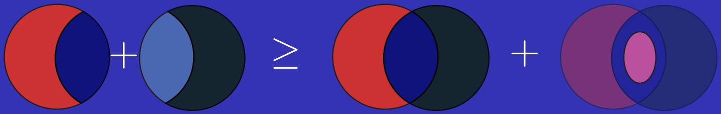

Mathematical Properties of Submodularity and Applications to Machine Learning

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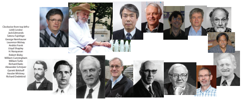
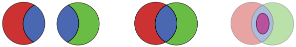
Friday, May 2nd, 2014

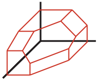
Goals of the Tutorial



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

$= f(A_r) + 2f(C) + f(B_r)$ $\quad = f(A_r) + f(C) + f(B_r)$ $\quad = f(A \cap B)$





- 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.

Submodularity

- Definition: given a finite ground set V, a function $f : 2^V \to \mathbb{R}$ is said to be submodular if

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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
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Outline of Part 2: Theory

Outline of Part 3: Algorithms

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Sets and set functions

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

$V =$ 

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

Sets and set functions

Subset $A \subseteq V$ of objects:

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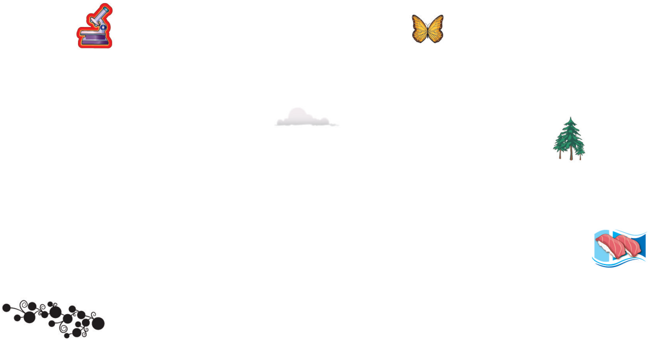
Subset $B \subseteq V$ of objects:

$B = \{$  $\}$

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Two Equivalent Submodular Definitions

Definition (submodular)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{2}$$

An alternate and equivalent definition is:

Definition (submodular (diminishing returns))

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

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \tag{3}$$

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.

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- $f(x) : \{0,1\}^V \to \mathbb{R}$ is a pseudo-Boolean function. A submodular function is a special case.

Modular functions, and vectors in $\mathbb{R}^V$

- Any set function $m : 2^V \to \mathbb{R}$ whose valuations, for $A \subseteq V$, take form

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- If f is both submodular and supermodular, then it is modular.

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- When f is submodular, Eq. (9) is polytime, and Eq. (10) is constant-factor approximable.

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- Constrained discrete optimization problems:

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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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  - 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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SET COVER and MAXIMUM COVERAGE

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

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

SET COVER and MAXIMUM COVERAGE

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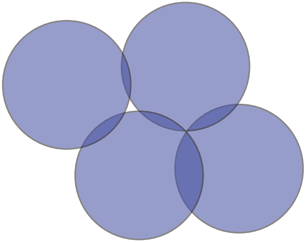
- Both SET COVER and MAXIMUM COVERAGE are well known to be NP-hard, but have a fast greedy approximation algorithm.
- The set cover function $f(A) = |\bigcup_{a \in A} V_a|$ is submodular!

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 $\text{area}(v)$ 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:

$$f(A) = f(\{a_1, a_2, a_3, a_4\})$$

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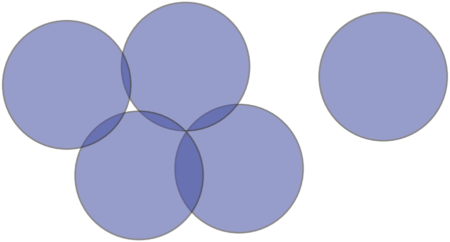

Area of A along with with v:

$$f(A \cup \{v\}) = f(\{a_1, a_2, a_3, a_4\} \cup \{v\})$$

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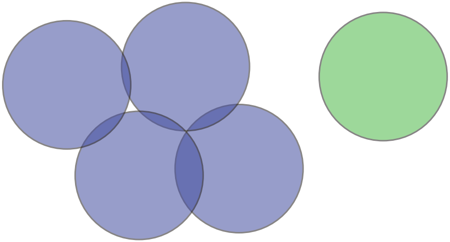
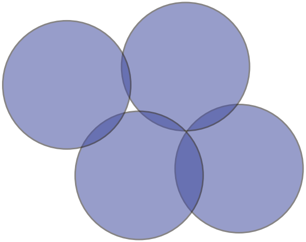


Gain (value) of v in context of A:

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

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.

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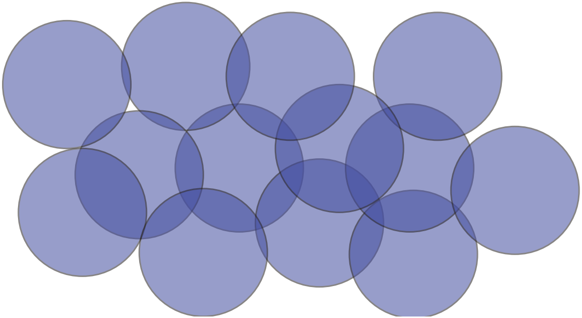
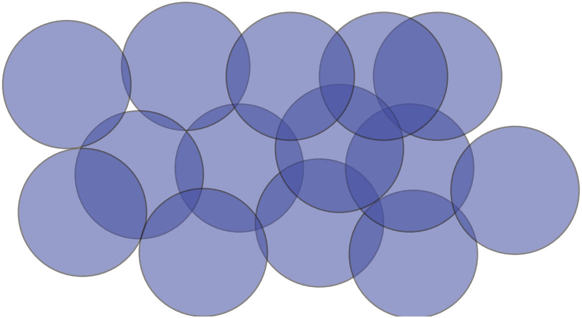


Union of areas of elements of $B \supset A$, where v is not included:

$$f(B) \text{ where } v \notin B \text{ and where } A \subseteq B$$

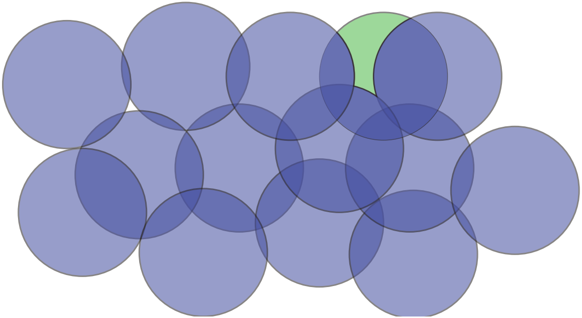
Area of the union of areas indexed by A



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 $B \supseteq A$.

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- Consider an urn containing colored balls. Given a set S of balls, $f(S)$ counts the number of distinct colors.

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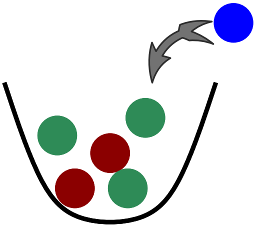
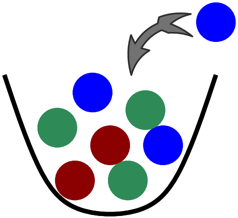


Initial value: 2 (colors in urn).
New value with added blue ball: 3



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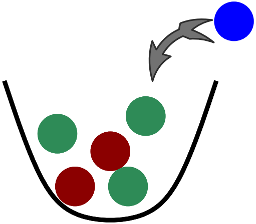

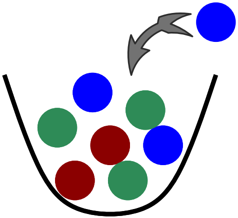

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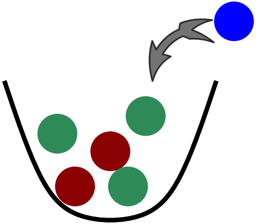

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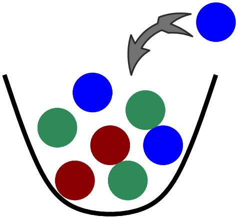

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- Thus, f is submodular.

Vertex and Edge Covers

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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.

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Graph Cut Problems

- Given a graph $G = (V, E)$, let $f : 2^V \to \mathbb{R}_+$ 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 $V \setminus X$.

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$$f(X) = w\Big(\{(u, v) \in E : u \in X, v \in V \setminus X\}\Big) \tag{14}$$

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- Both functions (Equations (13) and (14)) are submodular.

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

Extractive Document Summarization

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

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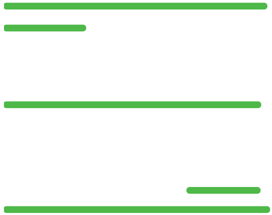

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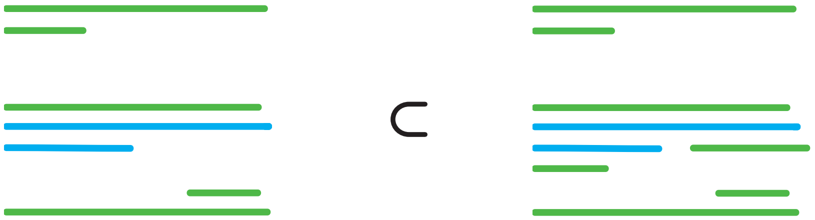

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- **diminishing returns** $\leftrightarrow$ **submodularity**

Image collections

Many images, also that have a higher level gestalt than just a few.

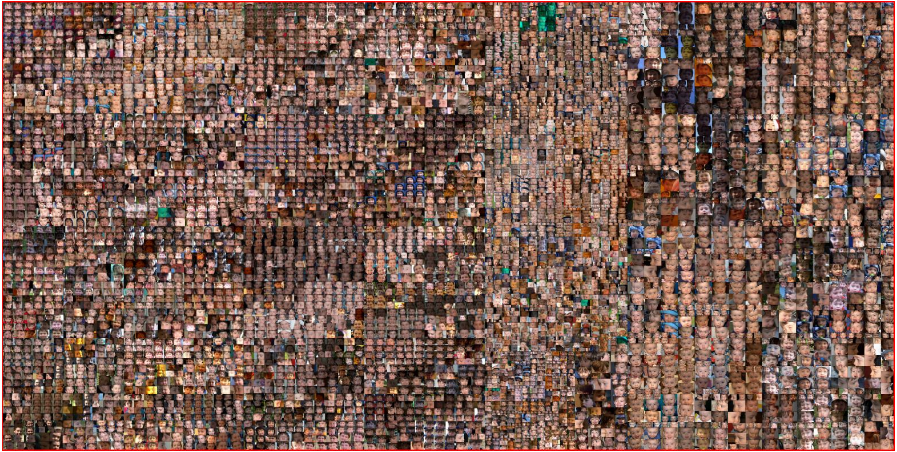

Image Summarization

10×10 image collection:

3 best summaries:

3 medium summaries:

3 worst summaries:

The three best summaries exhibit diversity. The three worst summaries exhibit redundancy.

Feature Selection in Pattern Classification

- 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 $\Pr(Y, X_1, X_2, \ldots, X_n)$.

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- The mutual information function $f(A) = I(Y; X_A)$ where

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

measures how well features A are for predicting Y (entropy reduction, reduction of uncertainty of Y)

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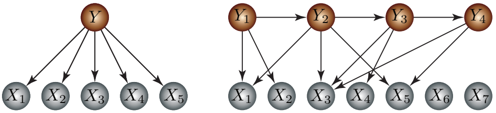

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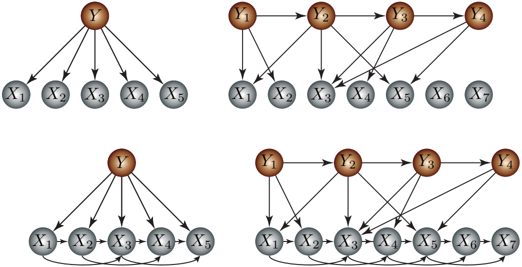
- If not, $f(A)$ is naturally expressed as a difference of two submodular functions.



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- 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.

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- 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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- $f(X)$ measures X's ability to represent set of features U as measured by $m_u(X)$, with diminishing returns function g, and importance weights α_u.

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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- Consider the KL-divergence between these two distributions:

$$\begin{aligned} D(p||\{\bar{m}_u(X)\}) &= \sum_{u \in U} p_u \log p_u - \sum_{u \in U} p_u \log(\bar{m}_u(X)) \qquad (23) \\ &= \sum_{u \in U} p_u \log p_u - \sum_{u \in U} p_u \log(m_u(X)) + \log(m(X)) \\ &= -H(p) + \log m(X) - \sum_{u \in U} p_u \log(m_u(X)) \qquad (24) \end{aligned}$$

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- Alternatively, if we define

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

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., $D(p||\{\bar{m}_u(X)\})$).

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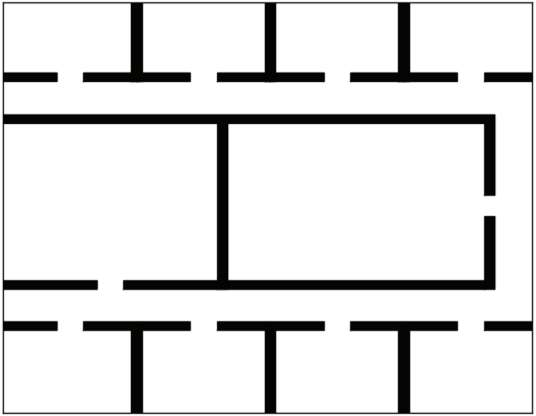
- Environment could be a floor of a building, water network, monitored ecological preservation.

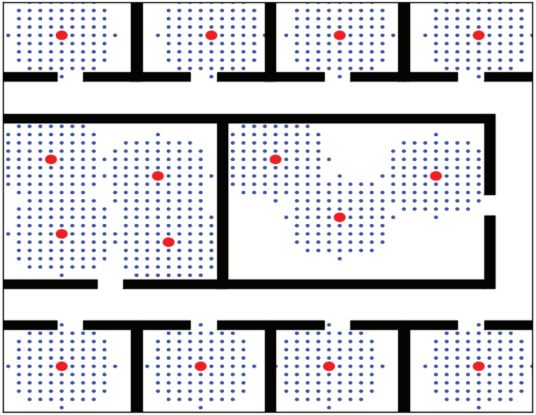
Sensor Placement within Buildings

- 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.



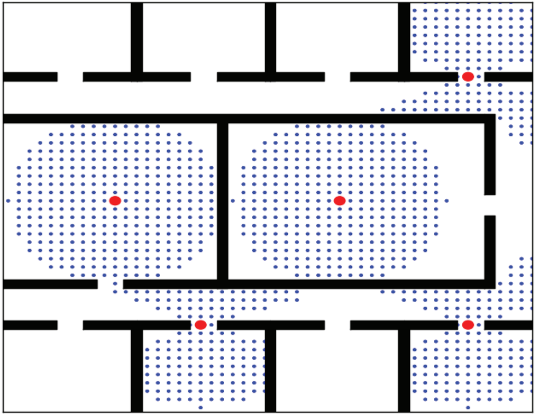
Sensor Placement within Buildings

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



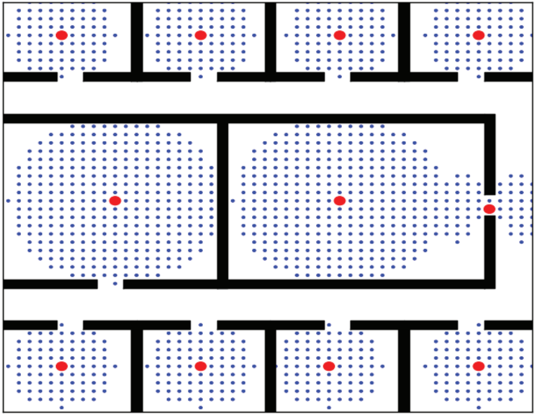
Sensor Placement within Buildings

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



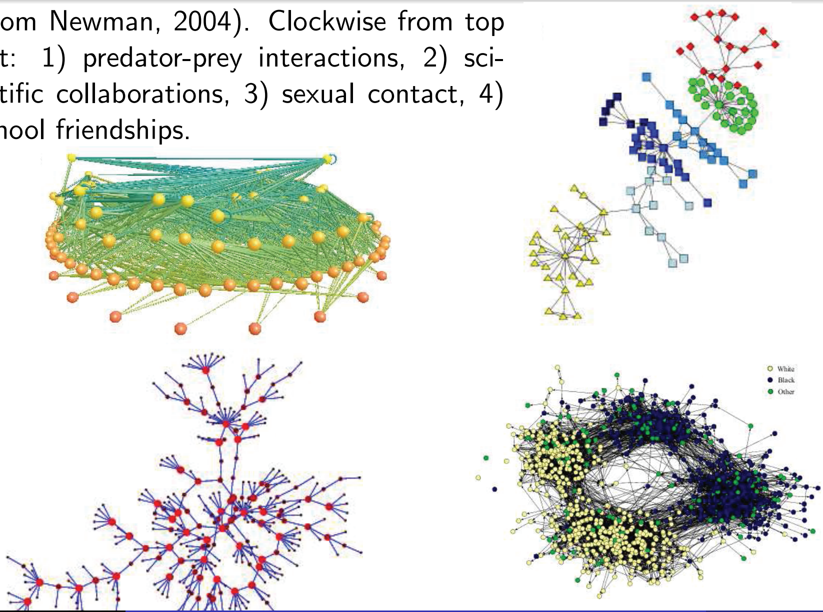
Sensor Placement within Buildings

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



Social Networks

(from Newman, 2004). Clockwise from top left: 1) predator-prey interactions, 2) scientific collaborations, 3) sexual contact, 4) school friendships.



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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).
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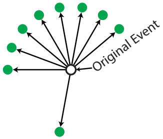

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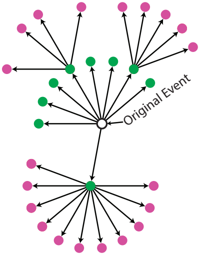

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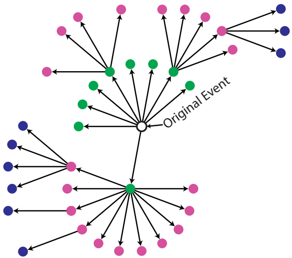

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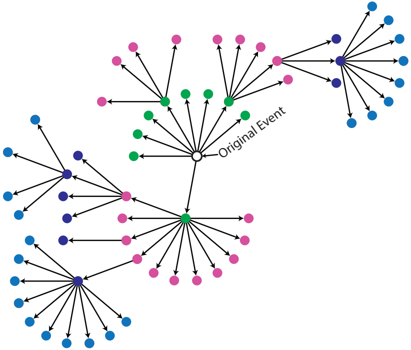

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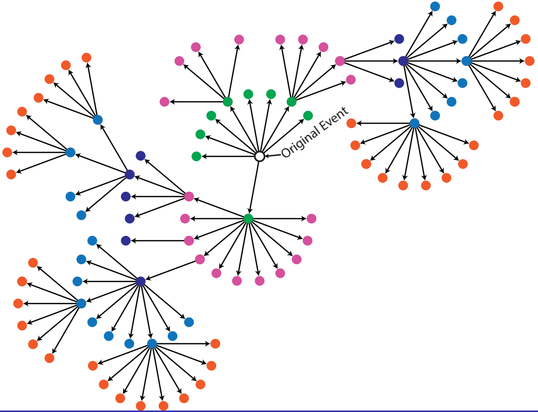

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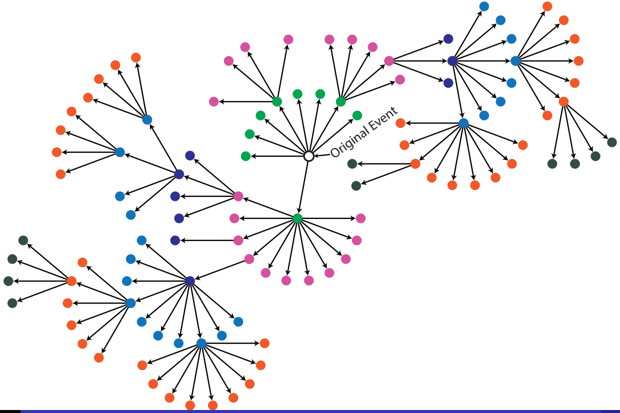

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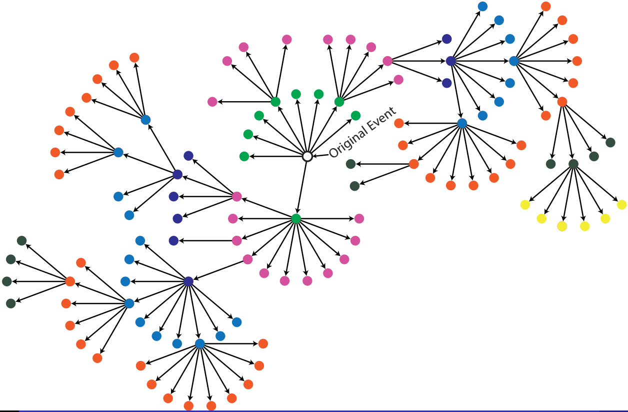

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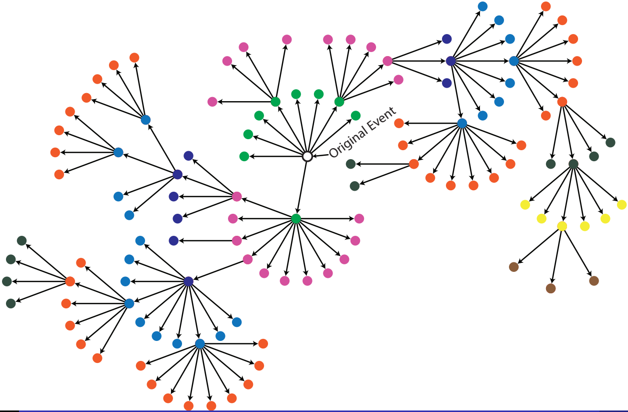

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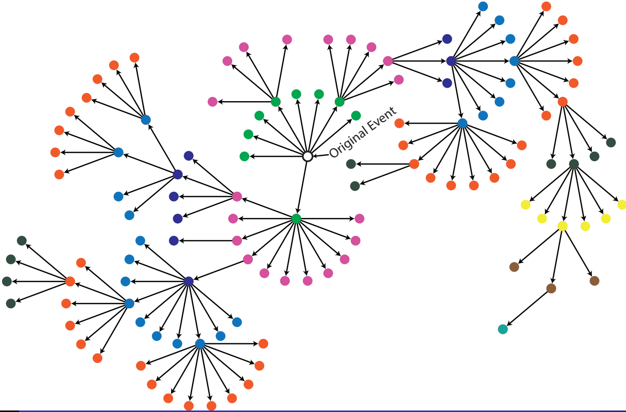

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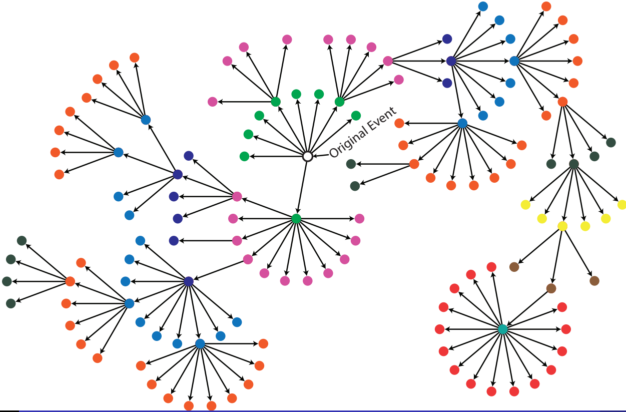

A model of influence in social networks

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

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- 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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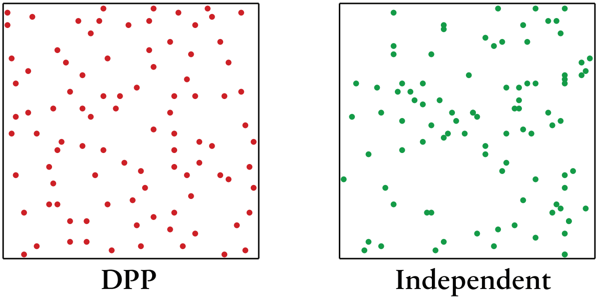

(Kulesza & Taskar, 2011)

Determinantal Point Processes (DPPs)

- Sometimes we wish not only to valuate subsets $A \subseteq V$ but to induce probability distributions over all subsets.
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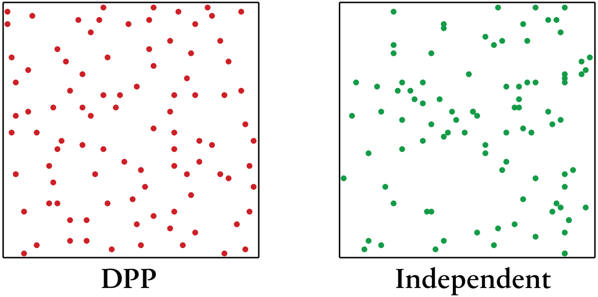

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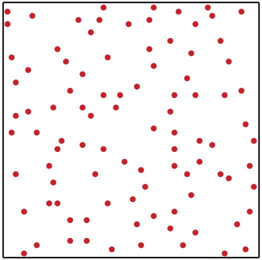
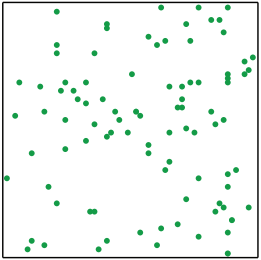


DPP



Independent

(Kulesza & Taskar, 2011)

- 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.

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- Given positive definite matrix M, function $f : 2^V \to \mathbb{R}$ with $f(A) = \log |M_A|$ (the logdet function) is submodular.

Graphical Model Structure Learning

- A probability distribution on binary vectors $p : \{0,1\}^V \to [0,1]$:

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- 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

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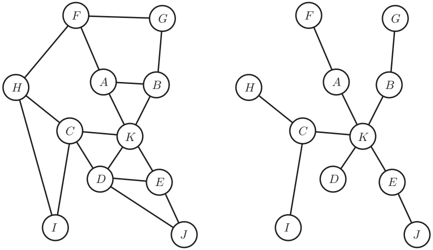

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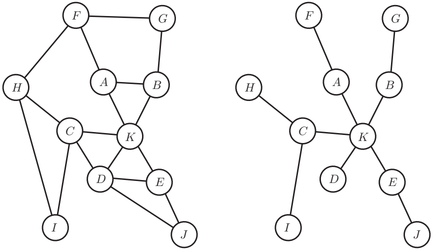

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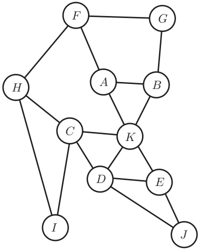

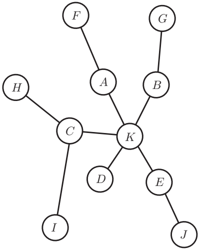

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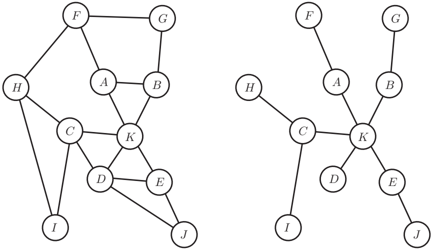

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- Then finding the maximum weight base of the matroid is solved by the greedy algorithm, and also finds the optimal tree (Chow & Liu, 1968)

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

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

$$E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in \mathcal{E}(G)} e_{ij}(x_i, x_j) \tag{32}$$

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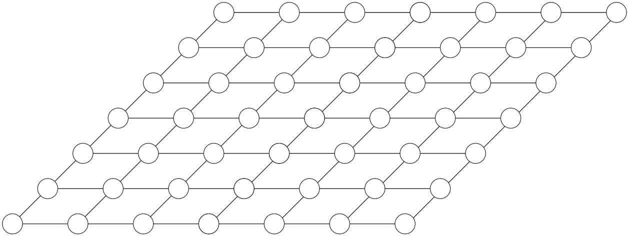
- When G is a 2D grid graph, we have

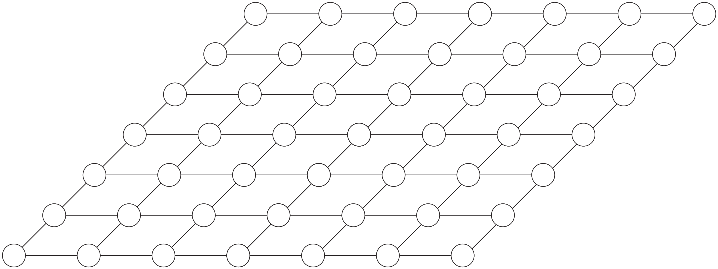


Auxiliary (s, t)-graph

- 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., $G_a = (V \cup \{s, t\}, E + \cup_{v \in V}((s, v) \cup (v, t)))$.

Transformation from graphical model to auxiliary graph

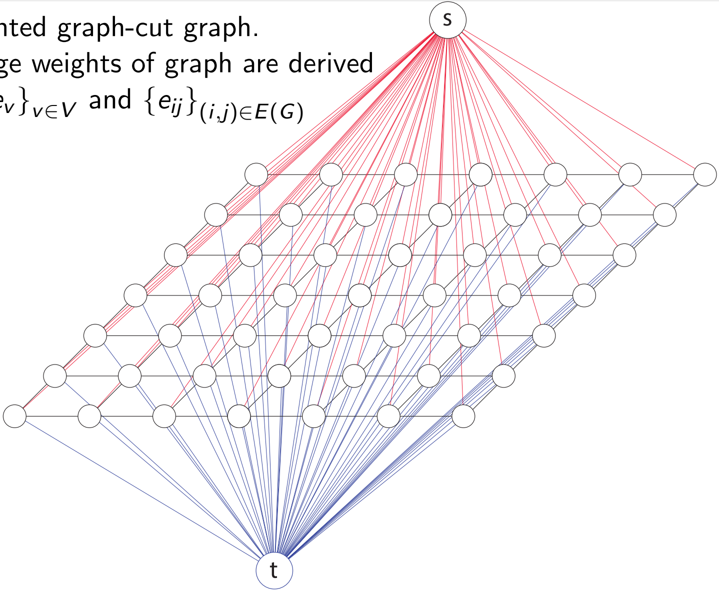
Original Graph: $E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j)$



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 $\{e_{ij}\}_{(i,j) \in E(G)}$



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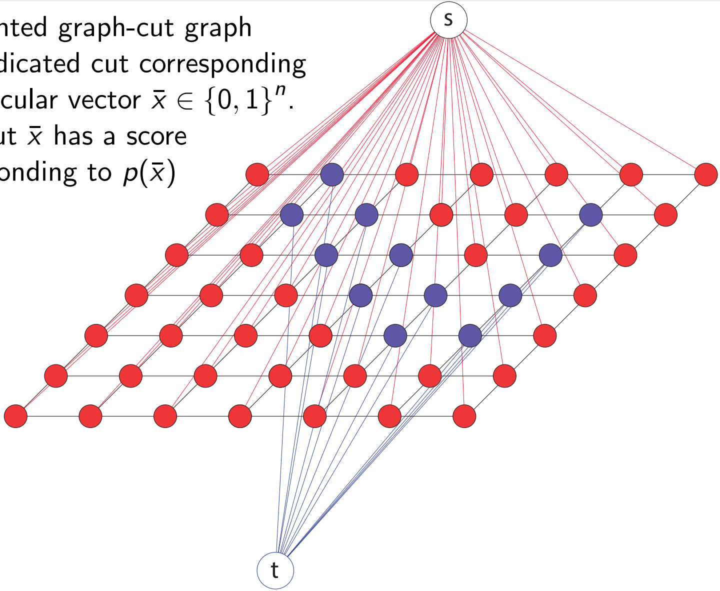

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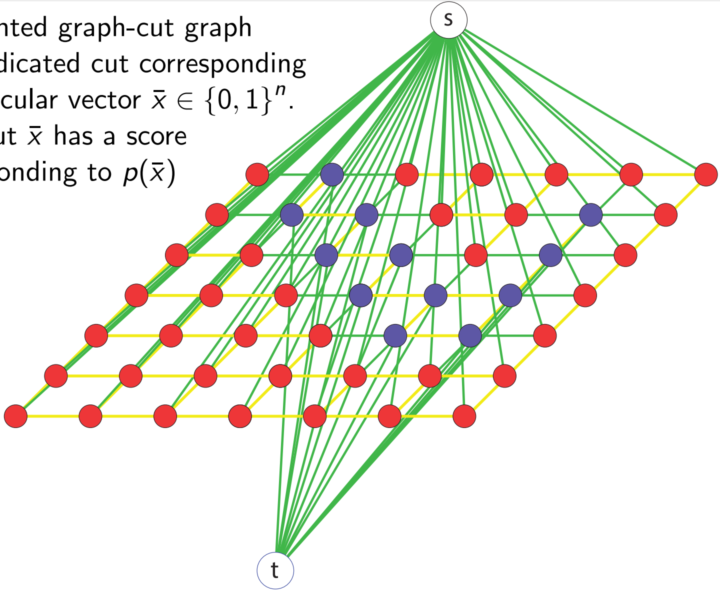

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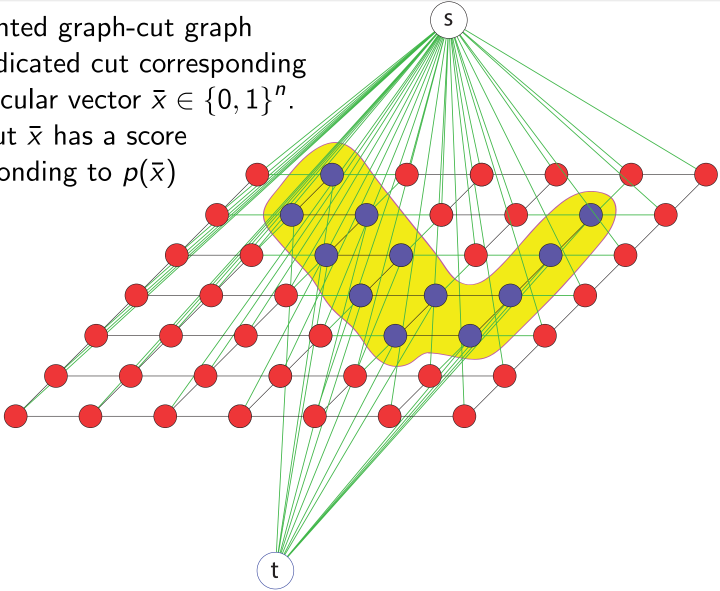

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Edge weight assignments:

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

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- For (s, v) with $v \in V(G)$, set edge $w_{s,v} = (e_v(1) - e_v(0))\mathbf{1}(e_v(1) > e_v(0))$
- For (v, t) with $v \in V(G)$, set edge $w_{v,t} = (e_v(0) - e_v(1))\mathbf{1}(e_v(0) \geq e_v(1))$

Setting of the weights in the auxiliary cut graph

- 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 $E(x) = \log p(\bar{x}) + \text{const.}$.
- If weights of all edges, except those involving terminals s and t, are non-negative, graph cut computable in polynomial time via max-flow!
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- For original edge $(i,j) \in E$, $i,j \in V$, set weight $w_{i,j} = e_{ij}(1,0) + e_{ij}(0,1) - e_{ij}(1,1) - e_{ij}(0,0)$.

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:

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- Weights w_{ij} in s,t-graph above are always non-negative, so graph-cut solvable.

On log-supermodular vs. log-submodular distributions

- Log-supermodular distributions.

$$\log \Pr(x) = f(x) + \text{const.} = -E(x) + \text{const.} \tag{35}$$

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.

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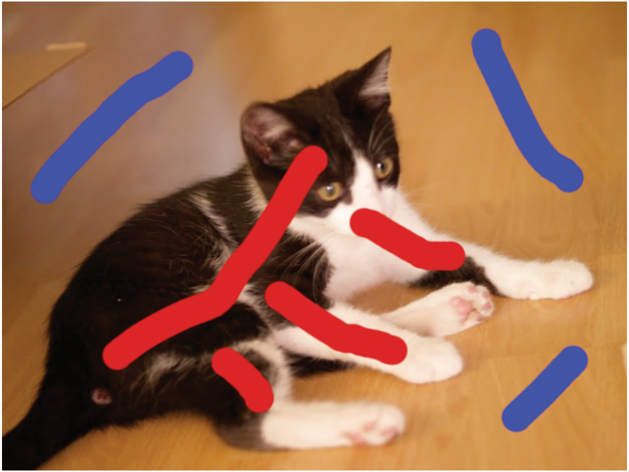
Submodular potentials in GMs: Image Segmentation

- an image needing to be segmented.

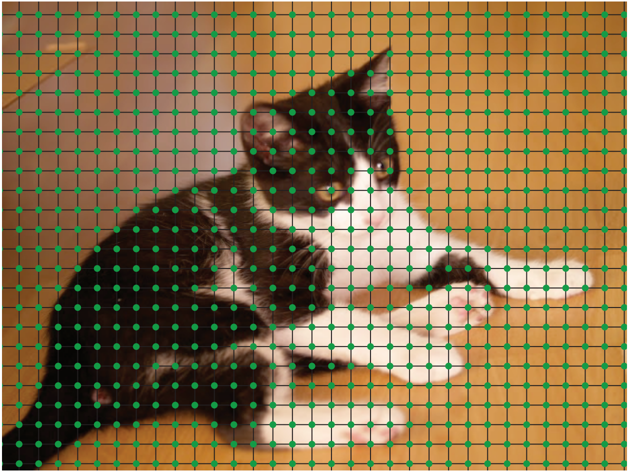
Submodular potentials in GMs: Image Segmentation

- labeled data, some pixels being marked foreground (red) and others marked background (blue) to train the unaries $\{e_v(x_v)\}_{v \in V}$.



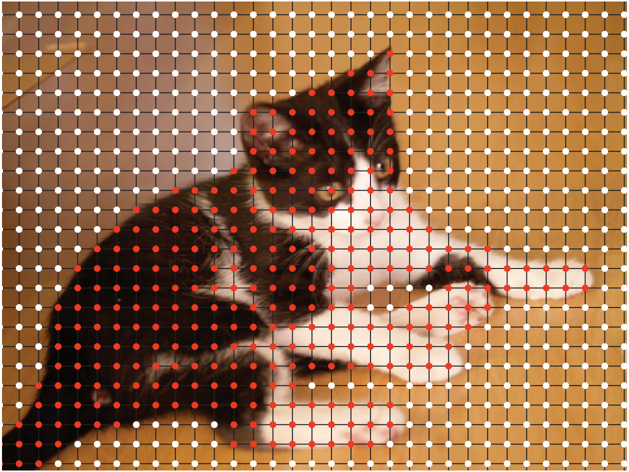
Submodular potentials in GMs: Image Segmentation

- Set of a graph over the image, graph shows binary pixel labels.



Submodular potentials in GMs: Image Segmentation

- Run graph-cut to segment the image, foreground in red, background in white.



Submodular potentials in GMs: Image Segmentation

- the foreground is removed from the background.

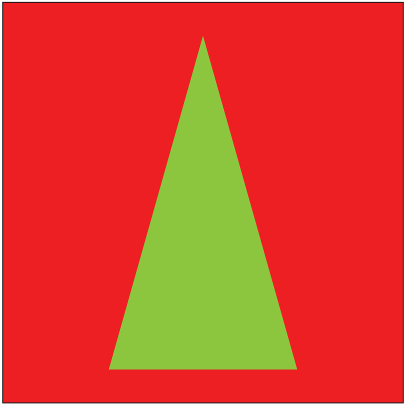
Shrinking bias in graph cut image segmentation

What does graph-cut based image segmentation do with elongated structures (top) or contrast gradients (bottom)?

Shrinking bias in graph cut image segmentation

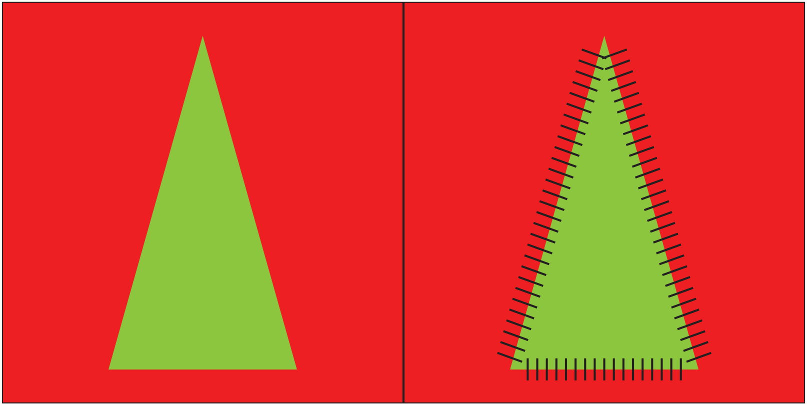
Shrinking bias in image segmentation

- An image needing to be segmented
- Clear high-contrast boundaries



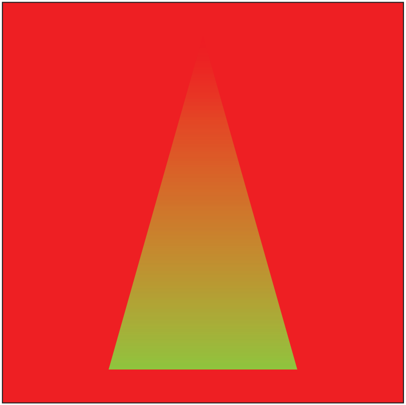
Shrinking bias in image segmentation

- Graph-cut (MRF with submodular edge potentials) works well.



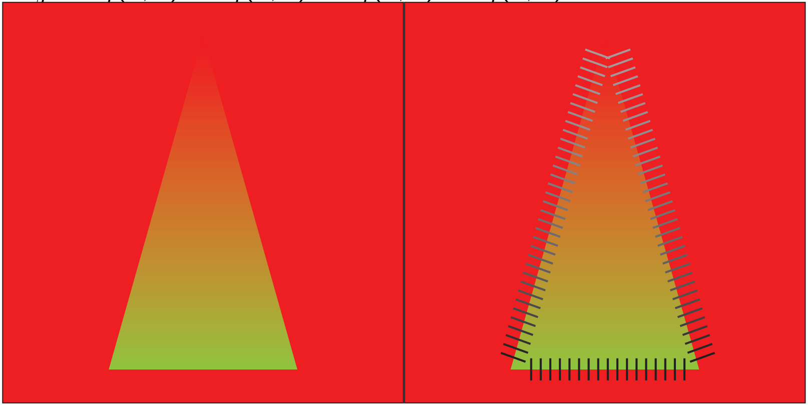
Shrinking bias in image segmentation

- Now with contrast gradient (less clear segment as we move up).
- The "elongated structure" also poses a challenge.



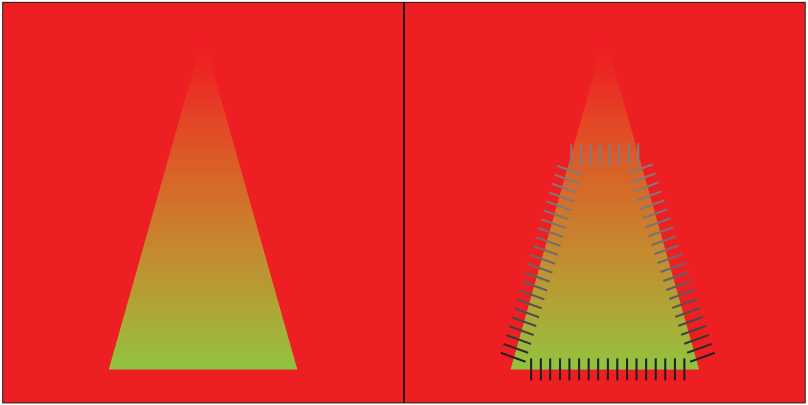
Shrinking bias in image segmentation

- Unary potentials $\{e_v(x_v)\}_{v \in V}$ prefer a different segmentation.
- Edge weights are the same regardless of where they are $w_{i,j} = e_{ij}(1,0) + e_{ij}(0,1) - e_{ij}(1,1) - e_{ij}(0,0) \geq 0$.



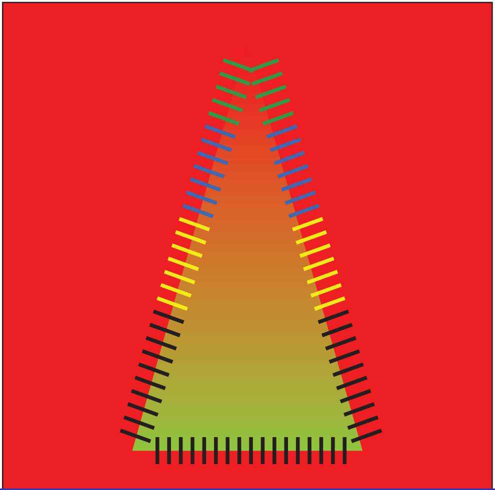
Shrinking bias in image segmentation

- 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.



Addressing shrinking bias with edge submodularity

- 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.

$$f_w(X) = w\Big(\{(u, v) \in E : u \in X, v \in V \setminus X\}\Big) \tag{37}$$

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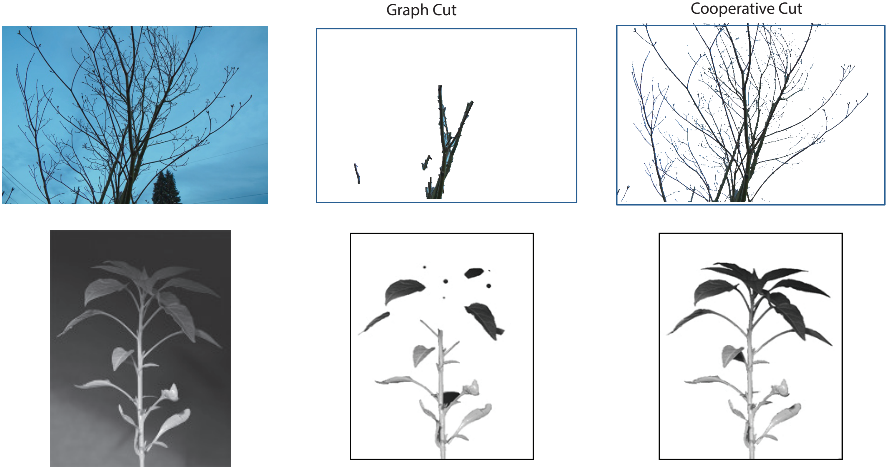
- $\Rightarrow$ cooperative-cut (Jegelka & Bilmes, 2011).

Graph-cut vs. cooperative-cut comparisons



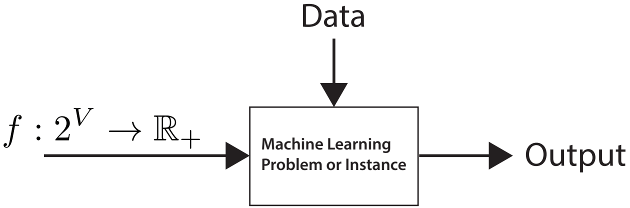
(Jegelka&Bilmes,'11). There are fast algorithms for solving as well (as we'll see tomorrow).

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

A submodular function as a parameter

- In some cases, it may be useful to view a submodular function $f : 2^V \to \mathbb{R}$ as a input "parameter" to a machine learning algorithm.



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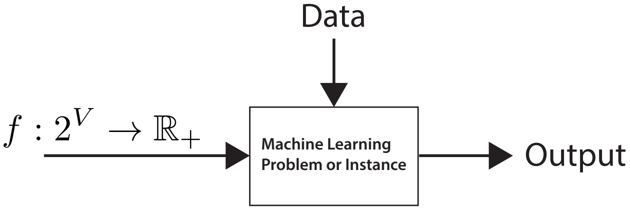

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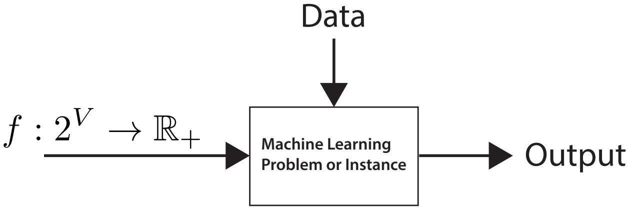

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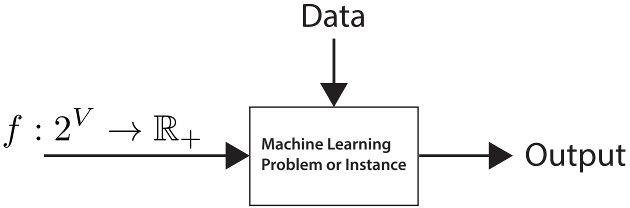

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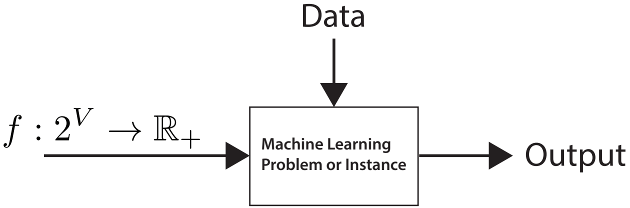

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- We next see how f parameterizes problems in ML, and then address learning.

Supervised And Unsupervised Machine 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:

$$\min_{w \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^{m} \ell(y_i, w^\intercal x_i) + \lambda \Omega(w), \tag{39}$$

where $\ell(\cdot)$ is a loss function (e.g., squared error) and $\Omega(w)$ is a norm.

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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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- When data has multiple responses only that are observed, $(y_i) \in R^k$ we get dictionary learning (Krause & Guestrin, Das & Kempe):

$$\min_{x_1, \dots, x_m} \min_{w^1, \dots, w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^k, (w^k)^\intercal x_i) + \lambda \Omega(w^k), \tag{41}$$

Norms, sparse norms, and computer vision

- 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:

$$\Omega(w) = \sum_{i=2}^{N} |w_i - w_{i-1}| \tag{42}$$

- Points of difference should be "sparse" (frequently zero).

(Rodriguez, 2009)

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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

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

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

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- and a notion of "conditional independence" , i.e., $A \perp\!\!\!\perp B | C$:

$$f(A \cup B \cup C) + f(C) = f(A \cup C) + f(B \cup C) \tag{45}$$

Submodular Generalized Dependence

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- and two notions of "information amongst a collection of sets":

$$I_f(S_1; S_2; \dots; S_k) = \sum_{i=1}^{k} f(S_k) - f(S_1 \cup S_2 \cup \dots \cup S_k) \tag{47}$$

$$I'_f(S_1; S_2; \dots; S_k) = \sum_{A \subseteq \{1,2,\dots,k\}} (-1)^{|A|+1} f(\bigcup_{j \in A} S_j) \tag{48}$$

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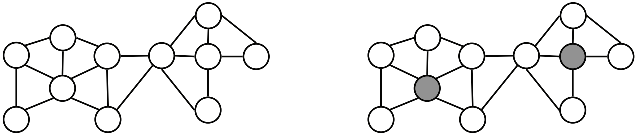
- Hence, family of clustering algorithms parameterized by f.

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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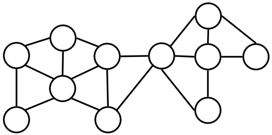

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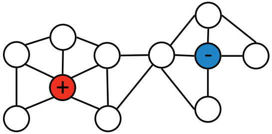

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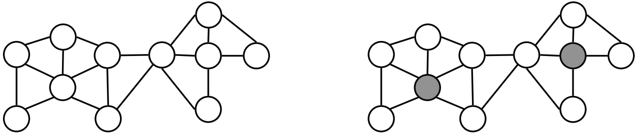

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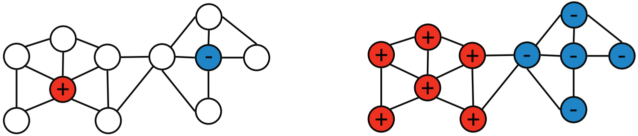
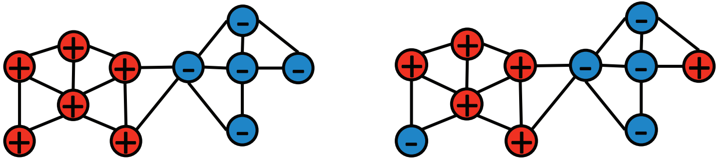


- Learner suffers loss $\|\hat{y} - y\|_1$, here $\|\hat{y} - y\|_1 = 2$.



Choosing labels: how to select L

- Consider the following objective

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

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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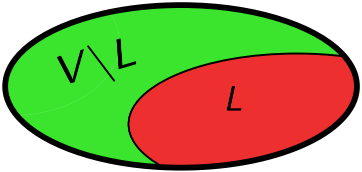

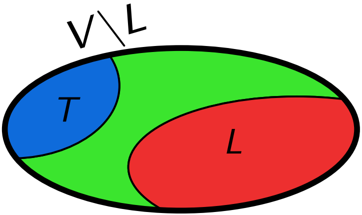

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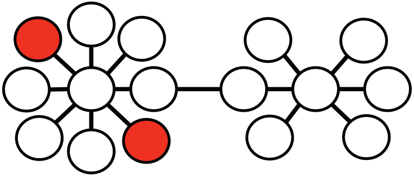

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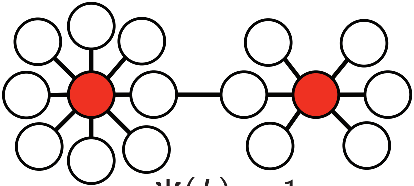

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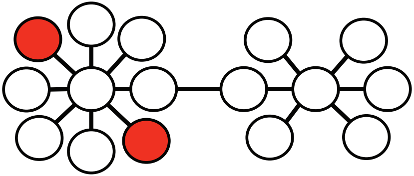

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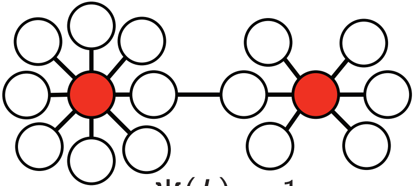

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- This suggests choosing (bounded cost) L that maximizes $\Psi(L)$.

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

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

$$\|\hat{y} - y\|_1 \leq 2\frac{\Gamma(Y(y))}{\Psi(L)} \tag{51}$$

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

- All is defined in terms of the symmetric submodular function Γ (need not be graph cut), where:

$$\Psi(S) = \min_{T \subseteq V \setminus S : T \neq \emptyset} \frac{\Gamma(T)}{|T|} \tag{52}$$

- $\Gamma(T) = f(S) + f(V \setminus S) - f(V)$ is determined by arbitrary submodular function f, giving different error bound for each.
- Joint algorithm is "parameterized" by a submodular function f.

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- General: Hamming, Recall, Precision, Cond. MI, Sq. Hamming, etc.

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

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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.
- 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 $D = \left\{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\right\}_i$ where $\mathbf{x}^{(i)} \in \mathcal{X}$, $\mathbf{y}^{(i)} \in \mathcal{Y}$.
- $\mathbf{f} : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^M$ is a (fixed) vector of functions, and $\mathbf{w} \in \mathbb{R}^M$ is a vector of parameters to learn.
- Score function: $s(\mathbf{x}, \mathbf{y}) = \mathbf{w}^\intercal \mathbf{f}(\mathbf{x}, \mathbf{y}) = \sum_i w_i f_i(\mathbf{x}, \mathbf{y})$.
- Decision making (inference) for a given $\bar{\mathbf{x}}$ is based on:

$$\hat{\mathbf{y}} \in h_{\mathbf{w}}(\bar{\mathbf{x}}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} s(\bar{\mathbf{x}}, \mathbf{y}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} \mathbf{w}^\intercal \mathbf{f}(\bar{\mathbf{x}}, \mathbf{y}) \tag{55}$$

- Goal of learning: optimize $\mathbf{w}$ so that such decision making is "good"
- Let $\ell : \mathcal{Y} \times Y \to \mathbb{R}_+$ be a loss function. I.e., $\ell_{\mathbf{y}}(\hat{\mathbf{y}})$ is cost of deciding $\hat{\mathbf{y}}$ when truth is $\mathbf{y}$.
- Empirical risk minimization: adjust $\mathbf{w}$ so that $\sum_i \ell_{\mathbf{y}}(h_{\mathbf{w}}(\mathbf{x}^{(i)}))$ is small subject to other conditions (e.g., regularization).

Structured Prediction: Approach with inference

- Constraints specified in inference form:

$$\underset{\mathbf{w},\xi_t}{\text{minimize}} \quad \frac{1}{T}\sum_t \xi_t + \frac{\lambda}{2}\|\mathbf{w}\|^2 \tag{56}$$

$$\text{subject to} \quad \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) \geq \max_{\mathbf{y}\in\mathcal{Y}_t}\left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y})\right) - \xi_t, \forall t \tag{57}$$

$$\xi_t \geq 0, \forall t. \tag{58}$$

- Exponential set of constraints reduced to an embedded optimization problem, "inference."

Learning Submodular Mixtures: Unconstrained Form

- 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 $\mathbf{w}$, of the following

$$\max_{\mathbf{y} \in \mathcal{Y}_t} \left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y}) \right) - \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) + \frac{\lambda}{2} \|\mathbf{w}\|^2 \tag{61}$$

can be found by computing or approximating

$$\mathbf{y}^* \in \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}_t} \left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y}) \right) - \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) \tag{62}$$

and then finding subgradient of

$$\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^*) + \ell_t(\mathbf{y}^*) - \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) + \frac{\lambda}{2} \|\mathbf{w}\|^2 \tag{63}$$

which has the form

$$\mathbf{f}_t(\mathbf{y}^*) - \mathbf{f}_t(\mathbf{y}^{(t)}) + \lambda \mathbf{w}. \tag{64}$$

Structured Prediction: Subgradient Learning

Algorithm 1: Subgradient descent learning

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

$w_0 = 0$;

for $t = 1, \cdots, T$ **do**

  Loss augmented inference: $\mathbf{y}_t^* \in \text{argmax}_{\mathbf{y} \in \mathcal{Y}_t} \mathbf{w}_{t-1}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y})$;

  Compute the subgradient: $\mathbf{g}_t = \lambda \mathbf{w}_{t-1} + \mathbf{f}_t(\mathbf{y}^*) - \mathbf{f}_t(\mathbf{y}^{(t)})$;

  Update the weights: $\mathbf{w}_t = \mathbf{w}_{t-1} - \eta_t \mathbf{g}_t$;

Return : the averaged parameters $\frac{1}{T} \sum_t \mathbf{w}_t$.

Outline

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- Any function can be expressed as the difference between two submodular functions.
- Hence, rather than minimize $E(x)$ (hard), we can minimize $E_f(x) \geq E(x)$ (relatively easy), which is an upper bound.

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

Ex. Submodular: Consumer Costs of Living

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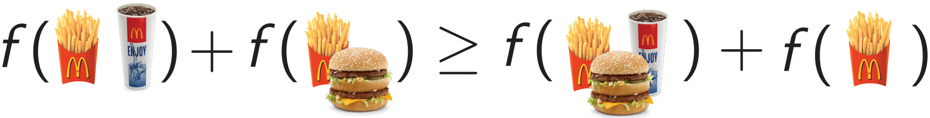

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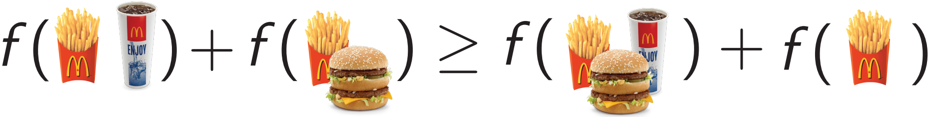

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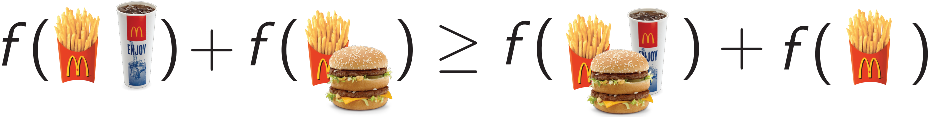

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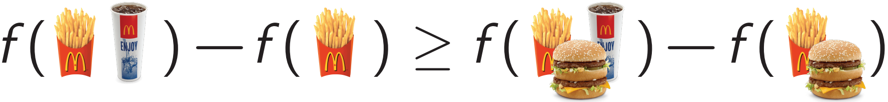

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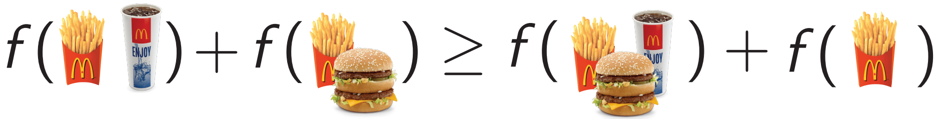

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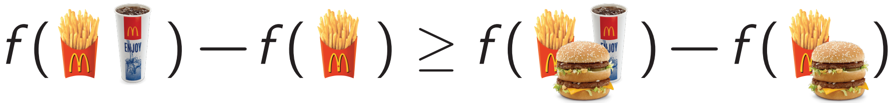

- This is very common: The additional cost of a coke is, say, free if you add it to fries and a hamburger, but when added just to an order of fries, the coke is not free.

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- Shared fixed costs are submodular: $f(v_1) + f(v_2) \geq f(v_1, v_2) + f(\emptyset)$

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- So diminishing returns (a submodular function) would be a good model.

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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:

$$\begin{array}{c} \\ \mathbf{X} = \end{array} \begin{array}{c} \begin{array}{cccccc} 1 & 2 & 3 & 4 & & m \end{array} \\ \begin{pmatrix} | & | & | & | & & | \\ x_1 & x_2 & x_3 & x_4 & \dots & x_m \\ | & | & | & | & & | \end{pmatrix} \end{array} \tag{67}$$

- Let set $V = \{1, 2, \dots, m\}$ 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 4×8 matrix, so $V = \{1, 2, 3, 4, 5, 6, 7, 8\}$.

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

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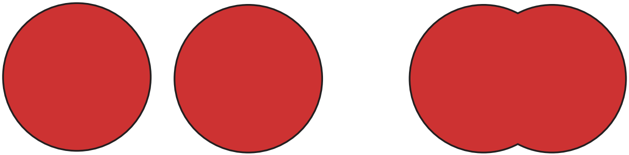

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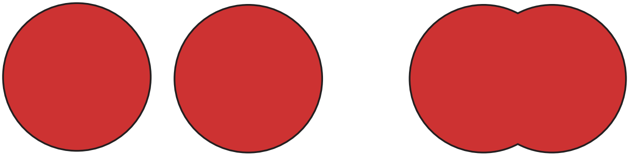

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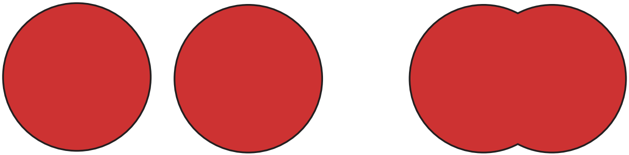

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- Any function where the above inequality is true for all $A, B \subseteq V$ is called subadditive.

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

$$r(A \cup B) = r(A_r) + r(C) + r(B_r) \tag{69}$$

Rank functions of a matrix

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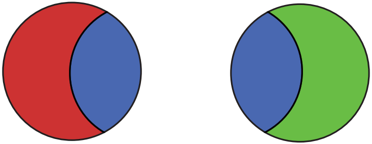
$$r(A) + r(B) = r(A_r) + 2r(C) + r(B_r)$$



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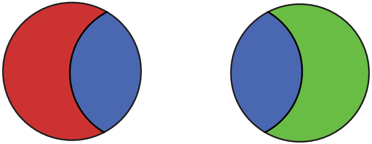

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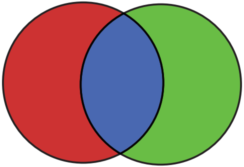

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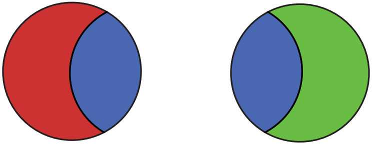

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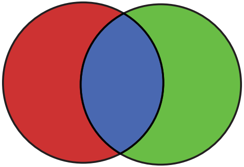
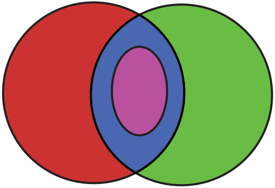


- Thus, we have subadditivity: $r(A) + r(B) \geq r(A \cup B)$. Can we add more to the r.h.s. and still have an inequality? Yes.

Rank function of a matrix

- 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).

$$r(C) \geq r(A \cap B)$$



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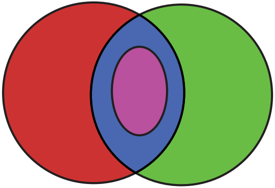

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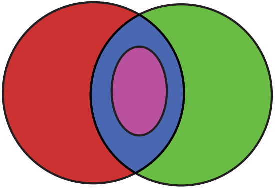
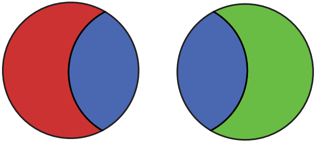


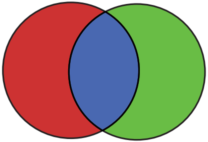
In short:

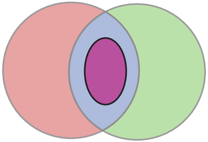
- Common span (blue) is "more" (no less) than span of common index (magenta).
- More generally, common information (blue) is "more" (no less) than information within common index (magenta).

The Venn and Art of Submodularity

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







Polymatroid function and its polyhedron.

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

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

$$= \left\{ y \in \mathbb{R}^V : y \geq 0, y(A) \leq f(A) \text{ for all } A \subseteq V \right\} \tag{71}$$

Chains of sets

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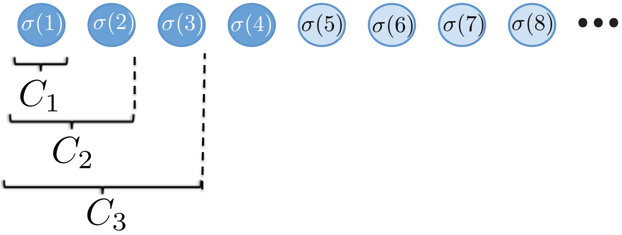
$$C_i = \{\sigma_1, \sigma_2, \ldots, \sigma_i\}, \quad \text{for } i = 1 \ldots n \tag{72}$$



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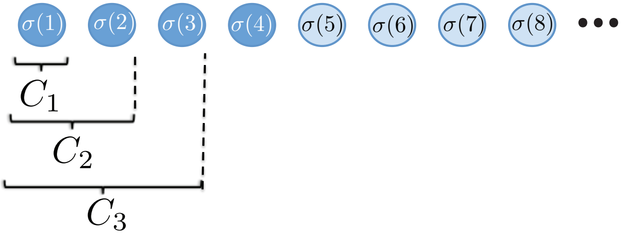

- Can also form a chain from a vector $w \in \mathbb{R}^V$ sorted in descending order. Choose σ so that $w(\sigma_1) \geq w(\sigma_2) \geq \cdots \geq w(\sigma_n)$.

Gain

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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{aligned}
f(A \cup \{j\}) - f(A) &\triangleq \rho_j(A) && (73)\\
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- We'll use $f(j|A)$. Also, $f(A|B) = f(A \cup B) - f(B)$.
- Submodularity's diminishing returns definition can be stated as saying that $f(j|A)$ is a monotone non-increasing function of A, since $f(j|A) \geq f(j|B)$ whenever $A \subseteq B$ (conditioning reduces valuation).

Polymatroidal polyhedron and greedy

- Suppose we wish to solve the following linear programming problem:

$$\begin{aligned} &\underset{x \in \mathbb{R}^V}{\text{maximize}} && w^\intercal x \\ &\text{subject to} && x \in \left\{ y \in \mathbb{R}_+^V : y(A) \leq f(A) \text{ for all } A \subseteq V \right\} \end{aligned} \tag{78}$$

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

$$x(v_i) = f(V_i) - f(V_{i-1}) = f(v_i | V_{i-1}) \tag{80}$$

Polymatroidal polyhedron and greedy

- We have the following very powerful result (which generalizes a similar one that is true for matroids).

Theorem

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

Polymatroid extreme points

Greedy does more than this. In fact, we have:

Theorem

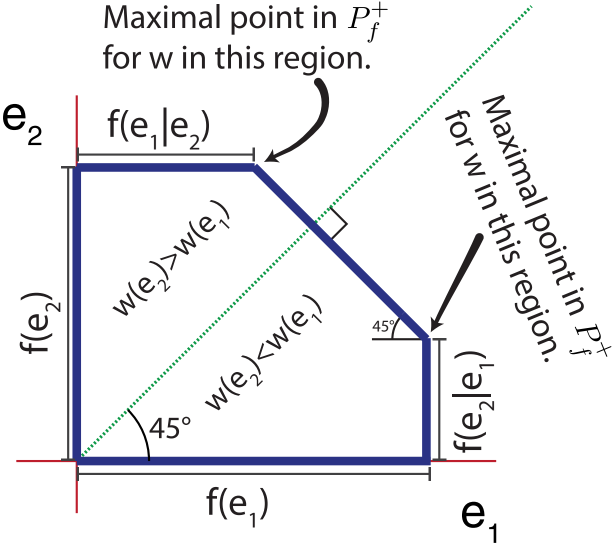
For a given ordering $V = (v_1, \dots, v_m)$ of V and a given V_i and x generated by V_i using the greedy procedure, then x is an extreme point of P_f

Corollary

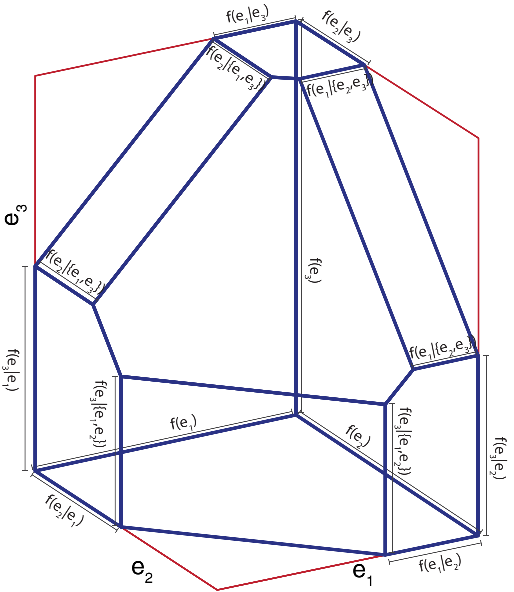
If x is an extreme point of P_f and $B \subseteq V$ is given such that $\{v \in V : x(v) \neq 0\} \subseteq B \subseteq \cup(A : x(A) = f(A))$, then x is generated using greedy by some ordering of B.

Intuition: why greedy works with polymatroids

- Given w, the goal is to find $x = (x(e_1), x(e_2))$ that maximizes $x^\intercal w = x(e_1)w(e_1) + x(e_2)w(e_2)$.
- If $w(e_2) > w(e_1)$ the upper extreme point indicated maximizes $x^\intercal w$ over $x \in P_f^+$.
- If $w(e_2) < w(e_1)$ the lower extreme point indicated maximizes $x^\intercal w$ over $x \in P_f^+$.



Polymatroid with labeled edge lengths



A polymatroid function's polyhedron vs. a polymatroid.

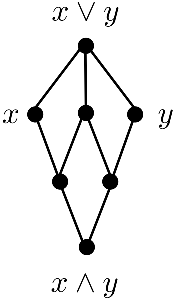
- Given these results, we can conclude that a polymatroid is really an extremely natural polyhedral generalization of a matroid. This was all realized by Jack Edmonds in the mid 1960s (and published in 1969 in his landmark paper "Submodular Functions, Matroids, and Certain Polyhedra").

- Jack Edmonds NIPS talk, 2011 http://videolectures.net/nipsworkshops2011_edmonds_polymatroids/

Outline: Part 2

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.

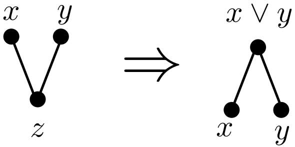


height
3
2
1
0

submodularity
h(x)+h(y)
> h($x \vee y$)
+ h($x \wedge y$)

$2 + 2 > 3 + 0$

- Such lattices require that for all x, y, z,



- The lattice is upper-semimodular (submodular), height function is submodular on the lattice.

Submodular Definitions

Definition (submodular)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{81}$$

- General submodular function, f need not be monotone, non-negative, nor normalized (i.e., $f(\emptyset)$ need not be $= 0$).

Normalized Submodular Function

- Given any submodular function $f : 2^V \to \mathbb{R}$, form a normalized variant $f' : 2^V \to \mathbb{R}$, with

$$f'(A) = f(A) - f(\emptyset) \tag{82}$$

- 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.

Submodular Polymatroidal Decomposition

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

$$f(A) = \underbrace{f(A) - m(A)}_{\bar{f}(A)} + m(A) = \bar{f}(A) + m(A) \tag{83}$$

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

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

$$\bar{f}(a|A) = f(a|A) - f(a|V \setminus \{a\}) \geq 0 \tag{85}$$

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

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- m is like a unary score, $\bar{f}$ is where things interact . All of the real structure is in $\bar{f}$
- Hence, any submodular function is a sum of polymatroid and modular.

Telescoping Summation

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

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- 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:

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

Submodular Definitions

Theorem

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \text{ for all } A, B \subseteq V \qquad \text{(SC)}$$

if and only if

$$f(v|X) \geq f(v|Y) \text{ for all } X \subseteq Y \subseteq V \text{ and } v \notin B \qquad \text{(DR)}$$

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Proof.

(SC)⇒(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)⇒(SC): Order $A \setminus B = \{v_1, v_2, \ldots, v_r\}$ arbitrarily. Then $f(v_i|A \cap B \cup \{v_1, v_2, \ldots, v_{i-1}\}) \geq f(v_1|B \cup \{v_1, v_2, \ldots, v_{i-1}\}), \ i \in [r-1]$

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

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$$f(j|S) \geq f(j|S \cup \{k\}), \; \forall S \subseteq V \text{ with } j \in V \setminus (S \cup \{k\}) \tag{92}$$

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Basic ops: Sums, Restrictions, Conditioning

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

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- Therefore, h can be used as a submodular surrogate for the "or" of multiple submodular functions.

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- Convex/Concave have many nice properties of composition (see Boyd & Vandenberghe, "Convex Optimization")
- 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.
- However, we have a number of forms of composition results that preserve submodularity, which we turn to next:

Grouping elements, set cover, and bipartite neighborhoods

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- In fact, all integral polymatroid functions can be obtained in g above for f a matroid rank function and $\{V_d\}$ appropriately chosen.

Concave composed with polymatroid

We also have the following composition property with concave functions:

Theorem

Given functions $f : 2^V \to \mathbb{R}$ *and* $g : \mathbb{R} \to \mathbb{R}$*, the composition* $h = f \circ g : 2^V \to \mathbb{R}$ *(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 $m : 2^V \to \mathbb{R}_+$, then $f : 2^V \to \mathbb{R}$ defined as $f(A) = g(m(A))$ is submodular*
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- However, Vondrak showed that a graphic matroid rank function over K_4 can't be represented in this fashion.

Weighted Matroid Rank Functions

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$$f(B) = \max \{|A| : A \subseteq B \text{ and } A \in \mathcal{I}\} \tag{101}$$

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- Take a 1-partition matroid with limit 1, we get the max function:

$$f(B) = \max_{b \in B} m(b) \tag{104}$$

Facility Location

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

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

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- 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:

$$f(A) = \sum_{i \in V} \max_{a \in A} w_{ai} \tag{106}$$

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

$$\begin{aligned} &I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B}) \\ &= H(X_A) + H(X_B) - H(X_{A \cup B}) - H(X_{A \cap B}) \geq 0 \end{aligned} \tag{108}$$

Submodular Generalized Dependence

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

$$f(A \cup B) = f(A) + f(B), \tag{44}$$

- and a notion of "conditional independence" , i.e., $A \perp\!\!\!\perp B | C$:

$$f(A \cup B \cup C) + f(C) = f(A \cup C) + f(B \cup C) \tag{45}$$

- and a notion of "dependence" (conditioning reduces valuation):

$$f(A|B) \triangleq f(A \cup B) - f(B) < f(A), \tag{46}$$

- and a notion of "conditional mutual information"

$$I_f(A; B|C) \triangleq f(A \cup C) + f(B \cup C) - f(A \cup B \cup C) - f(C) \geq 0$$

- and two notions of "information amongst a collection of sets":

$$I_f(S_1; S_2; \ldots; S_k) = \sum_{i=1}^{k} f(S_k) - f(S_1 \cup S_2 \cup \cdots \cup S_k) \tag{47}$$

$$I'_f(S_1; S_2; \ldots; S_k) = \sum_{A \subseteq \{1,2,\ldots,k\}} (-1)^{|A|+1} f(\bigcup_{j \in A} S_j) \tag{48}$$

Gaussian entropy, and the log-determinant function

Definition (differential entropy $h(X)$)

$$h(X) = -\int_S f(x) \log f(x) dx \tag{109}$$

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

$$h(X) = \log \sqrt{|2\pi e \mathbf{\Sigma}|} = \log \sqrt{(2\pi e)^n |\mathbf{\Sigma}|} \tag{110}$$

and in particular, for a variable subset A and a constant γ,

$$f(A) = h(X_A) = \log \sqrt{(2\pi e)^{|A|} |\mathbf{\Sigma}_A|} = \gamma |A| + \frac{1}{2} \log |\mathbf{\Sigma}_A| \tag{111}$$

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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?

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No, entropy functions must also satisfy the following:

Theorem (Yeung)

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

$$I(X; Y) = I(X; Y|Z) = 0 \tag{112}$$

implies that

$$I(X; Y|Z, U) \leq I(Z; U|X, Y) + I(X; Y|U) \tag{113}$$

where $I(\cdot; \cdot|\cdot)$ *is the standard Shannon mutual information function.*

- This is not required for all polymatroid-based conditional mutual information functions $I_f(\cdot; \cdot|\cdot)$.

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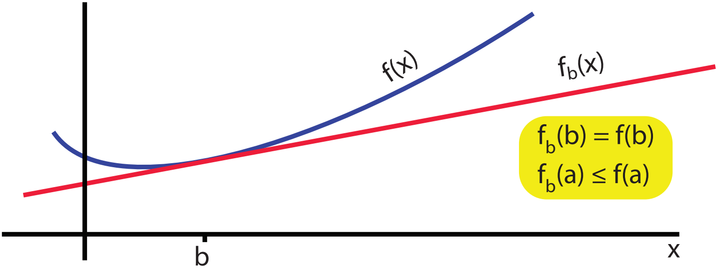
- Thanks to the properties of matrix algebra (e.g., determinants), DPPs are computationally extremely attractive and are now widely used in ML.

Outline: Part 3

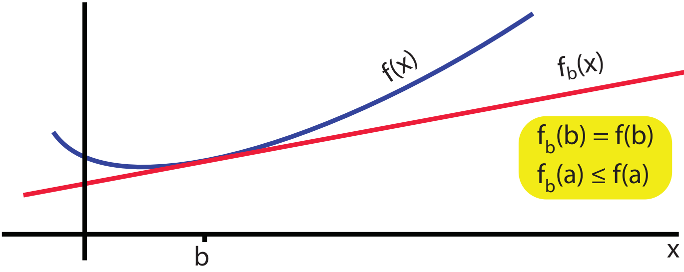
Convex Functions and Tight Subgradients



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

$$f(x) - f(b) \geq \langle f_b, x - b \rangle, \forall x. \tag{114}$$

Concave Functions and Tight Supergradients



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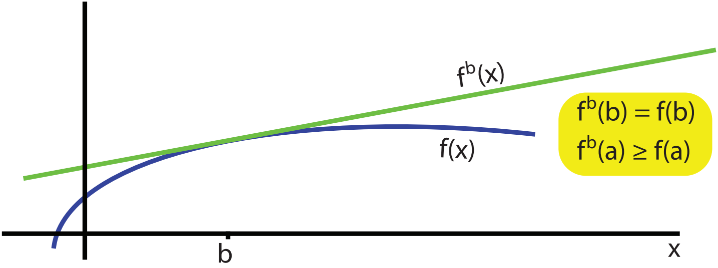
Convex Functions and Tight Subgradients



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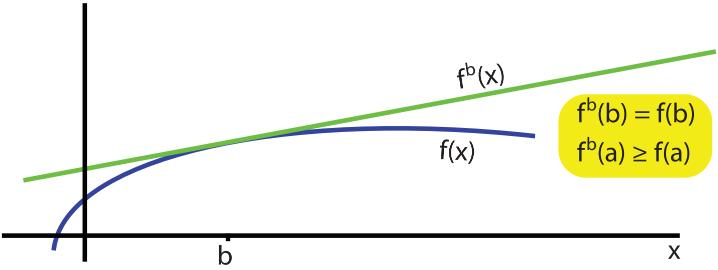

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- We have that $f(x)$ is concave, $f^b(x)$ is affine, and is a tight supergradient (tight at b, affine upper bound on $f(x)$).

Trivial additive upper/lower bounds

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

$$m_f(A) \leq f(A) \leq m^f(A) \tag{116}$$

where

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

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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:

$$\partial f(X) = \{x \in \mathbb{R}^V : \forall Y \subseteq V, x(Y) - x(X) \leq f(Y) - f(X)\} \quad (119)$$

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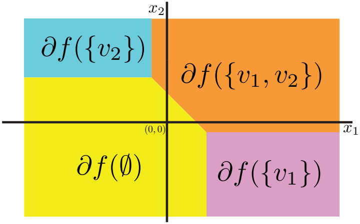

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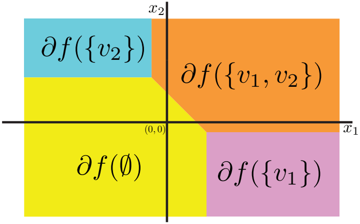

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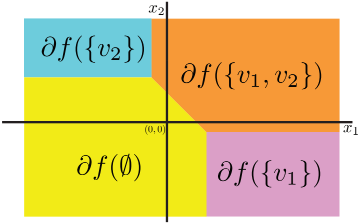

- Extreme points are easy to get via Edmonds's greedy algorithm:

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 $y(S_i \setminus S_{i-1}) = y(S_i) - y(S_{i-1}) = f(S_i) - f(S_{i-1})$.

The Submodular Subgradients (Fujishige 2005)

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

$$h^f_{Y,\sigma}(\sigma(i)) = \begin{cases} f(S_1^\sigma) & \text{if } i = 1 \\ f(S_i^\sigma) - f(S_{i-1}^\sigma) & \text{otherwise} \end{cases} .$$

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

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

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

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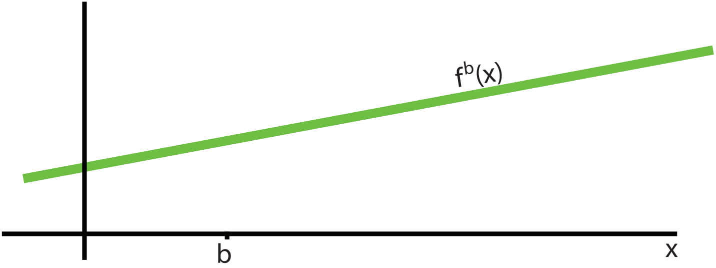

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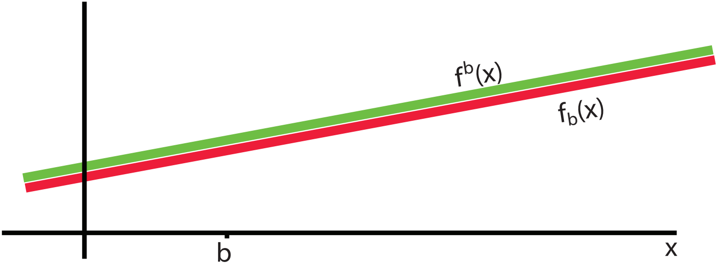

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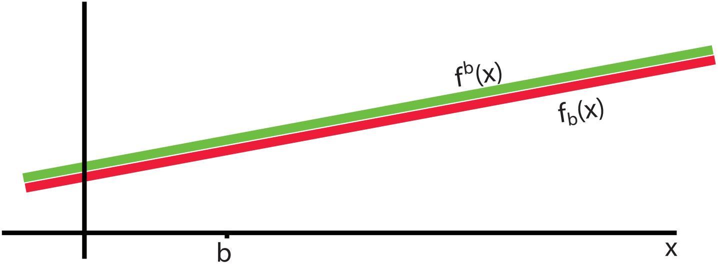

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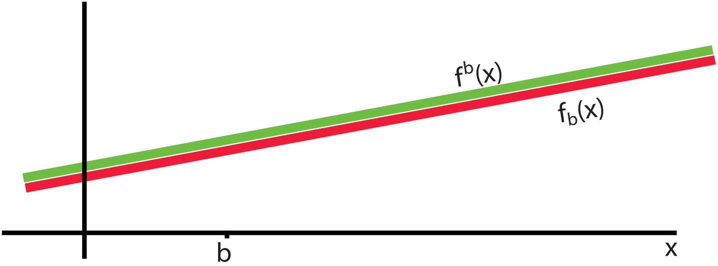

- If a continuous function has both a sub- and super-gradient at a point, then the function must be affine.
- What about discrete set functions?

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):

$$f(Y) \leq f(X) - \sum_{j \in X \setminus Y} f(j|X \setminus j) + \sum_{j \in Y \setminus X} f(j|X \cap Y),$$

$$f(Y) \leq f(X) - \sum_{j \in X \setminus Y} f(j|(X \cup Y) \setminus j) + \sum_{j \in Y \setminus X} f(j|X)$$

Recall that $f(A|B) \triangleq f(A \cup B) - f(B)$ is the gain of adding A in the context of B.

Submodular and Supergradients

- Using submodularity further, these can be relaxed to produce two tight modular upper bounds (Jegelka & Bilmes, 2011, Iyer & Bilmes 2013):

$$f(Y) \leq m^f_{X,1}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j|X \setminus j) + \sum_{j \in Y \setminus X} f(j|\emptyset),$$
$$f(Y) \leq m^f_{X,2}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j|V \setminus j) + \sum_{j \in Y \setminus X} f(j|X).$$

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

Optimizing difference of submodular functions

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., cooperative cut, submodular on edges, see Jegelka & Bilmes 2011)
- Opens the doors to first-order methods for discrete optimization.

Outline: Part 3

Continuous Extensions of Discrete Set Functions

- Any function $f : 2^V \to \mathbb{R}$ (equivalently $f : \{0,1\}^V \to \mathbb{R}$) can be extended to a continuous function $\tilde{f} : [0,1]^V \to \mathbb{R}$.

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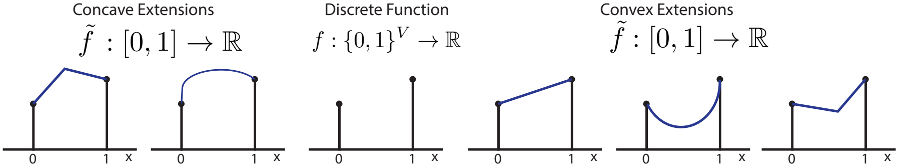
- In fact, any such discrete function defined on the vertices of the n-D hypercube $\{0,1\}^n$ has a variety of both convex and concave extensions tight at the vertices (Crama & Hammer). Example $n = 1$,



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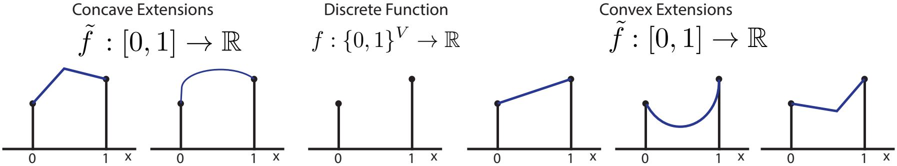

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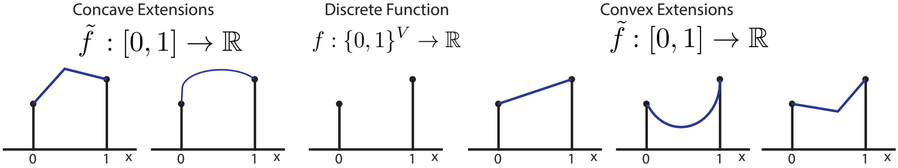

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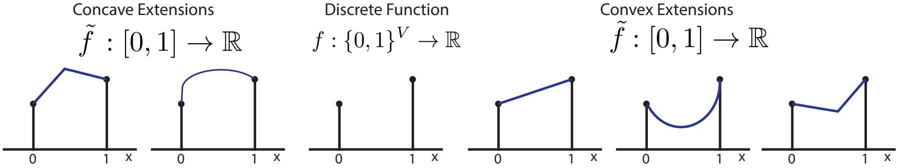

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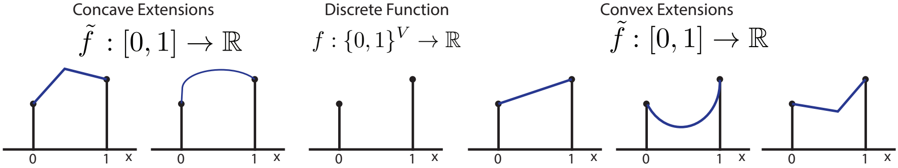

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  3. When are they useful for something practical?

A continuous extension of f

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

$$\tilde{f}(w)$$

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$$= w(v_m) f(V_m) + \sum_{i=1}^{m-1} (w(v_i) - w(v_{i+1})) f(V_i) \tag{123}$$

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

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

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

$$\text{for } i \in \{1, \dots, m\}, \quad \lambda_i = \begin{cases} w(v_i) - w(v_{i+1}) & \text{if } i < m \\ w(v_m) & \text{if } i = m \end{cases} \tag{128}$$

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

An extension of f

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

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- Note that $w = \sum_{i=1}^m \lambda_i \mathbf{1}_{V_i}$ 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 Extension, Submodularity and Convexity

Lovász proved the following important theorem.

Theorem

A function $f : 2^V \to \mathbb{R}$ is submodular iff its its continuous extension defined above as $\tilde{f}(w) = \sum_{i=1}^m \lambda_i f(V_i)$ with $w = \sum_{i=1}^m \lambda_i \mathbf{1}_{V_i}$ 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 $w^* \in \operatorname{argmin}\left\{\tilde{f}(w)|w \in [0,1]^V\right\}$ and let $A^* \in \operatorname{argmin}\{f(A)|A \subseteq V\}$.

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- Define chain $\{V_i^*\}$ based on descending sort of w^*. Then by greedy evaluation of L.E. we have

$$\tilde{f}(w^*) = \sum_i \lambda_i^* f(V_i^*) = f(A^*) = \min\{f(A)|A \subseteq V\} \tag{129}$$

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- Then we can show that, for each i s.t. $\lambda_i > 0$,

$$f(V_i^*) = f(A^*) \tag{130}$$

So such $\{V_i^*\}$ are also minimizers.

Duality: convex minimization of L.E. and min-norm alg.

- Let f be a submodular function with $\tilde{f}$ it's Lovász extension. Then the following two problems are duals:

$$\underset{w \in \mathbb{R}^V}{\text{minimize}} \; \tilde{f}(w) + \frac{1}{2}\|w\|_2^2 \tag{131}$$

$$\begin{aligned} &\text{maximize} && -\|x\|_2^2 && \text{(132a)} \\ &\text{subject to} && x \in B_f && \text{(132b)} \end{aligned}$$

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.

- Minimum-norm point algorithm (Fujishige-1991, Fujishige-2005, Fujishige-2011, Bach-2013) is essentially an active-set procedure for quadratic programming, and uses Edmonds's greedy algorithm to make it efficient.
- Unknown worst-case running time, although in practice it usually performs quite well.

Other applications of Lovász Extension

- "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).

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Definition

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

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

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- 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.

Outline: Part 3

Submodular: Concave? Convex? Neither? Both?

- 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 $f : 2^V \to \mathbb{R}$ be a submodular function and $g : 2^V \to \mathbb{R}$ be a supermodular function such that for all $A \subseteq V$,

$$g(A) \leq f(A) \tag{134}$$

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

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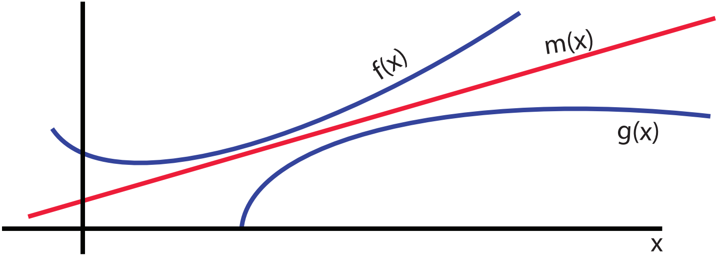
- Compare to convex/concave case.



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- **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 $A, B \in \operatorname{argmin}_{A \subseteq V} f(A)$ then $A \cup B \in \operatorname{argmin}_{A \subseteq V} f(A)$ and $A \cap B \in \operatorname{argmin}_{A \subseteq V} f(A)$

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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 $j, k \in V$

$$f(X + j) + f(X + k) \geq f(X + j + k) + f(X) \tag{136}$$

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- With the gain defined as $\nabla_j(X) = f(X + j) - f(X)$, 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:

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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

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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.

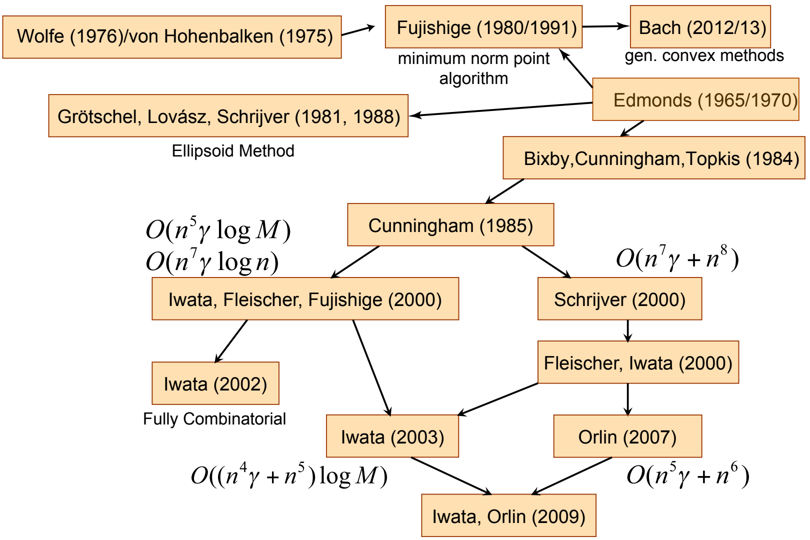
Outline: Part 3

Submodular Optimization Results Summary

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

SFM Summary (modified from S. Iwata's slides)

General Submodular Function Minimization



Theoretical Results: Constrained Submodular Min

$$\text{minimize} \quad f(S) : S \in \mathcal{S} \tag{138}$$

- Constraint set $\mathcal{S}$ might either be cuts, paths, matchings, cardinality constraints, etc.

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- In general, how good are the algorithms? Depends on the constraint:

Constraint:	**MMin**	**EA**	**Lower bound**
trees/matchings	n	$\sqrt{m}$	n
cuts	m	$\sqrt{m}$	$\sqrt{m}$
paths	n	$\sqrt{m}$	$n^{2/3}$
cardinality	k	$\sqrt{n}$	$\sqrt{n}$

Goel et al (09), Goemans et al (2009), Jegelka-Bilmes (11) ...

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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:

Algorithm 2: The Greedy Algorithm

Set $S_0 \leftarrow \emptyset$;
for $i \leftarrow 0 \ldots |V| - 1$ **do**
  Choose v_i as follows: $v_i = \left\{ \operatorname{argmax}_{v \in V \setminus S_i} f(S_i \cup \{v\}) \right\}$;
  Set $S_{i+1} \leftarrow S_i \cup \{v_i\}$;

- has a strong guarantee:

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

Constraint	Approximation	Hardness	Technique
$\|S\| \leq k$	$1 - 1/e$	$1 - 1/e$	greedy
matroid	$1 - 1/e$	$1 - 1/e$	multilinear ext.
$O(1)$ knapsacks	$1 - 1/e$	$1 - 1/e$	multilinear ext.
k matroids	$k + \epsilon$	$k/\log k$	local search
k matroids and $O(1)$ knapsacks	$O(k)$	$k/\log k$	multilinear ext.

Nonmonotone Maximization

Constraint	Approximation	Hardness	Technique
Unconstrained	$1/2$	$1/2$	combinatorial
matroid	$1/e$	0.48	multilinear ext.
$O(1)$ knapsacks	$1/e$	0.49	multilinear ext.
k matroids	$k + O(1)$	$k/\log k$	local search
k matroids and $O(1)$ knapsacks	$O(k)$	$k/\log k$	multilinear ext.

, compiled by J. Vondrak

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Constraints	Method	Approximation bound	Lower bound
Cardinality	Greedy	$\frac{1}{\kappa_f}(1 - e^{-\kappa_f})$	$\frac{1}{\kappa_f}(1 - e^{-\kappa_f})$
Matroid	Greedy	$1/(1 + \kappa_f)$	$\frac{1}{\kappa_f}(1 - e^{-\kappa_f})$
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Knapsack	Greedy	$1-1/e$	$1-1/e$

- Improve curvature independent bounds when $\kappa_f < 1$.

Curvature Dependent Bounds for Constraint Minimization

- Minimization bounds take the form:

$$f(\widehat{X}) \leq \frac{|X^*|}{1 + (|X^*| - 1)(1 - \kappa_f(X^*))} f(X^*) \leq \frac{1}{1 - \kappa_f(X^*)} f(X^*)$$

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Constraint	Semigradient	Curvature-Ind.	Lower bound
Card. LB	$\frac{k}{1+(k-1)(1-\kappa_f)}$	$\theta(n^{1/2})$	$\tilde{\Omega}(\frac{\sqrt{n}}{1+(\sqrt{n}-1)(1-\kappa_f)})$
Spanning Tree	$\frac{n}{1+(n-1)(1-\kappa_f)}$	$\theta(n)$	$\tilde{\Omega}(\frac{n}{1+(n-1)(1-\kappa_f)})$
Matchings	$\frac{n}{2+(n-2)(1-\kappa_f)}$	$\theta(n)$	$\tilde{\Omega}(\frac{n}{1+(n-1)(1-\kappa_f)})$
s-t path	$\frac{n}{1+(n-1)(1-\kappa_f)}$	$\theta(n^{2/3})$	$\tilde{\Omega}(\frac{n^{2/3}}{1+(n^{2/3}-1)(1-\kappa_f)})$
s-t cut	$\frac{m}{1+(m-1)(1-\kappa_f)}$	$\theta(n^{2/3})$	$\tilde{\Omega}(\frac{n^{2/3}}{1+(n^{2/3}-1)(1-\kappa_f)})$
s-t cut	$\frac{m}{1+(m-1)(1-\kappa_f)}$	$\theta(\sqrt{n})$	$\tilde{\Omega}(\frac{\sqrt{n}}{1+(\sqrt{n}-1)(1-\kappa_f)})$

Summary of results for constrained minimization (Iyer, Jegelka, Bilmes, 2013).

Outline: Part 3

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-I", 1978
- Lovász's paper, "Submodular functions and convexity", from 1983.

Classic 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.

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!
- Andreas Krause's web page http://submodularity.org.
- Stefanie Jegelka and Andreas Krause's ICML 2013 tutorial http://techtalks.tv/talks/submodularity-in-machine-learning-new-directions-part-i/58125/
- 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

The End: Thank you!