Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 2 —

http://www.ee.washington.edu/people/faculty/bilmes/classes/ee596b_spring_2016/

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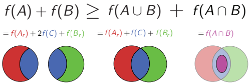
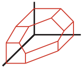
Mar 30th, 2016





Cumulative Outstanding Reading

- Read chapter 1 from Fujishige's book.

Announcements, Assignments, and Reminders

- Weekly Office Hours: Mondays, 3:30-4:30, or by skype or google hangout (set up meeting via our our discussion board (https://canvas.uw.edu/courses/1039754/discussion_topics)).

Class Road Map - IT-I

- L1(3/28): Motivation, Applications, & Basic Definitions
- L2(3/30):
- L3(4/4):
- L4(4/6):
- L5(4/11):
- L6(4/13):
- L7(4/18):
- L8(4/20):
- L9(4/25):
- L10(4/27):
- L11(5/2):
- L12(5/4):
- L13(5/9):
- L14(5/11):
- L15(5/16):
- L16(5/18):
- L17(5/23):
- L18(5/25):
- L19(6/1):
- L20(6/6): Final Presentations maximization.

Finals Week: June 6th-10th, 2016.

Two Equivalent Submodular Definitions

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)

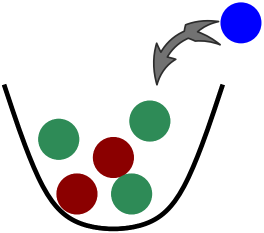
A function $f : 2^V \to \mathbb{R}$ is submodular if for any $A \subseteq B \subset V$, and $v \in V \setminus B$, we have that:

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

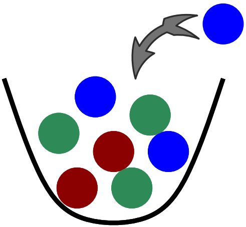
The incremental "value", "gain", or "cost" of v decreases (diminishes) as the context in which v is considered grows from A to B.

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:

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Definition 2.2.2 (supermodular (improving returns))

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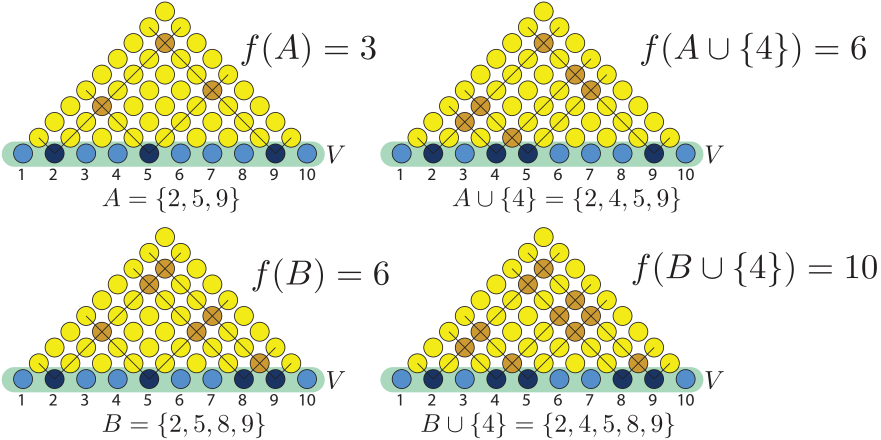
- Incremental "value", "gain", or "cost" of v increases (improves) as the context in which v is considered grows from A to B.
- A function f is submodular iff $-f$ is supermodular.
- If f both submodular and supermodular, then f is said to be **modular**, and $f(A) = c + \sum_{a \in A} f(a)$ (often $c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

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.



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- 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,

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  - Also, we can "relax" a problem to a submodular one where it can be efficiently solved and offer a bounded quality solution.
  - 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.

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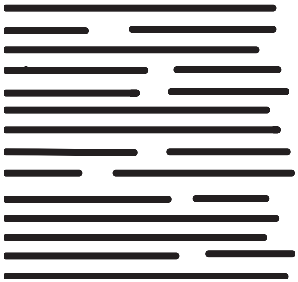
- Random sample has probability of poorly representing normally underrepresented groups.

Extractive Document Summarization

- The figure below represents the sentences of a document



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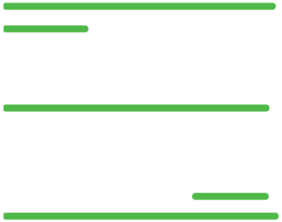

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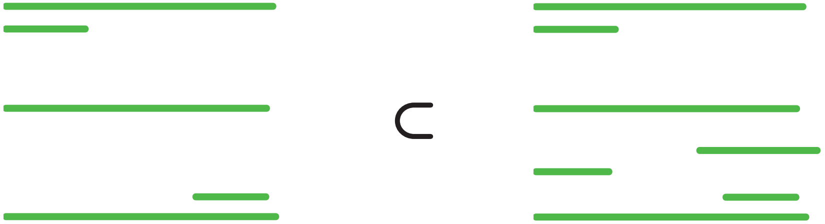

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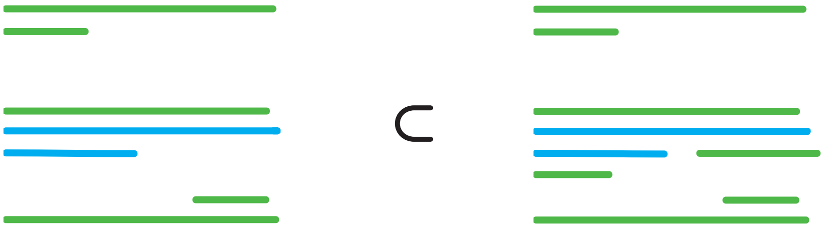

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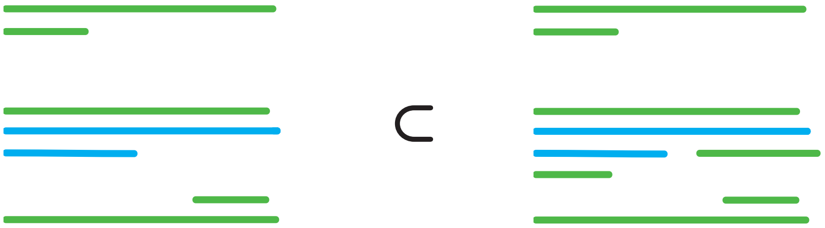

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- **diminishing returns** $\leftrightarrow$ **submodularity**

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.

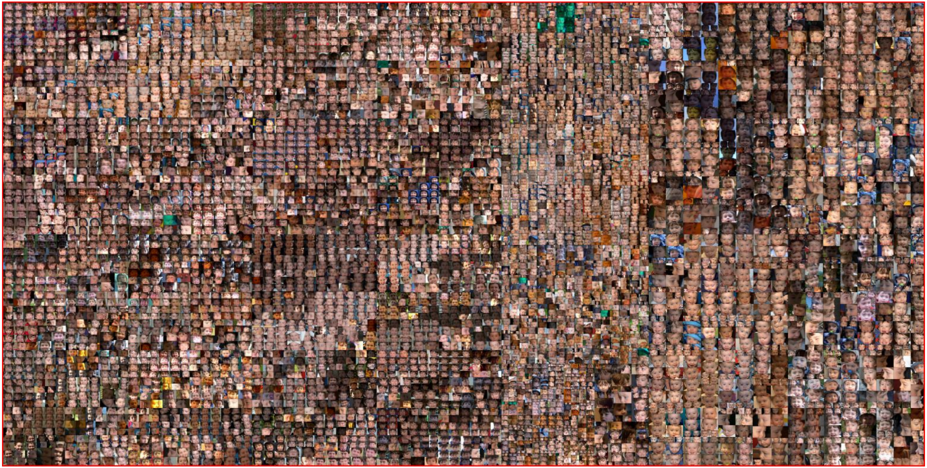

Image Summarization

10×10 image collection:

3 good summaries (diverse):

3 ok summaries:

3 poor summaries (redundant):

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

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

$$= H(X_A) - H(X_A|Y) = H(X_A) + H(Y) - H(X_A, Y) \tag{2.2}$$

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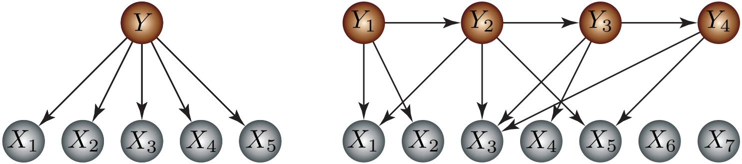
- Applicable in pattern recognition, also in sensor coverage problem, where Y is whatever question we wish to ask about environment.

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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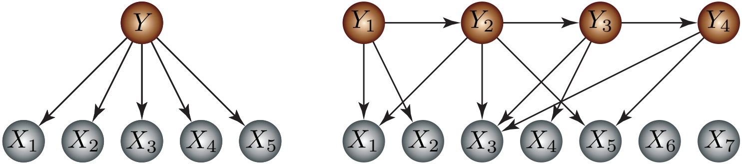

- When $X_A \perp\!\!\!\perp X_B | Y$ for all A, B (the Naïve Bayes assumption holds), then

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

is submodular (submodular minus modular).

Variable Selection in Pattern Classification

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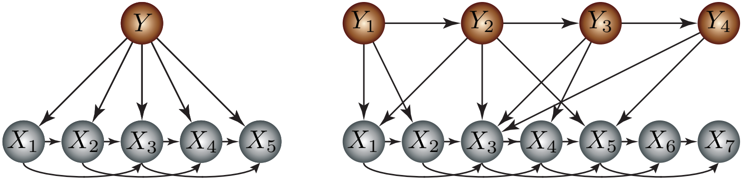

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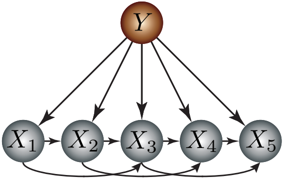

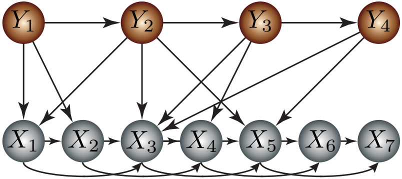

- $f(A)$ naturally expressed as a difference of two submodular functions

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

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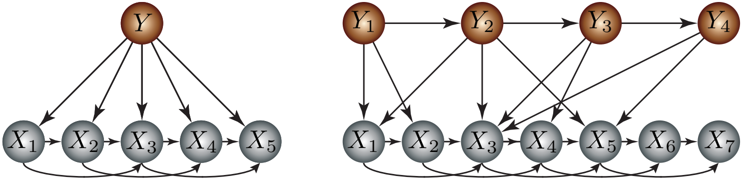

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- Alternatively, when Naïve Bayes assumption is false, we can make a submodular approximation (Peng-2005). E.g., functions of the form:

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

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

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Variable Selection: Linear Regression Case

- Next, let Z be continuous. Predictor is linear $\tilde{Z}_A = \sum_{i \in A} \alpha_i X_i$.
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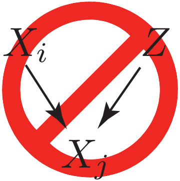
- When there are no "suppressor" variables (essentially, no v-structures that converge on X_j with parents X_i and Z), then

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

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



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- 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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- Example: U might be a set of textual features (e.g., ngrams), and $m_u(v)$ is the number of ngrams of type u in sentence v. E.g., if a document consists of the sentence

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

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

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

Data Subset Selection, KL-divergence

- Let $p = \{p_u\}_{u \in U}$ be a desired probability distribution over features (i.e., $\sum_u p_u = 1$ and $p_u \geq 0$ for all $u \in U$).

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- Consider the KL-divergence between these two distributions:

$$D(p||\{\bar{m}_u(X)\}_{u \in U}) = \sum_{u \in U} p_u \log p_u - \sum_{u \in U} p_u \log(\bar{m}_u(X)) \tag{2.11}$$

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

$$= -H(p) + \log m(X) - \sum_{u \in U} p_u \log(m_u(X)) \tag{2.12}$$

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

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- Alternatively, if we define (Shinohara, 2014)

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

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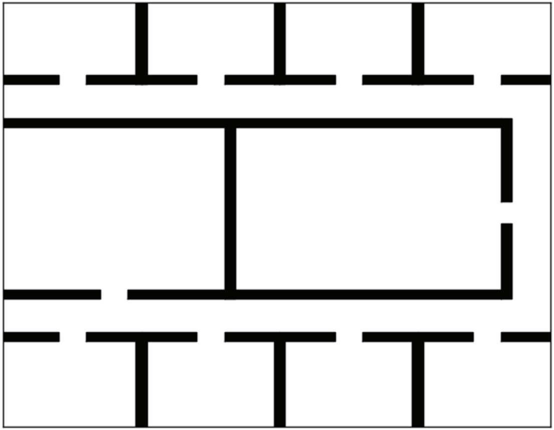
- Environment could be a floor of a building, water network, monitored ecological preservation.

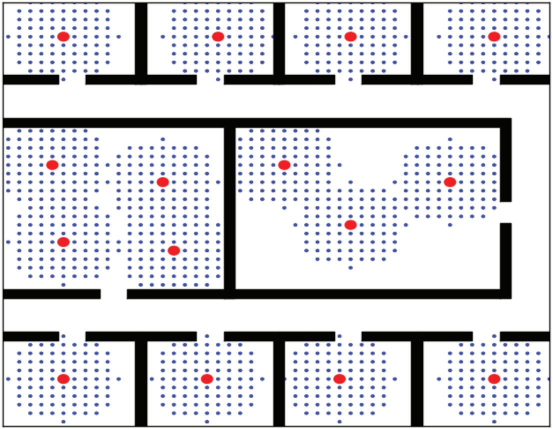
Sensor Placement within Buildings

- 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.



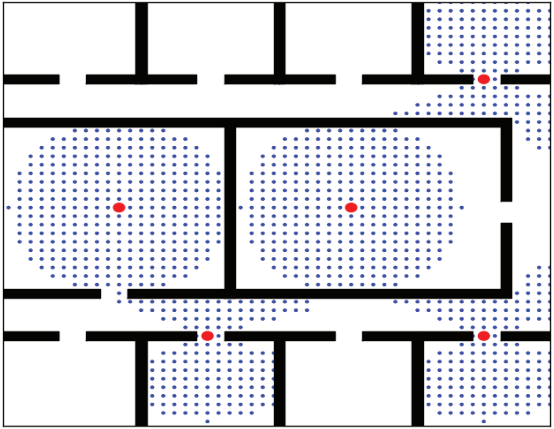
Sensor Placement within Buildings

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



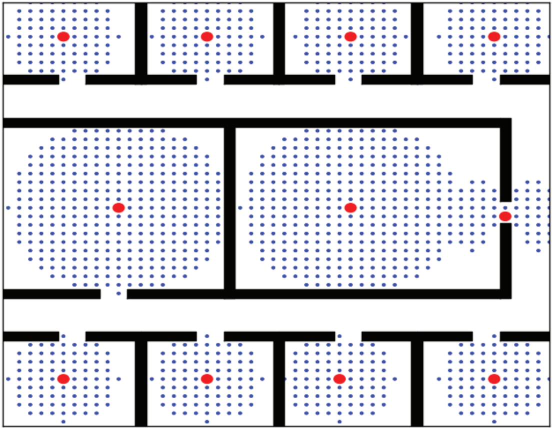
Sensor Placement within Buildings

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



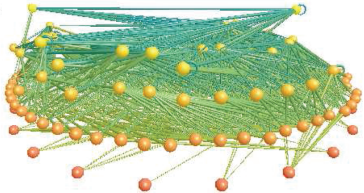
Sensor Placement within Buildings

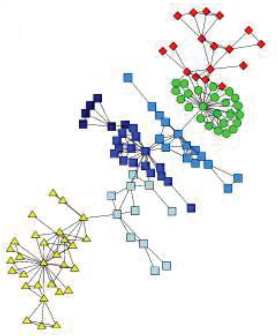
- Example sensor placement using mixed range sensors (located at red dots).

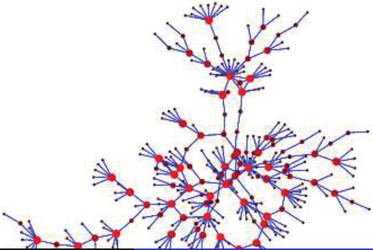


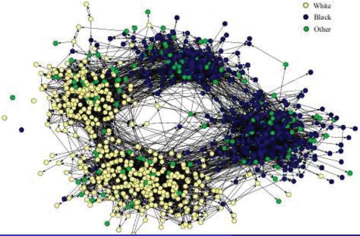
Social Networks

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









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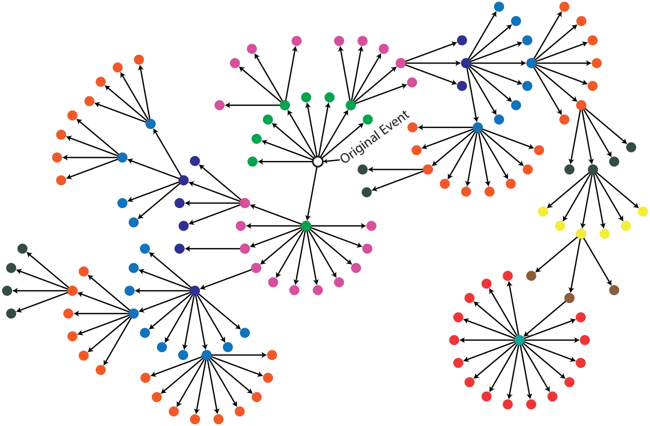
- Which is a better model?

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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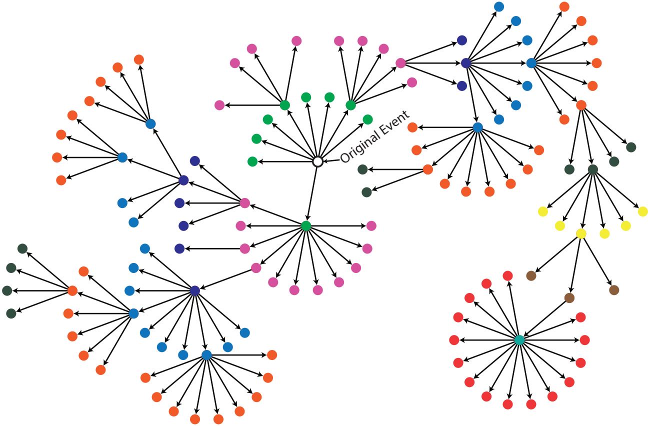

- Goal: How to find the most influential sources, the ones that often set off cascades, which are like large "waves" of information flow?

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., $f_v(A) = f_v(A \cap \Gamma(v))$.
- Goal - Viral Marketing: find a small subset $S \subseteq V$ of individuals to directly influence, and thus indirectly influence the greatest number of possible other individuals (via the social network G).
- 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,
  - activate new nodes $v \in V \setminus S$ if $f_v(S \cap \Gamma_v) \geq U[0, 1]$, where $U[0, 1]$ is a uniform random number between 0 and 1, and Γ_v are the neighbors of v.
- For many f_v (including simple linear functions, and where f_v is submodular itself), we can show f is submodular (Kempe, Kleinberg, Tardos 1993).

Graphical Model Structure Learning

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

$$p(x) = \frac{1}{Z} \exp(-E(x)) \tag{2.15}$$

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

Graphical Models: Learning Tree Distributions

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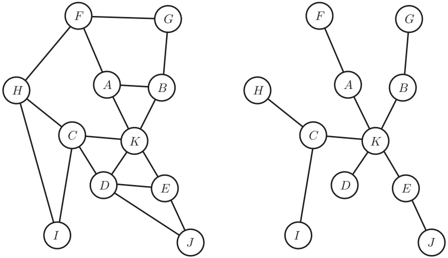

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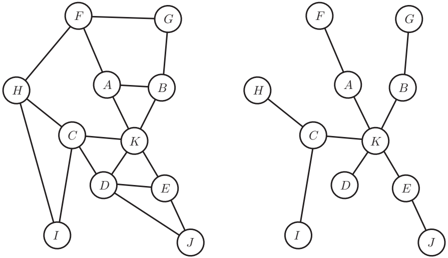

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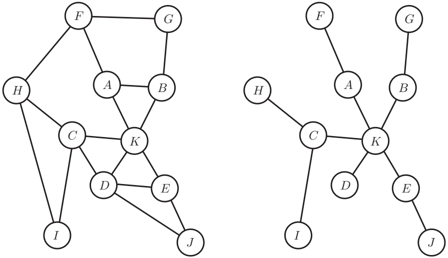

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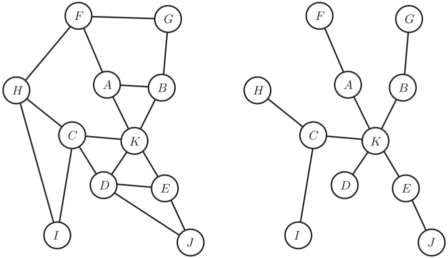

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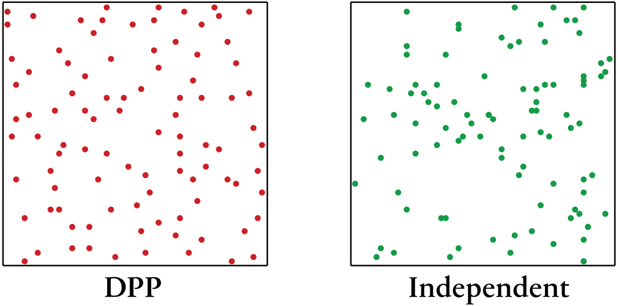

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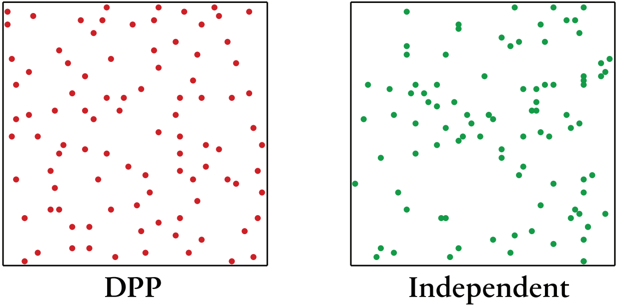

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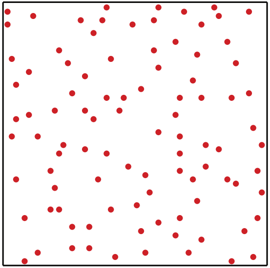
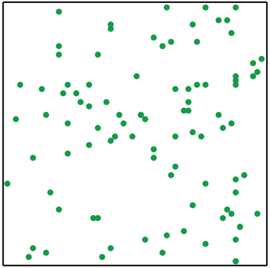


DPP



Independent

(Kulesza, Gillenwater, & Taskar, 2011)

- A Determinantal point processes (DPPs) is a probability distribution over subsets A of V where the "energy" function is submodular.
- More "diverse" or "complex" samples are given higher probability.

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

Graphical Models and fast MAP Inference

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$$p(x) = \frac{1}{Z}\exp(-E(x)) \tag{2.19}$$

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

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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 $p \in \mathcal{F}(G, \mathcal{M}^{(\mathsf{f})})$ 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 $\text{D}_{X_v} = \{0, 1\}$ (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.,

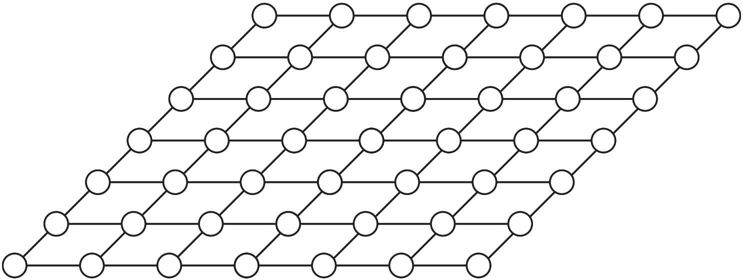
$$\min_{x \in \{0,1\}^V} E(x) \tag{2.22}$$

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

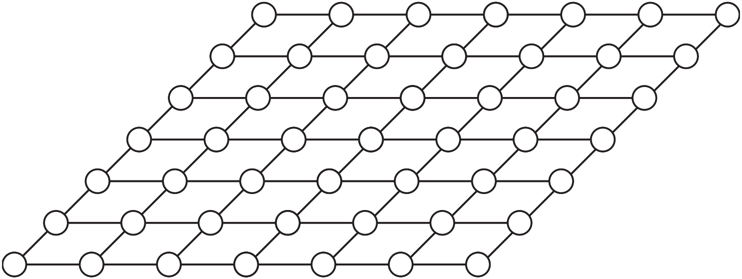


Create an auxiliary graph

- 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

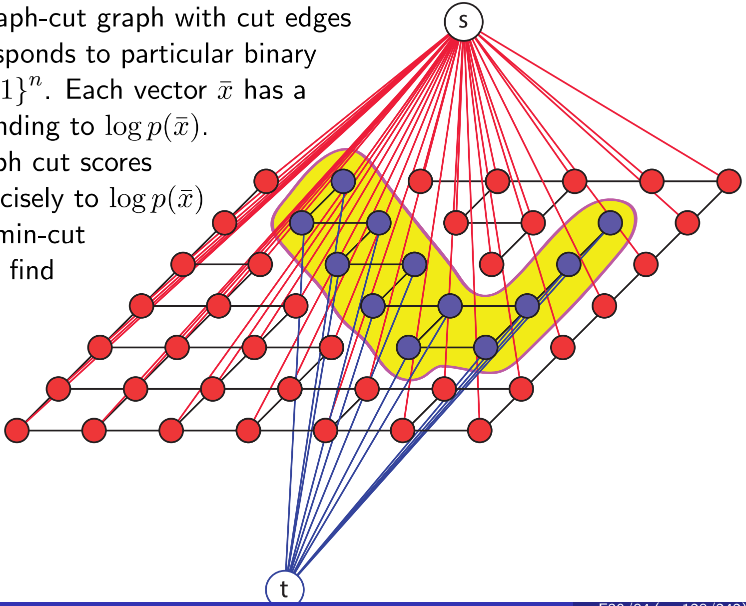
Original 2D-grid graphical model G and energy function $E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j)$ needing to be minimized over $x \in \{0,1\}^V$. Recall, tree-width is $O(\sqrt{|V|})$.



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:

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

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

$$f(X) = \sum_{\{i,j\} \in \mathcal{E}(G)} f_{i,j}(X \cap \{i,j\}) \tag{2.32}$$

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

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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.

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.

- Log-submodular distributions:

$$\log \Pr(x) = f(x) + \text{const.} \tag{2.34}$$

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

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

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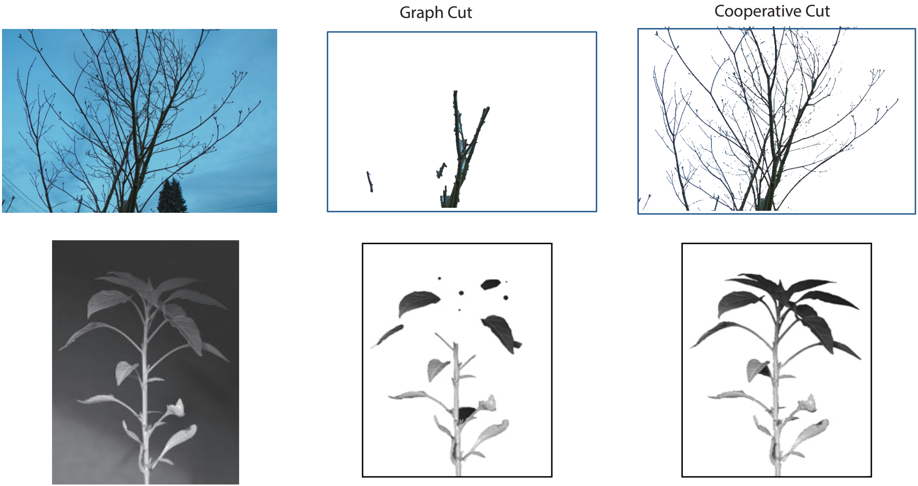
- $\Rightarrow$ cooperative-cut (Jegelka & B., 2011).

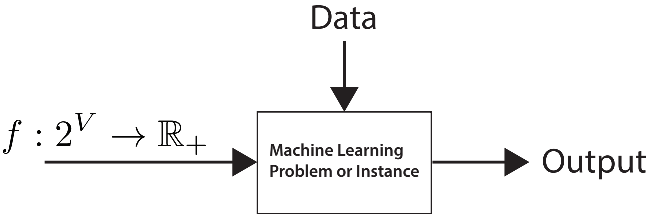
Graph-cut vs. cooperative-cut comparisons



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

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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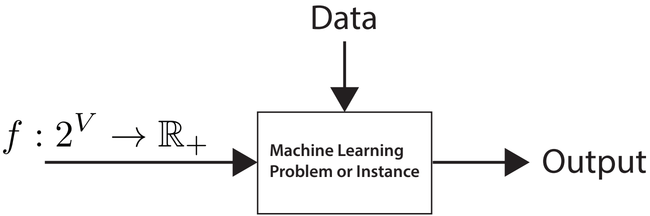

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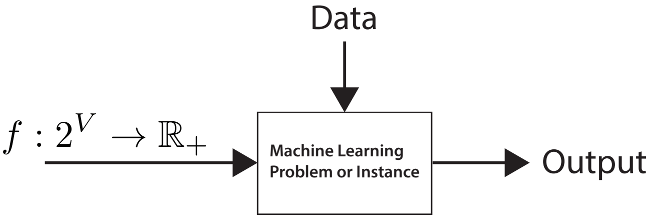

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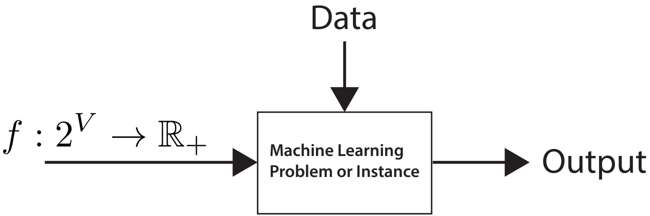

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- $\mathbb{S}$ is a submodular cone since submodularity is closed under non-negative (conic) combinations.
- 2^n-dimensional since for certain $f \in \mathbb{S}$, there exists $f_\epsilon \in \mathbb{R}^{2^n}$ having no zero elements with $f + f_\epsilon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

$$\min_{w \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, w^\intercal x_i) + \lambda\Omega(w) = \min_{w \in \mathbb{R}^p} L(y, Xw) + \lambda\Omega(w) \qquad (2.37)$$

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

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  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, $y = (y^1, \dots, y^k) \in R^{n \times k}$, we get:

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

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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$$\tilde{f}(w) = \sum_{i=1}^{n} w_{\sigma_i}(f(\sigma_1, \ldots, \sigma_i) - f(\sigma_1, \ldots, \sigma_{i-1})) \tag{2.42}$$

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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":

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

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

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- 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

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- Batch active learning: choose a subset $S \subset V$ so that only the labels $\{y_i\}_{i \in S}$ should be acquired.

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Active Learning and Semi-Supervised Learning

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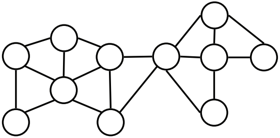
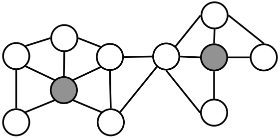
- Semi-supervised (transductive) learning: Once we have $\{y_i\}_{i \in S}$, infer the remaining labels $\{y_i\}_{i \in V \setminus S}$.

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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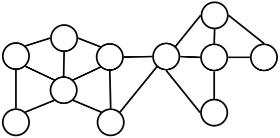
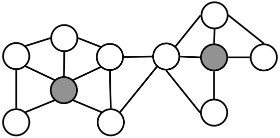

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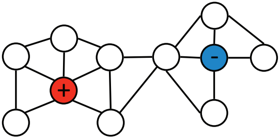
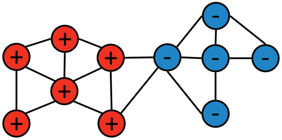

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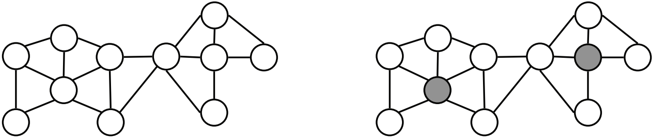

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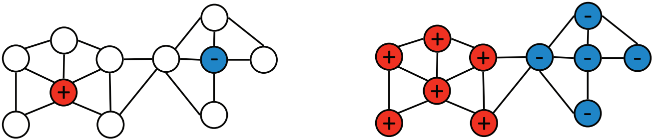
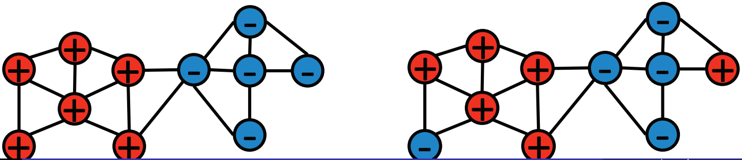


- Learner suffers loss $\|\hat{y} - y\|_1$, where y is truth. Below, $\|\hat{y} - y\|_1 = 2$.



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- 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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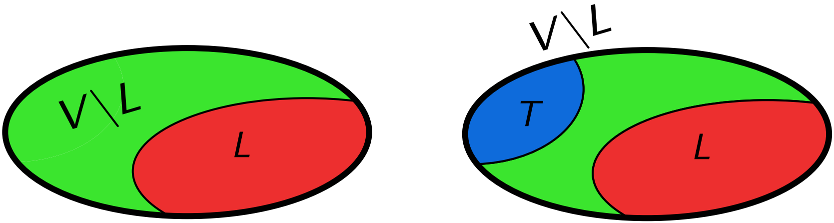

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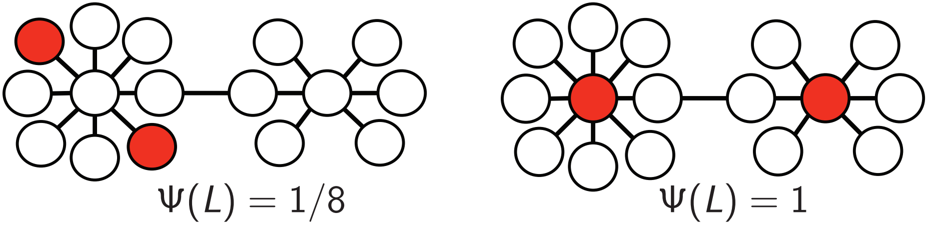

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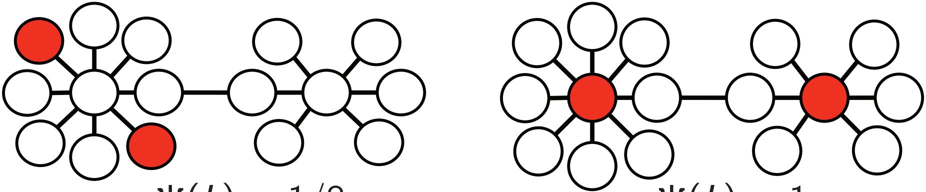

$\Psi(L) = 1/8$ $\Psi(L) = 1$

- 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*

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

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:

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

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

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

Structured Learning of Submodular Mixtures

- Constraints specified in inference form:

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$$\text{subject to} \quad \mathbf{w}^\top \mathbf{f}_t(\mathbf{y}^{(t)}) \geq \max_{\mathbf{y}\in\mathcal{Y}_t}\left(\mathbf{w}^\top \mathbf{f}_t(\mathbf{y}) + \ell_t(\mathbf{y})\right) - \xi_t, \forall t \tag{2.55}$$

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

  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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- For example, "deviation from submodularity" can be measured using the submodularity ratio (Das & Kempe):

$$\gamma_{U,k}(f) = \min_{L \subseteq U, S : |S| \leq k, S \cap L = \emptyset} \frac{\sum_{s \in S} f(x|L)}{f(S|L)} \tag{2.58}$$

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- Sometimes the quality of solutions to non-submodular problems can be analyzed via submodularity.
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- This gradually get worse as we move away from an objective being submodular (see Das & Kempe, 2011).
- Other analogous concepts: curvature of a submodular function, and also the submodular degree.

Monge Matrices

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

$$c_{ij} + c_{rs} \leq c_{is} + c_{rj} \tag{2.60}$$

for all $1 \leq i < r \leq m$ and $1 \leq j < s \leq n$.

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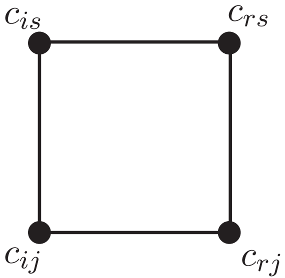
- Consider four elements of the matrix:



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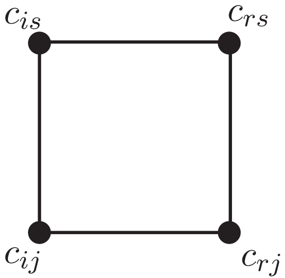
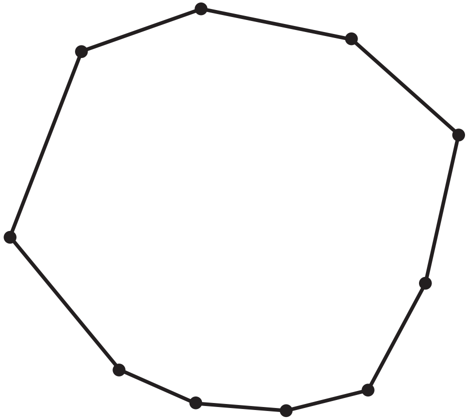


- Useful for speeding up certain dynamic programming problems.

Monge Matrices

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



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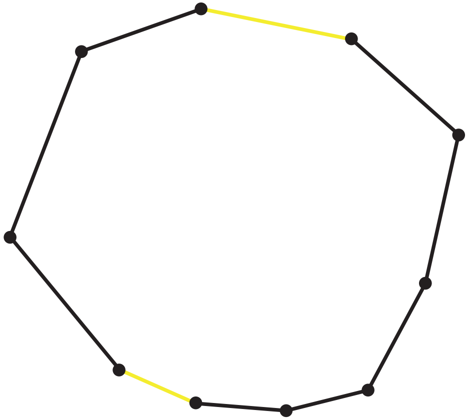

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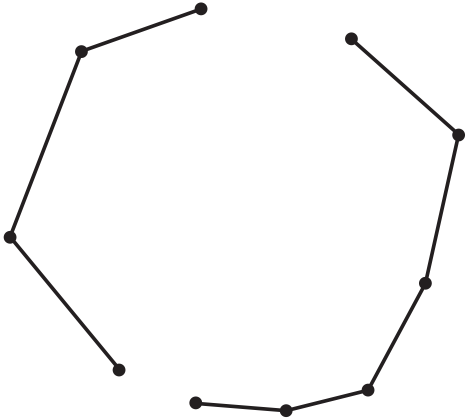

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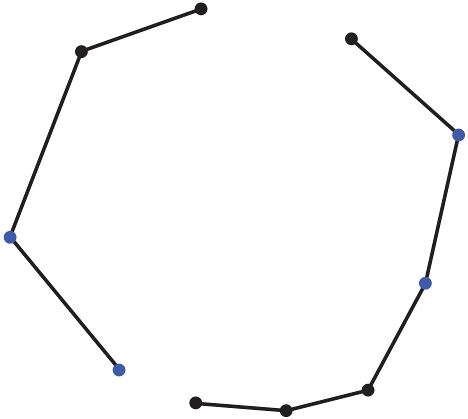

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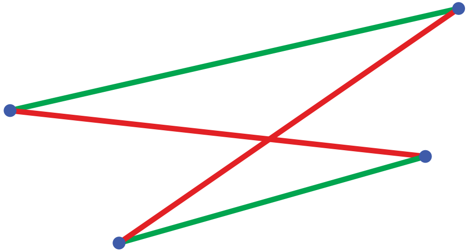


Example Submodular: Entropy from Information Theory

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

$$f(A) = H(X_A) = -\sum_{x_A} p(x_A) \log p(x_A) \tag{2.61}$$

is submodular.

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

$$H(X_v | X_B) = H(X_{B+v}) - H(X_B) \tag{2.62}$$

$$\leq H(X_{A+v}) - H(X_A) = H(X_v | X_A) \tag{2.63}$$

Information Theory: Block Coding

- Given a set of random variables $\{X_i\}_{i \in V}$ indexed by set V, how do we partition them so that we can best block-code them within each block.

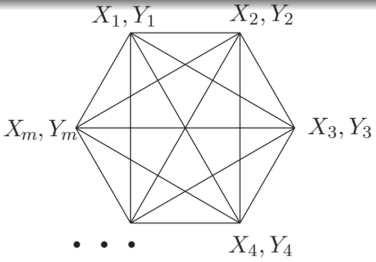
Information Theory: Block Coding

- Given a set of random variables $\{X_i\}_{i \in V}$ indexed by set V, how do we partition them so that we can best block-code them within each block.
- I.e., how do we form $S \subseteq V$ such that $I(X_S; X_{V \setminus S})$ is as small as possible, where $I(X_A; X_B)$ is the mutual information between random variables X_A and X_B, i.e.,

$$I(X_A; X_B) = H(X_A) + H(X_B) - H(X_A, X_B) \tag{2.64}$$

and $H(X_A) = -\sum_{x_A} p(x_A) \log p(x_A)$ is the joint entropy of the set X_A of random variables.

Information Theory: Network Communication



- A network of senders/receivers
- Each sender X_i is trying to communicate simultaneously with each receiver Y_i (i.e., for all i, X_i is sending to $\{Y_i\}_i$
- The X_i are not necessarily independent.

- Communication rates from i to j are $R^{(i \to j)}$ to send message $W^{(i \to j)} \in \left\{1, 2, \ldots, 2^{nR^{(i \to j)}}\right\}$.
- Goal: necessary and sufficient conditions for achievability.
- I.e., can we find functions f such that any rates must satisfy

$$\forall S \subseteq V, \quad \sum_{i \in S, j \in V \setminus S} R^{(i \to j)} \leq f(S) \tag{2.65}$$

- Special cases MAC (Multi-Access Channel) for communication over $p(y|x_1, x_2)$ and Slepian-Wolf compression (independent compression of X and Y but at joint rate $H(X, Y)$).

Example Submodular: Entropy from Information Theory

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

$$I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B}) = \sum_{x_{A \cup B}} p(x_{A \cup B}) \log \frac{p(x_{A \setminus B}, x_{B \setminus A} | x_{A \cap B})}{p(x_{A \setminus B} | x_{A \cap B}) p(x_{B \setminus A} | x_{A \cap B})}$$

$$= \sum_{x_{A \cup B}} p(x_{A \cup B}) \log \frac{p(x_{A \cup B}) p(x_{A \cap B})}{p(x_A) p(x_B)} \geq 0 \quad (2.66)$$

then

$$I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B})$$
$$= H(X_A) + H(X_B) - H(X_{A \cup B}) - H(X_{A \cap B}) \geq 0 \quad (2.67)$$

so entropy satisfies

$$H(X_A) + H(X_B) \geq H(X_{A \cup B}) + H(X_{A \cap B}) \quad (2.68)$$

Example Submodular: Mutual Information

- Also, symmetric mutual information is submodular,

$$f(A) = I(X_A; X_{V \setminus A}) = H(X_A) + H(X_{V \setminus A}) - H(X_V) \qquad (2.69)$$

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

Two Equivalent Submodular Definitions

Definition 2.11.1 (submodular concave)

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

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

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

Definition 2.11.2 (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:

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

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

Subadditive Definitions

Definition 2.11.1 (subadditive)

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

$$f(A) + f(B) \geq f(A \cup B) \tag{2.70}$$

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

Two Equivalent Supermodular Definitions

Definition 2.11.1 (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 2.11.2 (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:

$$f(A \cup \{v\}) - f(A) \leq f(B \cup \{v\}) - f(B) \tag{2.9}$$

- 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 $c = 0$).

Superadditive Definitions

Definition 2.11.2 (superadditive)

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

$$f(A) + f(B) \leq f(A \cup B) \tag{2.71}$$

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Superadditive Definitions

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- This means that the "whole" is greater than the sum of the parts.
- In general, submodular and subadditive (and supermodular and superadditive) are different properties.

Modular Definitions

Definition 2.11.3 (modular)

A function that is both submodular and supermodular is called **modular**

If f is a modular function, than for any $A, B \subseteq V$, we have

$$f(A) + f(B) = f(A \cap B) + f(A \cup B) \tag{2.72}$$

In modular functions, elements do not interact (or cooperate, or compete, or influence each other), and have value based only on singleton values.

Proposition 2.11.4

If f is modular, it may be written as

$$f(A) = f(\emptyset) + \sum_{a \in A} \Big(f(\{a\}) - f(\emptyset) \Big) \tag{2.73}$$

Modular Definitions

Proof.

We inductively construct the value for $A = \{a_1, a_2, \ldots, a_k\}$.
For $k = 2$,

$$f(a_1) + f(a_2) = f(a_1, a_2) + f(\emptyset) \tag{2.74}$$

$$\text{implies } f(a_1, a_2) = f(a_1) - f(\emptyset) + f(a_2) - f(\emptyset) + f(\emptyset) \tag{2.75}$$

then for $k = 3$,

$$f(a_1, a_2) + f(a_3) = f(a_1, a_2, a_3) + f(\emptyset) \tag{2.76}$$

$$\text{implies } f(a_1, a_2, a_3) = f(a_1, a_2) - f(\emptyset) + f(a_3) - f(\emptyset) + f(\emptyset) \tag{2.77}$$

$$= f(\emptyset) + \sum_{i=1}^{3} \big(f(a_i) - f(\emptyset) \big) \tag{2.78}$$

and so on …

□

Complement function

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

Proposition 2.11.5

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

Proof.

$$\bar{f}(A) + \bar{f}(B) \geq \bar{f}(A \cup B) + \bar{f}(A \cap B) \tag{2.79}$$

follows from

$$f(V \setminus A) + f(V \setminus B) \geq f(V \setminus (A \cup B)) + f(V \setminus (A \cap B)) \tag{2.80}$$

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