cascades, diffusion networks
- Graphical models: tree distributions, factors, and image segmentation
- Diversity and its models
- NLP: Natural language processing: document summarization, web search, information retrieval
- ML: Machine Learning: active/semi-supervised learning
- Economics: markets, economies of scale


## Set Cover and Maximum Coverage

- We are given a finite set $V$ of $n$ elements and a set of subsets $\mathcal{V}=\left\{V_{1}, V_{2}, \ldots, V_{m}\right\}$ of $m$ subsets of $V$, so that $V_{i} \subseteq V$ and $\bigcup_{i} V_{i}=V$.


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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 $\left\{a_{1}, a_{2}, \ldots, a_{k}\right\}$ with $a_{i} \in[m]$ such that $\left|\bigcup_{i=1}^{k} V_{a_{i}}\right|$ is maximized.


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- Both Set cover and maximum coverage are well known to be NP-hard, but have a fast greedy approximation algorithm.


## Other Covers

## Definition 1.5.1 (vertex cover)

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

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


## Definition 1.5.2 (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 $|V|(F)=|V|$.


## Graph Cut Problems

- Minimum cut: Given a graph $G=(V, E)$, find a set of vertices $S \subseteq V$ that minimize the cut (set of edges) between $S$ and $V \backslash S$.



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


## Facility/Plant Location (uncapacitated)

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



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## Facility/Plant Location (uncapacitated)

- Let $F=\{1, \ldots, f\}$ be a set of possible factory/plant locations for facilities to be built.
- $S=\{1, \ldots, s\}$ is a set of sites needing to be serviced (e.g., cities, clients).
- Let $c_{i j}$ be the "benefit" (e.g., $1 / c_{i j}$ is the cost) of servicing site $i$ with facility location $j$.
- Let $m_{j}$ be the benefit (e.g., either $1 / m_{j}$ is the cost or $-m_{j}$ is the cost) to build a plant at location $j$.
- Each site needs to be serviced by only one plant but no less than one.
- Define $f(A)$ as the "delivery benefit" plus "construction benefit" when the locations $A \subset F$ are to be constructed.
- We can def ne $f(A)=\sum_{j \in A} m_{j}+\sum_{i \in F} \max _{j \in A} c_{i j}$.
- Goal is to find aset 4 that maximizes $f(A)$ (the henefit) placing a bound on the number of plants $A$ (e.g., $|A| \leq k$ ).


## Sensor Placement

- 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).



## Sensor Placement within Buildings

- Example sensor placement using mixed range sensors (located at red dots).



## Information Gain and Feature Selection

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- Given subset of features $A \subseteq V$, prediction based on $p\left(y \mid x_{A}\right)$.
- Goal: choose the smallest set of features that retains accuracy.


## Information Gain and Feature Selection

- Task: pattern recognition based on (at most) features $X_{V}$ to predict random variable $Y$. True model is $p\left(Y, X_{V}\right)$, where $V$ is a finite set of feature indices.
- Given subset of features $A \subseteq V$, prediction based on $p\left(y \mid x_{A}\right)$.
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- Information gain is defined as:

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\begin{equation*}
f(A)=I\left(Y ; X_{A}\right)=H(Y)-H\left(Y \mid X_{A}\right)=H\left(X_{A}\right)-H\left(X_{A} \mid Y\right) \tag{1.6}
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- Goal is to find a subset $A$ of size $k$ that has high 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 the room.


## Information Theory: Block Coding

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- l.e., how do we form $S \subseteq V$ such that $I\left(X_{S} ; X_{V \backslash S}\right)$ is as small as possible, where $I\left(X_{A} ; X_{B}\right)$ is the mutual information between random variables $X_{A}$ and $X_{B}$, i.e.,

$$
\begin{equation*}
I\left(X_{A} ; X_{B}\right)=H\left(X_{A}\right)+H\left(X_{B}\right)-H\left(X_{A}, X_{B}\right) \tag{1.7}
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and $H\left(X_{A}\right)=-\sum_{x_{A}} p\left(x_{A}\right) \log p\left(x_{A}\right)$ is the joint entropy of the set $X_{A}$ of random variables.

## Information Theory: Networks Communication



- A network of senders/receivers
- Each sender $X_{i}$ is trying to communicate simultaneously with each receiver $Y_{i}$ (i.e., for all $i, X_{i}$ is sending to $\left\{Y_{i}\right\}_{i}$
- The $X_{i}$ are not necessarily independent.
- Communication rates from $i$ to $j$ are $R^{(i \rightarrow j)}$ to send message $W^{(i \rightarrow j)} \in\left\{1,2, \ldots, 2^{n R^{(i \rightarrow j)}}\right\}$.
- Goal: necessary and sufficient conditions for achievability as we've done for other channels.
- l.e., can we find functions $f$ such that any rates must satisfy

$$
\begin{equation*}
\forall S \subseteq V, \quad \sum \quad R^{(i \rightarrow j)} \leq f(S) \tag{1.8}
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$$

## Monge Matrices

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

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c_{i j}+c_{r s} \leq c_{i s}+c_{r j} \tag{1.9}
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- Consider four elements of the matrix:

- Useful for speeding up certain dynamic programming problems.


## Monge Matrices

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



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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., $f_{v}(A)=f_{v}(A \cap \Gamma(v))$.


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- 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 $v \in V \backslash S$ if $f_{v}(S) \geq U[0,1]$ (where $U[0,1]$ is a uniform random number between 0 and 1).


## The value of a friend

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- Let $f(S)$ be the value of the set of friends $S$. Is submodular or supermodular a good model?


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## Diffusion Networks

- Information propagation: when blogs or news stories break, and creates an information cascade over multiple other blogs/newspapers/magazines.
- Viral marketing: What is the pattern of trendsetters that cause an individual to purchase a product?
- Epidemiology: who got sick from whom, and what is the network of such links?
- How can we infer the connectivity of a network (of memes, purchase decisions, virusus, etc.) based only on diffusion traces (the time that each node is "infected")? How to find the most likely tree?


## Graphical Models: Tree Distributions

- Family of probability distributions $p:\{0,1\}^{V} \rightarrow[0,1]$ :

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\begin{equation*}
p(x)=\frac{1}{Z} \exp (f(x)) \tag{1.10}
\end{equation*}
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- Given a graphical model $G=(V, E)$ and a family of probability distributions $p \in \mathcal{F}(G, \mathcal{M})$ that factor w.r.t. that distribution. I.e., $f(x)=\sum_{c \in \mathcal{C}} f_{c}\left(x_{c}\right)$ where $\mathcal{C}$ are a set of cliques.


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- 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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& T=(V, F) \text { is a tree } \tag{1.11}
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- Discrete problem: Choose the right subset of edges from $E$ that make up a tree (i.e., find a spanning tree of $G$ of best quality).


## Graphical Models: Image Segmentation

- an image needing to be segmented.



## Graphical Models: Image Segmentation

- labeled data in the form of some pixels being marked foreground (red). and others being marked background (blue).



## Graphical Models: Image Segmentation

- the foreground is removed from the background.



## Markov random fields and image segmentation

Markov random field

$$
\begin{equation*}
\log p(x) \propto \sum_{v \in V(G)} e_{v}\left(x_{v}\right)+\sum_{(i, j) \in E(G)} e_{i j}\left(x_{i}, x_{j}\right) \tag{1.12}
\end{equation*}
$$

When $G$ is a 2D grid graph, we have


## Markov random fields and image segmentation

- We can create auxiliary graph that involves two new nodes $s$ and $t$ and connect each of $s$ and $t$ to all of the original nodes.
- I.e., $G_{a}=\left(V \cup\{s, t\}, E+\cup_{v \in V}((s, v) \cup(v, t))\right)$.


## Markov random fields and image segmentation

Original Graph: $\log p(x) \propto \sum_{v \in V(G)} e_{v}\left(x_{v}\right)+\sum_{(i, j) \in E(G)} e_{i j}\left(x_{i}, x_{j}\right)$


## Markov random fields and image segmentation

Augmented graph-cut graph.
The edge weights of graph are derived from $\left\{e_{v}\right\}_{v \in V}$ and $\left\{e_{i j}\right\}_{(i, j) \in E(G)}$


## Markov random fields and image segmentation

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 $p(\bar{x})$


## Other applications in or related to computer vision

- Image denoising, total variation, structured convex norms.

$$
\begin{equation*}
g(w)=\sum_{i=2}^{N}\left|w_{i}-w_{i-1}\right| \tag{1.13}
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$$



- Multi-label graph cuts
- graphical model inference, computing the Viterbi (or the MPE or the MAP) assignment of a set of random variables.
- Clustering of data sets.


## Diversity Functions

- Diverse web search. Given search term (e.g., "jaguar") but no other information, one probably does not want only articles about cars.


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- How do we choose the smallest set $S$ that maintains a given quality of diversity?
- Goal of diversity: ensure proper representation in chosen set that, say otherwise in a random sample, could lead to poor representation of normally underrepresented groups.


## Extractive Document Summarization

- The figure below represents the sentences of a document



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- We extract sentences (green) as a summary of the full document



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- diminishing returns $\leftrightarrow$ submodularity


## Web search and information retrieval

- A web search is a form of summarization based on query.
- Goal of a web search engine is to produce a ranked list of web pages that, conditioned on the text query entered, summarizes the most important links on the web.
- Information retrieval (the science of automatically acquiring information), book and music recommendation systems -
- Overall goal: user should quickly find information that is informative, concise, accurate, relevant (to the user's needs), and comprehensive.


## Active Learning and Semi-Supervised Learning

- Given training data $\mathcal{D}_{V}=\left\{\left(x_{i}, y_{i}\right)\right\}_{i \in V}$ of $(x, y)$ pairs where $x$ is a query (data item) and $y$ is an answer (label), goal is to learn a good mapping $y=h(x)$.


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- Semi-supervised (transductive) learning: Once we have $\left\{y_{i}\right\}_{i \in S}$, infer the remaining labels $\left\{y_{i}\right\}_{i \in V \backslash S}$.


## Markets: Supply Side Economies of scale

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- If you already make a good, making a similar good is easier than if you start from scratch (e.g., Apple making both iPod and iPhone).
- An argument in favor of free trade is that it opens up larger markets to firms in (especially otherwise small markets), thereby enabling better economies of scale, and hence greater efficiency (lower costs and resources per unit of good produced).


## Supply Side Economies of scale: 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 $S$.


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- 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.
$f($ green, blue, yellow $)-f$ (blue, yellow) $<=f($ green, blue) $-f$ (blue)


## Demand side Economies of Scale: Network Externalities

- consumers of a good derive positive value when size of the market increases.


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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 (or there is human capital investment), the total benefits derived from a good will depend on the number of consumers who adopt compatible products in the future.


## Positive Network Externalities

- railroad - standard rail format and shared access


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- any widely used standard (job training now is useful in the future)
- Concepts like the "tipping point", and "winner take all" markets.


## Other Network Externalities

## No Network Externalities

- food/drink - (should be) independent of how many others are eating the type of food.


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## Optimization Problem Involving Network Externalities

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- and let $S_{k^{*}}$ be the saturation point, lowest value of $k$ such that $S_{k}=S_{k+1}$
- Goal: find $A$ and $p$ to maximize $p \times\left|S_{k^{*}}\right|$.


## Anecdote

From David Brooks, NYTs column, March 28th, 2011 on "Tools for Thinking". In response to Steven Pinker (Harvard) asking a number of people "What scientific concept would improve everybody's cognitive toolkit?"

Emergent systems are ones in which many different elements interact. The pattern of interaction then produces a new element that is greater than the sum of the parts, which then exercises a top-down influence on the constituent elements.

## Submodular Motivation Recap

- Given a set of objects $V=\left\{v_{1}, \ldots, v_{n}\right\}$ and a function $f: 2^{V} \rightarrow \mathbb{R}$ that returns a real value for any subset $S \subseteq V$.
- Suppose we are interested in finding the subset that either maximizes or minimizes the function, e.g., $\operatorname{argmax}_{S \subseteq V} f(S)$, possibly subject to some constraints.
- In general, this problem has exponential time complexity.
- Example: $f$ might correspond to the value (e.g., information gain) of a set of sensor locations in an environment, and we wish to find the best set $S \subseteq V$ of sensors locations given a fixed upper limit on the number of sensors $|S|$.
- In many cases (such as above) $f$ has properties that make its optimization tractable to either exactly or approximately compute.
- One such property is submodularity.


## Submodular Definitions

## Definition 1.6.1 (submodular concave)

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

$$
\begin{equation*}
f(A)+f(B) \geq f(A \cup B)+f(A \cap B) \tag{1.2}
\end{equation*}
$$

An alternate and (as we see in lecture 3) equivalent definition is:

## Definition 1.6.2 (diminishing returns)

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

$$
\begin{equation*}
f(A \cup\{v\})-f(A) \geq f(B \cup\{v\})-f(B) \tag{1.3}
\end{equation*}
$$

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 $B$.

## Subadditive Definitions

## Definition 1.6.1 (subadditive)

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

$$
\begin{equation*}
f(A)+f(B) \geq f(A \cup B) \tag{1.15}
\end{equation*}
$$

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

## Supermodular Definitions

## Definition 1.6.2 (supermodular convex)

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

$$
\begin{equation*}
f(A)+f(B) \leq f(A \cup B)+f(A \cap B) \tag{1.16}
\end{equation*}
$$

An alternate and equivalent definition is:

## Definition 1.6.3 (increasing returns)

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

$$
\begin{equation*}
f(A \cup\{v\})-f(A) \leq f(B \cup\{v\})-f(B) \tag{1.17}
\end{equation*}
$$

The incremental "value", "gain", or "cost" of $v$ increases as the context in which $v$ is considered grows from $A$ to $B$.

## Submodular vs. Supermodular

- Submodular and supermodular functions are closely related.


## Submodular vs. Supermodular

- Submodular and supermodular functions are closely related.
- In fact, $f$ is submodular iff $-f$ is supermodular.


## Superadditive Definitions

## Definition 1.6 .4 (superadditive)

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

$$
\begin{equation*}
f(A)+f(B) \leq f(A \cup B) \tag{1.18}
\end{equation*}
$$

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

## Modular Definitions

## Definition 1.6.5 (modular)

A function that is both submodular and supermodular is called modular
If $f$ is a modular function, than for any $A, B \subseteq V$, we have

$$
\begin{equation*}
f(A)+f(B)=f(A \cap B)+f(A \cup B) \tag{1.19}
\end{equation*}
$$

Modular functions have no interaction, and have value based only on singleton values.

## Proposition 1.6.6

If $f$ is modular, it may be written as

$$
\begin{equation*}
f(A)=f(\emptyset)+\sum_{a \in A}(f(\{a\})-f(\emptyset)) \tag{1.20}
\end{equation*}
$$

## Modular Definitions

## Proof.

We inductively construct the value for $A=\left\{a_{1}, a_{2}, \ldots, a_{k}\right\}$.

$$
\begin{align*}
& f\left(a_{1}\right)+f\left(a_{2}\right)=f\left(a_{1}, a_{2}\right)+f(\emptyset)  \tag{1.21}\\
\text { implies } & f\left(a_{1}, a_{2}\right)=f\left(a_{1}\right)-f(\emptyset)+f\left(a_{2}\right)-f(\emptyset)+f(\emptyset) \tag{1.22}
\end{align*}
$$

then

$$
\begin{equation*}
f\left(a_{1}, a_{2}\right)+f\left(a_{3}\right)=f\left(a_{1}, a_{2}, a_{3}\right)+f(\emptyset) \tag{1.23}
\end{equation*}
$$

$$
\begin{equation*}
\text { implies } f\left(a_{1}, a_{2}, a_{3}\right)=f\left(a_{1}, a_{2}\right)-f(\emptyset)+f\left(a_{3}\right)-f(\emptyset)+f(\emptyset) \tag{1.24}
\end{equation*}
$$

$$
\begin{equation*}
=f(\emptyset)+\sum_{i=1}^{3} f\left(a_{i}\right)-f(\emptyset) \tag{1.25}
\end{equation*}
$$

## Complement function

Given a function $f: 2^{V} \rightarrow \mathbb{R}$, we can find a complement function $\bar{f}: 2^{V} \rightarrow \mathbb{R}$ as $\bar{f}(A)=f(V \backslash A)$ for any $A$.

## Proposition 1.6.7

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

## Proof.

$$
\begin{equation*}
\bar{f}(A)+\bar{f}(B) \geq \bar{f}(A \cup B)+\bar{f}(A \cap B) \tag{1.26}
\end{equation*}
$$

follows from

$$
\begin{equation*}
f(V \backslash A)+f(V \backslash B) \geq f(V \backslash(A \cup B))+f(V \backslash(A \cap B)) \tag{1.27}
\end{equation*}
$$

which is true because $V \backslash(A \cup B)=(V \backslash A) \cap(V \backslash B)$ and $V \backslash(A \cap B)=(V \backslash A) \cup(V \backslash B)$.

## Submodularity

- Submodular functions have a long history in economics, game theory, combinatorial optimization, electrical networks, and operations research.
- They are gaining importance in machine learning as well (one of our main motivations for offering this course).
- Arbitrary set functions are hopelessly difficult to optimize, while the minimum of submodular functions can be found in polynomial time, and the maximum can be constant-factor approximated in low-order polynomial time.
- Submodular functions share properties in common with both convex and concave functions.


## Attractions of Convex Functions

Why do we like Convex Functions? (Quoting Lovász 1983):
(1) Convex functions occur in many mathematical models in economy, engineering, and other sciences. Convexity is a very natural property of various functions and domains occurring in such models; quite often the only non-trivial property which can be stated in general.

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(3) Convex functions and domains exhibit sufficient structure so that a mathematically beautiful and practically useful theory can be developed.
(1) There are theoretically and practically (reasonably) efficient methods to find the minimum of a convex function.

## Attractions of Submodular Functions

In this course, we wish to demonstrate that submodular functions also possess attractions of these four sorts as well.

## Example Submodular: Number of Colors of Balls in Urns

- 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).
New value with added blue ball: 3


Initial value: 3 (colors in urn).
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- Thus, $f$ is submodular.


## Ex. Submodular: Consumer Costs of Living

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## Ex. Submodular: Consumer Costs of Living

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- 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.


## Area of the union of areas indexed by $A$

- Let $V$ be a set of indices, and each $v \in V$ indexes a given sub-area of some region. Let area $(v)$ be the area corresponding to item $v$.
- Let $f(S)=\bigcup_{s \in S}$ 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:

$$
f(A)=f\left(\left\{a_{1}, a_{2}, a_{3}, a_{4}\right\}\right)
$$

## Area of the union of areas indexed by $A$



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

$$
f(A \cup\{v\})=f\left(\left\{a_{1}, a_{2}, a_{3}, a_{4}\right\} \cup\{v\}\right)
$$

## 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.

$$
f(A)=f\left(\left\{a_{1}, a_{2}, a_{3}, a_{4}\right\}\right)
$$

## Area of the union of areas indexed by $A$



Union of areas of elements of $B \supset A$, where $v$ is not included: $f(B)$ where $v \notin B$ 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 $B \supseteq A$.

## Example Submodular: Entropy from Information Theory

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

$$
\begin{equation*}
f(A)=H\left(X_{A}\right)=-\sum_{x_{A}} p\left(x_{A}\right) \log p\left(x_{A}\right) \tag{1.28}
\end{equation*}
$$

is submodular.

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

$$
\begin{align*}
H\left(X_{v} \mid X_{B}\right) & =H\left(X_{B+v}\right)-H\left(X_{B}\right)  \tag{1.29}\\
& \leq H\left(X_{A+v}\right)-H\left(X_{A}\right)=H\left(X_{v} \mid X_{A}\right) \tag{1.30}
\end{align*}
$$

## Example Submodular: Entropy from Information Theory

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

$$
\begin{align*}
I\left(X_{A \backslash B} ; X_{B \backslash A} \mid X_{A \cap B}\right) & =\sum_{x_{A \cup B}} p\left(x_{A \cup B}\right) \log \frac{p\left(x_{A \backslash B}, x_{B \backslash A} \mid x_{A \cap B}\right)}{p\left(x_{A \backslash B} \mid x_{A \cap B}\right) p\left(x_{B \backslash A} \mid x_{A \cap B}\right)} \\
& =\sum_{x_{A \cup B}} p\left(x_{A \cup B}\right) \log \frac{p\left(x_{A \cup B}\right) p\left(x_{A \cap B}\right)}{p\left(x_{A}\right) p\left(x_{B}\right)} \geq 0 \tag{1.31}
\end{align*}
$$

then

$$
\begin{align*}
& I\left(X_{A \backslash B} ; X_{B \backslash A} \mid X_{A \cap B}\right) \\
& \quad=H\left(X_{A}\right)+H\left(X_{B}\right)-H\left(X_{A \cup B}\right)-H\left(X_{A \cap B}\right) \geq 0 \tag{1.32}
\end{align*}
$$

so entropy satisfies

$$
\begin{equation*}
H\left(X_{A}\right)+H\left(X_{B}\right) \geq H\left(X_{A \cup B}\right)+H\left(X_{A \cap B}\right) \tag{1.33}
\end{equation*}
$$

## Example Submodular: Mutual Information

- Also, symmetric mutual information is submodular,

$$
\begin{equation*}
f(A)=I\left(X_{A} ; X_{V \backslash A}\right)=H\left(X_{A}\right)+H\left(X_{V \backslash A}\right)-H\left(X_{V}\right) \tag{1.34}
\end{equation*}
$$

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

