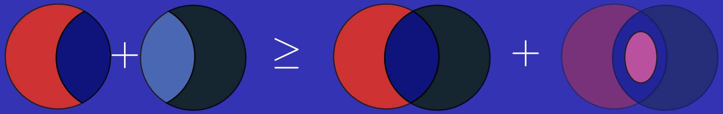

Submodularity in Machine Learning Applications

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Departments of Electrical Engineering
& Computer Science and Engineering
University of Washington, Seattle
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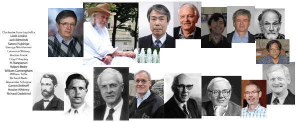
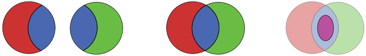
Monday, January 26th, 2015

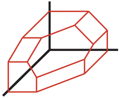
Goals of the Tutorial



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

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





- Intuitive sense for and familiarity with submodular functions.
- Survey a variety of applications of submodularity in machine learning and beyond.
- Realize why submodularity is important, worthy of study, and should be a standard tool in the tool chest of ML and AI.

On The Submodularity Tutorial

- The definition of submodularity is fairly simple: given a finite ground set V, a function $f : 2^V \to \mathbb{R}$ is said to be submodular if

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V, \tag{1}$$

we will revisit this in many forms today

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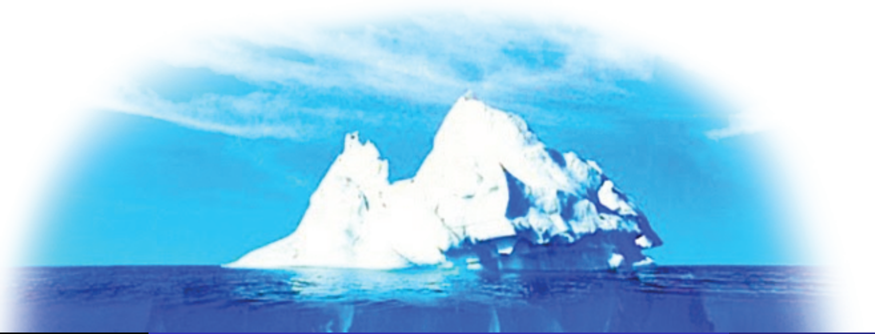
we will revisit this in many forms today

- The definition, however, is only the tip of the iceberg — this simple definition can lead to great mathematical and practical richness.



Overall Outline of Tutorial

1. Part 1: Basics, Examples, and Properties
2. Part 2: Applications

Outline of Part 1: Basics, Examples, and Properties

Outline of Part 2: Submodular Applications in ML

5. Submodular Applications in Machine Learning
   - Where is submodularity useful?
6. As a model of diversity, coverage, span, or information
7. As a model of cooperative costs, complexity, roughness, and irregularity
8. As a Parameter for an ML algorithm
9. Itself, as a target for learning
10. Surrogates for optimization and analysis
11. Reading
    - Refs

Acknowledgments

Thanks to the following people (former & current students, and current colleagues):

Mukund Narasimhan, Hui Lin, Andrew Guillory, Stefanie Jegelka, Sebastian Tschiatschek, Kai Wei, Yuzong Liu, Rishabh Iyer, Jennifer Gillenwater, Yoshinobu Kawahara, Katrin Kirchhoff, Carlos Guestrin, & Bill Noble.

Outline: Part 1

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:

$A = \{$

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Ex: $f(A) = 1$

Sets and set functions

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Ex: $f(B) = 6$

Simple Costs

- Grocery store: finite set of items V that one can purchase.

Simple Costs

FUNNYRECEIPTS.com

TRADER JOE'S

[redacted]

Store [redacted]

OPEN 9:00AM TO 10:00PM DAILY

TJ'S PLAIN SOY MILK	1.69
EGGS BROWN	1.79
VEG TEMPEH ORGANIC 3 GRAIN	1.69
VEG SOY CHORIZO	1.99
PLAIN ORGANIC NONFAT YOGURT 32	2.99
LARGE BABY NON TAXABLE	1.99
GROCERY	0.49
3 @ 3 FOR 0.49	
SUBTOTAL	$12.63
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$$m(A) = \sum_{a \in A} m(a), \tag{2}$$

the sum of individual item costs (no two-for-one discounts).

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- This is known as a modular function.

Discounted Costs

- Let f be the cost of purchasing a set of items (consumer cost).

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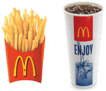
$f($  $) + f($  $) \geq f($  $) + f($  $)$

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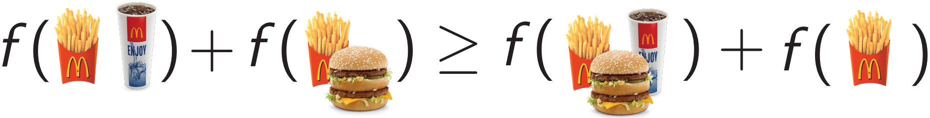

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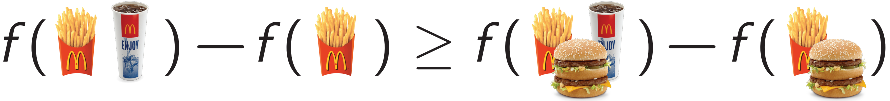

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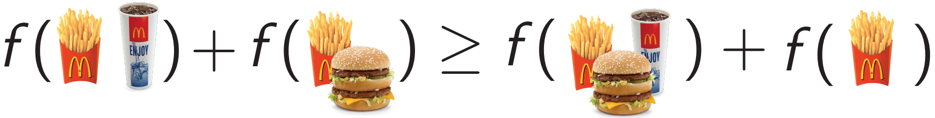

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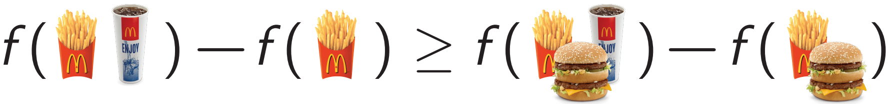

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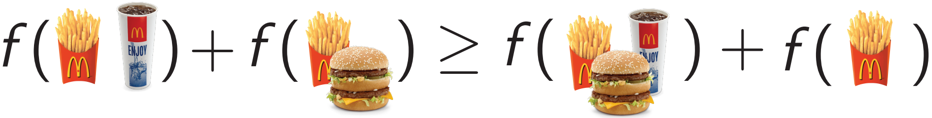

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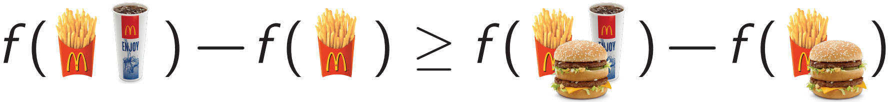

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Shared Fixed Costs (interacting costs)

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- But $f(\{v_1, v_2\}) = c_d + c_m + c_h < 2c_d + c_m + c_h$ since c_d (driving) is a shared fixed cost.
- Shared fixed costs are submodular: $f(v_1) + f(v_2) \geq f(v_1, v_2) + f(\emptyset)$

Supply Side Economies of scale

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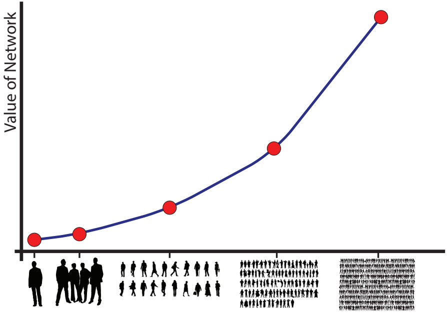
- So diminishing returns (a submodular function) would be a good model.

Demand side Economies of Scale: Network Externalities

- Value of a network to a user depends on the number of other users in that network. External use benefits internal use.



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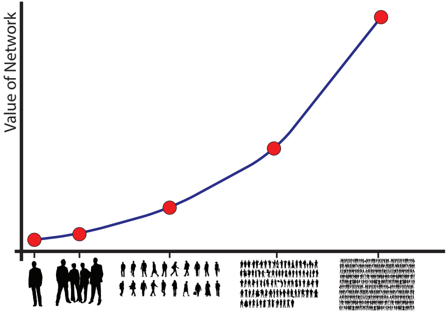

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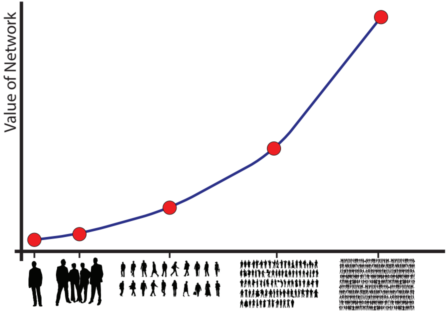

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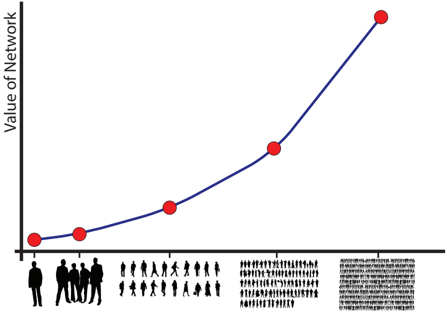

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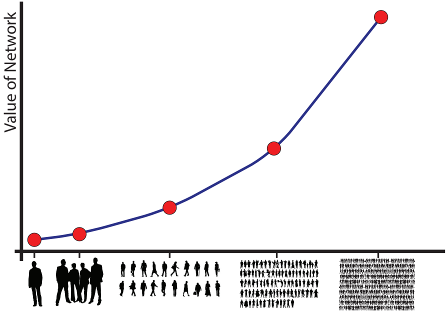

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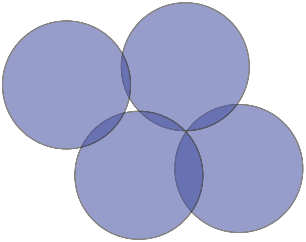
- Ex: durable goods (e.g., a car or phone), software (facebook, smartphone apps), and technology-specific human capital investment (e.g., education in a skill).
- Let V be a set of goods, A a subset and $v \notin A$. Incremental gain of good $f(A+v) - f(A)$ gets larger as size of market A grows. This is known as a supermodular function.

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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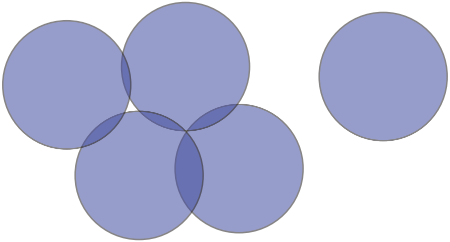

Area of A along with with v:

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

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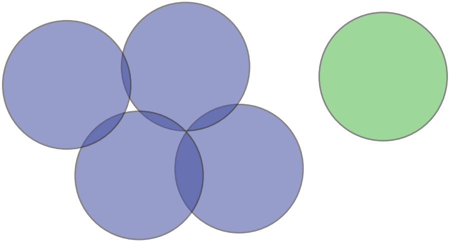
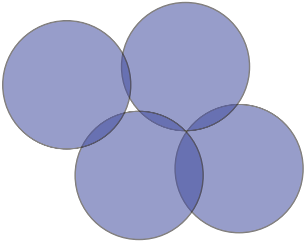


Gain (value) of v in context of A:

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

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

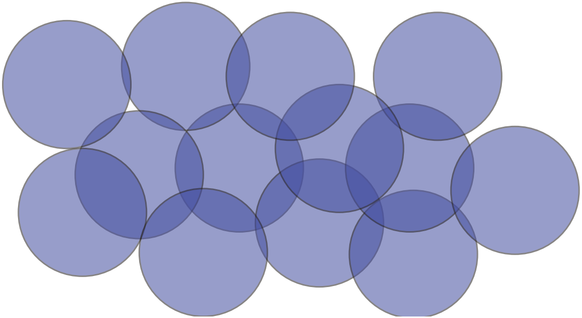
Area of the union of areas indexed by A



Area of A once again.

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

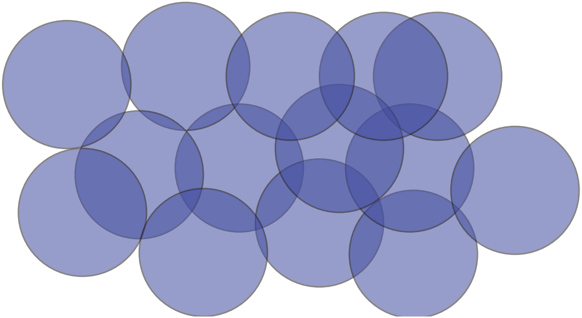
Area of the union of areas indexed by A



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

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

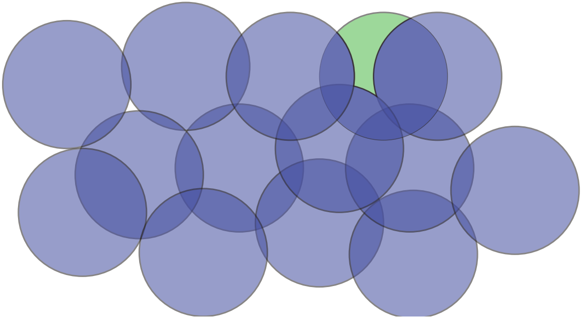
Area of the union of areas indexed by A



Area of B now also including v:

$$f(B \cup \{v\})$$

Area of the union of areas indexed by A



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

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

So benefit of v in the context of A is greater than the benefit of v in the context of $B \supseteq A$.

Example Submodular: Number of Colors of Balls in Urns

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

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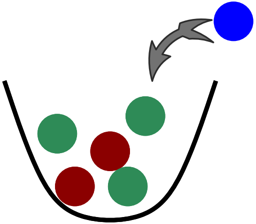
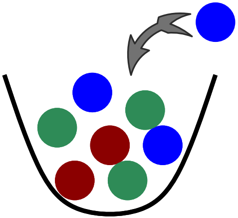


Initial value: 2 (colors in urn).
New value with added blue ball: 3



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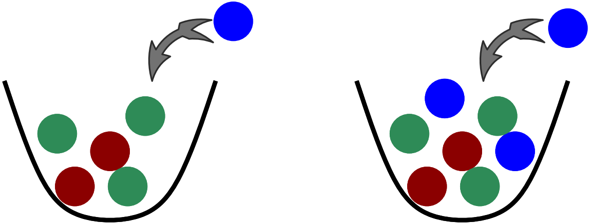

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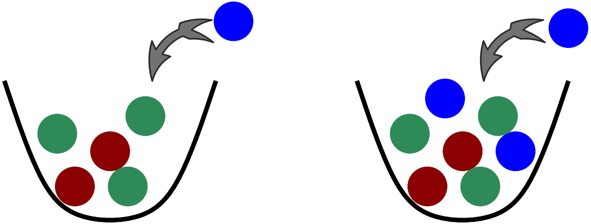

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- Thus, f is submodular.

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:

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{3}$$

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:

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \tag{4}$$

- Incremental “value”, “gain”, or “cost” of v decreases (diminishes) as the context in which v is considered grows from A to B.

Two Equivalent Supermodular Definitions

Definition (submodular)

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

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Definition (supermodular (improving returns))

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

$$f(A \cup \{v\}) - f(A) \leq f(B \cup \{v\}) - f(B) \qquad (6)$$

- The incremental "value", "gain", or "cost" of v increases (improves) as the context in which v is considered grows from A to B.
- A function f is submodular iff $-f$ is supermodular.

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- $f(x) : \{0,1\}^V \to \mathbb{R}$ is a pseudo-Boolean function. A submodular function is a special case.
- Also, it is a bit tedious to write $A \cup \{v\}$ so we instead occasionally write $A + v$.

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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A function $f : 2^V \rightarrow \mathbb{R}$ is said to be monotone nondecreasing if:

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- Thus, a polymatroid function is non-negative since $f(A) \geq f(\emptyset) = 0$.
- Any submodular function can be written as a difference between a polymatroid function and a modular function. I.e., for any submodular f, we can write:

$$f(A) = f_p(A) - m(A) \tag{12}$$

where f_p is a polymatroid function and m is a modular function.

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- superadditive means that $f(A) + f(B) \leq f(A \cup B)$.

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$$f(A \cup \{j\}) - f(A) \triangleq \rho_j(A) \tag{14}$$

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- We'll use $f(j|A)$. Also, $f(A|B) = f(A \cup B) - f(B)$.
- Submodularity's diminishing returns stated using gain:

$$\forall j,\ f(j|A) \text{ is a monotone non-increasing function of } A. \tag{19}$$

True since submodularity means $f(j|A) \geq f(j|B)$ whenever $A \subseteq B$.

Recap: Basic Submodular/Supermodular Definitions

- Set function: map from any subset A of a ground set V to a real number:

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

- Submodular functions

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

$$\text{for all } A \subseteq B \subseteq V, v \notin B, \quad f(v|A) \geq f(v|B)$$

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"What's in a name? That which we call a submodular function, by any other name, would optimize as quickly"

Outline: Part 1

Set Cover and Maximum Coverage

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- $f(A) = \mu(\bigcup_{i=1}^k U_{a_i})$ is still submodular if we take $U \subseteq \mathbb{R}^\ell$ and $U_i \subseteq U$ and $\mu(\cdot)$ is an additive measure (e.g., the Lebesgue measure).

Vertex and Edge Covers

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- 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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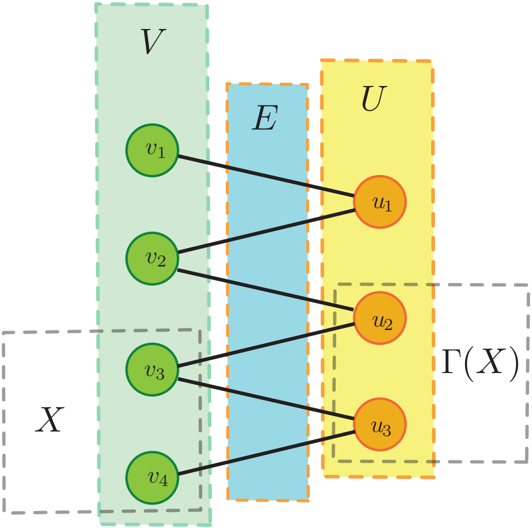
Bipartite Neighborhood Function

- Let $G = (V, U, E, w)$ be a weighted bipartite graph, where V (resp. U) is a set of left (resp. right) nodes, E is a set of edges, and $w : 2^U \to \mathbb{R}_+$ is a modular function on right nodes.



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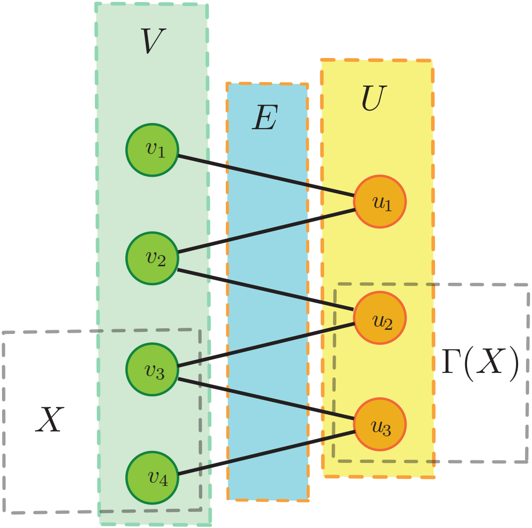

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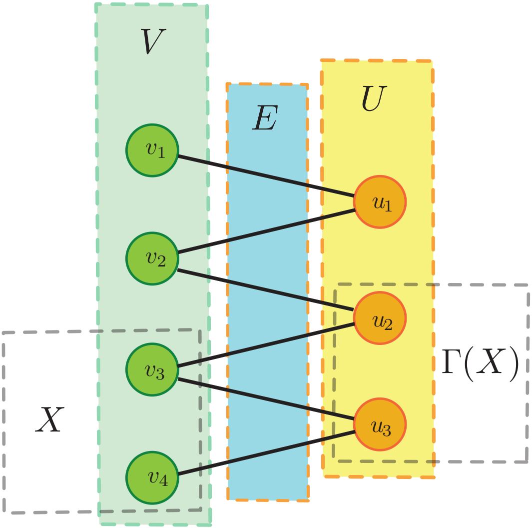

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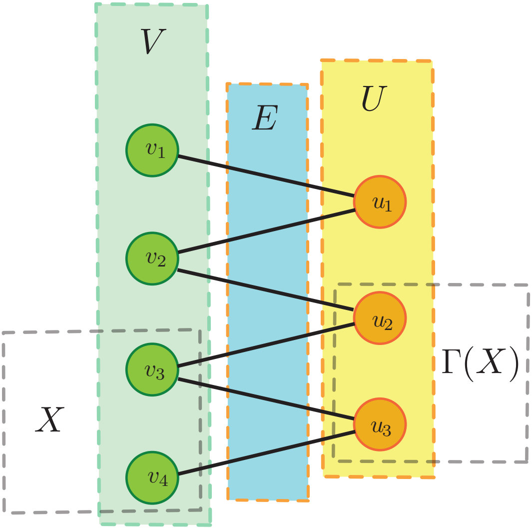
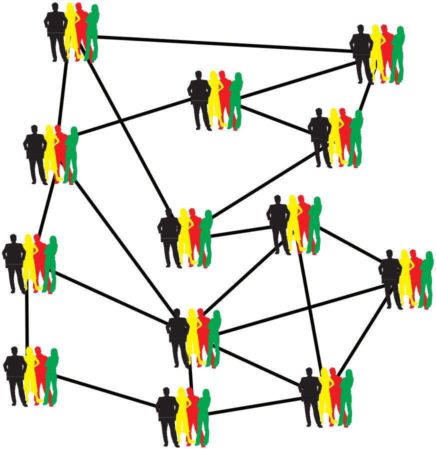


Facility/Plant Location (uncapacitated)

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



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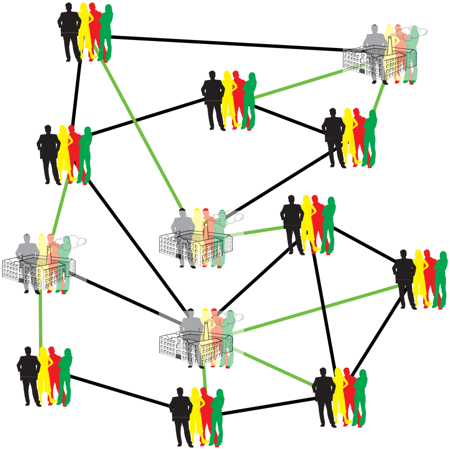

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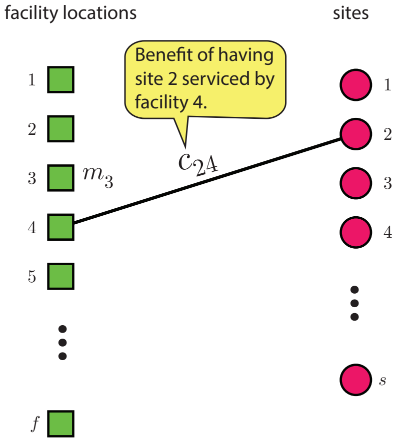
- We can model this with a weighted bipartite graph $G = (F, S, E, c)$ where F is set of possible factory/plant locations, S is set of sites needing service, E are edges indicating (factory,site) service possibility pairs, and $c : E \to \mathbb{R}_+$ is the benefit of a given pair.
- Facility location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

$$f(A) = \sum_{i \in F} \max_{j \in A} c_{ij}. \qquad (32)$$



Square root of cardinality

- Define a function $f : 2^V \to \mathbb{R}_+$ as follows:

  $$f(A) = \sqrt{|A|},$$

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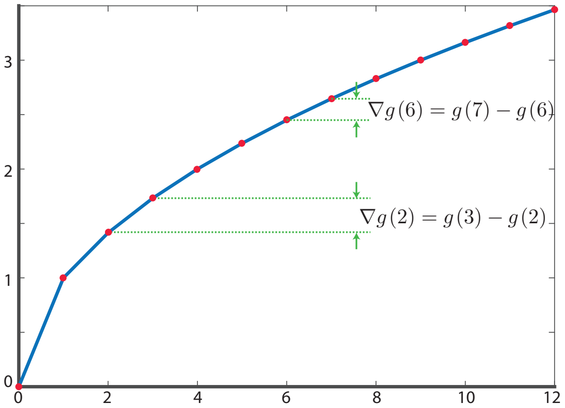

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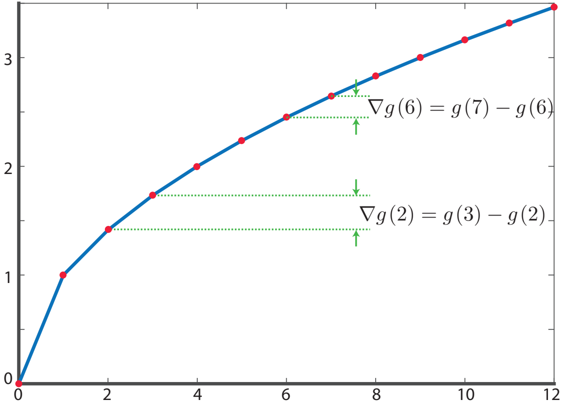

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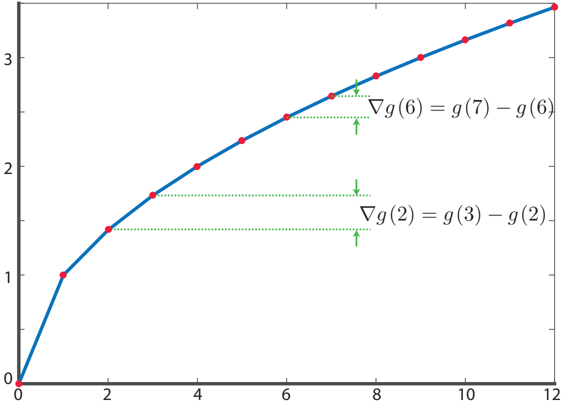

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- $\nabla g(i) > \nabla g(j)$ for $j > i$ by concavity, so f is a submodular function.

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- Very large class of functions, including graph cut, bipartite neighborhoods, set cover (Stobbe & Krause).
- However, Vondrak showed that a simple matroid rank function (defined below) which is submodular is not a member.

Example: Rank function of a matrix

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

$$\mathbf{X} = \begin{pmatrix} 1 & 2 & 3 & 4 & & m \\ | & | & | & | & & | \\ x_1 & x_2 & x_3 & x_4 & \dots & x_m \\ | & | & | & | & & | \end{pmatrix} \tag{35}$$

- 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

Ex: a 4×8 matrix with column index set $V = \{1, 2, 3, 4, 5, 6, 7, 8\}$.

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- Let $A = \{1, 2, 3\}$, $B = \{3, 4, 5\}$, $C = \{6, 7\}$, $A_r = \{1\}$, $B_r = \{5\}$.
- Then $r(A) = 3$, $r(B) = 3$, $r(C) = 2$.
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=
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\begin{pmatrix} | & | & | & | & | & | & | & | \\ x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \\ | & | & | & | & | & | & | & | \end{pmatrix} \end{array}
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$$
\begin{array}{c}
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\begin{array}{c}
\begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{matrix} \\
\begin{pmatrix}
0 & 2 & 2 & 3 & 0 & 1 & 3 & 1 \\
0 & 3 & 0 & 4 & 0 & 0 & 2 & 4 \\
0 & 0 & 0 & 0 & 3 & 0 & 0 & 5 \\
2 & 0 & 0 & 0 & 0 & 0 & 0 & 5
\end{pmatrix}
\end{array}
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| & | & | & | & | & | & | & | \\
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- $6 = r(A) + r(B) > r(A \cup B) + r(A \cap B) = 5$

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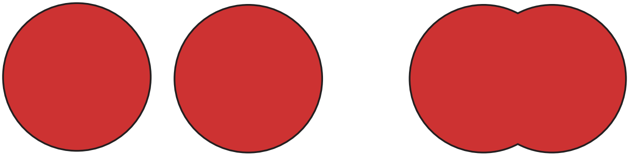
$$r(A) \quad + \quad r(B) \qquad \geq \qquad r(A \cup B)$$



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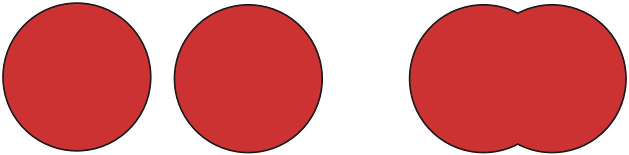
$$r(A) \quad + \quad r(B) \qquad \geq \qquad r(A \cup B)$$



- If some of the dimensions spanned by A overlap some of the dimensions spanned by B (i.e., if $\exists$ common span), then that area is counted twice in $r(A) + r(B)$, so the inequality will be strict.

Rank function of a matrix

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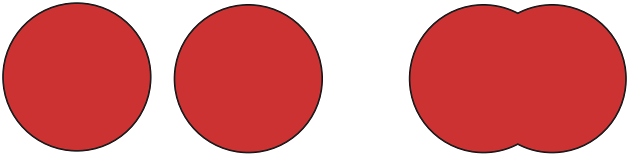

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- Any function where the above inequality is true for all $A, B \subseteq V$ is called subadditive.

Rank functions of a matrix

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

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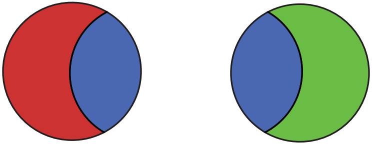

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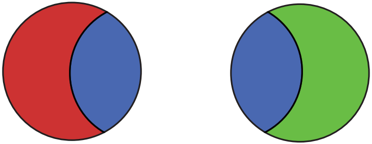

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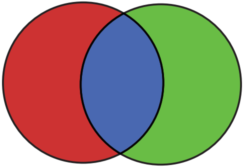

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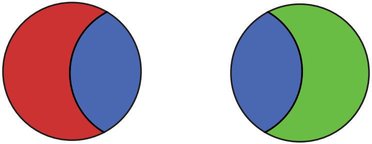

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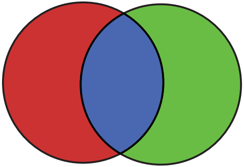

- Thus, we have subadditivity: $r(A) + r(B) \geq r(A \cup B)$. Can we add more to the r.h.s. and still have an inequality? Yes.

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).

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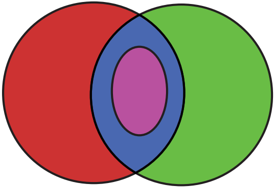

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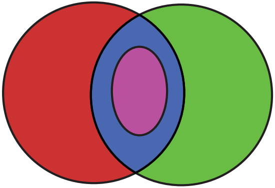

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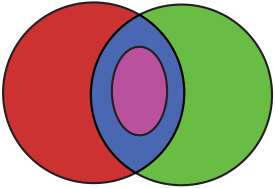

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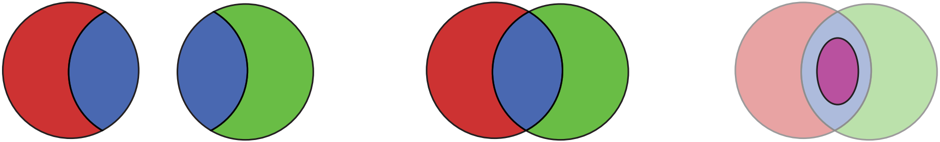
- More generally, common information (blue) is "more" (no less) than information within common index (magenta).

The Venn and Art of Submodularity

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



Matroid

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A set system $(V, \mathcal{I})$ is an independence system if

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(I3) $\forall I, J \in \mathcal{I}$, with $|I| = |J| + 1$, then $\exists\, x \in I \setminus J$ s.t. $J \cup \{x\} \in \mathcal{I}$.

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We can a bit more formally define the rank function this way.

Definition

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Lemma

The rank function $r : 2^V \to \mathbb{Z}_+$ of a matroid is submodular, that is $r(A) + r(B) \geq r(A \cup B) + r(A \cap B)$

Example: Partition Matroid

Ground set of objects, $V = \Bigg\{$

$\Bigg\}$

Example: Partition Matroid

Partition of V into six blocks, $V_1, V_2, \dots, V_6$

Example: Partition Matroid

Limit associated with each block, $\{k_1, k_2, \ldots, k_6\}$

Example: Partition Matroid

Independent subset but not maximally independent.

Example: Partition Matroid

Maximally independent subset, what is called a base.

Example: Partition Matroid

Not independent since over limit in set six.

Information and Complexity functions

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- This was realized as early as 1954 (McGill) but it was not called submodularity then.

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Definition (differential entropy $h(X)$)

$$h(X) = -\int_S f(x) \log f(x) dx \tag{38}$$

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

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- Hence, logdet function $f(A) = \log \det(\Sigma_A)$ is submodular.

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  is a submodular function.
- This covers not only logdet, but also generalizes and shows submodularity of quantum entropy (used in quantum physics) with $g(x) = x \ln x$ and other functions such as $g(x) = x^p$ for $0 < p < 1$.

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No, entropy functions must also satisfy the following:

Theorem (Yeung, 1998)

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

$$I(X;Y) = I(X;Y|Z) = 0 \tag{42}$$

implies that

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

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- Open: Are all polymatroid functions spectral functions of a matrix?

Outline: Part 1

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- Are there other properties, besides their ubiquity, that are useful?
- Also, as this tutorial ultimately will cover, they seem to be useful for a variety of problems in machine learning.

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- Without knowing anything about f, it takes 2^n queries to be able to offer any quality assurance on a candidate solution. Otherwise, solution can be unboundedly poor.

Discrete Optimization

- We are given a finite set of objects V of size $n = |V|$.
- There are 2^n such subsets (denoted 2^V) of the form $A \subseteq V$.
- We have a function $f : 2^V \to \mathbb{R}$ that judges the quality (or value, or cost, or etc.) of each subset. $f(A) =$ some real number.
- Unconstrained minimization & maximization:

$$\min_{X \subseteq V} f(X) \quad (44) \qquad\qquad \max_{X \subseteq V} f(X) \quad (45)$$

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- When f is submodular, Eq. (44) is polytime, and Eq. (45) is constant-factor approximable.

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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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- This yields a chain of sets $\emptyset = S_0 \subset S_1 \subset S_2 \subset \cdots \subset S_n = V$, with $|S_i| = i$, having very nice properties.

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- The greedy chain also addresses the problem:

$$\text{minimize } |A| \text{ subject to } f(A) \geq \alpha \tag{48}$$

i.e., the submodular set cover problem (approximation factor $O(\log(\max_{s \in V} f(s)))$.

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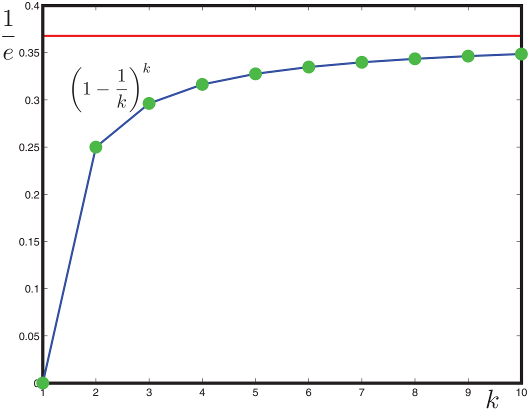

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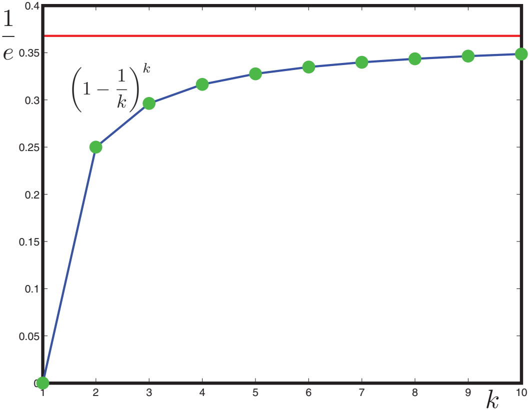

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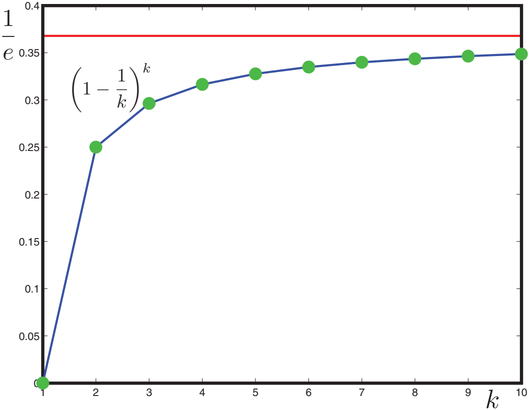

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- Frankenstein Cuts (Kawahara, Iyer, & B): $h(X) = f(X) + g(X)$ where f is submodular and g is a supermodular tree (submodular optimization for f, dynamic programming for g).

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  - Non-submodular problems can be analyzed via submodularity.

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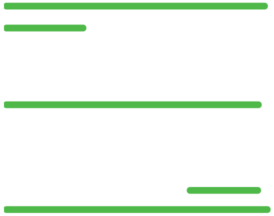

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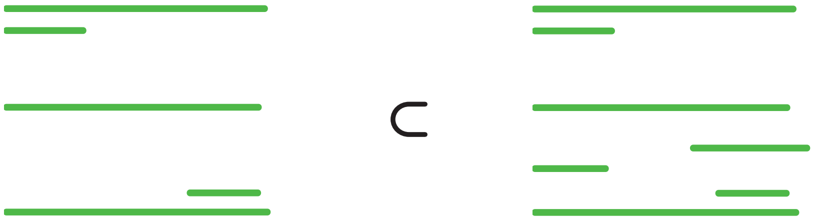

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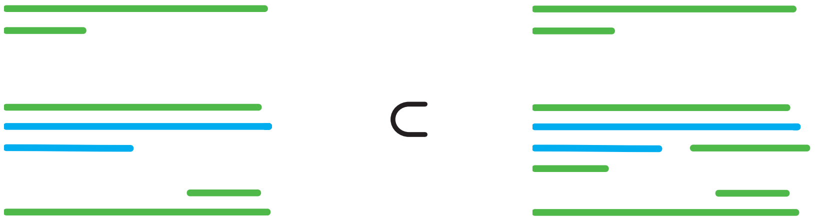

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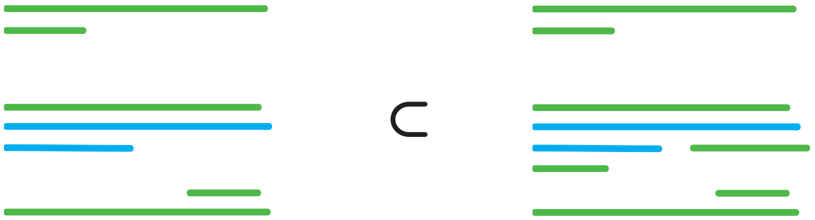

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Image collections

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

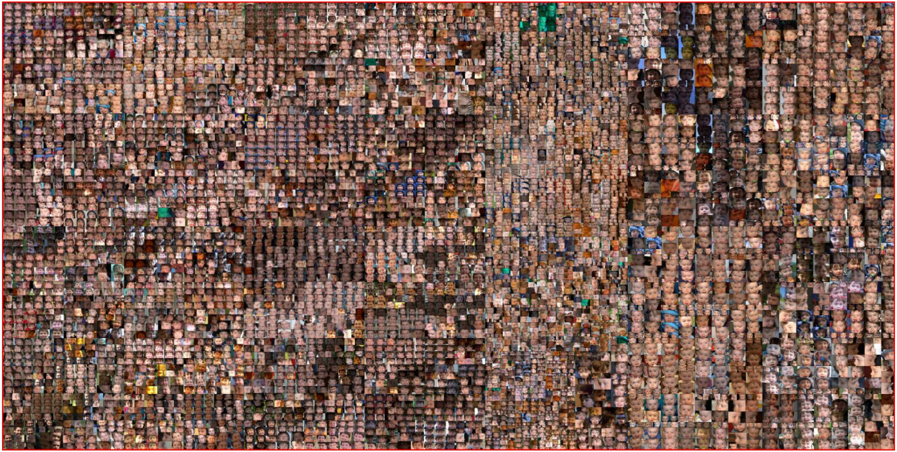

Image Summarization

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 (Tschiatschek, Iyer, & B, NIPS 2014).

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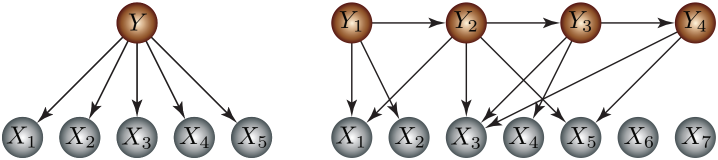
$$I(Y; X_A) = \sum_{y, x_A} \Pr(y, x_A) \log \frac{\Pr(y, x_A)}{\Pr(y) \Pr(x_A)} = H(Y) - H(Y|X_A) \quad (51)$$

$$= H(X_A) - H(X_A|Y) = H(X_A) + H(Y) - H(X_A, Y) \quad (52)$$

Feature Selection in Pattern Classification: Naïve Bayes

- Naïve Bayes property: $X_A \perp\!\!\!\perp X_B | Y$ for all A, B.



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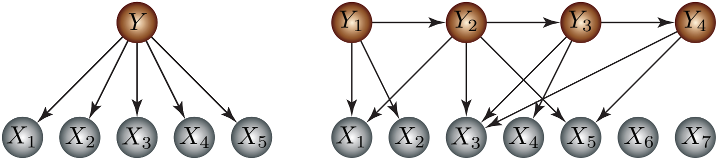

- When $X_A \perp\!\!\!\perp X_B | Y$ for all A, B (the Naïve Bayes assumption holds), then

$$f(A) = I(Y; X_A) = H(X_A) - H(X_A|Y) = H(X_A) - \sum_{a \in A} H(X_a|Y) \tag{53}$$

is submodular (submodular minus modular).

Variable Selection in Pattern Classification

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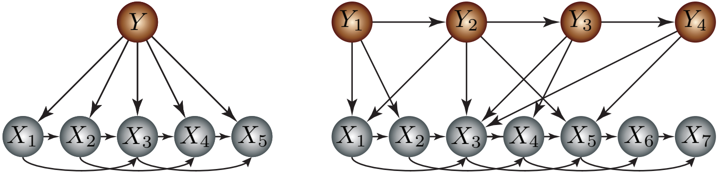

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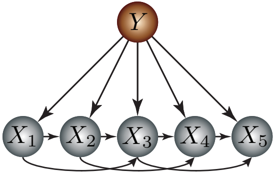

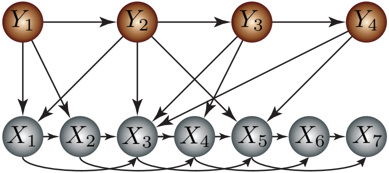

- $f(A)$ naturally expressed as a difference of two submodular functions

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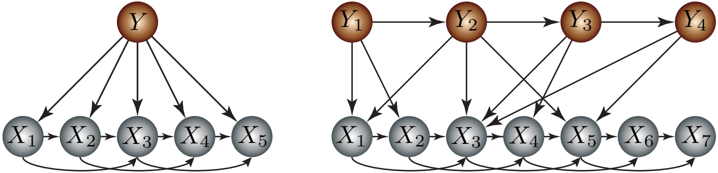

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- Alternatively, when Naïve Bayes assumption is false, we can make a submodular approximation (Peng-2005). E.g., functions of the form:

$$f(A) = \sum_{a \in A} I(X_a; Y) - \lambda \sum_{a,a' \in A} I(X_a; X_{a'}|Y) \tag{55}$$

where $\lambda \geq 0$ is a tradeoff constant.

Variable Selection: Linear Regression Case

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- $R^2_{Z,A}$'s minimizing parameters, for a given A, can be easily computed ($R^2_{Z,A} = {b_A}^\intercal (C_A^{-1})^\intercal b_A$ when Var$Z = 1$, where $b_i = \text{Cov}(Z, X_i)$ and $C = E[(X - E[X])^\intercal (X - E[X])]$ is the covariance matrix).

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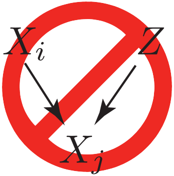
- When there are no "suppressor" variables (essentially, no v-structures that converge on X_j with parents X_i and Z), then

$$f(A) = R^2_{Z,A} = b_A{}^\intercal (C_A^{-1})^\intercal b_A \tag{57}$$



is a polymatroid function (so the greedy algorithm gives the $1 - 1/e$ guarantee). (Das&Kempe).

Data Subset Selection

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- 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

  $v =$ "Whenever I go to New York City, I visit the New York City museum."

  then $m_{\text{'the'}}(v) = 1$ while $m_{\text{'New York City'}}(v) = 2$.

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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 $p = \{p_u\}_{u \in U}$ be a desired 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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$$\bar{m}_u(X) = \frac{m_u(X)}{\sum_{u' \in U} m_{u'}(X)} = \frac{m_u(X)}{m(X)} \tag{60}$$

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- Consider the KL-divergence between these two distributions:

$$D(p||\{\bar{m}_u(X)\}_{u \in U}) = \sum_{u \in U} p_u \log p_u - \sum_{u \in U} p_u \log(\bar{m}_u(X)) \tag{61}$$

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

$$= -H(p) + \log m(X) - \sum_{u \in U} p_u \log(m_u(X)) \tag{62}$$

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- Alternatively, if we define (Shinohara, 2014)

$$g(X) \triangleq \log m(X) - D(p||\{\bar{m}_u(X)\}) = \sum_{u \in U} p_u \log(m_u(X)) \quad (64)$$

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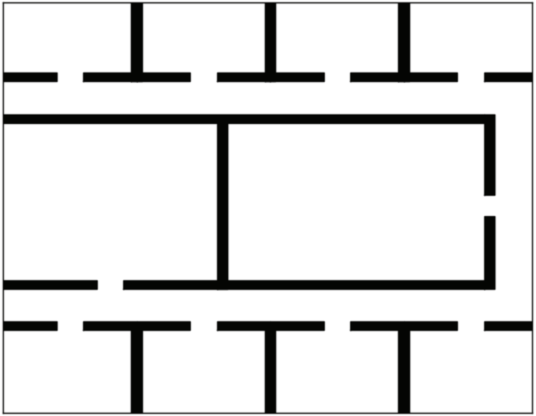
- Environment could be a floor of a building, water network, monitored ecological preservation.

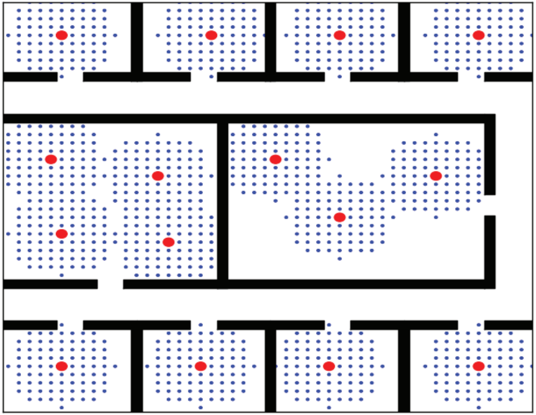
Sensor Placement within Buildings

- 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.



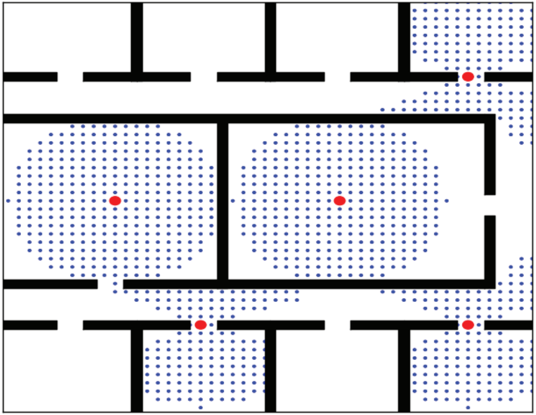
Sensor Placement within Buildings

- 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).



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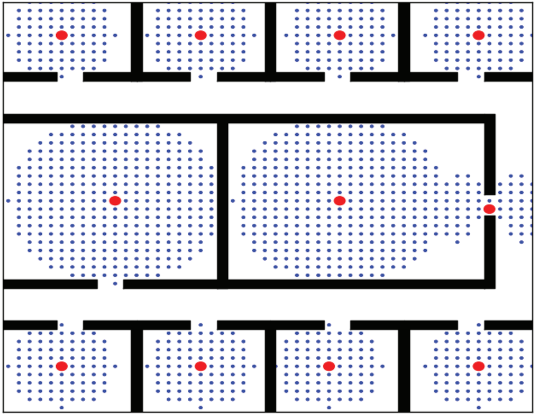
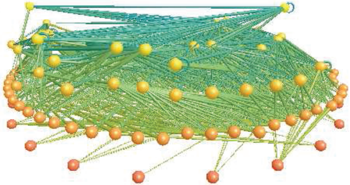
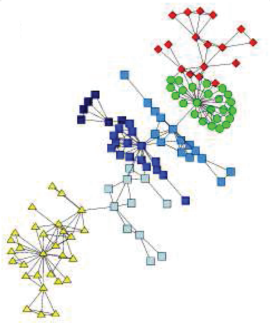
- Example sensor placement using mixed range sensors (located at red dots).

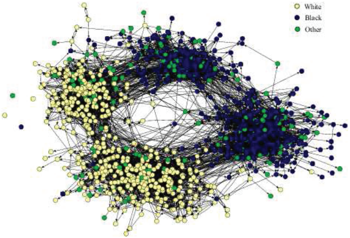


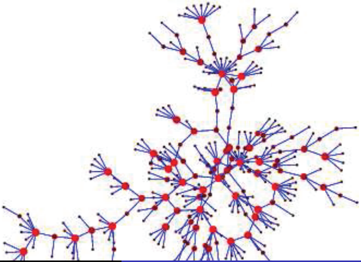
Social Networks

(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

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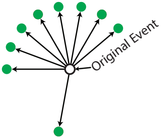

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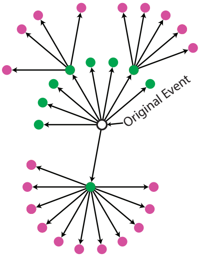

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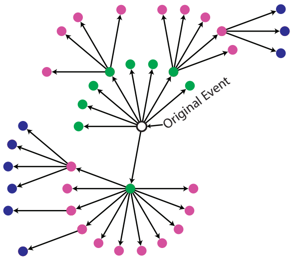

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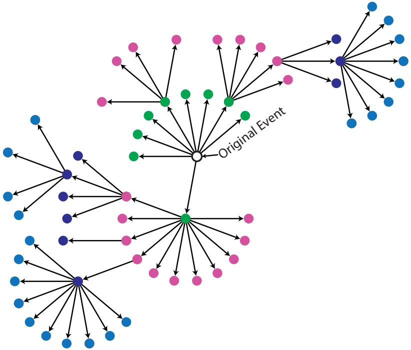

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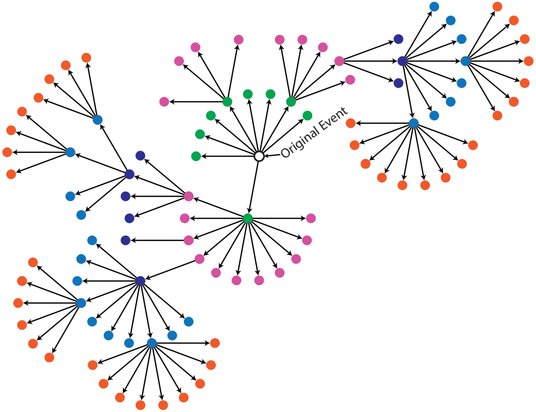

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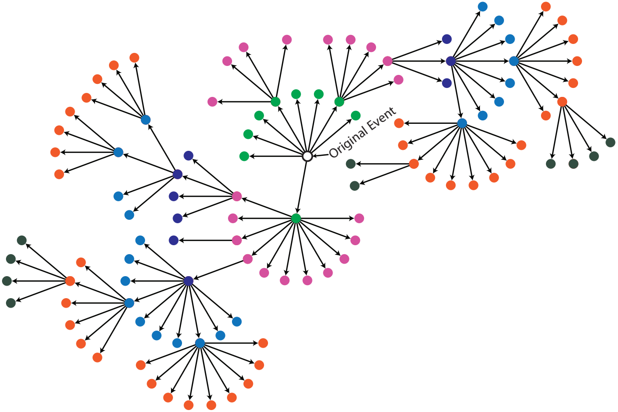

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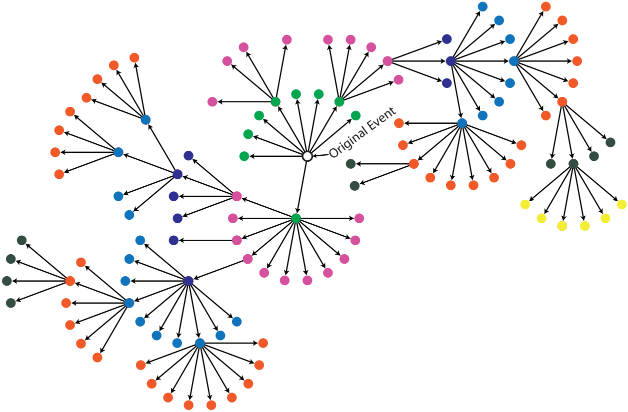

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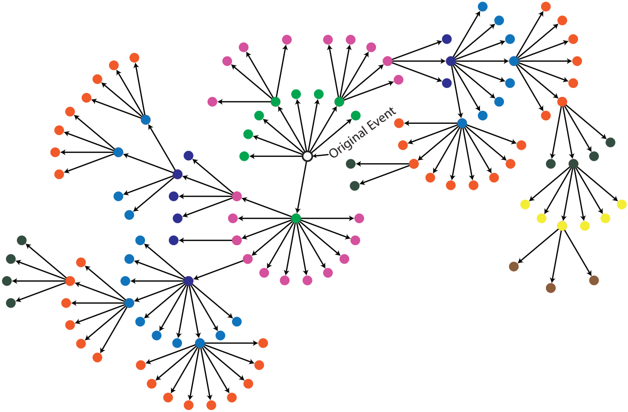

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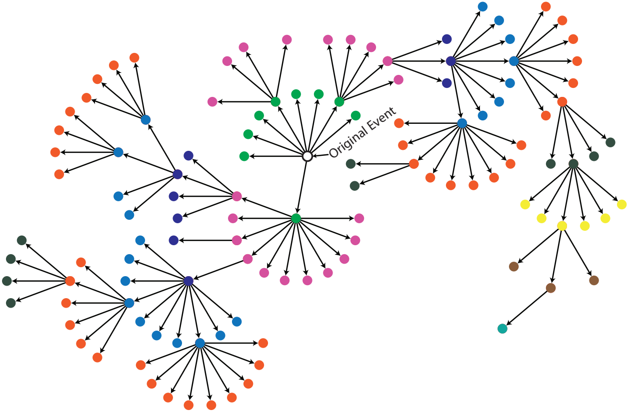

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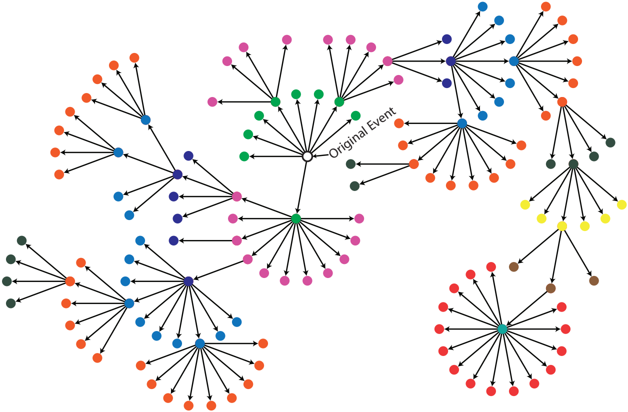

- Goal: How to find the most influential sources, the ones that often set off cascades, which are like large "waves" of information flow?

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).

Graphical Model Structure Learning

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$$p(x) = \frac{1}{Z}\exp(-E(x)) \tag{65}$$

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

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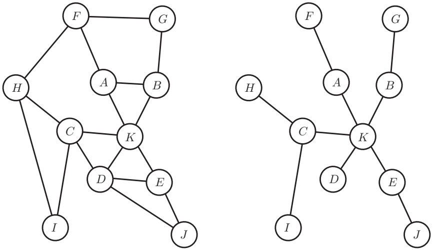

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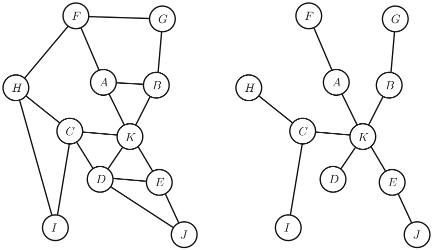

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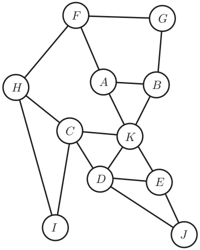

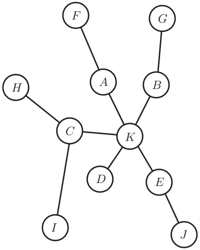

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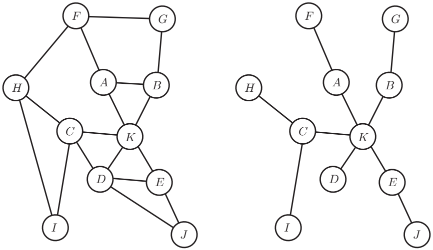

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- Then finding the maximum weight base of the matroid is solved by the greedy algorithm, and also finds the optimal tree (Chow & Liu, 1968)

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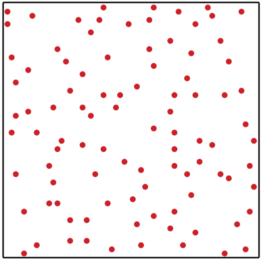
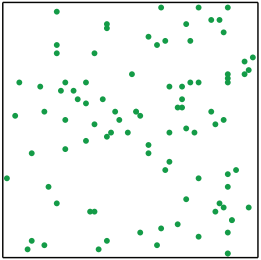


DPP



Independent

(Kulesza, Gillen-water, & Taskar, 2011)

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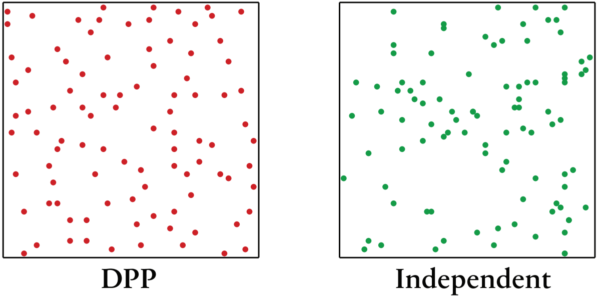

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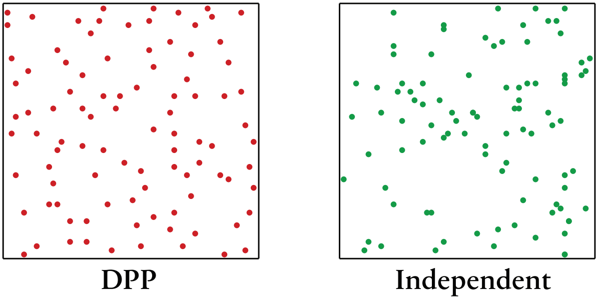

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- Therefore, a DPP is a log-submodular probability distribution.

Outline: Part 2

Graphical Models and fast MAP Inference

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

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where $E(x) = \sum_{c \in \mathcal{C}} E_c(x_c)$ and $\mathcal{C}$ are cliques of graph $G = (V, \mathcal{E})$.

- MAP inference problem is important in ML: compute

$$x^* \in \operatorname*{argmax}_{x \in \{0,1\}^V} p(x) \quad (70)$$

- Easy when G a tree, exponential in k (tree-width of G) in general.
- Even worse, NP-hard to find the tree-width.
- Tree-width can be large even when degree is small (e.g., regular grid graphs have low-degree but $\Omega(\sqrt{n})$ tree-width).
- Many approximate inference strategies utilize additional factorization assumptions (e.g., mean-field, variational inference, expectation propagation, etc).
- Can we do exact MAP inference in polynomial time regardless of the tree-width, without even knowing the tree-width?

Order-two (edge) graphical models

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

$$E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \tag{71}$$

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- Further, say that $\mathsf{D}_{X_v} = \{0, 1\}$ (binary), so we have binary random vectors distributed according to $p(x)$.
- Thus, $x \in \{0, 1\}^V$, and finding MPE solution is setting some of the variables to 0 and some to 1, i.e.,

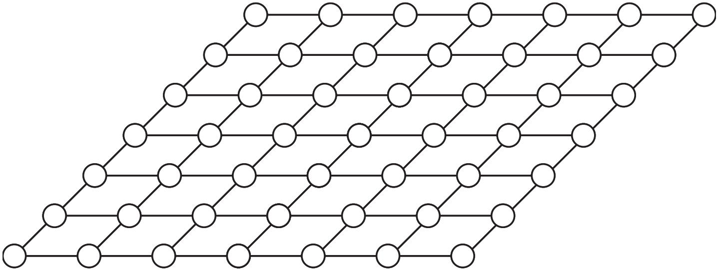
$$\min_{x \in \{0,1\}^V} E(x) \tag{72}$$

MRF example

Markov random field

$$\log p(x) \propto \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \tag{73}$$

When G is a 2D grid graph, we have

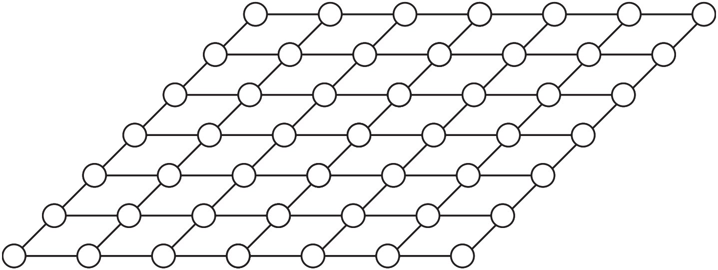


Create an auxiliary graph

- We can create auxiliary graph G_a that involves two new "terminal" nodes s and t and all of the original "non-terminal" nodes $v \in V(G)$.
- The non-terminal nodes represent the original random variables $x_v, v \in V$.
- Starting with the original grid-graph amongst the vertices $v \in V$, we connect each of s and t to all of the original nodes.
- I.e., we form $G_a = (V \cup \{s,t\}, E + \cup_{v \in V}((s,v) \cup (v,t)))$.

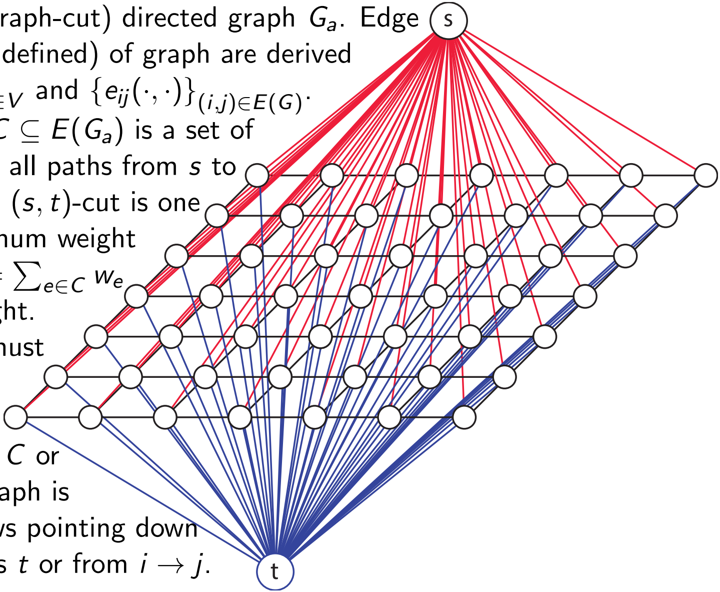
Transformation from graphical model to auxiliary graph

Original 2D-grid graphical model G and energy function $E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j)$ needing to be minimized over $x \in \{0,1\}^V$. Recall, tree-width is $O(\sqrt{|V|})$.



Transformation from graphical model to auxiliary graph

Augmented (graph-cut) directed graph G_a. Edge weights (soon defined) of graph are derived from $\{e_v(\cdot)\}_{v \in V}$ and $\{e_{ij}(\cdot,\cdot)\}_{(i,j)\in E(G)}$. An (s,t)-cut $C \subseteq E(G_a)$ is a set of edges that cut all paths from s to t. A minimum (s,t)-cut is one that has minimum weight where $w(C) = \sum_{e \in C} w_e$ is the cut weight. To be a cut, must have that, for every $v \in V$, either $(s,v) \in C$ or $(v,t) \in C$. Graph is directed, arrows pointing down from s towards t or from $i \to j$.



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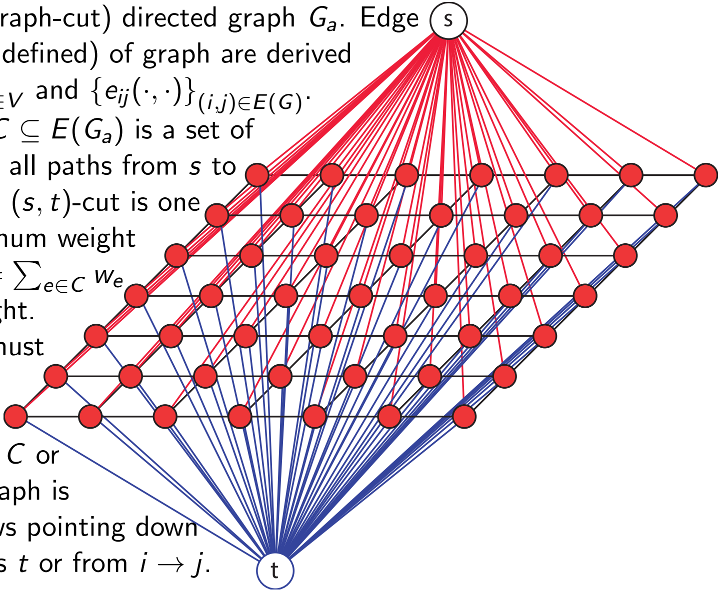
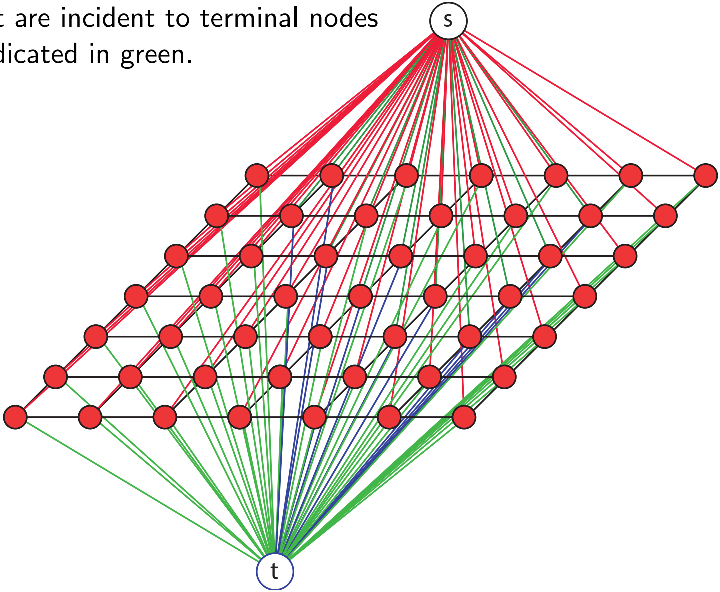


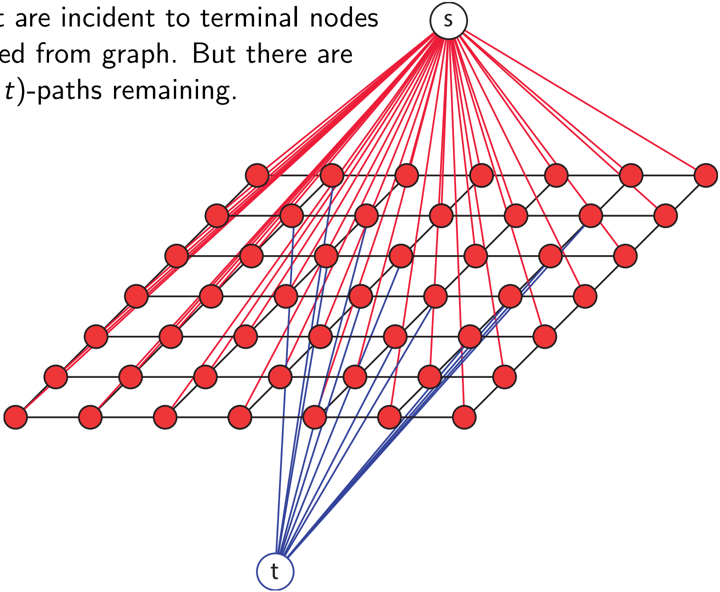
Transformation from graphical model to auxiliary graph

Cut edges that are incident to terminal nodes s and t are indicated in green.



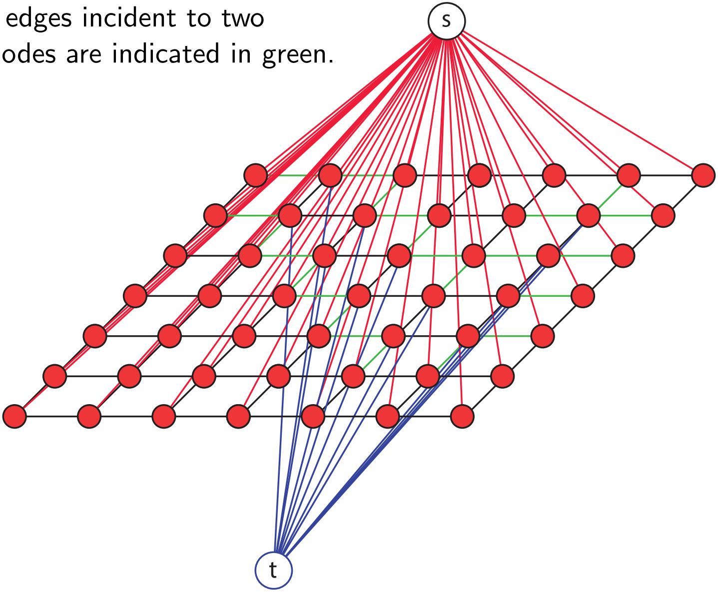
Transformation from graphical model to auxiliary graph

Cut edges that are incident to terminal nodes s and t removed from graph. But there are still un-cut (s, t)-paths remaining.



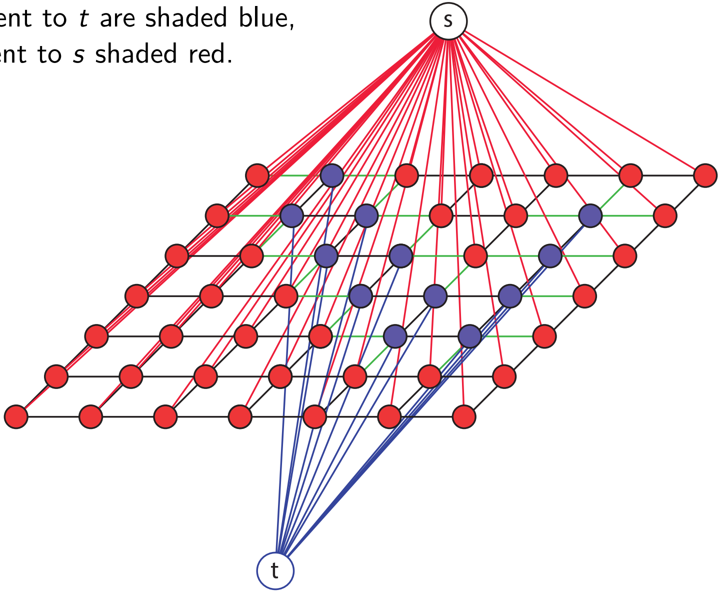
Transformation from graphical model to auxiliary graph

Additional cut edges incident to two non-terminal nodes are indicated in green.



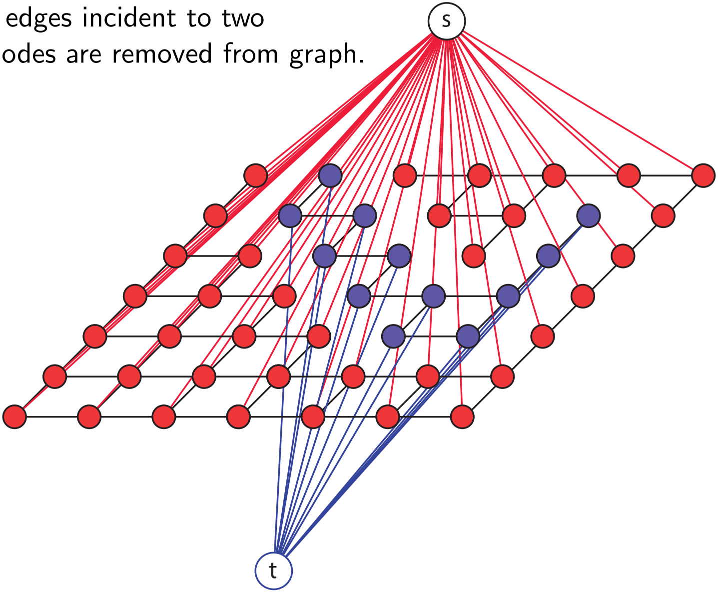
Transformation from graphical model to auxiliary graph

Vertices adjacent to t are shaded blue, vertices adjacent to s shaded red.



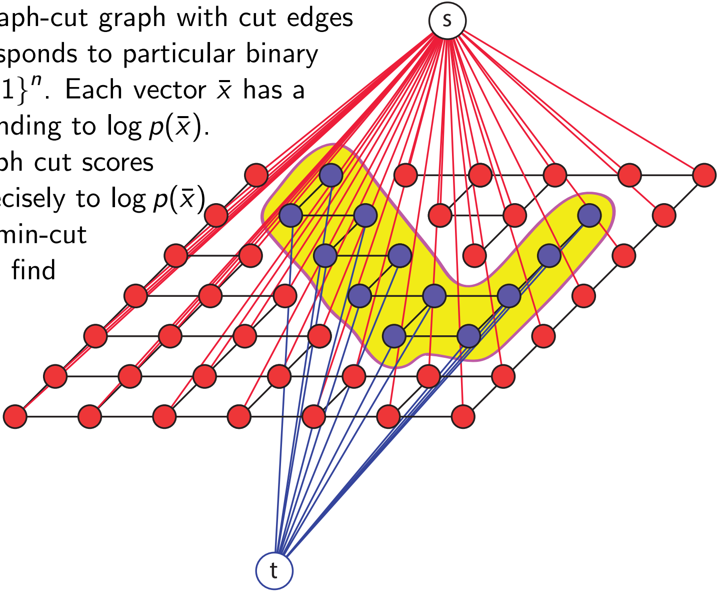
Transformation from graphical model to auxiliary graph

Additional cut edges incident to two non-terminal nodes are removed from graph.



Transformation from graphical model to auxiliary graph

Augmented graph-cut graph with cut edges removed corresponds to particular binary vector $\bar{x} \in \{0,1\}^n$. Each vector $\bar{x}$ has a score corresponding to $\log p(\bar{x})$. When can graph cut scores correspond precisely to $\log p(\bar{x})$ in a way that min-cut algorithms can find minimum of energy $E(x)$?



Setting of the weights in the auxiliary cut graph

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- Hence, poly time graph cut, can find the optimal MPE assignment, regardless of the graphical model's tree-width!
- In general, finding MPE is an NP-hard optimization problem.

Setting of the weights in the auxiliary cut graph

Edge weight assignments. Start with all weights set to zero.

- For (s, v) with $v \in V(G)$, set edge

$$w_{s,v} = (e_v(1) - e_v(0))\mathbf{1}(e_v(1) > e_v(0)) \tag{74}$$

- For (v, t) with $v \in V(G)$, set edge

$$w_{v,t} = (e_v(0) - e_v(1))\mathbf{1}(e_v(0) \geq e_v(1)) \tag{75}$$

- For original edge $(i, j) \in E$, $i, j \in V$, set weight

$$w_{i,j} = e_{ij}(1,0) + e_{ij}(0,1) - e_{ij}(1,1) - e_{ij}(0,0) \tag{76}$$

and if $e_{ij}(1,0) > e_{ij}(0,0)$, and $e_{ij}(1,1) > e_{ij}(0,1)$,

$$w_{s,i} \leftarrow w_{s,i} + (e_{ij}(1,0) - e_{ij}(0,0)) \tag{77}$$

$$w_{j,t} \leftarrow w_{j,t} + (e_{ij}(1,1) - e_{ij}(0,1)) \tag{78}$$

and analogous increments if inequalities are flipped.

Non-negative edge weights

- The inequalities ensures that we are adding non-negative weights to each of the edges. I.e., we do $w_{s,i} \leftarrow w_{s,i} + (e_{ij}(1,0) - e_{ij}(0,0))$ only if $e_{ij}(1,0) > e_{ij}(0,0)$.

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

Submodular potentials

- Edge functions must be submodular (in the binary case, equivalent to "associative", "attractive", "regular", "Potts", or "ferromagnetic"): for all $(i, j) \in E(G)$, must have:

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- As a set function, this is the same as:

$$f(X) = \sum_{\{i,j\} \in \mathcal{E}(G)} f_{i,j}(X \cap \{i,j\}) \tag{82}$$

which is submodular if each of the $f_{i,j}$'s are submodular!

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  which is submodular if each of the $f_{i,j}$'s are submodular!
- A special case of more general submodular functions – unconstrained submodular function minimization is solvable in polytime.

On log-supermodular vs. log-submodular distributions

- Log-supermodular distributions.

$$\log \Pr(x) = f(x) + \text{const.} = -E(x) + \text{const.} \tag{83}$$

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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- Log-submodular distributions:

$$\log \Pr(x) = f(x) + \text{const.} \tag{84}$$

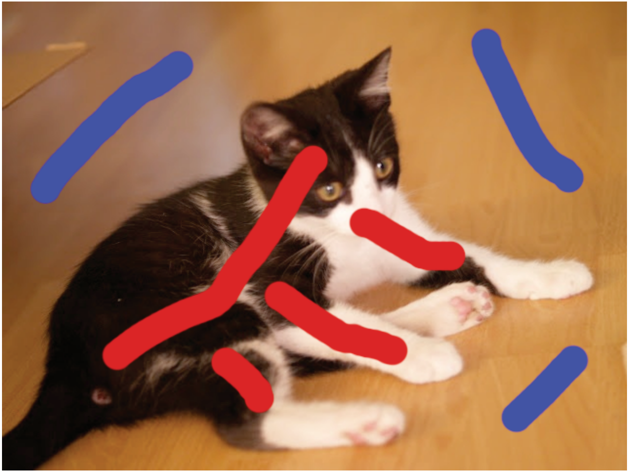
where f is submodular. MAP or high-probable assignments should be "diverse", or "complex", or "covering", like in determinantal point processes.

Submodular potentials in GMs: Image Segmentation

- an image needing to be segmented.

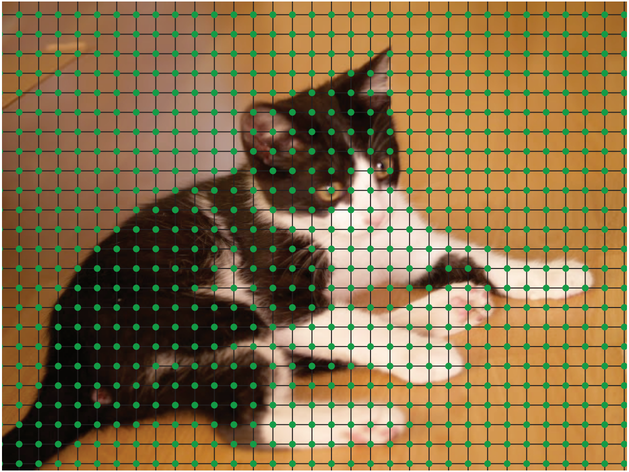
Submodular potentials in GMs: Image Segmentation

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



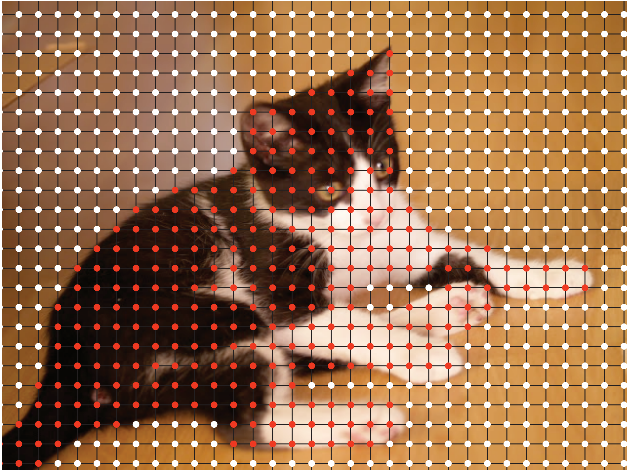
Submodular potentials in GMs: Image Segmentation

- 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.

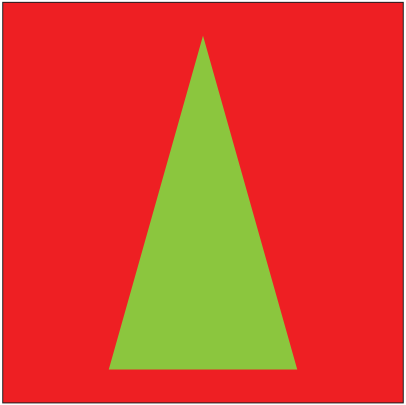
Shrinking bias in graph cut image segmentation

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

Shrinking bias in graph cut image segmentation

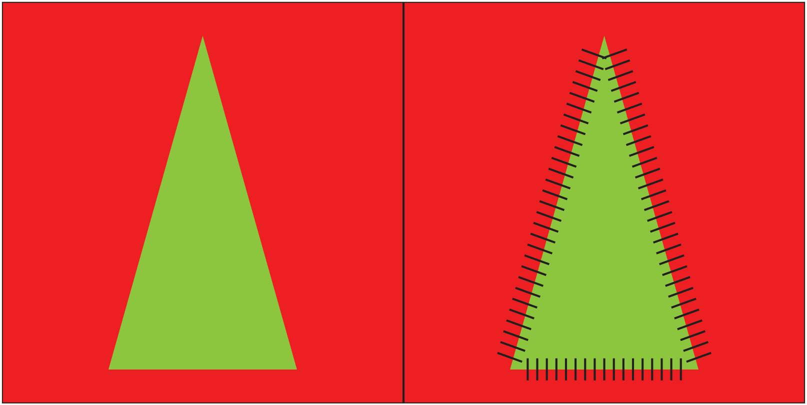
Shrinking bias in image segmentation

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



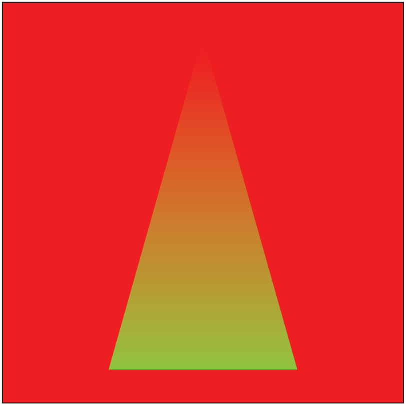
Shrinking bias in image segmentation

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



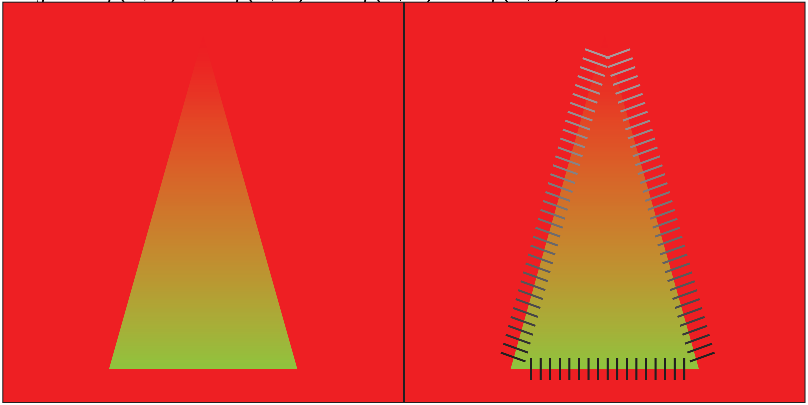
Shrinking bias in image segmentation

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



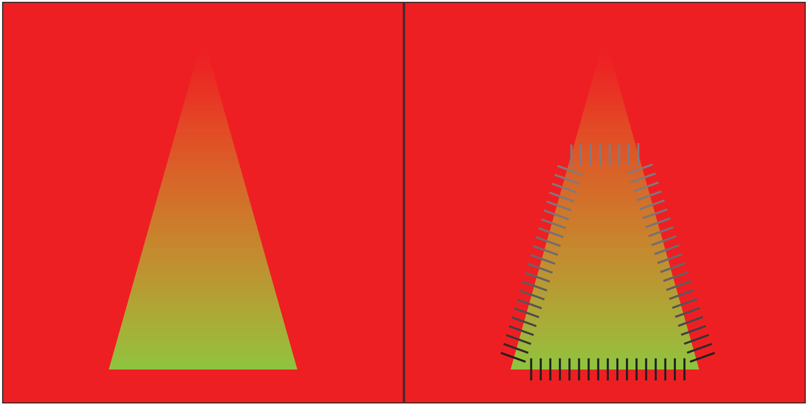
Shrinking bias in image segmentation

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



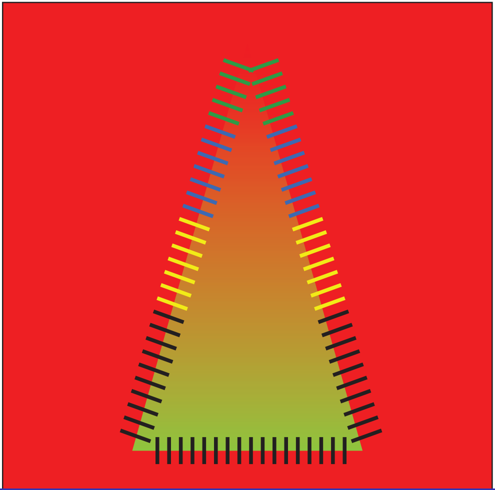
Shrinking bias in image segmentation

- 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.

$$f_w(X) = w\Big(\{(u, v) \in E : u \in X, v \in V \setminus X\}\Big) \tag{85}$$

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- Instead, we can use a submodular function $g : 2^E \rightarrow \mathbb{R}_+$ defined on the edges to express cooperative costs.

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- Seen as a node function, $f_g : 2^V \to \mathbb{R}_+$ is not submodular, but it uses submodularity internally to solve the shrinking bias problem.

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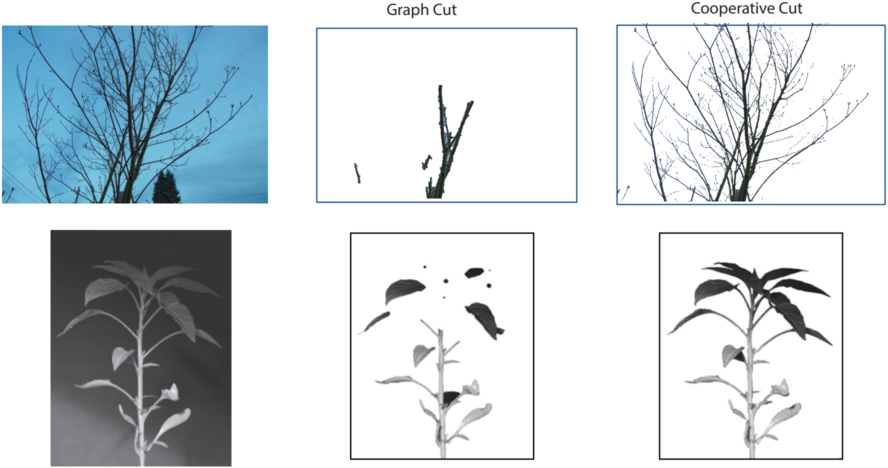
$$f_g(X) = g\Big(\{(u,v) \in E : u \in X, v \in V \setminus X\}\Big) \tag{86}$$

- Seen as a node function, $f_g : 2^V \to \mathbb{R}_+$ is not submodular, but it uses submodularity internally to solve the shrinking bias problem.
- $\Rightarrow$ cooperative-cut (Jegelka & B., 2011).

Graph-cut vs. cooperative-cut comparisons

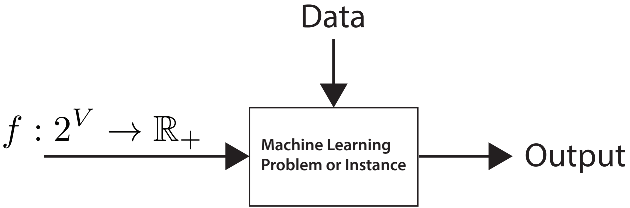


(Jegelka&Bilmes,'11). There are fast algorithms for solving as well.

Outline: Part 2

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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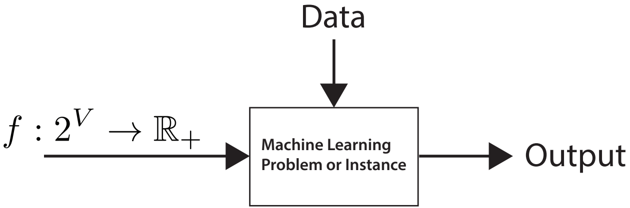

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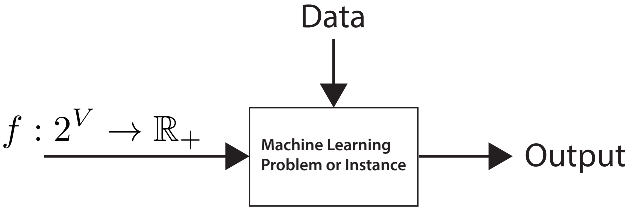

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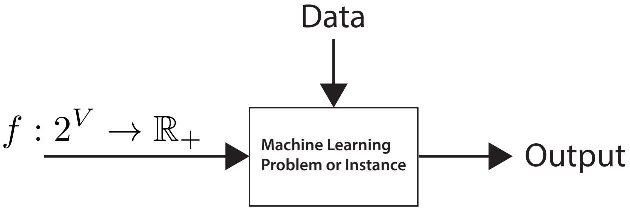

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- $\mathbb{S}$ is a submodular cone since submodularity is closed under non-negative (conic) combinations.
- 2^n-dimensional since for certain $f \in \mathbb{S}$, there exists $f_\epsilon \in \mathbb{R}^{2^n}$ having no zero elements with $f + f_\epsilon \in \mathbb{S}$.

Supervised 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:

$$\min_{w \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^m \ell(y_i, w^\intercal x_i) + \lambda \Omega(w), \tag{87}$$

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 (k) responses $(x_i, y_i) \in \mathbb{R}^n \times \mathbb{R}^k$ for each of the m samples, learning becomes:

$$\min_{w^1, \ldots, w^k \in \mathbb{R}^n} \sum_{j=1}^{k} \frac{1}{m} \sum_{i=1}^{m} \ell(y_i^j, (w^j)^\intercal x_i) + \lambda \Omega(w^j), \tag{88}$$

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- When only the multiple responses $\{y_i\}_{i \in [m]}$ are observed, we get either dictionary learning

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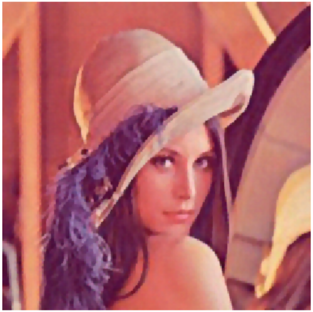
- In each case of the above cases, the regularizer $\Omega(\cdot)$ is critical.

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:

$$\Omega(w) = \sum_{i=2}^{N} |w_i - w_{i-1}| \tag{91}$$

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

(Rodriguez, 2009)

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

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- Hence, family of clustering algorithms parameterized by f.

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8. Submodular functions may be more general than clustering objectives (submodularity allows high-order interactions between elements).

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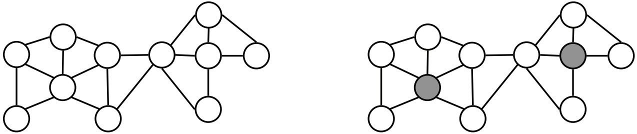
- Batch/Offline **active learning**: Given a set V of unlabeled data items, learner chooses subset $L \subseteq V$ of items to be labeled



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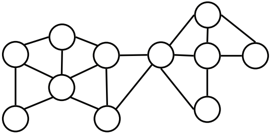
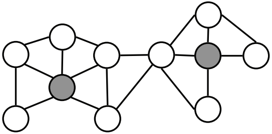

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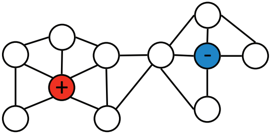
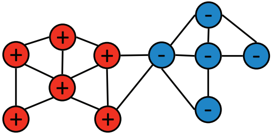

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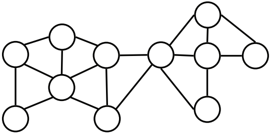
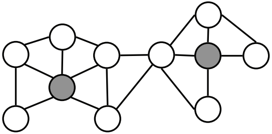

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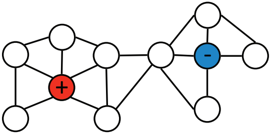
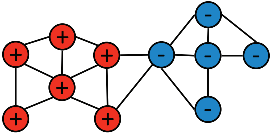
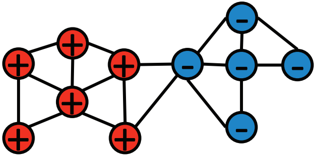
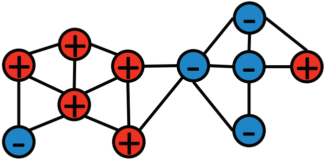



- Learner suffers loss $\|\hat{y} - y\|_1$, where y is truth. Below, $\|\hat{y} - y\|_1 = 2$.

Choosing labels: how to select L

- Consider the following objective

$$\Psi(L) = \min_{T \subseteq V \setminus L : T \neq \emptyset} \frac{\Gamma(T)}{|T|} \tag{96}$$

where $\Gamma(T) = I_f(T; V \setminus T) = f(T) + f(V \setminus T) - f(V)$ is an arbitrary symmetric submodular function (e.g., graph cut value between T and $V \setminus T$, or combinatorial mutual information).

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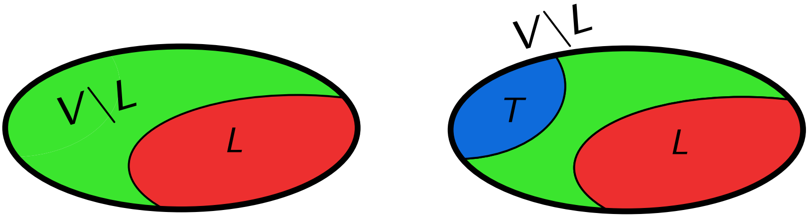

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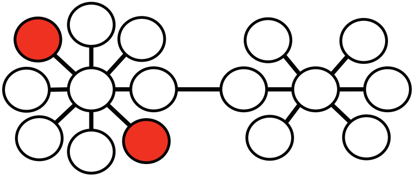

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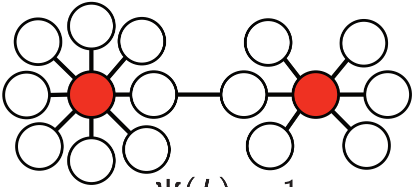

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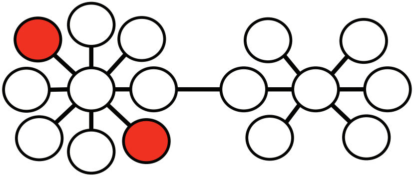

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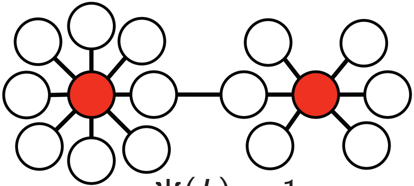

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- This suggests choosing (bounded cost) L that maximizes $\Psi(L)$.

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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 & B., '11)

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

$$\|\hat{y} - y\|_1 \leq 2\frac{\Gamma(Y(y))}{\Psi(L)} \tag{98}$$

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:

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- $\Gamma(T) = I_f(T; V \setminus T) = f(S) + f(V \setminus S) - f(V)$ determined by arbitrary submodular function f, 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.

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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 Learning of Submodular Mixtures

- Constraints specified in inference form:

$$\underset{\mathbf{w},\xi_t}{\text{minimize}} \quad \frac{1}{T}\sum_t \xi_t + \frac{\lambda}{2}\|\mathbf{w}\|^2 \tag{102}$$

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Structured Prediction: Subgradient Learning

- Solvable with simple sub-gradient descent algorithm using structured variant of hinge-loss (Taskar, 2004).
- Loss-augmented inference is either submodular optimization (Lin & B. 2012) or DS optimization (Tschiatschek, Iyer, & B. 2014).

Algorithm 7: 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 $\frac{1}{T} \sum_t \mathbf{w}_t$.

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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.

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- This gradually get worse as we move away from an objective being submodular (see Das & Kempe, 2011).

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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.

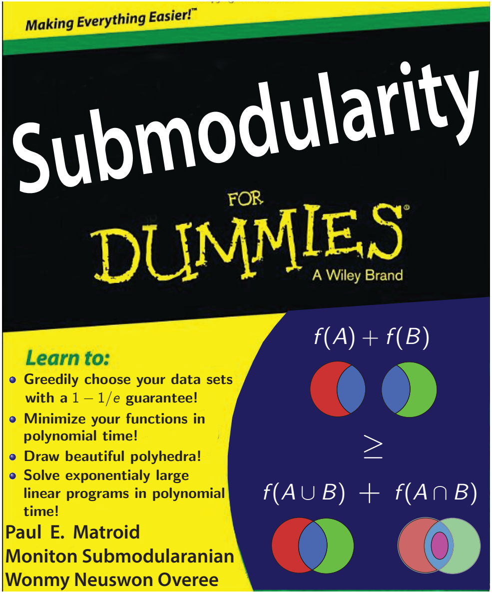
Classic Books

- 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/. Lectures available 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

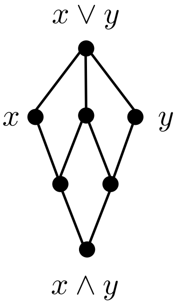
The End: Thank you!



Outline: Part 3

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.

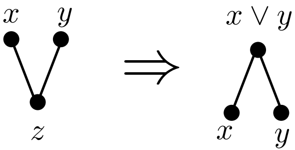


height
3
2
1
0

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:

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{108}$$

- 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

$$f'(A) = f(A) - f(\emptyset) \tag{109}$$

- 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

$$f(A) = \underbrace{f(A) - m(A)}_{\bar{f}(A)} + m(A) = \bar{f}(A) + m(A) \tag{110}$$

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

$$m(a) = f(a|V \setminus \{a\}) \tag{111}$$

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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

$$\bar{f}(a|A) = f(a|A) - f(a|V \setminus \{a\}) \geq 0 \tag{112}$$

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

$$P_f = \left\{x \in \mathbb{R}^V : x(A) \leq f(A), \forall A \subseteq V\right\} \tag{113}$$

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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

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Telescoping Summation

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- Then the telescoping summation property of the gains is as follows:

$$\sum_{i=1}^{r-1} f(A_{i+1}|A_i) = \sum_{i=2}^{r} f(A_i) - \sum_{i=1}^{r-1} f(A_i) = f(A_r) - f(A_1) \quad (115)$$

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:

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

□

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.,

$$f(A) = \sum_{i=1}^{k} \alpha_i f_i(A) \tag{116}$$

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Grouping elements, set cover, and bipartite neighborhoods

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- Neighbors defined as $\Gamma(X) = \{u \in U : |X \times \{u\} \cap E| \geq 1\}$ for $X \subseteq V$. Then $f(\Gamma(X))$ is submodular. Special case: set cover.
- In fact, all integral polymatroid functions can be obtained in g above for f a matroid rank function and $\{V_d\}$ appropriately chosen.

The "or" of two polymatroid functions

- Given two polymatroid functions f and g, suppose feasible A are defined as $\{A : f(A) \geq \alpha_f \text{ or } g(A) \geq \alpha_g\}$ for real α_f, α_g.

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

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- A submodular function $f : 2^V \to \mathbb{R}$ has a different type of input and output, so composing two submodular functions directly makes no sense.
- However, we have a number of forms of composition results that preserve submodularity, which we turn to next:

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

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

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

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

$$f(B) = \max_{b \in B} m(b) \tag{122}$$

Facility Location via sum of weighted matroid rank

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

$$f(A) = \sum_{i=1}^{k} \alpha_i \max \{ m_i(A) : A \subseteq B \text{ and } A \in \mathcal{I}_i \} \qquad (123)$$

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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:

$$f(A) = \sum_{i \in V} \max_{a \in A} w_{ai} \tag{124}$$

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- Given a set V of items, we might wish to measure the “information” or “complexity” in a subset $A \subset V$.
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  can measure partial independence.
- Entropy is submodular due to non-negativity of conditional mutual information. Given $A, B, C \subseteq V$,

$$I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B}) = H(X_A) + H(X_B) - H(X_{A \cup B}) - H(X_{A \cap B}) \geq 0 \tag{126}$$

Submodular Generalized Dependence

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

$$f(A \cup B) = f(A) + f(B), \tag{93}$$

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

$$f(A \cup B \cup C) + f(C) = f(A \cup C) + f(B \cup C) \tag{94}$$

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

$$f(A|B) \triangleq f(A \cup B) - f(B) < f(A), \tag{95}$$

- and a notion of "conditional mutual information"

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

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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

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

$$P_f^+ = \left\{ y \in \mathbb{R}_+^V : y(A) \leq f(A) \text{ for all } A \subseteq V \right\} \tag{127}$$

$$= \left\{ y \in \mathbb{R}^V : y \geq 0, y(A) \leq f(A) \text{ for all } A \subseteq V \right\} \tag{128}$$

Chains of sets

- Ground element $V = \{1, 2, \ldots, n\}$ set of integers w.l.o.g.

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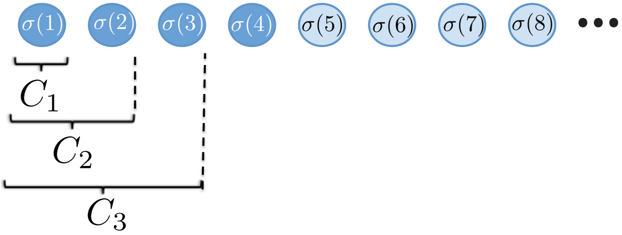
- From this we can form a chain of sets $\{C_i\}_i$ with $\emptyset = C_0 \subseteq C_1 \subseteq \cdots \subseteq C_n = V$ formed as:

$$C_i = \{\sigma_1, \sigma_2, \ldots, \sigma_i\}, \quad \text{for } i = 1 \ldots n \tag{129}$$



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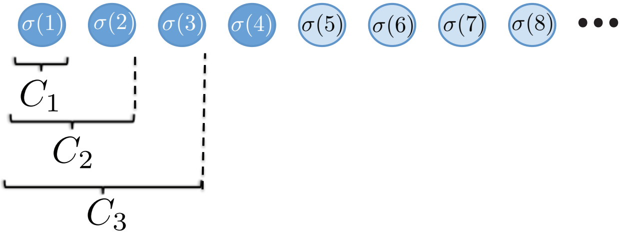

- Can also form a chain from a vector $w \in \mathbb{R}^V$ sorted in descending order. Choose σ so that $w(\sigma_1) \geq w(\sigma_2) \geq \cdots \geq w(\sigma_n)$.

Polymatroidal polyhedron and greedy

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

$$\begin{aligned} &\underset{x \in \mathbb{R}^V}{\text{maximize}} && w^\intercal x \\ &\text{subject to} && x \in \left\{ y \in \mathbb{R}_+^V : y(A) \leq f(A) \text{ for all } A \subseteq V \right\} \end{aligned} \tag{130}$$

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

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

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- Next, form chain of sets based on w sorted descended, giving:

$$V_i \stackrel{\text{def}}{=} \{v_1, v_2, \ldots v_i\} \tag{131}$$

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

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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:

$$x(v_i) = f(V_i) - f(V_{i-1}) = f(v_i | V_{i-1}) \tag{132}$$

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 $P = \{x \in \mathbb{R}_+^V : x(A) \leq f(A), \forall A \subseteq V\}$.
Then the greedy solution to the problem $\max(wx : x \in P)$ is optimal $\forall w$ iff f is monotone non-decreasing submodular (i.e., iff P is a polymatroid).

Polymatroid extreme points

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

Theorem

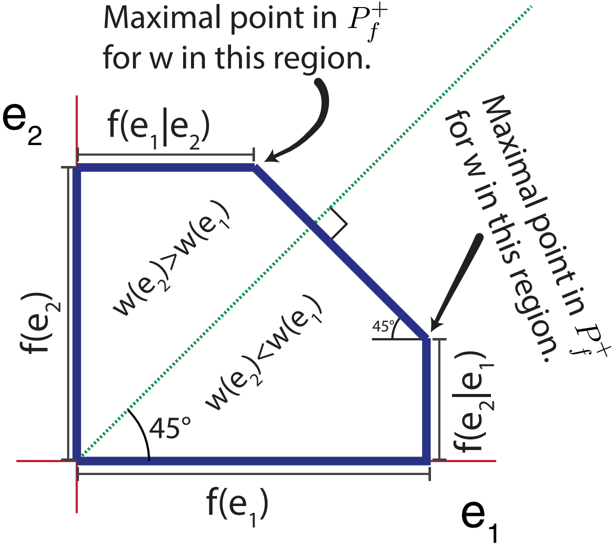
For a given ordering $V = (v_1, \dots, v_m)$ of V and a given V_i and x generated by V_i using the greedy procedure, then x is an extreme point of P_f

Corollary

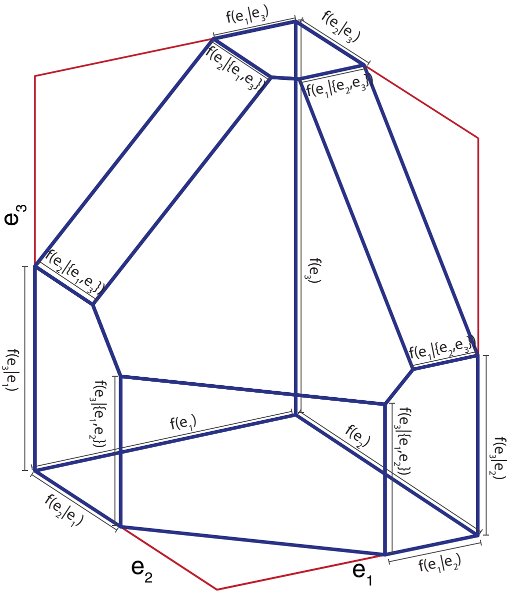
If x is an extreme point of P_f and $B \subseteq V$ is given such that $\{v \in V : x(v) \neq 0\} \subseteq B \subseteq \cup(A : x(A) = f(A))$, then x is generated using greedy by some ordering of B.

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



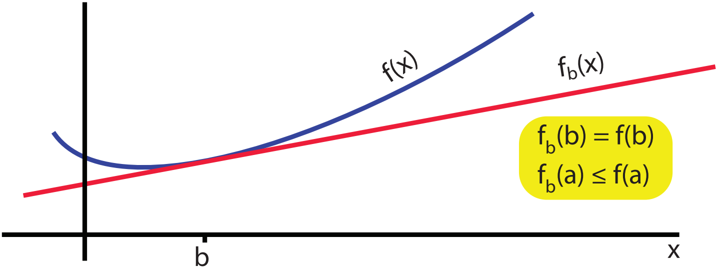
A polymatroid function's polyhedron vs. a polymatroid.

- 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 3

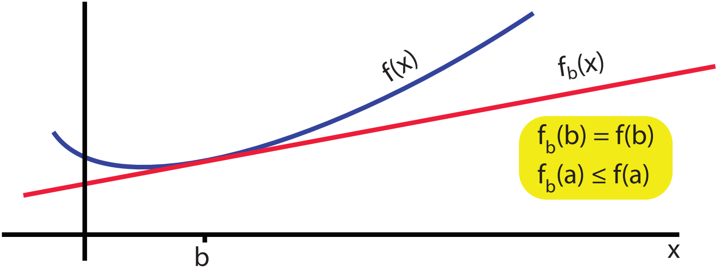
Convex Functions and Tight Subgradients



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

$$f(x) - f(b) \geq \langle f_b, x - b \rangle, \forall x. \tag{133}$$

Concave Functions and Tight Supergradients



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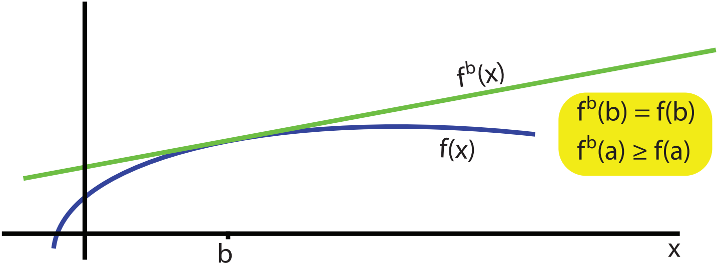
Convex Functions and Tight Subgradients



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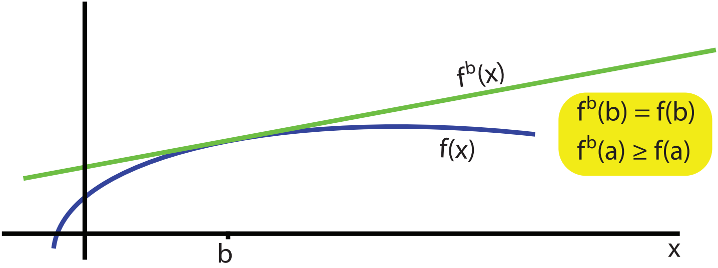

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- We have that $f(x)$ is concave, $f^b(x)$ is affine, and is a tight supergradient (tight at b, affine upper bound on $f(x)$).

Trivial additive upper/lower bounds

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

$$m_f(A) \leq f(A) \leq m^f(A) \tag{135}$$

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- $m^f \in \mathbb{R}^V$ and $m_f \in \mathbb{R}^V$ are both modular (or additive) functions.
- 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:

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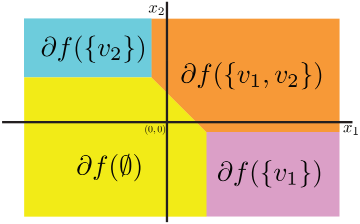

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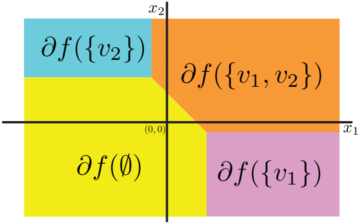

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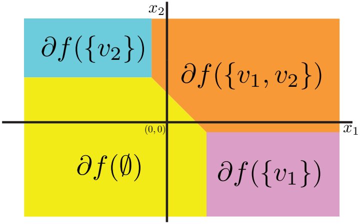

- Extreme points are easy to get via Edmonds's greedy algorithm:

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 $h^f_{Y,\sigma}(Y) = f(Y)$.

Convexity and Tight Sub- and Super-gradients?

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

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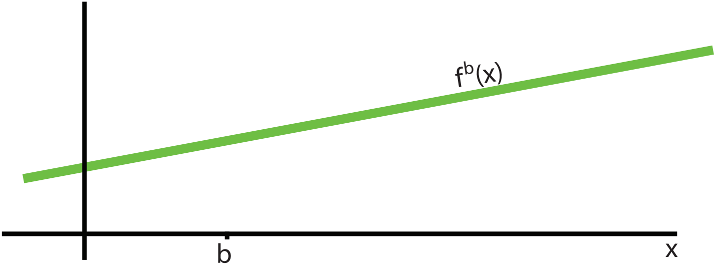

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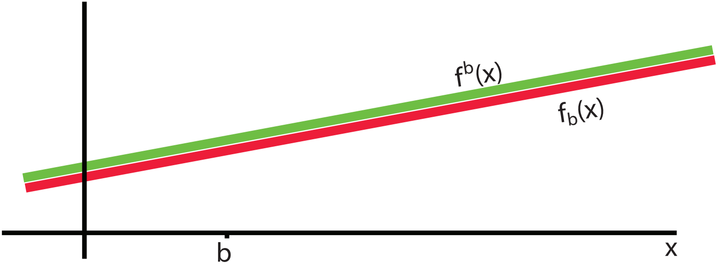

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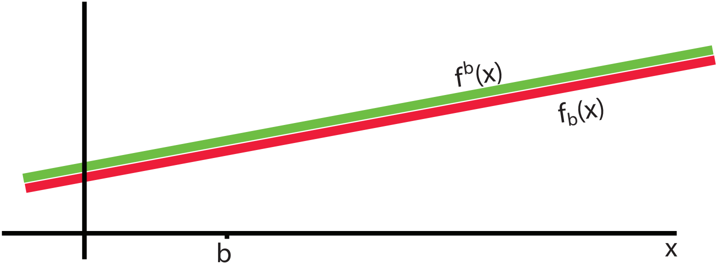

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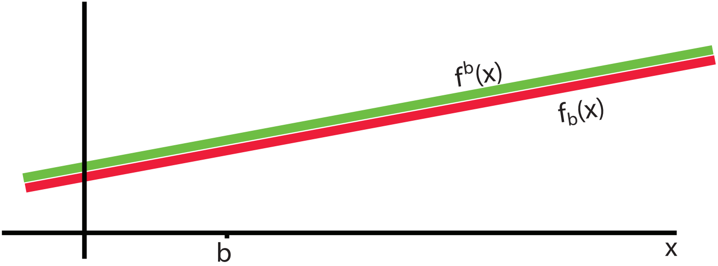

- If a continuous function has both a sub- and super-gradient at a point, then the function must be affine.
- What about discrete set functions?

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 & B., 2011, Iyer & B. 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 & B., 2012).
- Similar strategy used for other combinatorial constraints (.e., cooperative cut, submodular on edges, see Jegelka & B. 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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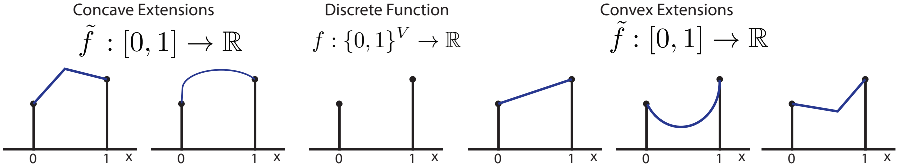
- In fact, any such discrete function defined on the vertices of the n-D hypercube $\{0,1\}^n$ has a variety of both convex and concave extensions tight at the vertices (Crama & Hammer). Example $n = 1$,



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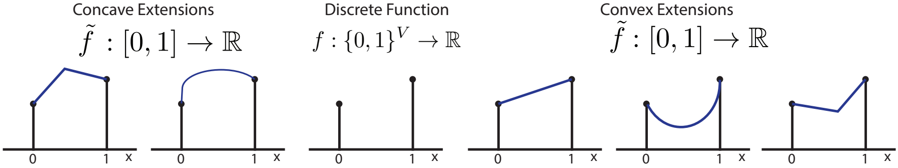

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Continuous Extensions of Discrete Set Functions

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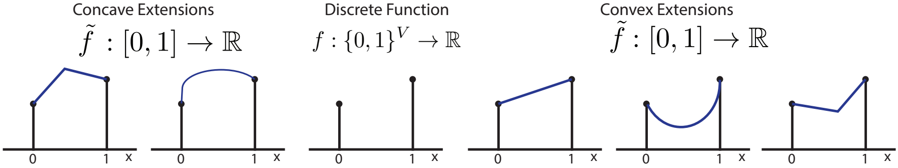

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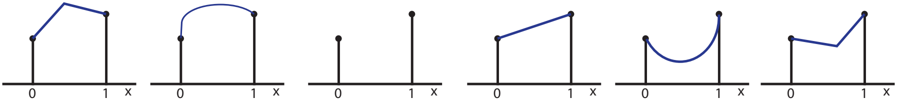
Concave Extensions $\tilde{f} : [0,1] \to \mathbb{R}$ — Discrete Function $f : \{0,1\}^V \to \mathbb{R}$ — Convex Extensions $\tilde{f} : [0,1] \to \mathbb{R}$



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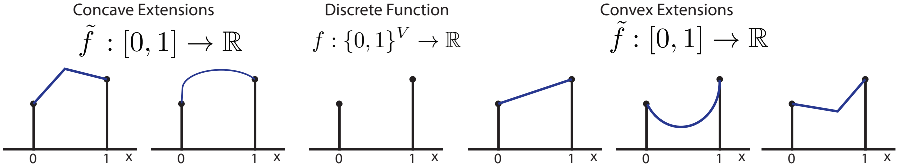

- Since there are an exponential number of vertices $\{0,1\}^n$, important questions regarding such extensions is:
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  3. When are they useful for something practical?

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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- 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

$$\tilde{f}(w) = \sum_{i=1}^{m} \lambda_i f(V_i) \tag{146}$$

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

$$\text{for } i \in \{1, \ldots, m\}, \quad \lambda_i = \begin{cases} w(v_i) - w(v_{i+1}) & \text{if } i < m \\ w(v_m) & \text{if } i = m \end{cases} \tag{147}$$

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

$$\tilde{f}(w^*) = \sum_i \lambda_i^* f(V_i^*) = f(A^*) = \min \{f(A)|A \subseteq V\} \qquad (148)$$

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

$$f(V_i^*) = f(A^*) \tag{149}$$

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:

$$\underset{w \in \mathbb{R}^V}{\text{minimize}} \; \tilde{f}(w) + \frac{1}{2}\|w\|_2^2 \tag{150}$$

$$\text{maximize} \quad -\|x\|_2^2 \tag{151a}$$

$$\text{subject to} \quad x \in B_f \tag{151b}$$

where $B_f = P_f \cap \left\{x \in \mathbb{R}^V : x(V) = f(V)\right\}$ 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

$$F(x) = \sum_{S \subseteq V} f(S) \prod_{i \in S} x_i \prod_{j \in V \setminus S} (1 - x_j) \quad (152)$$

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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 $A \subseteq V$,

$$g(A) \le f(A) \tag{153}$$

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

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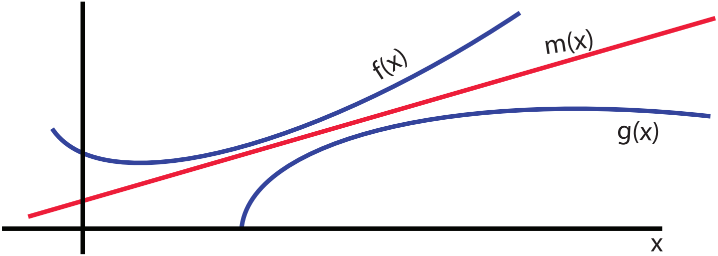
- Compare to convex/concave case.



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

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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 $j, k \in V$

$$f(X + j) + f(X + k) \geq f(X + j + k) + f(X) \qquad (155)$$

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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 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.

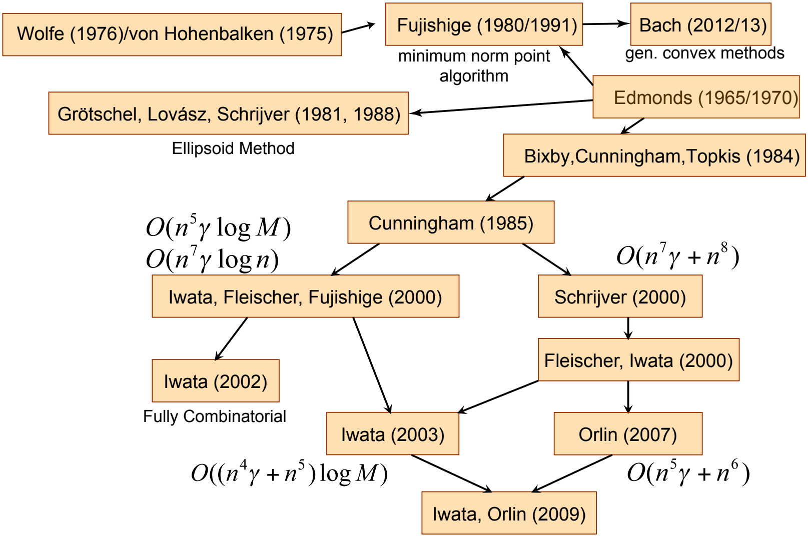
Outline: Part 3

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

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- Constraint set $\mathcal{S}$ might either be cuts, paths, matchings, cardinality constraints, etc.
- Minimization algorithms should have multiplicative approximation guarantee, i.e,. $f(S) \leq \alpha f(S^*)$ where S^* is optimal solution, $\alpha \geq 1$.

Theoretical Results: Constrained Submodular Min

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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	$\sqrt{n}$	$\sqrt{n}$

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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 8: The Greedy Algorithm

Set $S_0 \leftarrow \emptyset$;
for $i \leftarrow 0 \dots |V| - 1$ **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
$\lvert S \rvert \leq k$	$1 - 1/e$	$1 - 1/e$	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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The solutions $\widehat{X}$ then have guarantees in terms of curvature κ_f:

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- Curvature dependent constrained maximization bounds:

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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- 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	$\frac{m}{1+(m-1)(1-\kappa_f)}$	$\theta(\sqrt{n})$	$\tilde{\Omega}(\frac{\sqrt{n}}{1+(\sqrt{n}-1)(1-\kappa_f)})$

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