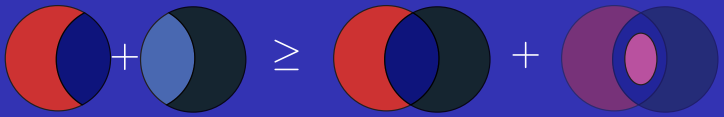

NOML: Submodularity in Machine Learning

June 17th, 2015: Intro and Applications

Jeffrey A. Bilmes and Rishabh Iyer

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& Computer Science and Engineering
University of Washington, Seattle
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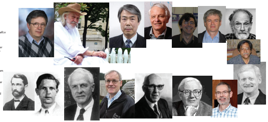
June 17th-19th, 2015

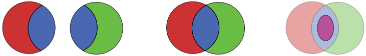
Goals of the Tutorial

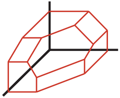
Clockwise from top left:v
Lásló Lovász
Jack Edmonds
Satoru Fujishige
George Nemhauser
Laurence Wolsey
András Frank
Lloyd Shapley
H. Narayanan
Robert Bixby
William Cunningham
William Tutte
Richard Rado
Alexander Schrijver
Garrett Birkhoff
Hassler Whitney
Richard Dedekind



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

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





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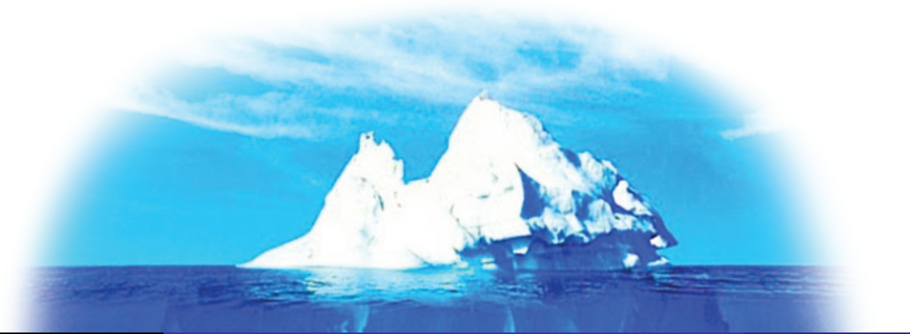
- The definition, however, is only the tip of the iceberg — this simple definition can lead to great mathematical and practical richness.



Overall Outline of Tutorial

1. Today (Wednesady): Basics, Examples, Properties, and Applications (presented by myself, Jeff Bilmes)
2. Tomorrow: Algorithms for constrained and unconstrained submodular optimization, details of semidifferentials, many novel submodular strucures (presented by Dr. Rishabh Iyer)

Overall Outline of Today's 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:

$A = \Bigg\{$  $\Bigg\}$

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

Ex: $f(A) = 1$

Sets and set functions

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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
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GROCERY	0.49
3 @ 3 FOR 0.49	
SUBTOTAL	$12.63
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- This is known as a modular function.

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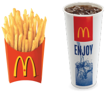
$f($ 

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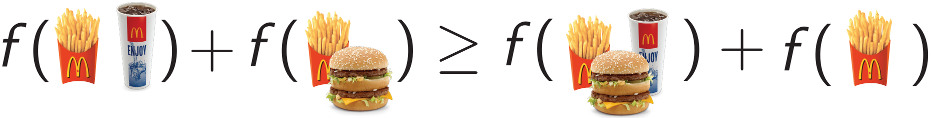

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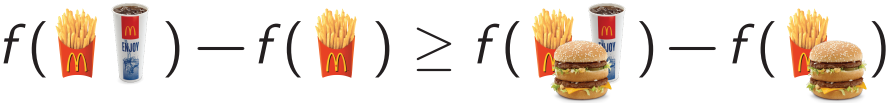

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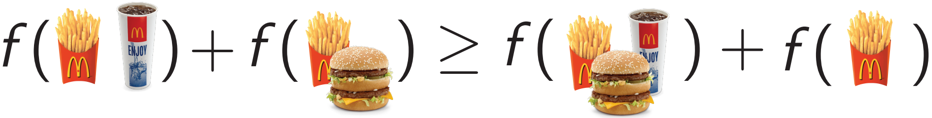

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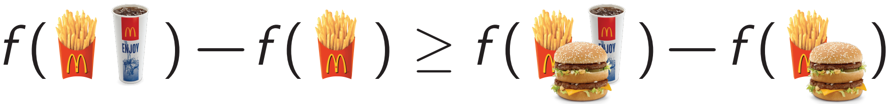

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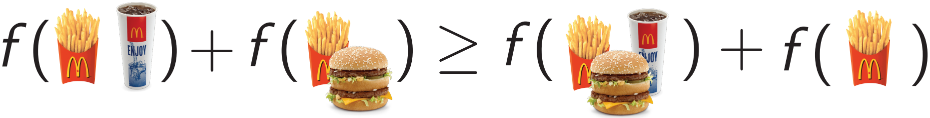

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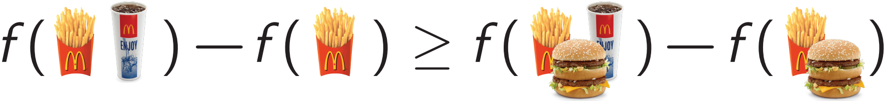

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- But $f(\{v_1, v_2\}) = c_d + c_m + c_h < 2c_d + c_m + c_h$ since c_d (driving) is a shared fixed cost.
- Shared fixed costs are submodular: $f(v_1) + f(v_2) \geq f(v_1, v_2) + f(\emptyset)$

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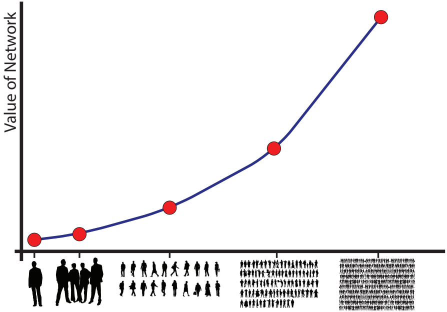
- So diminishing returns (a submodular function) would be a good model.

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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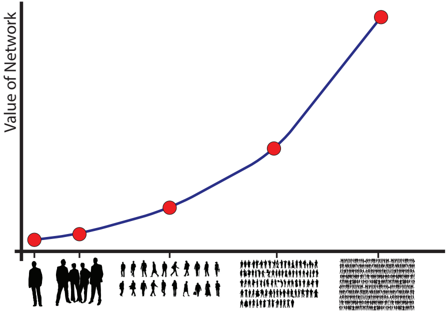

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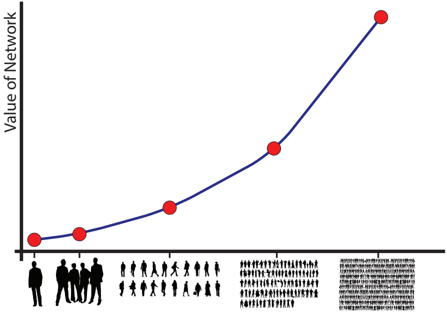

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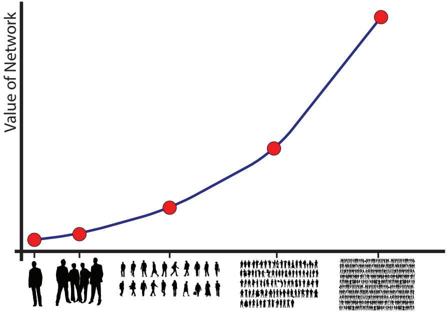

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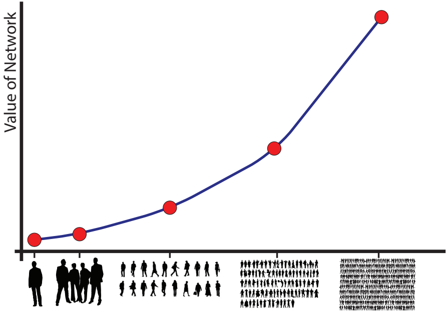

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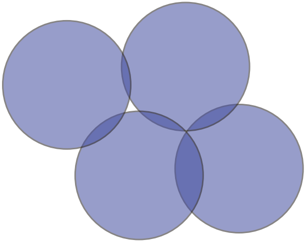
- Ex: durable goods (e.g., a car or phone), software (facebook, smartphone apps), and technology-specific human capital investment (e.g., education in a skill).
- Let V be a set of goods, A a subset and $v \notin A$. Incremental gain of good $f(A+v) - f(A)$ gets larger as size of market A grows. This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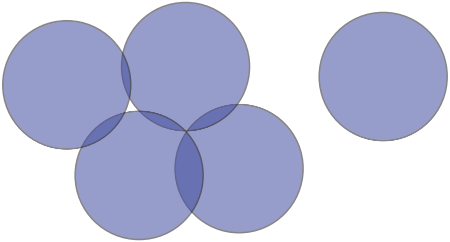
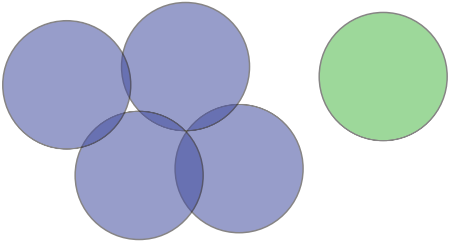


Area of A along with with v:

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

Area of the union of areas indexed by A

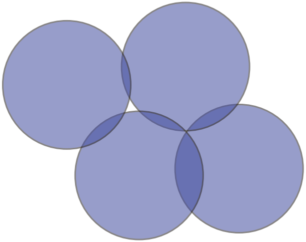


Gain (value) of v in context of A:

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

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

Area of the union of areas indexed by A



Area of A once again.

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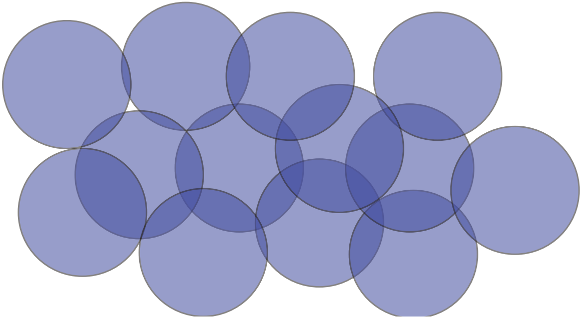
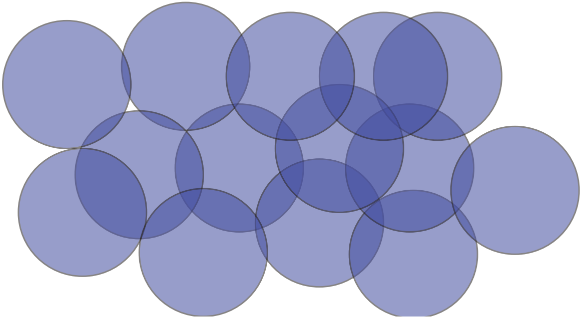


Union of areas of elements of $B \supset A$, where v is not included:

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

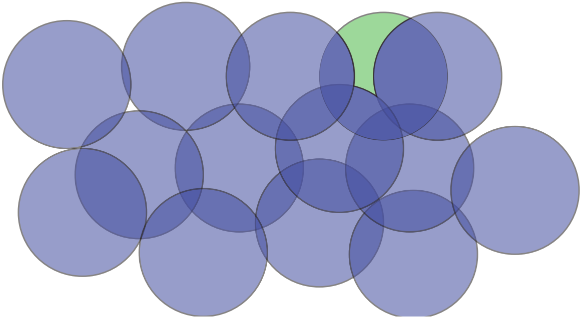
Area of the union of areas indexed by A



Area of B now also including v:

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

Area of the union of areas indexed by A



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

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

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

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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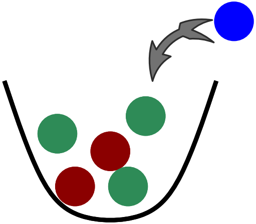
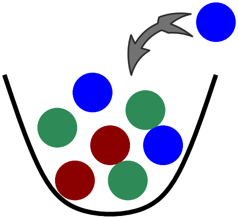


Initial value: 2 (colors in urn).
New value with added blue ball: 3



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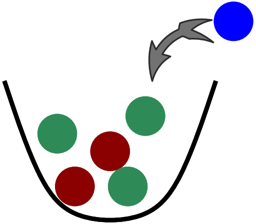

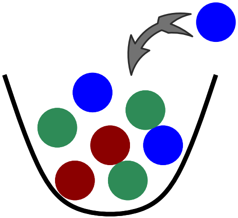

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- Submodularity: Incremental Value of Object Diminishes in a Larger Context (diminishing returns).

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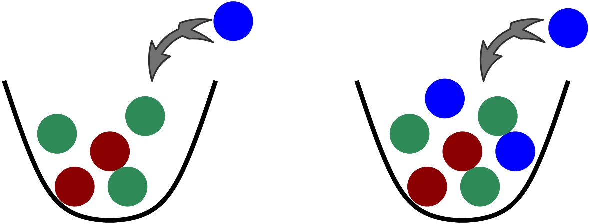

Initial value: 2 (colors in urn).
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- Submodularity: Incremental Value of Object Diminishes in a Larger Context (diminishing returns).
- Thus, f is submodular.

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.

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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))

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- 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.

Sets and Vectors: Some Notation Conventions

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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

$$m(A) = \sum_{a \in A} m(a) \tag{8}$$

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Definition (monotone function)

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

Subadditive Functions

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

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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:

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

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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- Associative
- Regular
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- Subadditive (but this is now known as something different)
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"What's in a name? That which we call a submodular function,

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).

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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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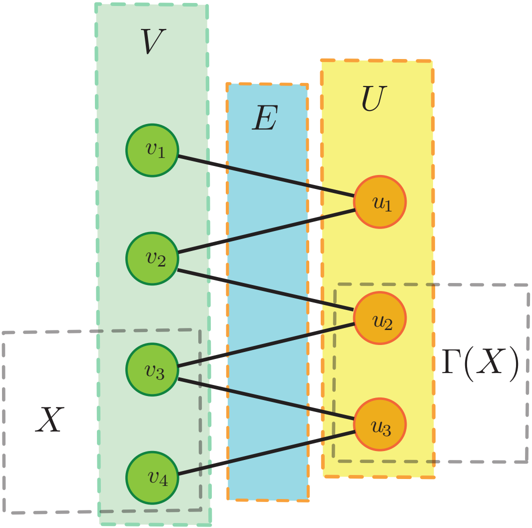
Bipartite Neighborhood Function

- 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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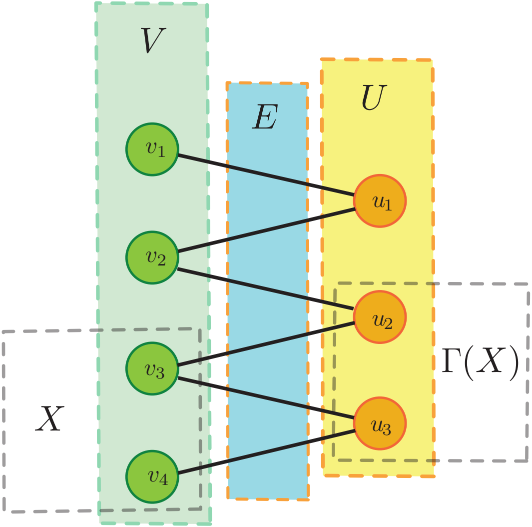

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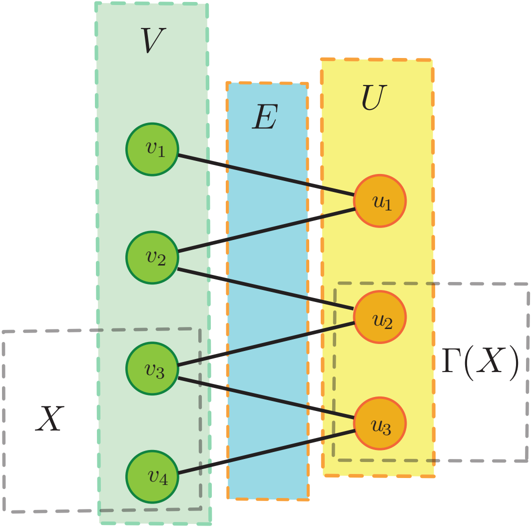

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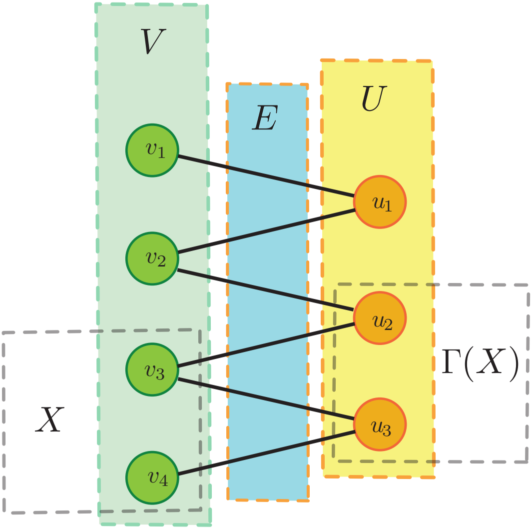
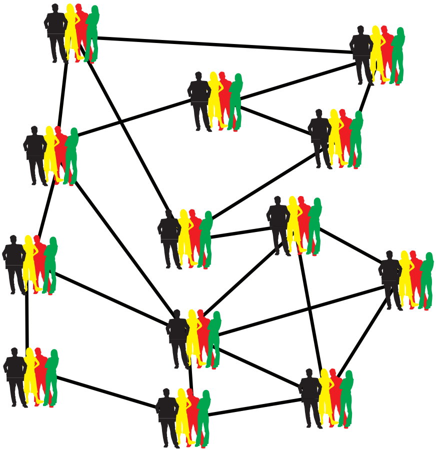


Facility/Plant Location (uncapacitated)

- 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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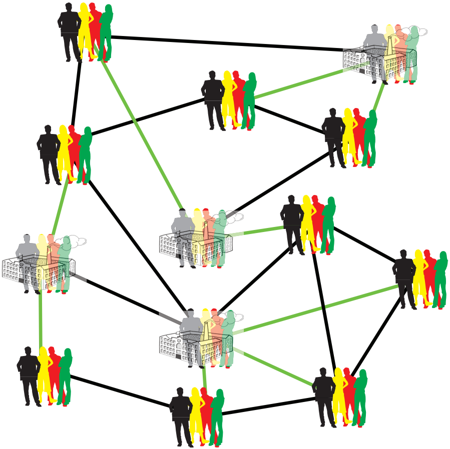

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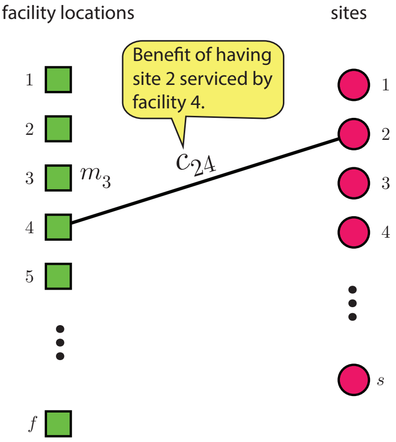
- We can model this with a weighted bipartite graph $G = (F, S, E, c)$ where F is set of possible factory/plant locations, S is set of sites needing service, E are edges indicating (factory,site) service possibility pairs, and $c : E \to \mathbb{R}_+$ is the benefit of a given pair.
- Facility location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

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



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

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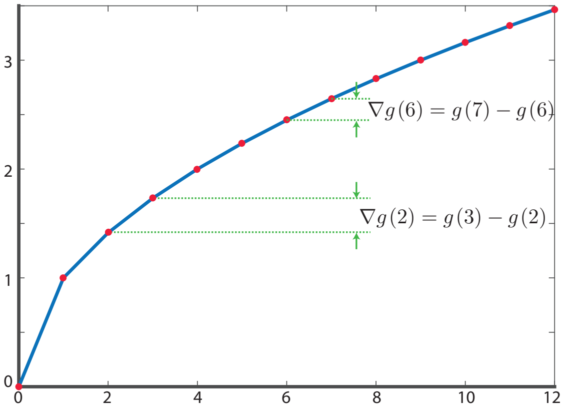

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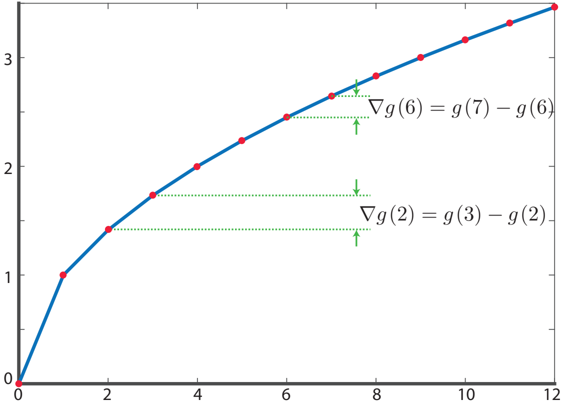

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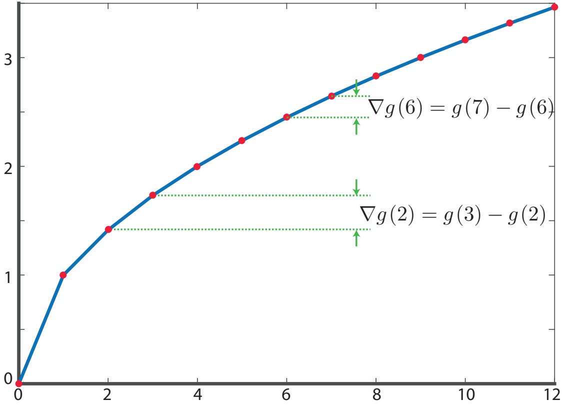

- This is a concave function (i.e., square root) composed with a modular function ($m(A) = \sum_{a \in A} m(a)$ where $m(a) = 1$).
- $\nabla g(i) > \nabla g(j)$ for $j > i$ by concavity, so f is a submodular function.

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- 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:

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

- 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 $V = \{1,2,3,4,5,6,7,8\}$.

$$\begin{array}{c|cccccccc} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ \hline 1 & & & & & & & & \\ 2 & \multicolumn{8}{c}{\left(\begin{array}{cccccccc} 0 & 2 & 2 & 3 & 0 & 1 & 3 & 1 \\ 0 & 3 & 0 & 4 & 0 & 0 & 2 & 4 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & 5 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 & 5 \end{array}\right)} \\ 3 & & & & & & & & \\ 4 & & & & & & & & \end{array}$$

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

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

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

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

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

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

- Let $A = \{1, 2, 3\}$, $B = \{3, 4, 5\}$, $C = \{6, 7\}$, $A_r = \{1\}$, $B_r = \{5\}$.
- Then $\boxed{r(A) = 3,}$ $\boxed{r(B) = 3,}$ $r(C) = 2$.
- $r(A \cup C) = 3$, $r(B \cup C) = 3$.
- $r(A \cup A_r) = 3$, $r(B \cup B_r) = 3$, $r(A \cup B_r) = 4$, $r(B \cup A_r) = 4$.
- $\boxed{r(A \cup B) = 4,}$ $\boxed{r(A \cap B) = 1}$ $< r(C) = 2$.
- $6 = \boxed{r(A) + r(B) > r(A \cup B) + r(A \cap B)} = 5$

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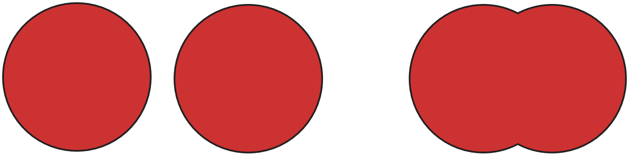

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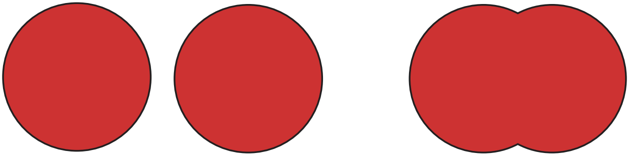

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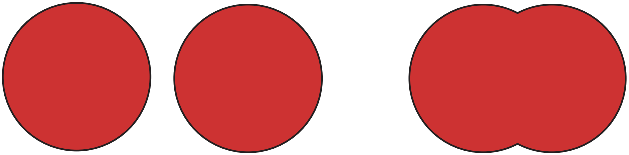

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- Any function where the above inequality is true for all $A, B \subseteq V$ is called subadditive.

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

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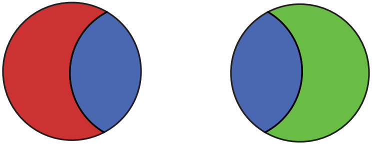

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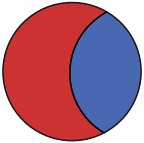

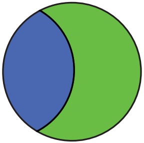

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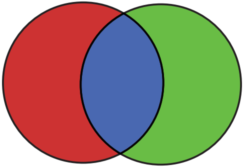

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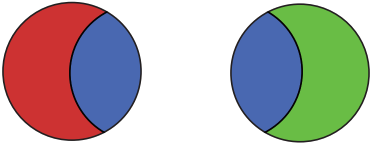

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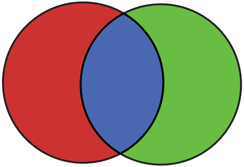

- Thus, we have subadditivity: $r(A) + r(B) \geq r(A \cup B)$. Can we add more to the r.h.s. and still have an inequality? Yes.

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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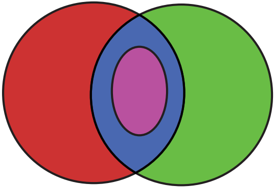

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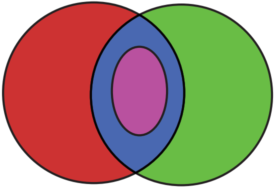

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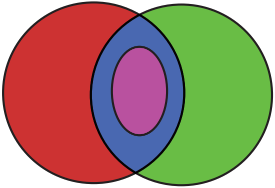

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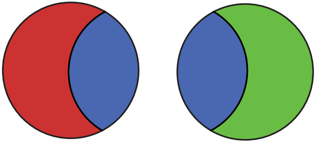
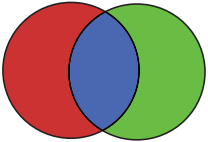
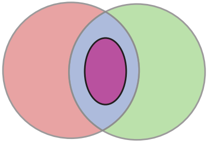
- More generally, common information (blue) is “more” (no less) than information within common index (magenta).

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. $J \cup \{x\} \in \mathcal{I}$.

A matroid rank function is submodular

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

Definition

The rank of a matroid is a function $r : 2^V \to \mathbb{Z}_+$ defined by

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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, $V = \{$

$\}$

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.

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

Gaussian entropy, and the log-determinant function

Definition (differential entropy $h(X)$)

$$h(X) = -\int_S f(x) \log f(x) dx \tag{40}$$

- 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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Gaussian entropy, and the log-determinant function

Definition (differential entropy $h(X)$)

$$h(X) = -\int_S f(x) \log f(x) dx \tag{40}$$

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

$$h(X) = \log \sqrt{|2\pi e \mathbf{\Sigma}|} = \log \sqrt{(2\pi e)^n |\mathbf{\Sigma}|} \tag{41}$$

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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*

$$I(X;Y) = I(X;Y|Z) = 0 \tag{44}$$

implies that

$$I(X;Y|Z,U) \leq I(Z;U|X,Y) + I(X;Y|U) \tag{45}$$

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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- When f is submodular, Eq. (46) is polytime, and Eq. (47) 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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Algorithm 5: The Greedy Algorithm

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

$$\text{minimize } |A| \text{ subject to } f(A) \geq \alpha \tag{50}$$

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

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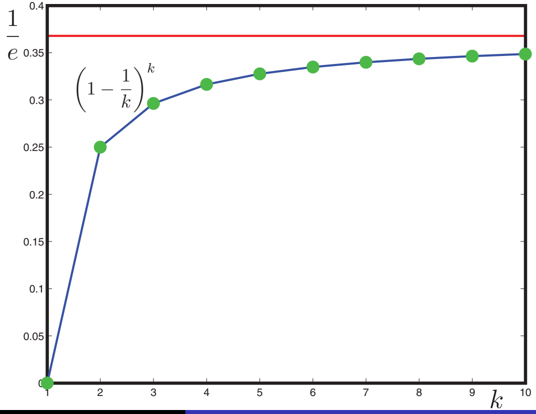

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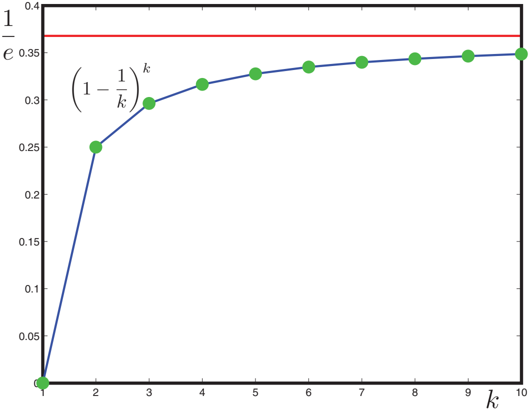

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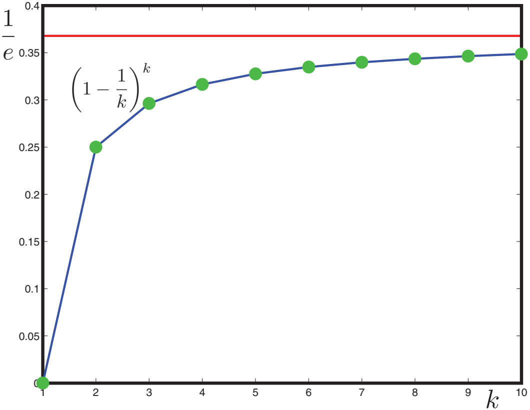

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- Frankenstein Cuts (Kawahara, Iyer, & B): $h(X) = f(X) + g(X)$ where f is submodular and g is a supermodular tree (submodular optimization for f, dynamic programming for g).

Outline: Part 2

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

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- A submodular function can act as a parameter for a machine learning strategy (active/semi-supervised learning, discrete divergence, convex norms for use in regularization).
- Itself, as an object or function to learn, based on data.
- A surrogate or relaxation strategy for optimization or analysis
  - An alternate to factorization, decomposition, or sum-product based simplification (as one typically finds in a graphical model). I.e., a means towards tractable surrogates for graphical models.

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  - Non-submodular problems can be analyzed via submodularity.

Outline: Part 2

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

Extractive Document Summarization

- The figure below represents the sentences of a document

Extractive Document Summarization

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

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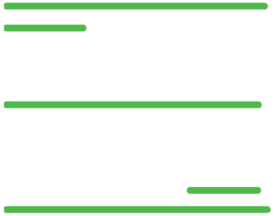

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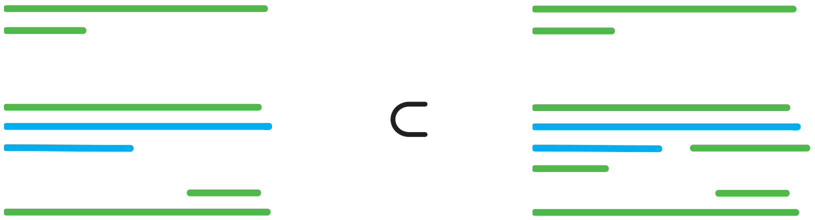

- The summary on the left is a subset of the summary on the right.
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- **diminishing returns** $\leftrightarrow$ **submodularity**

Image collections

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

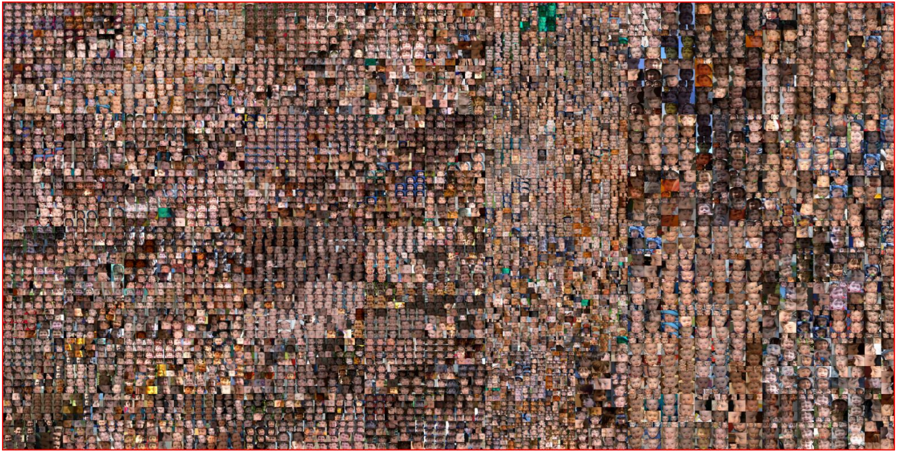

Image Summarization

10×10 image collection:

3 best summaries:

3 medium summaries:

3 worst summaries:

The three best summaries exhibit diversity. The three worst summaries exhibit redundancy (Tschiatschek, Iyer, & B, NIPS 2014).

Variable Selection in Classification/Regression

- Let Y be a random variable we wish to accurately predict based on at most n observed measurement variables $(X_1, X_2, \ldots, X_n) = X_V$ in a presumed probability model $\Pr(Y, X_1, X_2, \ldots, X_n)$.

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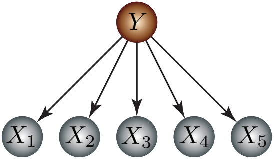
- The mutual information function $f(A) = I(Y; X_A)$ is defined as:

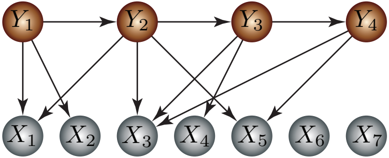
$$I(Y; X_A) = \sum_{y, x_A} \Pr(y, x_A) \log \frac{\Pr(y, x_A)}{\Pr(y)\Pr(x_A)} = H(Y) - H(Y|X_A) \quad (53)$$

$$= H(X_A) - H(X_A|Y) = H(X_A) + H(Y) - H(X_A, Y) \quad (54)$$

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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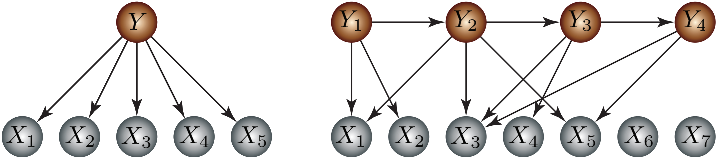

- When $X_A \perp\!\!\!\perp X_B | Y$ for all A, B (the Naïve Bayes assumption holds), then

$$f(A) = I(Y; X_A) = H(X_A) - H(X_A|Y) = H(X_A) - \sum_{a \in A} H(X_a|Y) \tag{55}$$

is submodular (submodular minus modular).

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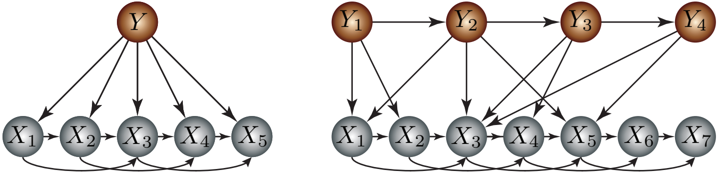

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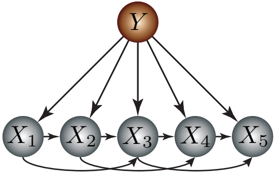

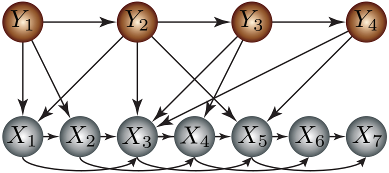

- $f(A)$ naturally expressed as a difference of two submodular functions

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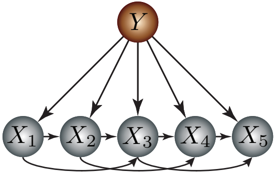

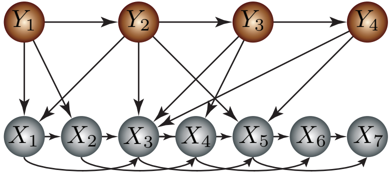

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- Alternatively, when Naïve Bayes assumption is false, we can make a submodular approximation (Peng-2005). E.g., functions of the form:

$$f(A) = \sum_{a \in A} I(X_a; Y) - \lambda \sum_{a, a' \in A} I(X_a; X_{a'}|Y) \tag{57}$$

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

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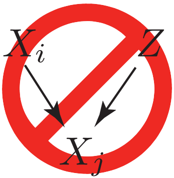
- When there are no "suppressor" variables (essentially, no v-structures that converge on X_j with parents X_i and Z), then

$$f(A) = R^2_{Z,A} = {b_A}^\intercal (C_A^{-1})^\intercal b_A \tag{59}$$



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

$$v = \text{“Whenever I go to New York City, I visit the New York City museum.”}$$

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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- Next, normalize the modular weights for each feature:

$$\bar{m}_u(X) = \frac{m_u(X)}{\sum_{u' \in U} m_{u'}(X)} = \frac{m_u(X)}{m(X)} \tag{62}$$

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- Consider the KL-divergence between these two distributions:

$$D(p||\{\bar{m}_u(X)\}_{u \in U}) = \sum_{u \in U} p_u \log p_u - \sum_{u \in U} p_u \log(\bar{m}_u(X)) \tag{63}$$

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

$$= -H(p) + \log m(X) - \sum_{u \in U} p_u \log(m_u(X)) \tag{64}$$

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- Alternatively, if we define (Shinohara, 2014)

$$g(X) \triangleq \log m(X) - D(p||\{\bar{m}_u(X)\}) = \sum_{u \in U} p_u \log(m_u(X)) \quad (66)$$

we have a submodular function g that represents a combination of its quantity of X via its features (i.e., $\log m(X)$) and its feature distribution closeness to some distribution p (i.e., $D(p||\{\bar{m}_u(X)\})$).

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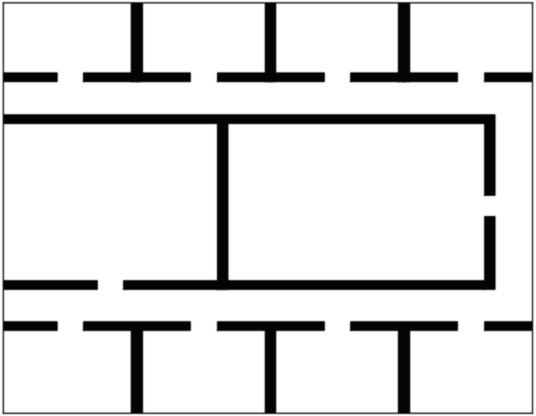
- Environment could be a floor of a building, water network, monitored ecological preservation.

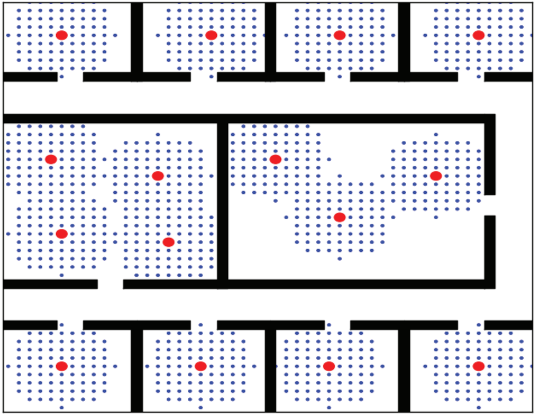
Sensor Placement within Buildings

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



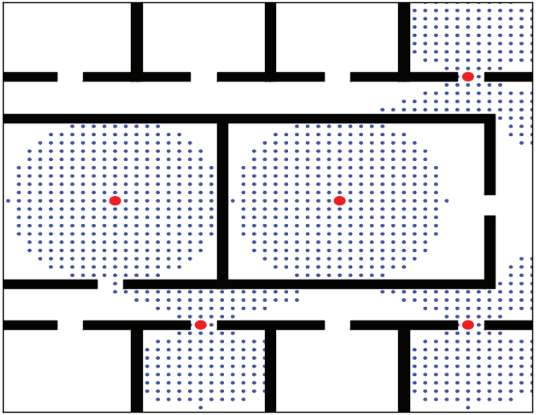
Sensor Placement within Buildings

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



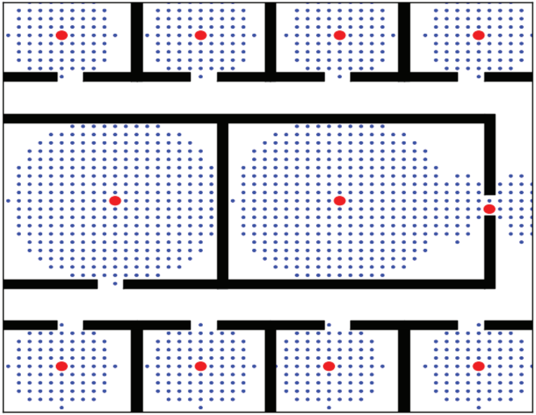
Sensor Placement within Buildings

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



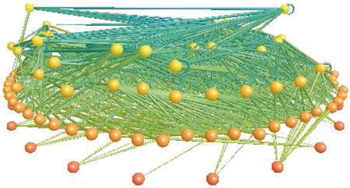
Sensor Placement within Buildings

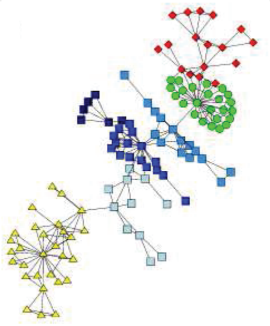
- Example sensor placement using mixed range sensors (located at red dots).

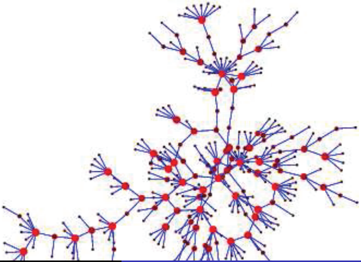


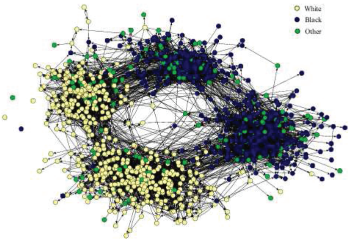
Social Networks

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









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- Which is a better model?

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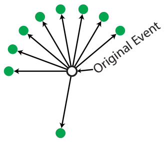

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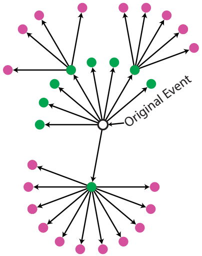

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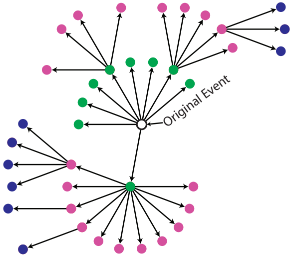

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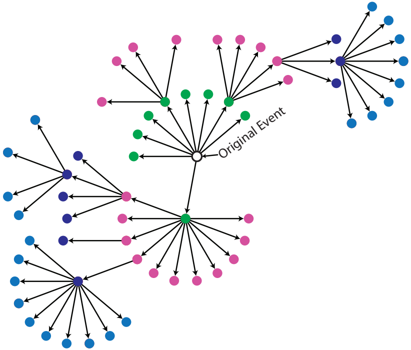

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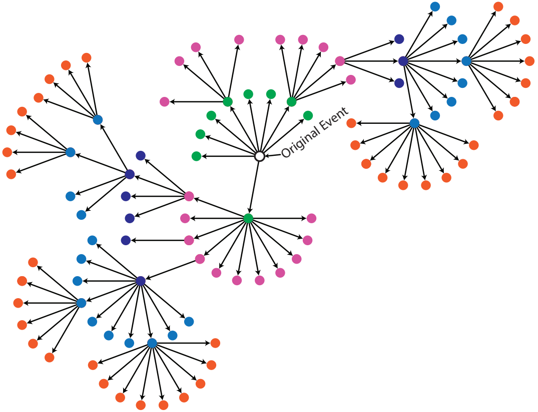

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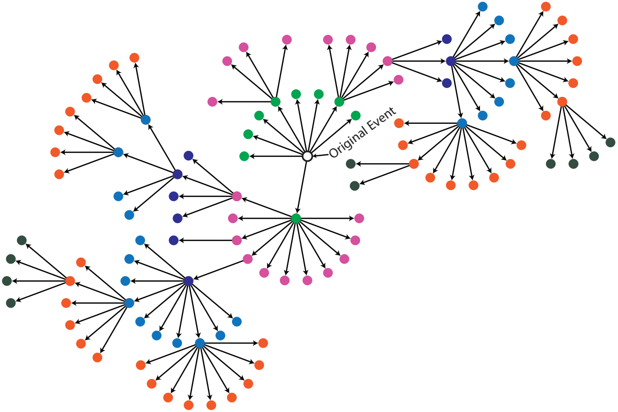

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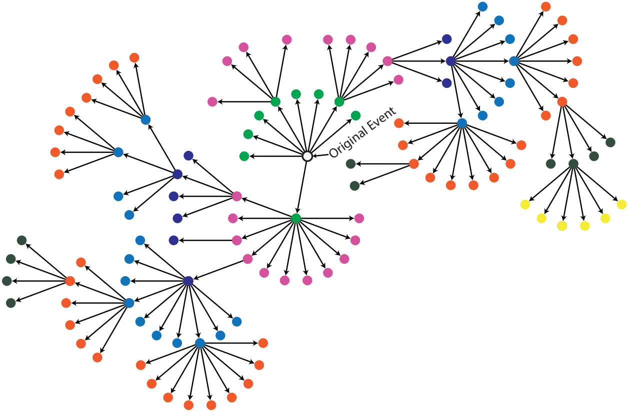

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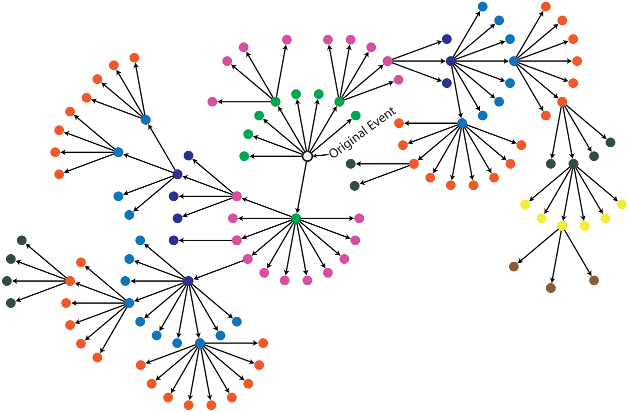

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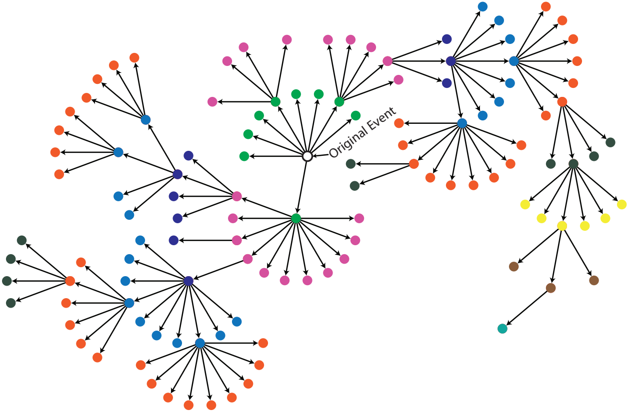

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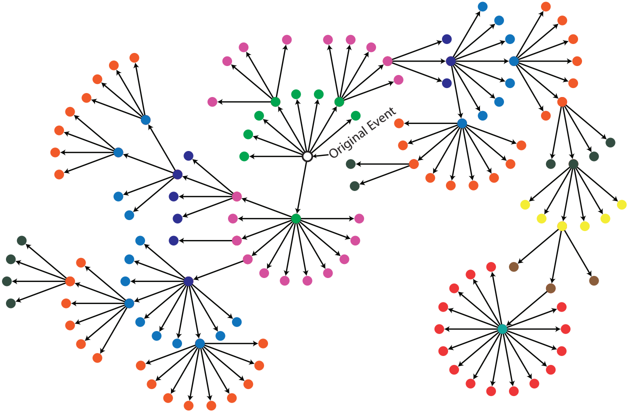

- Goal: How to find the most influential sources, the ones that often set off cascades, which are like large "waves" of information flow?

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

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

$$p(x) = \frac{1}{Z} \exp(-E(x)) \tag{67}$$

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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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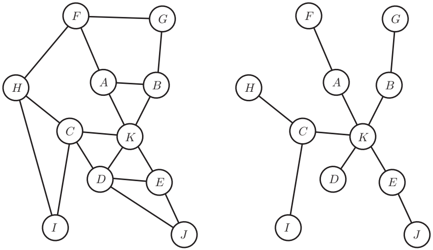

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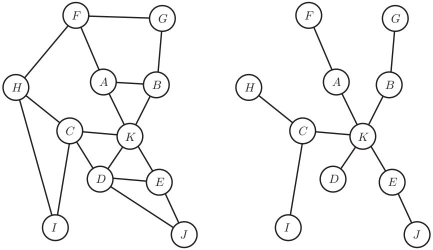

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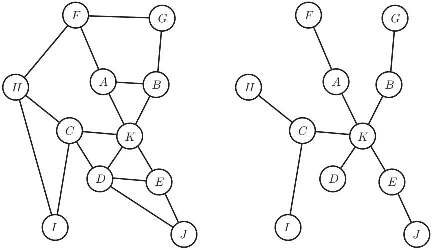

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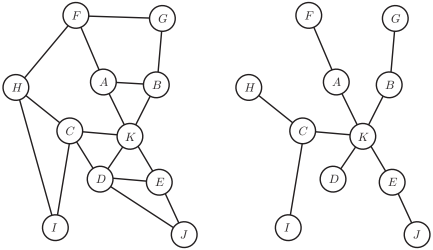

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- Then finding the maximum weight base of the matroid is solved by the greedy algorithm, and also finds the optimal tree (Chow & Liu, 1968)

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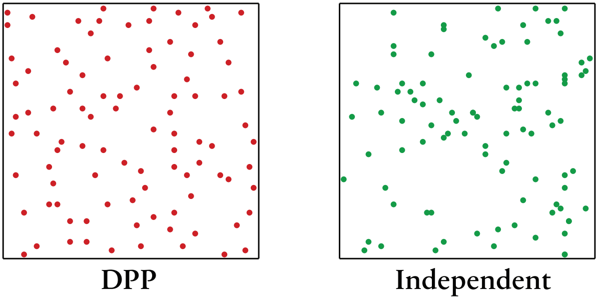

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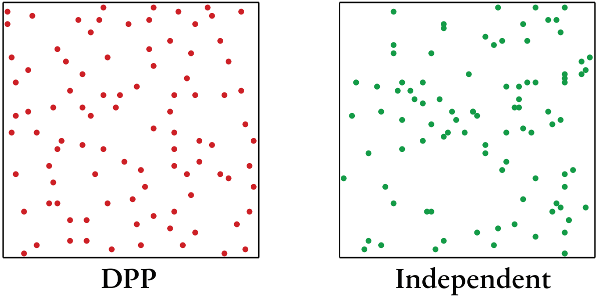

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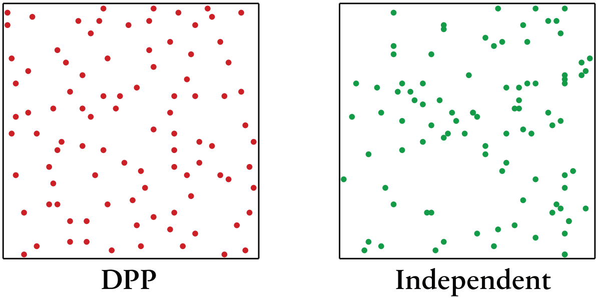

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- More "diverse" or "complex" samples are given higher probability.

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$$\Pr(\mathbf{X} = x) = \frac{|M_{X(x)}|}{|M + I|} = \exp\left(\log\left(\frac{|M_{X(x)}|}{|M + I|}\right)\right) \propto \det(M_{X(x)}) \quad (69)$$

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

Outline: Part 2

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

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- 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:

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- Further, say that $\mathrm{D}_{X_v} = \{0, 1\}$ (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.,

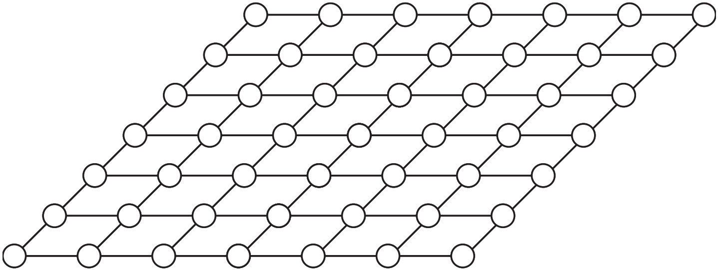
$$\min_{x \in \{0,1\}^V} E(x) \tag{74}$$

MRF example

Markov random field

$$\log p(x) \propto \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \tag{75}$$

When G is a 2D grid graph, we have

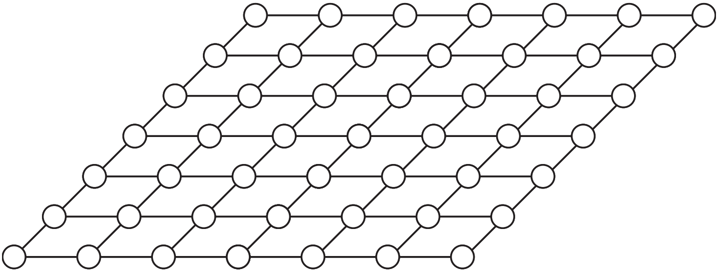


Create an auxiliary graph

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

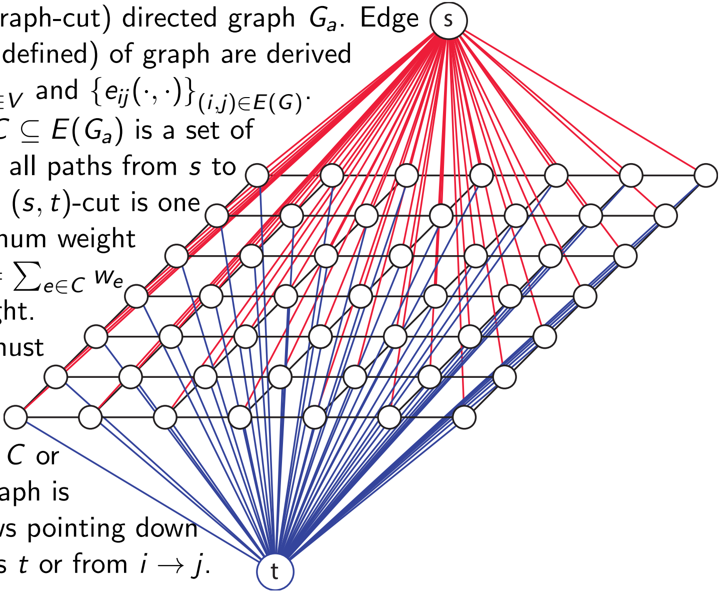
Transformation from graphical model to auxiliary graph

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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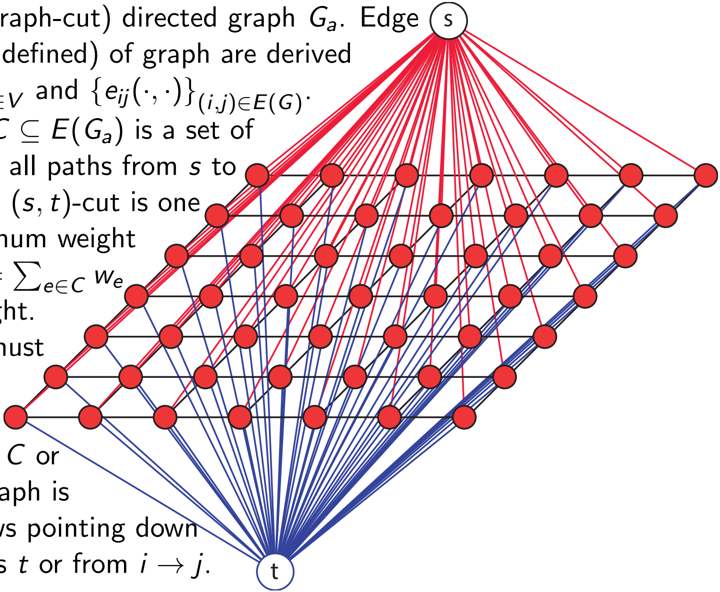
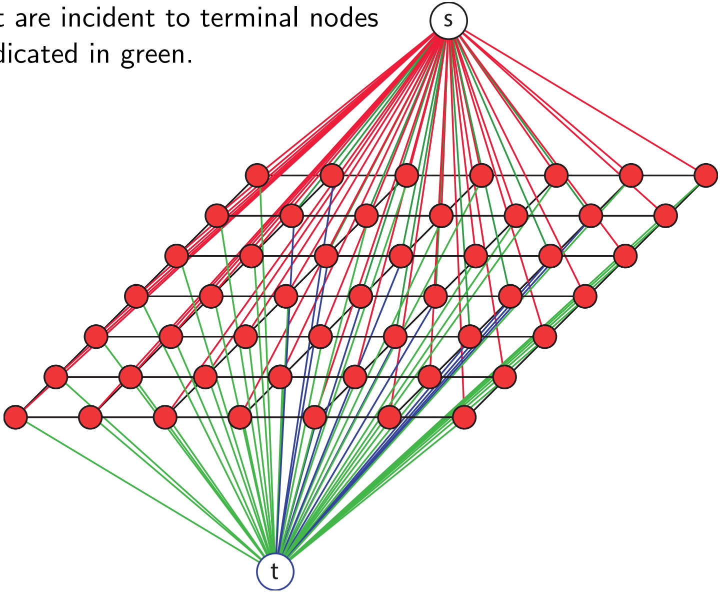


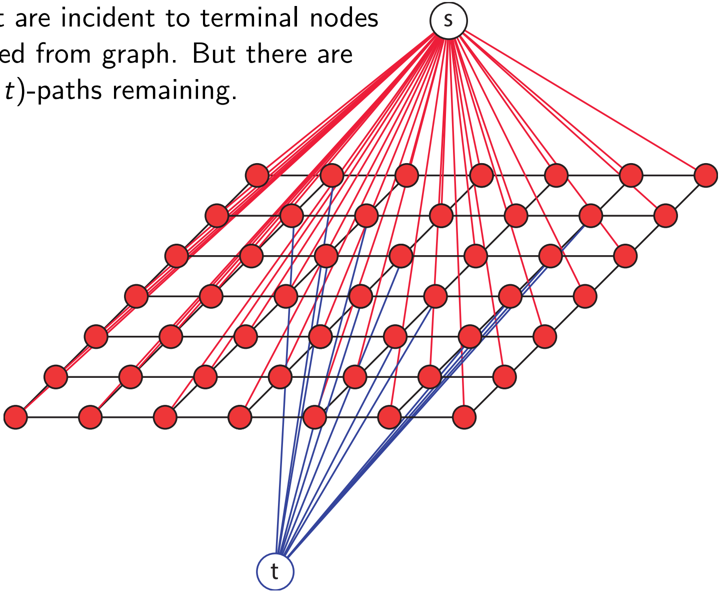
Transformation from graphical model to auxiliary graph

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



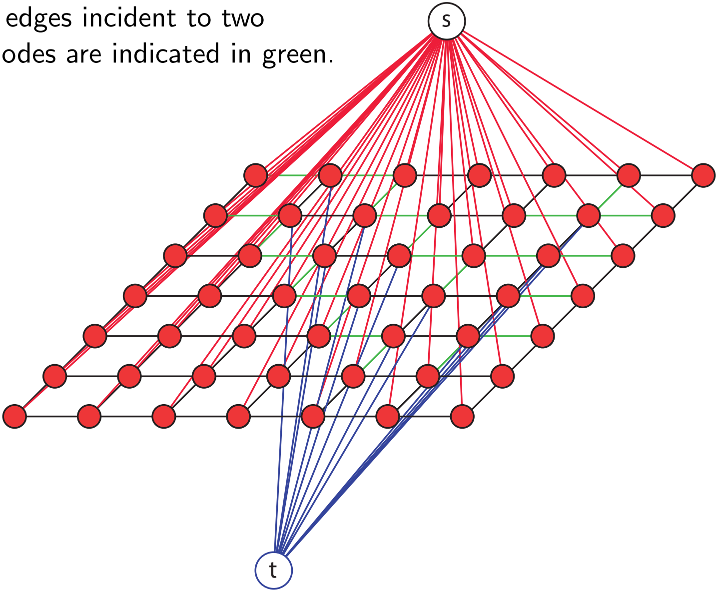
Transformation from graphical model to auxiliary graph

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



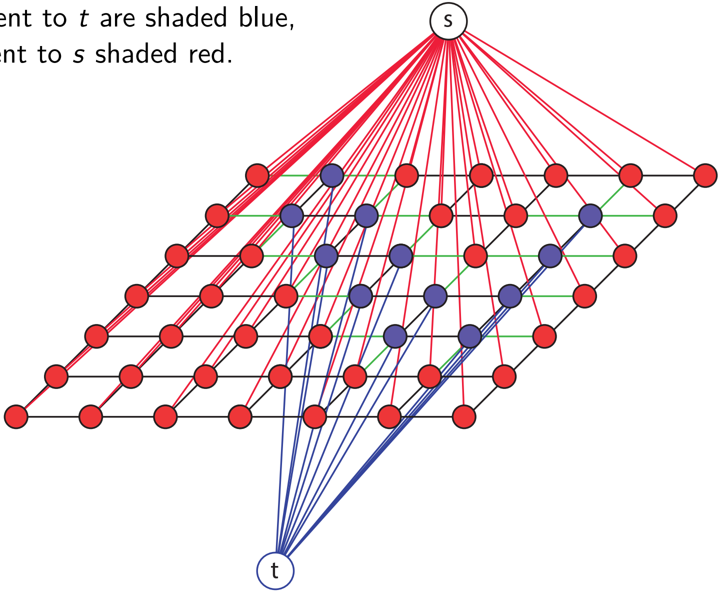
Transformation from graphical model to auxiliary graph

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.



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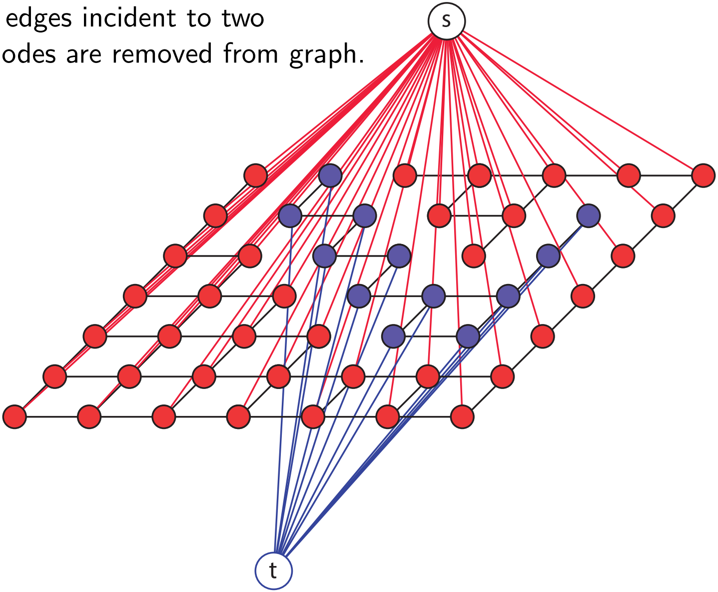
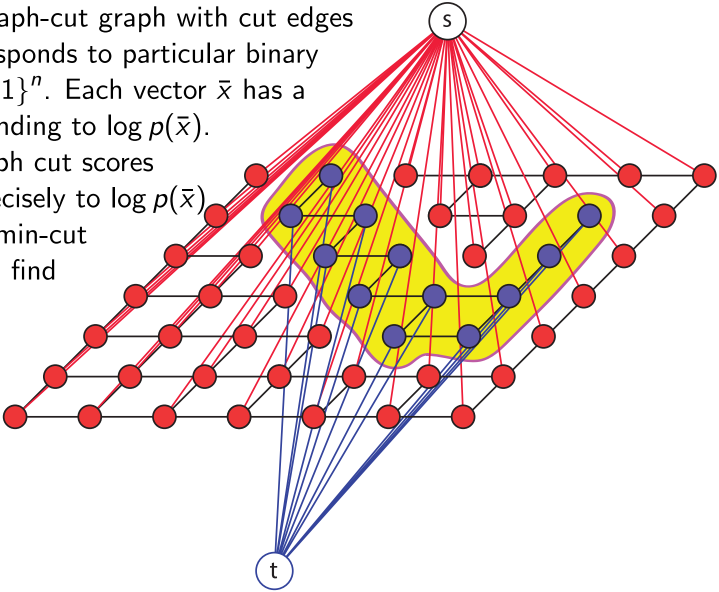


Transformation from graphical model to auxiliary graph

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 $E(x)$?



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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

$$w_{s,v} = (e_v(1) - e_v(0))\mathbf{1}(e_v(1) > e_v(0)) \tag{76}$$

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

$$w_{v,t} = (e_v(0) - e_v(1))\mathbf{1}(e_v(0) \geq e_v(1)) \tag{77}$$

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

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

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

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and analogous increments if inequalities are flipped.

Restricted clique functions

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

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- In probability form $p(x) \propto \prod \psi$, we get $\psi_{ij}(1,0)\psi_{ij}(0,1) \leq \psi_{ij}(0,0)\psi_{ij}(1,1)$, so geometric mean of factor scores (thus probability) is higher when neighboring pixels have the same value - reasonable assumption in natural scenes and signals.

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- So weights w_{ij} in s,t-graph above are always non-negative.

Theorem

If edge functions are submodular and edge weights in s,t-graph are set as above, then finding the minimum s,t-cut in the auxiliary graph will yield a variable assignment having maximum probability.

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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- 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.

$$\log \Pr(x) = f(x) + \text{const.} = -E(x) + \text{const.} \tag{86}$$

where f is supermodular ($E(x)$ is submodular). MAP (or high-probable) assignments should be "regular", "homogeneous", "smooth", "simple". E.g., attractive potentials in computer vision, ferromagnetic Potts models statistical physics.

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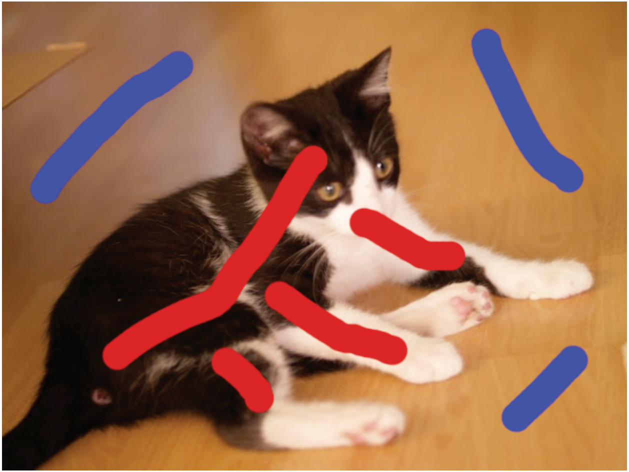
Submodular potentials in GMs: Image Segmentation

- an image needing to be segmented.

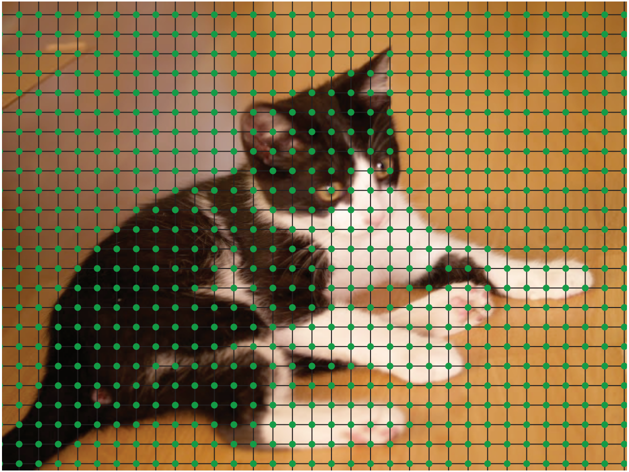
Submodular potentials in GMs: Image Segmentation

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



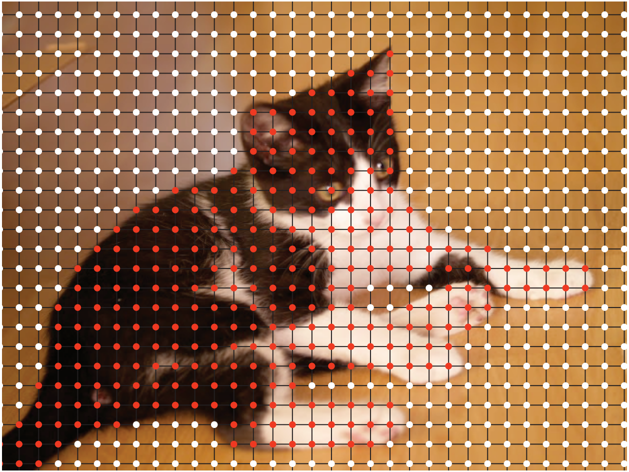
Submodular potentials in GMs: Image Segmentation

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



Submodular potentials in GMs: Image Segmentation

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



Submodular potentials in GMs: Image Segmentation

- the foreground is removed from the background.

Graph Cut Marginalization

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- On the other hand, for pairwise MRFs, computing partition function in submodular potential case is approximable (has low error with high probability).
- SPPs and log(SPP)s (Rishabh's talk) will also talk about how submodularity allows further approximations via semigradients.

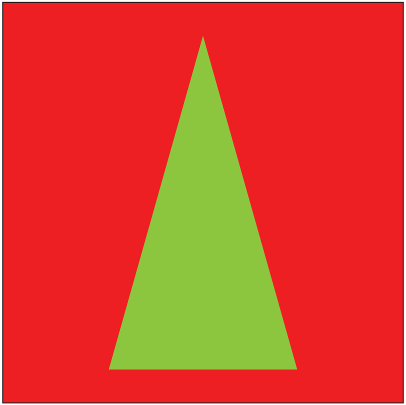
Shrinking bias in graph cut image segmentation

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

Shrinking bias in graph cut image segmentation

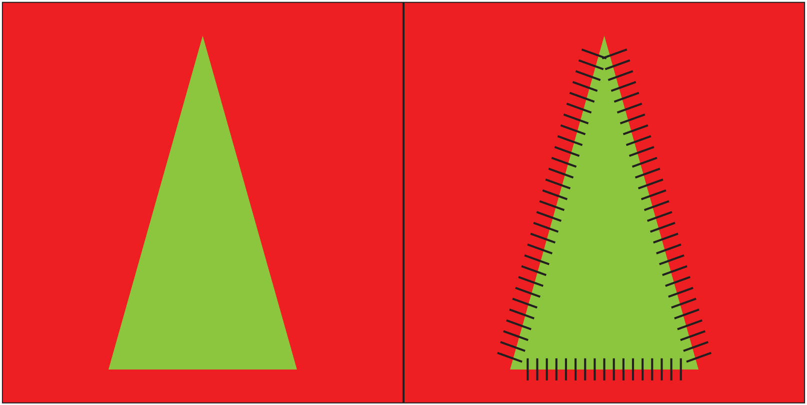
Shrinking bias in image segmentation

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



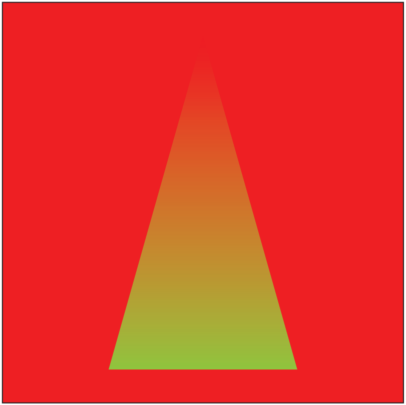
Shrinking bias in image segmentation

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



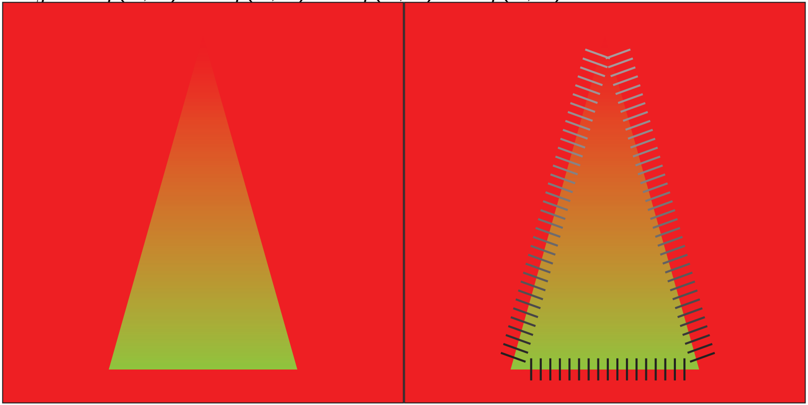
Shrinking bias in image segmentation

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



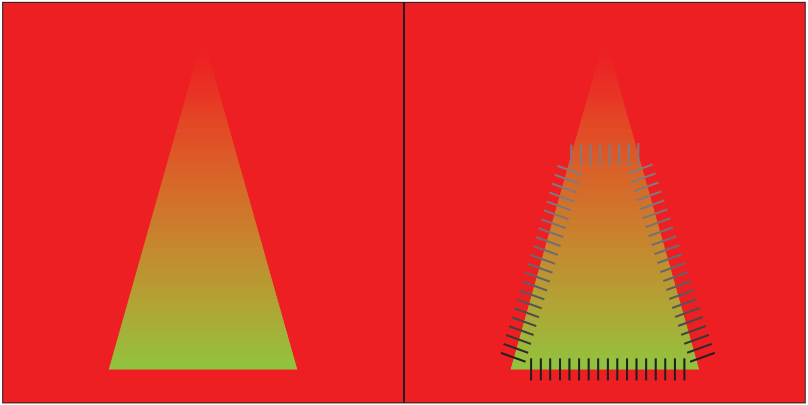
Shrinking bias in image segmentation

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



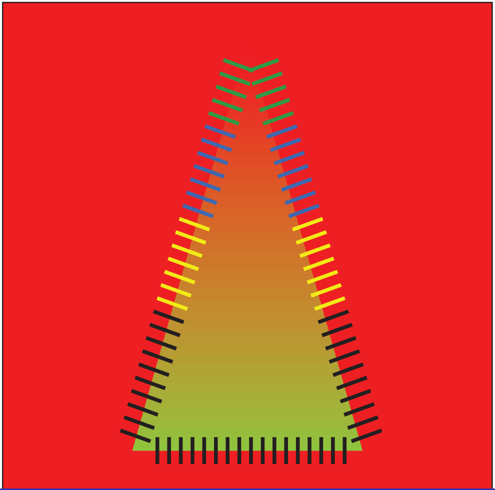
Shrinking bias in image segmentation

- 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.

$$f_w(X) = w\Big(\{(u, v) \in E : u \in X, v \in V \setminus X\}\Big) \tag{88}$$

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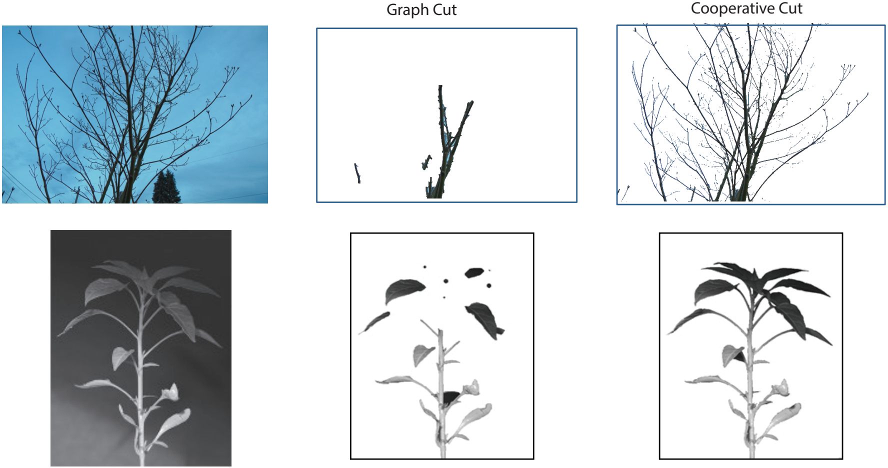
- $\Rightarrow$ cooperative-cut (Jegelka & B., 2011).

Graph-cut vs. cooperative-cut comparisons



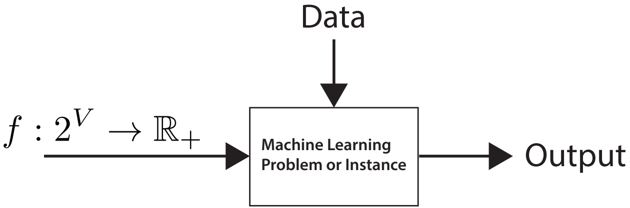
(Jegelka&Bilmes,'11). There are fast algorithms for solving as well.

Outline: Part 2

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

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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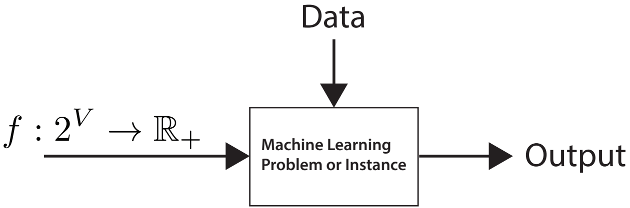

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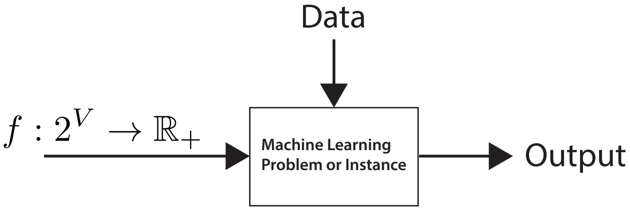

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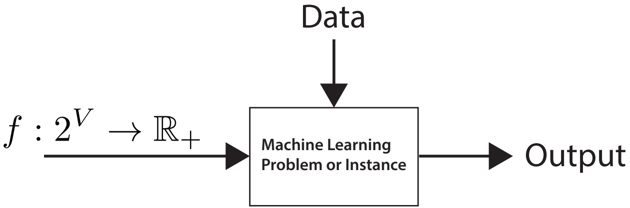

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- $\mathbb{S}$ is a submodular cone since submodularity is closed under non-negative (conic) combinations.
- 2^n-dimensional since for certain $f \in \mathbb{S}$, there exists $f_\epsilon \in \mathbb{R}^{2^n}$ having no zero elements with $f + f_\epsilon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

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:

$$\min_{w \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^m \ell(y_i, w^\intercal x_i) + \lambda \Omega(w), \tag{90}$$

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:

$$\min_{w^1, \dots, w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^j, (w^j)^\intercal x_i) + \lambda \Omega(w^j), \tag{91}$$

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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:

$$\Omega(w) = \sum_{i=2}^{N} |w_i - w_{i-1}| \tag{94}$$

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

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$$I'_f(S_1; S_2; \ldots; S_k) = \sum_{A \subseteq \{1,2,\ldots,k\}} (-1)^{|A|+1} f(\bigcup_{j \in A} S_j) \tag{100}$$

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- Hence, family of clustering algorithms parameterized by f.

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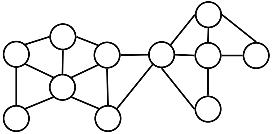
8. Submodular functions may be more general than clustering objectives (submodularity allows high-order interactions between elements).

Active Transductive Semi-Supervised Learning

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



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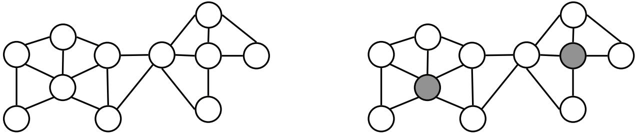

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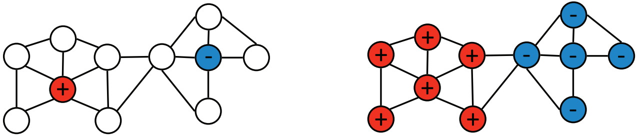

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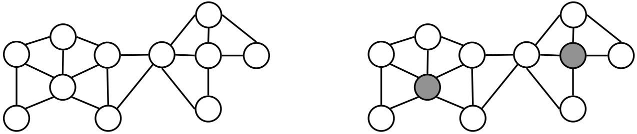

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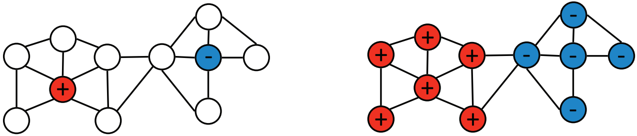
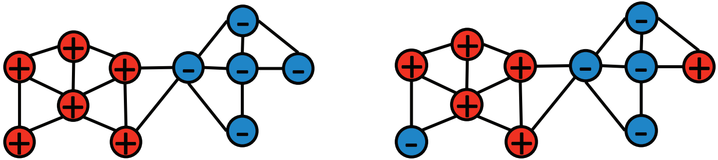


- Learner suffers loss $\|\hat{y} - y\|_1$, where y is truth. Below, $\|\hat{y} - y\|_1 = 2$.



Choosing labels: how to select L

- Consider the following objective

$$\Psi(L) = \min_{T \subseteq V \setminus L : T \neq \emptyset} \frac{\Gamma(T)}{|T|} \tag{101}$$

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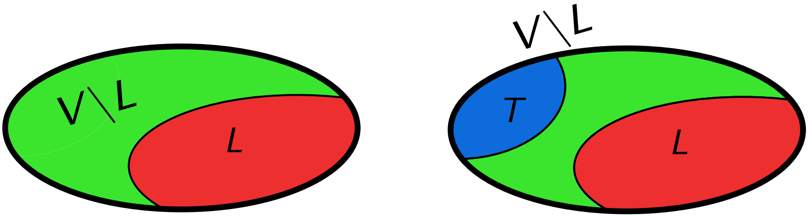

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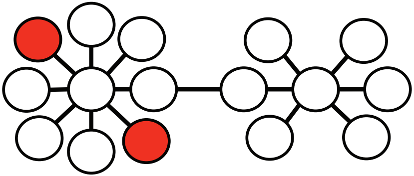

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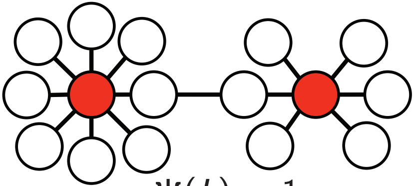

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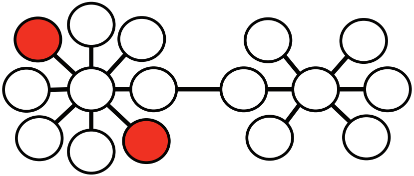

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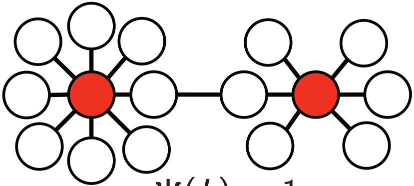

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- This suggests choosing (bounded cost) L that maximizes $\Psi(L)$.

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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

$$\|\hat{y} - y\|_1 \leq 2\frac{\Gamma(Y(y))}{\Psi(L)} \tag{103}$$

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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- Data subset (or core set) selection in machine learning (Lin & Bilmes, Wei & Bilmes). Data summarization, summarizing big redundant data.

examples: submodular parameterization

- Combinatorial independence, generalized entropy, and “information” or “complexity” functions (seen above).
- Simultaneous batch active-learning/semi-supervised learning (Guillory & Bilmes).
- Rank-order based divergences (Submodular Bregman Divergence, and the Lovász-Bregman Divergences) (Iyer & Bilmes, 2013).
- Feature and dictionary selection (Krause & Guestrin, Das & Kempe)
- Computer vision (Kolmogorov, Boykov, Kohli, Ladicky, Torr, etc.).
- Data subset (or core set) selection in machine learning (Lin & Bilmes, Wei & Bilmes). Data summarization, summarizing big redundant data.
- Influence determination in social networks (Kempe, Kleinberg, & Tardos)

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- Balcan & Harvey (2011): submodular function learning problem from a learning theory perspective, given a distribution on subsets. Negative result is that can't approximate in this setting to within a constant factor.
- But can we learn a subclass, perhaps non-negative weighted mixtures of submodular components?

Structured Prediction in Machine Learning

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

$$\hat{\mathbf{y}} \in h_{\mathbf{w}}(\bar{\mathbf{x}}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} s(\bar{\mathbf{x}}, \mathbf{y}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} \mathbf{w}^\intercal \mathbf{f}(\bar{\mathbf{x}}, \mathbf{y}) \tag{107}$$

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

Structured Learning of Submodular Mixtures

- Constraints specified in inference form:

$$\underset{\mathbf{w},\xi_t}{\text{minimize}} \quad \frac{1}{T}\sum_t \xi_t + \frac{\lambda}{2}\|\mathbf{w}\|^2 \tag{108}$$

$$\text{subject to} \quad \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) \geq \max_{\mathbf{y}\in\mathcal{Y}_t}\left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y})\right) - \xi_t, \forall t \tag{109}$$

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- If loss is supermodular, this is a difference-of-submodular (DS) function optimization.

Learning Submodular Mixtures: Unconstrained Form

- Unconstrained form uses a generalized hinge-loss (Taskar 2004), which is amenable to sub-gradient descent optimization:

$$\min_{\mathbf{w}\geq 0} \frac{1}{T} \sum_t \left[\max_{\mathbf{y}\in\mathcal{Y}_t} \left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y}) \right) - \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) \right] + \frac{\lambda}{2} \|\mathbf{w}\|^2 \quad (111)$$

- Note, $\mathbf{w} \geq 0$ critical to preserve submodularity.
- To compute a subgradient, must solve the following embedded optimization problem ("loss augmented inference"):

$$\max_{\mathbf{y}\in\mathcal{Y}_t} \left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y}) \right) \quad (112)$$

- The problem is convex in $\mathbf{w}$, and $\mathbf{w}^\top \mathbf{f}_t(\mathbf{y})$ is submodular (polymatroidal in fact), but what about $\ell_t(\mathbf{y})$?
- Often one uses Hamming loss (in general structured prediction problems) which is submodular (modular in fact).
- If loss $\ell_t(\mathbf{y})$, more generally, is submodular, then Eq. (112) can be solved at least approximately well.

Structured Prediction: Subgradient

- Subgradient, evaluated at $\mathbf{w}$, of the following

$$\max_{\mathbf{y}\in\mathcal{Y}_t}\left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y})\right) - \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) + \frac{\lambda}{2}\|\mathbf{w}\|^2 \tag{113}$$

can be found by computing or approximating

$$\mathbf{y}^* \in \operatorname*{argmax}_{\mathbf{y}\in\mathcal{Y}_t}\left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y})\right) - \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) \tag{114}$$

and then finding subgradient of

$$\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^*) + \ell_t(\mathbf{y}^*) - \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) + \frac{\lambda}{2}\|\mathbf{w}\|^2 \tag{115}$$

which has the form

$$\mathbf{f}_t(\mathbf{y}^*) - \mathbf{f}_t(\mathbf{y}^{(t)}) + \lambda\mathbf{w}. \tag{116}$$

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!