Submodular Functions, Optimization, and Applications to Machine Learning
— Spring Quarter, Lecture 2 —

http://www.ee.washington.edu/people/faculty/bilmes/classes/ee563_spring_2018/

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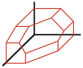
$f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$

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



Cumulative Outstanding Reading

- Read chapter 1 from Fujishige's book.

Class Road Map - EE563

- L1(3/26): Motivation, Applications, & Basic Definitions,
- L2(3/28): Machine Learning Apps (diversity, complexity, parameter, learning target, surrogate).
- L3(4/2):
- L4(4/4):
- L5(4/9):
- L6(4/11):
- L7(4/16):
- L8(4/18):
- L9(4/23):
- L10(4/25):
- L11(4/30):
- L12(5/2):
- L13(5/7):
- L14(5/9):
- L15(5/14):
- L16(5/16):
- L17(5/21):
- L18(5/23):
- L–(5/28): Memorial Day (holiday)
- L19(5/30):
- L21(6/4): Final Presentations maximization.

Last day of instruction, June 1st. Finals Week: June 2-8, 2018.

Two Equivalent Submodular Definitions

$|V|=n$

Definition 2.2.1 (submodular concave)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \quad (2.8)$$

An alternate and (as we will soon see) equivalent definition is:

Definition 2.2.2 (diminishing returns)

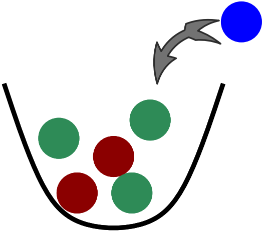
A function $f : 2^V \to \mathbb{R}$ is submodular if for any $A \subseteq B \subset V$, and $v \in V \setminus B$, we have that:

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \quad (2.9)$$

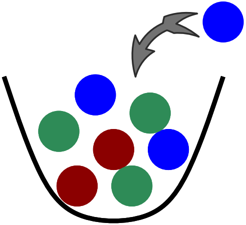
The incremental "value", "gain", or "cost" of v decreases (diminishes) as the context in which v is considered grows from A to B.

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 in S.



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



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

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

Two Equivalent Supermodular Definitions

Definition 2.2.1 (supermodular)

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

$$f(A) + f(B) \leq f(A \cup B) + f(A \cap B) \tag{2.8}$$

Definition 2.2.2 (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:

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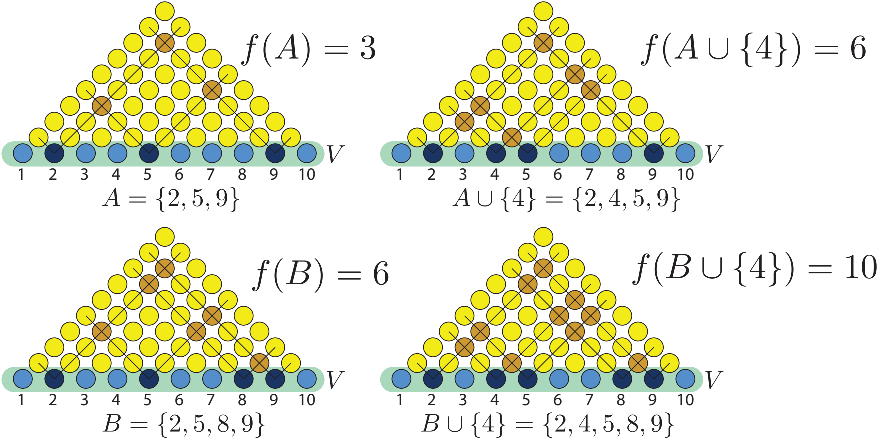
- Incremental "value", "gain", or "cost" of v increases (improves) as the context in which v is considered grows from A to B.
- A function f is submodular iff $-f$ is supermodular.
- If f both submodular and supermodular, then f is said to be **modular**, and $f(A) = c + \sum_{a \in A} f(a)$ (often $c = 0$).

Example Supermodular: Number of Balls with Two Lines

Given ball pyramid, bottom row V is size $n = |V|$. For subset $S \subseteq V$ of bottom-row balls, draw 45° and 135° diagonal lines from each $s \in S$. Let $f(S)$ be number of non-bottom-row balls with two lines $\Rightarrow f(S)$ is supermodular.



Review So far

- Machine learning paradigms should be: easy to define, mathematically rich, naturally applicable, and efficient/scalable.
- Convexity (continuous structures) and graphical models (based on factorization or additive separation) are two such modeling paradigms.
- Submodularity/supermodularity offer a distinct mathematically rich paradigm over discrete space that neither need be continous nor be additively additively separable,
- submodularity offers forms of structural decomposition, e.g., $h = f + g$, into potentially global (manner of interaction) terms.
- Set cover, supply and demand side economies of scale,

Submodularity's utility in ML

- A model of a physical process:
  - When maximizing, submodularity naturally models: diversity, coverage, span, and information.
  - When minimizing, submodularity naturally models: cooperative costs, complexity, roughness, and irregularity.
  - vice-versa for supermodularity.
- A submodular function can act as a parameter for a machine learning strategy (active/semi-supervised learning, discrete divergence, structured sparse 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.
  - Also, we can "relax" a problem to a submodular one where it can be efficiently solved and offer a bounded quality solution.
  - Non-submodular problems can be analyzed via submodularity.

Many different functions are submodular!

- We will see many applications of submodularity in machine learning.
- On next set of slides, we will state (without proof, for now) that many of the functions are submodular (or supermodular).
- In subsequent lectures, we will start showing how to prove submodularity.

Functions to Measure Diversity

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- How do we choose the smallest set S that maintains a given degree of diversity? Constrained minimization (i.e., $\min |A|$ s.t. $f(A) \geq \alpha$).

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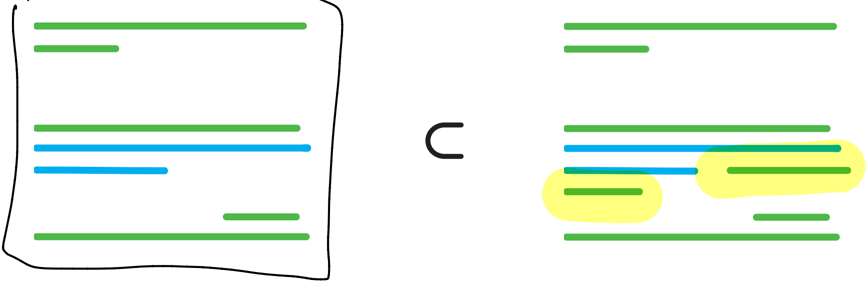
- How do we choose the smallest set S that maintains a given degree of diversity? Constrained minimization (i.e., $\min |A|$ s.t. $f(A) \geq \alpha$).
- Random sample has probability of poorly representing normally underrepresented groups.

Extractive Document Summarization

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



- The summary on the left is a subset of the summary on the right.
- Consider adding a new (blue) sentence to each of the two summaries.
- The marginal (incremental) benefit of adding the new (blue) sentence to the smaller (left) summary is no ~~more~~ less than the marginal benefit of adding the new sentence to the larger (right) summary.
- **diminishing returns $\leftrightarrow$ submodularity**

Large image collections need to be summarized

Many images, also that have a higher level gestalt than just a few, want a summary (subset of images) to represent the diversity in the large image set.

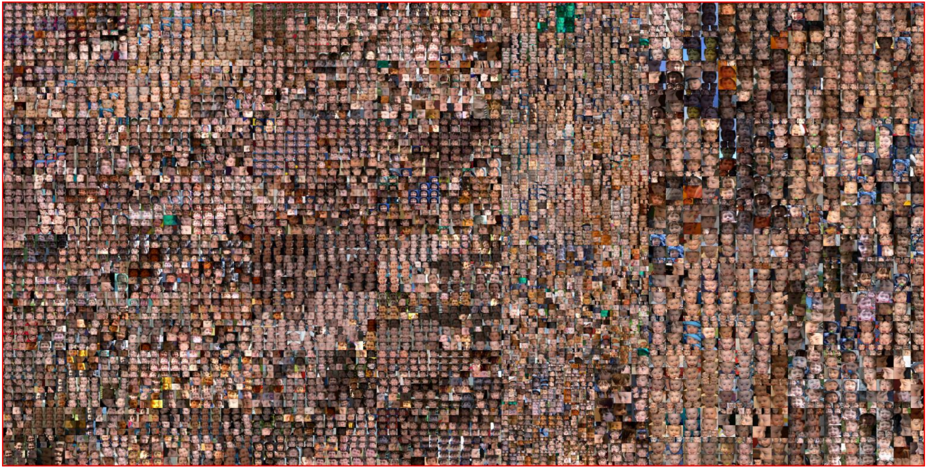


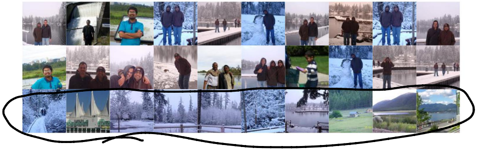
Image Summarization

10×10 image collection:

3 good summaries (diverse):

3 ok summaries:

3 poor summaries (redundant):



More Generally: Information and Summarization

- Let V be a set of information containing elements (V might say be any of words, sentences, documents, web pages, or blogs, sensor readings, etc.).

$f(v)$

- Each $v \in V$ is one (or a set of) element(s). The total amount of information in V is measure by a function $f(V)$, and any given subset $S \subseteq V$ measures the amount of information in S, given by $f(S)$.
- How informative is any given item v in different sized contexts? Any such real-world information function would exhibit diminishing returns, i.e., the value of v decreases when it is considered in a larger context.
- A submodular function is likely a good model.

Variable Selection in Classification/Regression

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

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- Too costly to use all V variables. Goal: choose subset $A \subseteq V$ of variables within budget $|A| \leq k$. Predictions based on only $\Pr(y|x_A)$, hence subset A should retain accuracy.

$x_A = \{x_{a_1}, x_{a_2}, \ldots, x_{a_{|A|}}\}$

$A = \{a_1, \ldots, a_{|A|}\}$

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

$$I(Y; X_A) = \sum_{y, x_A} \Pr(y, x_A) \log \frac{\Pr(y, x_A)}{\Pr(y) \Pr(x_A)} = H(Y) - H(Y|X_A) \quad (2.1)$$

$$= H(X_A) - H(X_A|Y) = H(X_A) + H(Y) - H(X_A, Y) \quad (2.2)$$

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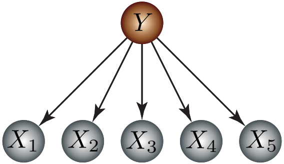
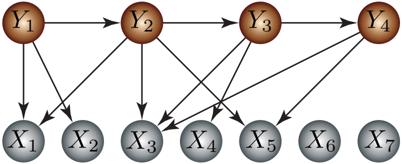
- Applicable in pattern recognition, also in sensor coverage problem, where Y is whatever question we wish to ask about environment.

Information Gain and 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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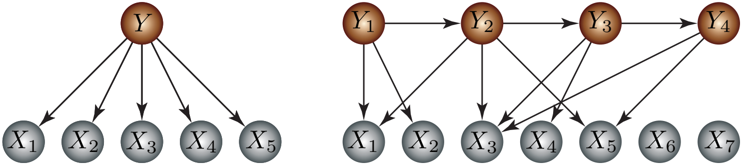


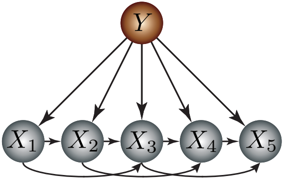
- When $X_A \perp\!\!\!\perp X_B | Y$ for all A, B (the Naïve Bayes assumption holds), then

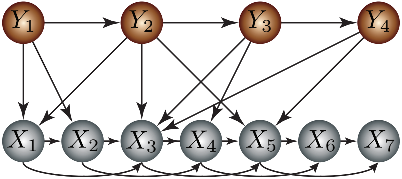
$$f(A) = I(Y; X_A) = H(X_A) - H(X_A|Y) = H(X_A) - \sum_{a \in A} H(X_a|Y) \tag{2.3}$$

is submodular (submodular minus modular).

Variable Selection in Pattern Classification

- Naïve Bayes property fails:





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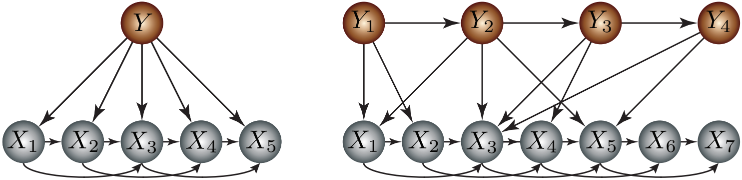

- $f(A)$ naturally expressed as a difference of two submodular functions

$$f(A) = I(Y; X_A) = H(X_A) - H(X_A|Y), \tag{2.4}$$

which is a DS (difference of submodular) function.

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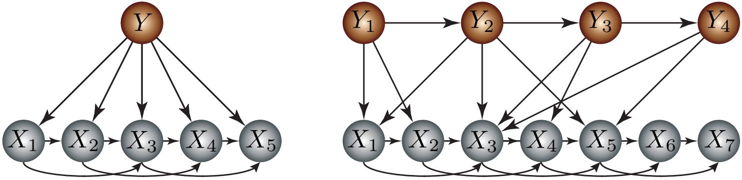

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- Alternatively, when Naïve Bayes assumption is false, we can make a submodular approximation (Peng-2005). E.g., functions of the form:

$$f(A) = \sum_{a \in A} I(X_a; Y) - \lambda \sum_{a, a' \in A} I(X_a; X_{a'}|Y) \tag{2.5}$$

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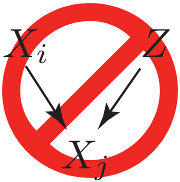
- When there are no "suppressor" variables (essentially, no v-structures that converge on X_j with parents X_i and Z), then

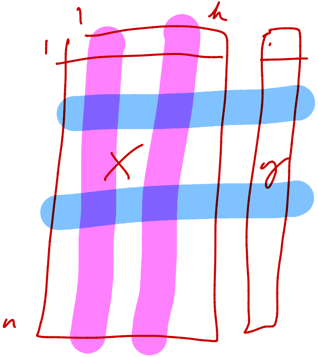
$$f(A) = R^2_{Z,A} = b_A{}^\intercal (C_A^{-1})^\intercal b_A \tag{2.7}$$

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



Data Subset Selection

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



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- Suppose moreover each data item $v \in V$ is described by a vector of non-negative scores for a set U of features (or "properties", or "concepts", etc.) of each data item.
- That is, for $u \in U$ and $v \in V$, let $m_u(v)$ $\in \mathbb{R}_+$ represent the "degree of u-ness" possessed by data item v. Then $m_u \in \mathbb{R}_+^V$ for all $u \in U$.

$m_u = (m_u(v_1), m_u(v_2), \ldots, m_u(v_n))$

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

additive
= modular function   a set function

$m : V \to \mathbb{R}$ $A \subseteq V$

$m(A) = \sum_{a \in A} m(a) + \text{const.}$

$m \in \mathbb{R}^V$

Linear function.

$f : \mathbb{R}^n \to \mathbb{R}$ $x_1, x_2 \in \mathbb{R}^n$

$f(\alpha x_1 + \beta x_2) = \alpha f(x_1) + \beta f(x_2)$

All linear functions take the form $f(1_X)$

$f(x) = a \cdot x$ + const. $a \in \mathbb{R}^n$ $= \sum_{i \in X} a_i$

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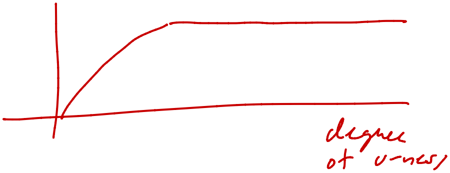

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- $f(X)$ measures X's ability to represent set of features U as measured by $m_u(X)$, with diminishing returns function g, and importance weights α_u.

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 $u \in U$).
- Next, normalize the modular weights for each feature:

$$0 \leq \bar{m}_u(X) \triangleq \frac{m_u(X)}{\sum_{u' \in U} m_{u'}(X)} = \frac{m_u(X)}{m(X)} \leq 1 \qquad (2.10)$$

where $m(X) \triangleq \sum_{u' \in U} m_{u'}(X)$.
- Then $\bar{m}_u(X)$ can also be seen as a distribution over features U since $\bar{m}_u(X) \geq 0$ and $\sum_{u \in U} \bar{m}_u(X) = 1$ for any $X \subseteq V$.
- Consider the KL-divergence between these two distributions:

$$\begin{aligned} D(p \| \{\bar{m}_u(X)\}_{u \in U}) &= \sum_{u \in U} p_u \log p_u - \sum_{u \in U} p_u \log(\bar{m}_u(X)) && (2.11) \\ &= \sum_{u \in U} p_u \log p_u - \sum_{u \in U} p_u \log(m_u(X)) + \log(m(X)) \\ &= -H(p) + \log m(X) - \sum_{u \in U} p_u \log(m_u(X)) && (2.12) \end{aligned}$$

Data Subset Selection, KL-divergence

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

$$D(p||\{\bar{m}_u(X)\}) = \text{const.} + \log m(X) - \sum_{u \in U} p_u \log(m_u(X)) \quad (2.13)$$

- But seen as a function of X, both $\log m(X)$ and $\sum_{u \in U} p_u \log m_u(X)$ are submodular functions.
- Hence the KL-divergence, seen as a function of X, i.e., $f(X) = D(p||\{\bar{m}_u(X)\})$ is quite naturally represented as a difference of submodular functions.
- Alternatively, if we define (Shinohara, 2014)

$$g(X) \triangleq \log m(X) - D(p||\{\bar{m}_u(X)\}) = \sum_{u \in U} p_u \log(m_u(X)) \quad (2.14)$$

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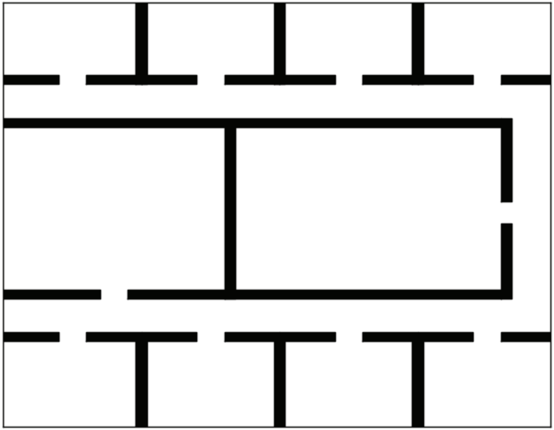
- Environment could be a floor of a building, water network, monitored ecological preservation.

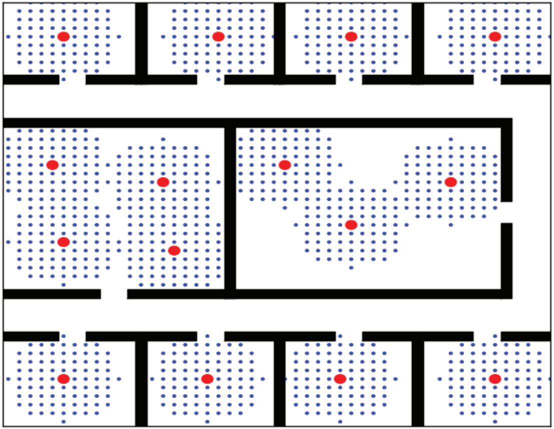
Sensor Placement within Buildings

- 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.



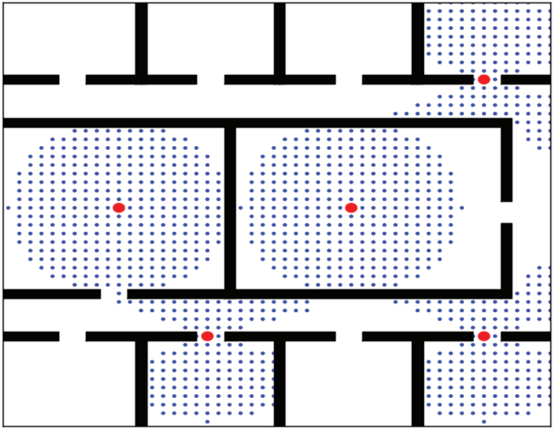
Sensor Placement within Buildings

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



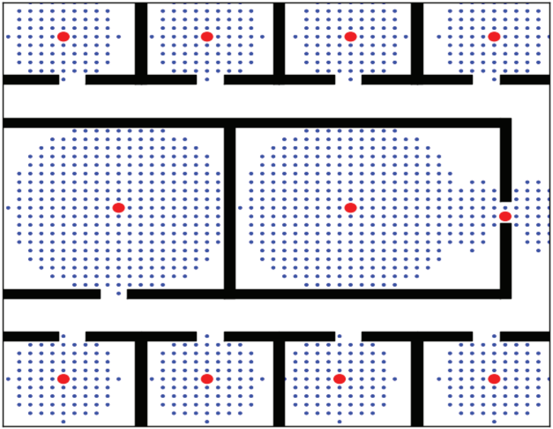
Sensor Placement within Buildings

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



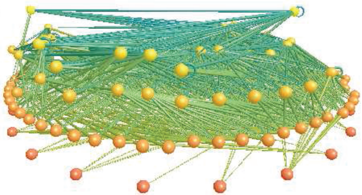
Sensor Placement within Buildings

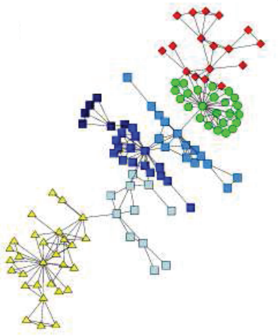
- Example sensor placement using mixed range sensors (located at red dots).

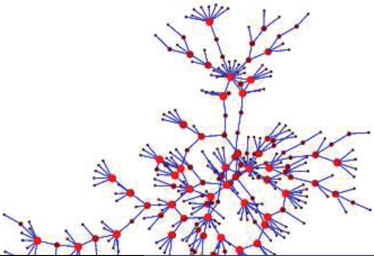


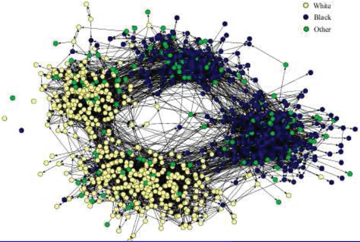
Social Networks

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









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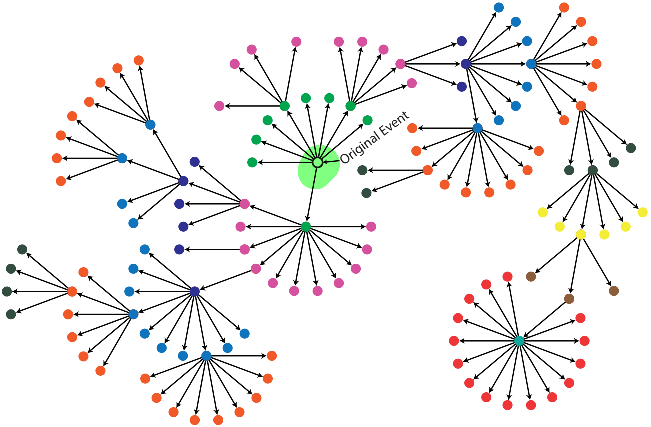
- Supermodular model: a friend becomes more valuable the more friends you have.
- Which is a better model?

Information Cascades, Diffusion Networks

- How to model flow of information from source to the point it reaches users — information used in its common sense (like news events).



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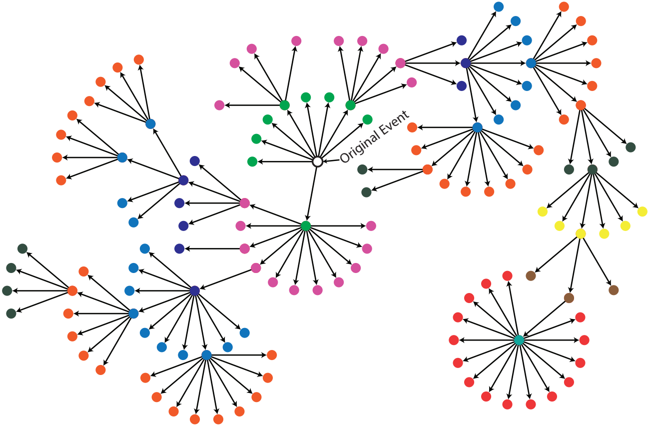


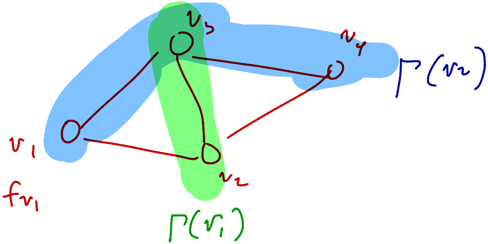
- Goal: How to find the most influential sources, the ones that often set off cascades, which are like large "waves" of information flow?

Diffusion Networks
Where are they useful?

- Information propagation: when blogs or news stories break, and creates an information cascade over multiple other blogs/newspapers/magazines.
- Viral marketing: What is the pattern of trendsetters that cause an individual to purchase a product?
- Epidemiology: who gets sick from whom? What is the infection network of such links? Given finite supply of vaccine, who to inoculate to protect overall population (cut the network)?
  - Infer the connectivity of a network (memes, purchase decisions, viruses, etc.) based only on diffusion traces (the time that each node is "infected")?
  - How to find the most likely tree or graph?

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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- Define function $f : 2^V \to \mathbb{Z}^+$ to model the ultimate influence of an initial infected nodes S. Use following iterative process; at each step:
  - Given previous set of infected nodes S that have not yet had their chance to infect their neighbors,
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- For many f_v (including simple ~~linear~~ modular functions, and where f_v is submodular itself), we can show f is submodular (Kempe, Kleinberg, Tardos ~~1998~~ 2003).

Optimization Problem Involving Network Externalities

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- Goal: find A and p to maximize $f_p(A) = \mathbb{E}[p \times |S_{k^*}|]$.

Graphical Model Structure Learning

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

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Graphical Models: Learning Tree Distributions

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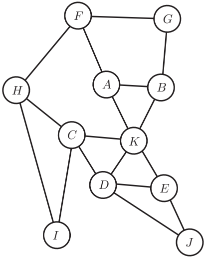

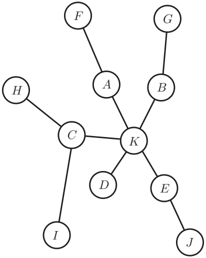

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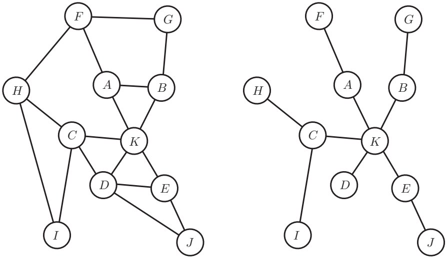

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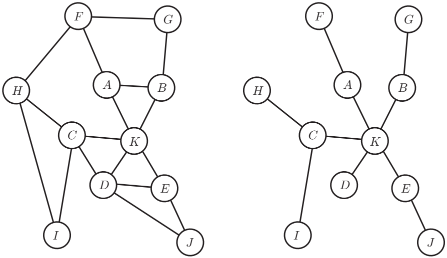

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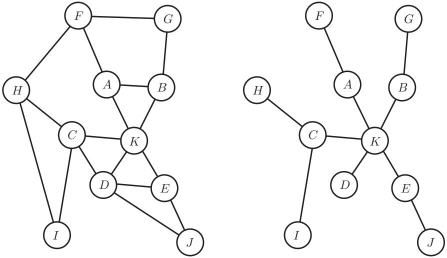

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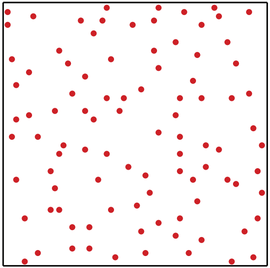
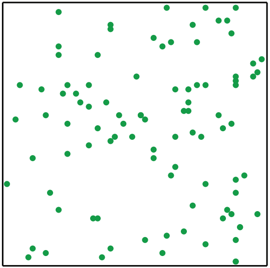


DPP



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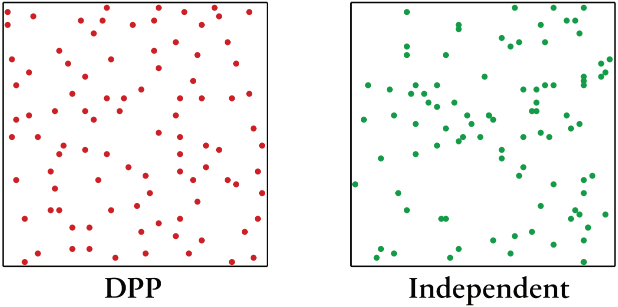

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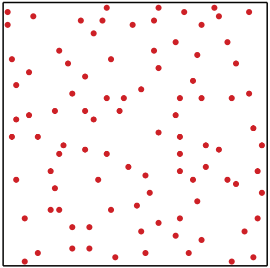

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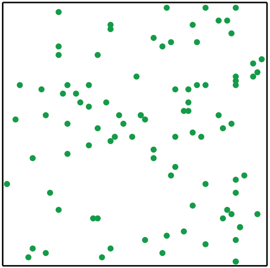

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- More "diverse" or "complex" samples are given higher probability.

DPPs and log-submodular probability distributions

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

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

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- Thus, $x \in \{0,1\}^V$, and finding MPE solution is setting some of the variables to 0 and some to 1, i.e.,

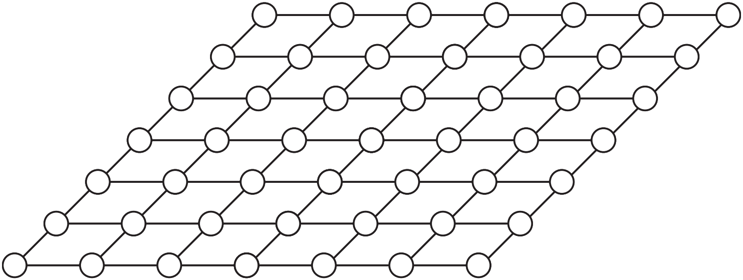
$$\min_{x \in \{0,1\}^V} E(x) \tag{2.22}$$

MRF example

Markov random field

$$\log p(x) \propto \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \tag{2.23}$$

When G is a 2D grid graph, we have

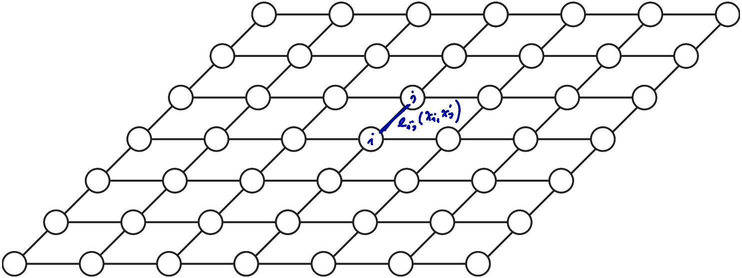


Create an auxiliary graph

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

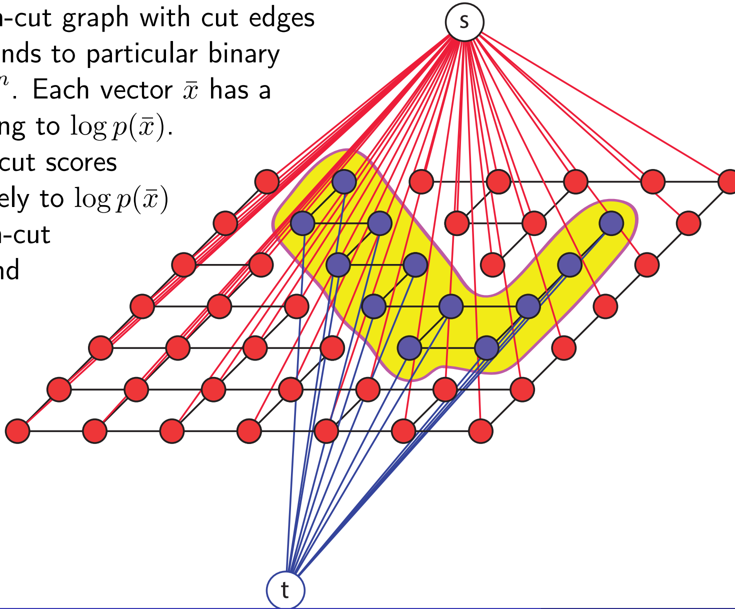
Transformation from graphical model to auxiliary graph

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 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

- Any graph cut corresponds to a vector $\bar{x} \in \{0,1\}^n$.
- If weights of all edges, except those involving terminals s and t, are non-negative, graph cut computable in polynomial time via max-flow (many algorithms, e.g., Edmonds&Karp $O(nm^2)$ or $O(n^2 m \log(nC))$; Goldberg&Tarjan $O(nm\log(n^2/m))$, see Schrijver, page 161).
- If weights are set correctly in the cut graph, and if edge functions e_{ij} satisfy certain properties, then graph-cut score corresponding to $\bar{x}$ can be made equivalent to $E(x) = \log p(\bar{x}) + \text{const.}$.
- 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.

Submodular potentials

submodularity is what allows graph cut to find exact solution

- 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:

$$\overset{v_1}{e_{ij}(0,1)} + \overset{v_2}{e_{ij}(1,0)} \geq e_{ij}(1,1) + e_{ij}(0,0) \tag{2.31}$$

$V = \{v_1, v_2\}$

$f(v_1) + f(v_2) \geq f(v_1 \cup v_2)$
$+ f(\underbrace{v_1 \cap v_2}_{\emptyset})$

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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.

$$\log \Pr(x) = g(x) + \text{const.} = -E(x) + \text{const.} \tag{2.33}$$

where g is supermodular ($E(x) = -g(x)$ 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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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

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.

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

Graph-cut vs. cooperative-cut comparisons

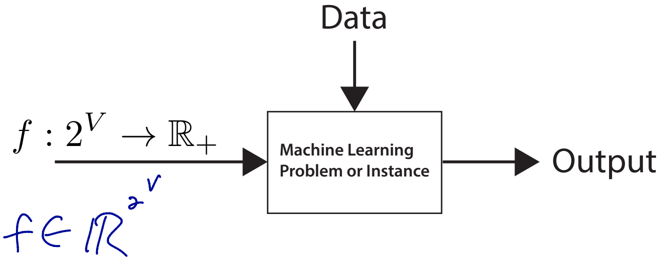
Graph Cut

Cooperative Cut

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

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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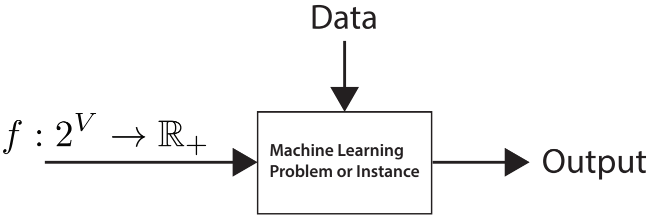

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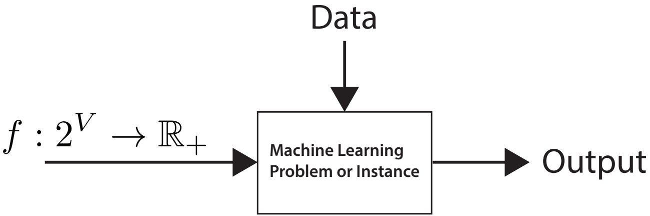

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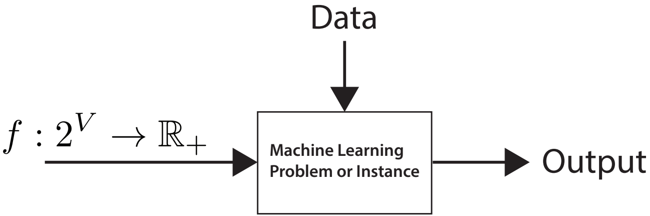

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- $\mathbb{S}$ is a submodular cone since submodularity is closed under non-negative (conic) combinations.
- 2^n-dimensional since for certain $f \in \mathbb{S}$, there exists $f_\epsilon \in \mathbb{R}^{2^n}$ having no zero elements with $f + f_\epsilon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

Supervised Machine Learning
From F. Bach

- We are given n samples of observed data $(x_i, y_i) \in \mathbb{R}^p \times \mathbb{R}$, $i \in [n]$.
  - Response vector $y = (y_1, \ldots, y_n)^\intercal \in \mathbb{R}^n$
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$$\min_{w \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, w^\intercal x_i) + \lambda \Omega(w) = \min_{w \in \mathbb{R}^p} L(y, Xw) + \lambda \Omega(w) \qquad (2.37)$$

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

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$\Omega(w) = LE(f)(w)$

relaxation of $f(\mathrm{supp}(w))$

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where $\ell(\cdot)$ is a loss function (e.g., squared error) and $\Omega(w)$ is a (perhaps sparse) norm.
- When data has multiple (k) responses, $y = (y^1, \ldots, y^k) \in R^{n \times k}$, we get:

$$\min_{w^1, \ldots, w^k \in \mathbb{R}^n} \sum_{j=1}^{k} \left\{ L(y^j, Xw^j) + \lambda \Omega(w^j) \right\} \tag{2.38}$$

Dictionary Learning and Selection

- When only the multiple responses $y = (y^1, \dots, y^k) \in \mathbb{R}^{n \times k}$ are observed, we get either dictionary learning

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- or when we select sub-dimensions of x, we get dictionary selection (Cevher & Krause, Das & Kempe).

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- This is a subset selection problem, and the regularizer $\Omega(\cdot)$ is critical (could be structured sparse convex norm, via Lovász extension!).

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:

$$\Omega(w) = \sum_{i=2}^{N} |w_i - w_{i-1}| \tag{2.41}$$

related to Lovász extension of a graph-cut submodular function.
- 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 two notions of "information amongst a collection of sets":

$$I_f(S_1; S_2; \ldots; S_k) = \sum_{i=1}^{k} f(S_k) - f(S_1 \cup S_2 \cup \cdots \cup S_k) \tag{2.46}$$

$$I'_f(S_1; S_2; \ldots; S_k) = \sum_{A \subseteq \{1,2,\ldots,k\}} (-1)^{|A|+1} f(\bigcup_{j \in A} S_j) \tag{2.47}$$

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- Recursively partition the partitions, we end up with a partition $V = V_1 \cup V_2 \cup \cdots \cup V_k$ that clusters the data.
- Each minimization can be done using Queyranne's algorithm (alternatively can construct a Gomory-Hu tree). This gives a partition no worse than factor 2 away from optimal partition. (Narasimhan&Bilmes, 2007).

Submodular Parameterized Clustering

- Given a submodular function $f : 2^V \to \mathbb{R}$, form the combinatorial dependence function $I_f(A; B) = f(A) + f(B) - f(A \cup B)$.
- Consider clustering algorithm: First find partition $A_1^* \in \operatorname{argmin}_{A \subseteq V} I_f(A; V \setminus A)$ and $A_2^* = V \setminus A_1^*$.
- Then partition the partitions: $A_{11}^* \in \operatorname{argmin}_{A \subseteq A_1^*} I_f(A; A_1^* \setminus A)$, $A_{12}^* = A_1^* \setminus A_{11}^*$, and $A_{21}^* \in \operatorname{argmin}_{A \subseteq A_2^*} I_f(A; A_2^* \setminus A)$, etc.
- Recursively partition the partitions, we end up with a partition $V = V_1 \cup V_2 \cup \cdots \cup V_k$ that clusters the data.
- Each minimization can be done using Queyranne's algorithm (alternatively can construct a Gomory-Hu tree). This gives a partition no worse than factor 2 away from optimal partition. (Narasimhan&Bilmes, 2007).
- Hence, family of clustering algorithms parameterized by f.

Is Submodular Maximization Just Clustering?

1. Clustering objectives often NP-hard and inapproximable, submodular maximization is approximable for any submodular function.
2. To have guarantee, clustering typically needs metricity, submodularity parameterized via any non-negative pairwise values.
3. Clustering often requires separate process to choose representatives within each cluster. Submodular max does this automatically. Can also do submodular data partitioning (like clustering).
4. Submodular max covers clustering objectives such as k-medoids.
5. Can learn submodular functions (hence, learn clustering objective).
6. We can choose quality guarantee for any submodular function via submodular set cover (only possible for some clustering algorithms).
7. Submodular max with constraints, ensures representatives are feasible (e.g., knapsack, matroid independence, combinatorial, submodular level set, etc.)
8. Submodular functions may be more general than clustering objectives (submodularity allows high-order interactions between elements).

Active Learning and Semi-Supervised Learning

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

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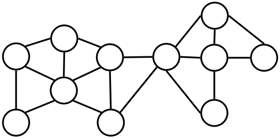
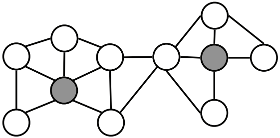
- Semi-supervised (transductive) learning: Once we have $\{y_i\}_{i \in S}$, infer the remaining labels $\{y_i\}_{i \in V \setminus S}$.

Active Transductive Semi-Supervised Learning

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

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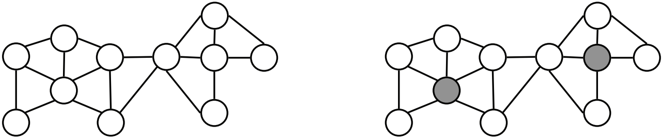
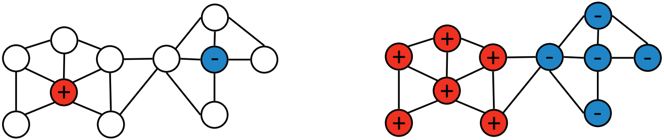


- Nature reveals labels $y_L \in \{0,1\}^L$, learner predicts labels $\hat{y} \in \{0,1\}^V$



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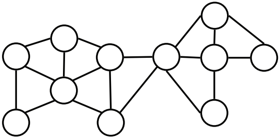
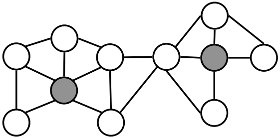

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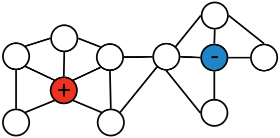
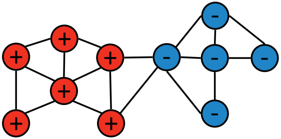
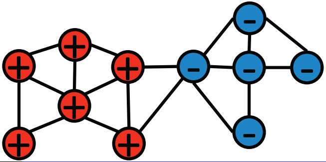
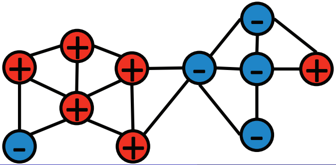



- Learner suffers loss $\|\hat{y} - y\|_1$, where y is truth. Below, $\|\hat{y} - y\|_1 = 2$.

Choosing labels: how to select L

- Consider the following objective

$$\Psi(L) = \min_{T \subseteq V \setminus L : T \neq \emptyset} \frac{\Gamma(T)}{|T|} \tag{2.48}$$

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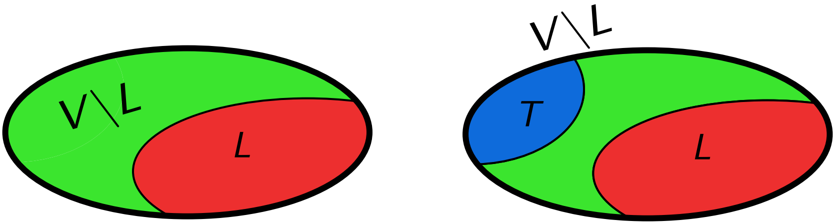

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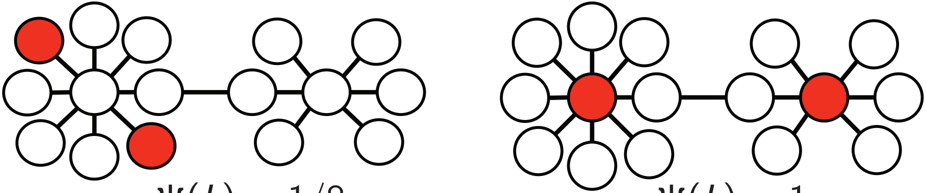

$\Psi(L) = 1/8$ $\Psi(L) = 1$

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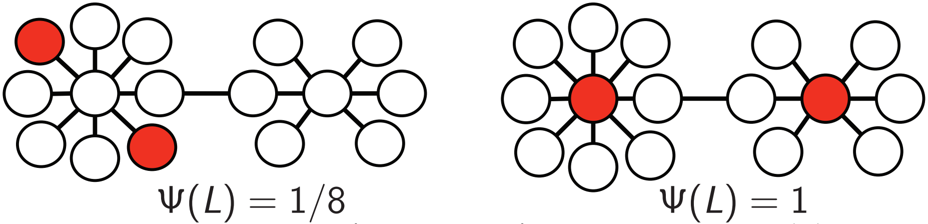

- This suggests choosing (bounded cost) L that maximizes $\Psi(L)$.

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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 2.6.1 (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*

$$\|\hat{y} - y\|_1 \leq 2\frac{\Gamma(Y(y))}{\Psi(L)} \tag{2.50}$$

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

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

$$\Psi(S) = \min_{T \subseteq V \setminus S : T \neq \emptyset} \frac{\Gamma(T)}{|T|} \tag{2.51}$$

- $\Gamma(T) = I_f(T; V \setminus T) = f(S) + f(V \setminus S) - f(V)$ 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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- One example: can we learn a subclass, perhaps non-negative weighted mixtures of submodular components?

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- Constraints specified in inference form:

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

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 1: Subgradient descent learning

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

$w_0 = 0$;

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

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

  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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where $E(x) = E_f(x) - E_g(x)$ and both of $E_f(x)$ and $E_g(x)$ are submodular.

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- Hence, rather than minimize $E(x)$ (hard), we can minimize $E_f(x) \geq E(x)$ (relatively easy), which is an upper bound.

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- Other analogous concepts: curvature of a submodular function, and also the submodular degree.

Recall

The next page shows a slide from Lecture 1

Submodular-Supermodular Decomposition

- As an alternative to graphical decomposition, we can decompose a function without resorting sums of local terms.

Theorem 2.8.1 (Additive Decomposition (Narasimhan & Bilmes, 2005))

*Let $h : 2^V \to \mathbb{R}$ be **any** set function. Then there exists a submodular function $f : 2^V \to \mathbb{R}$ and a supermodular function $g : 2^V \to \mathbb{R}$ such that h may be additively decomposed as follows: For all $A \subseteq V$,*

$$h(A) = f(A) + g(A) \tag{2.8}$$

- For many applications (as we will see), either the submodular or supermodular component is naturally zero.
- Sometimes more natural than a graphical decomposition.
- Sometimes $h(A)$ has structure in terms of submodular functions but is non additively decomposed (one example is $h(A) = f(A)/g(A)$).
- Complementary: simultaneous graphical/submodular-supermodular decomposition (i.e., submodular + supermodular tree).

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- Sensor placement with submodular costs. I.e., let V be a set of possible sensor locations, $f(A) = I(X_A; X_{V \setminus A})$ measures the quality of a subset A of placed sensors, and $c(A)$ the submodular cost. We have $f(A) - \lambda c(A)$ as the overall objective to maximize.

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- Graphical Model Inference. Finding x that maximizes $p(x) \propto \exp(-v(x))$ where $x \in \{0,1\}^n$ and v is a pseudo-Boolean function. When v is non-submodular, it can be represented as a difference between submodular functions.