

Submodular Functions, Optimization, and Applications to Machine Learning

— Fall Quarter, Lecture 2 —

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

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

$$-f(A) + 2f(C) + f(B), \quad -f(A) + f(C) + f(B), \quad -f(A \cap B)$$



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): Info theory exs, more apps, definitions, graph/combinatorial examples
- L4(4/4): Graph and Combinatorial Examples, Matrix Rank, Examples and Properties, visualizations
- L5(4/9): More Examples/Properties/ Other Submodular Defs., Independence,
- L6(4/11): Matroids, Matroid Examples, Matroid Rank, Partition/Laminar Matroids
- L7(4/16): Laminar Matroids, System of Distinct Reps, Transversal, Transversal Matroid, Matroid Representation, Dual Matroids
- L8(4/18): Dual Matroids, Other Matroid Properties, Combinatorial Geometries, Matroids and Greedy.
- L9(4/23): Polyhedra, Matroid Polytopes, Matroids \rightarrow Polymatroids
- L10(4/29): Matroids \rightarrow Polymatroids, Polymatroids and Greedy,
- L11(4/30): Polymatroids, Polymatroids and Greedy
- L12(5/2): Polymatroids and Greedy, Extreme Points, Cardinality Constrained Maximization
- L13(5/7): Constrained Submodular Maximization
- L14(5/9): Submodular Max w. Other Constraints, Cont. Extensions, Lovasz Extension
- L15(5/14): Cont. Extensions, Lovasz Extension, Choquet Integration, Properties
- L16(5/16): More Lovasz extension, Choquet, defs/props, examples, multilinear extension
- L17(5/21): Finish L.E., Multilinear Extension, Submodular Max/polyhedral approaches, Most Violated inequality, Still More on Matroids, Closure/Sat
- L-(5/28): Memorial Day (holiday)
- L18(5/30): Closure/Sat, Fund. Circuit/Dep
- L19(6/6): Fund. Circuit/Dep, Min-Norm Point Definitions, Review & Support for Min-Norm, Proof that min-norm gives optimal, Computing Min-Norm Vector for B_f maximization.

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

Class Road Map - EE563

- L1(9/30): Motivation, Applications, Definitions, Properties
- L2(10/5): Sums concave(modular), uses (diversity/costs, feature selection), information theory, Monge matrices, graph examples.
- L3(10/7):
- L4(10/12):
- L5(10/14):
- L6(10/19):
- L7(10/21):
- L8(10/26):
- L9(10/28):
- L10(11/2):
- L11(11/4):
- L12(11/9):
- L-(11/11): Veterans Day, Holiday
- L13(11/16):
- L14(11/18):
- L15(11/23):
- L16(11/25):
- L17(11/30):
- L18(12/2):
- L19(12/7):
- L20(12/9): maximization.

Last day of instruction, Fri. Dec 11th. Finals Week: Dec 12-18, 2020

Two Equivalent Submodular Definitions

Definition 2.2.1 (submodular concave)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \quad (2.7)$$

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

Definition 2.2.2 (diminishing returns)

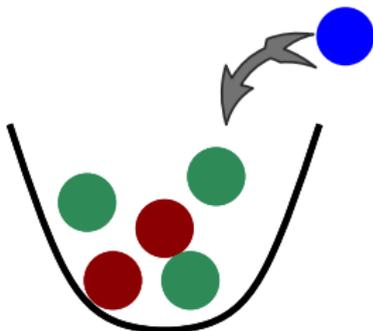
A function $f : 2^V \rightarrow \mathbb{R}$ is **submodular** if for any $A \subseteq B \subseteq V$, and $v \in V \setminus B$, we have that:

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \quad (2.8)$$

- The incremental “value”, “gain”, or “cost” of v decreases (diminishes) as the context in which v is considered grows from A to B .
- **Gain notation:** Define $f(v|A) \triangleq f(A + v) - f(A)$. Then function f is submodular if $f(v|A) \geq f(v|B)$ for all $A \subseteq B \subseteq V \setminus \{v\}$, $v \in V$.

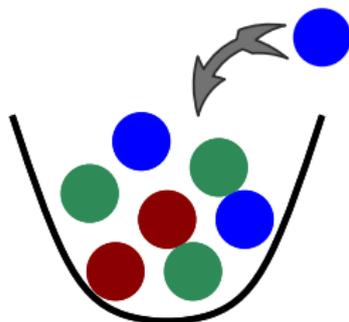
Example Submodular: Number of Colors of Balls in Urns

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

$$f(A) + f(B) \leq f(A \cup B) + f(A \cap B) \quad (2.7)$$

Definition 2.2.2 (supermodular (improving returns))

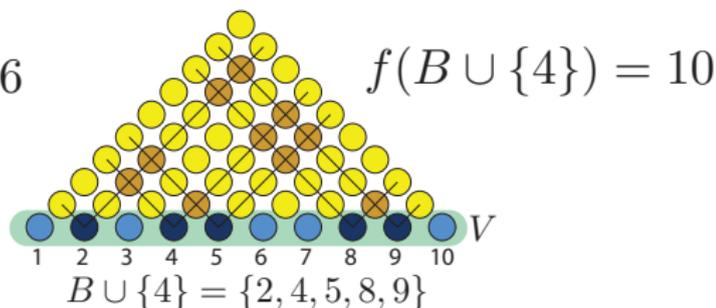
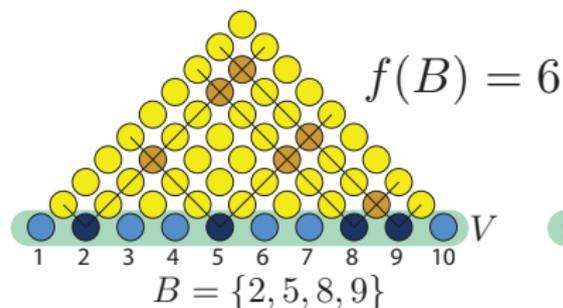
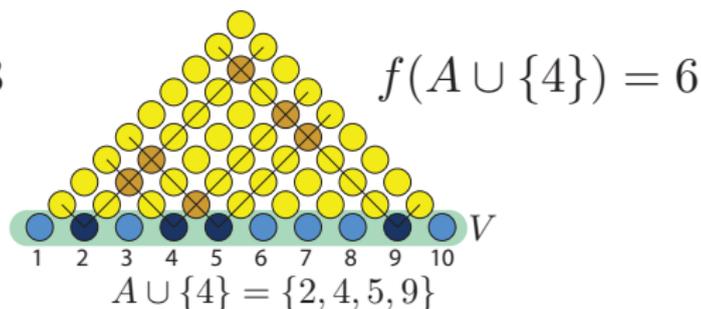
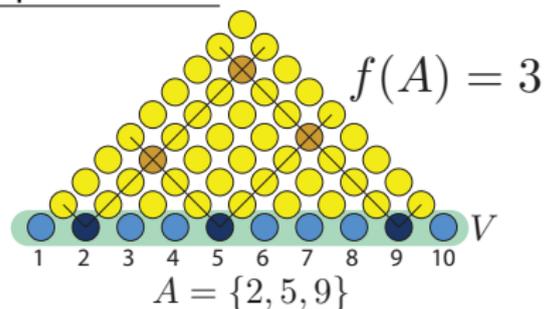
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- Incremental “value”, “gain”, or “cost” of v increases (improves) as the context in which v is considered grows from A to B .
- A function f is submodular iff $-f$ is supermodular.
- If f both submodular and supermodular, then f is said to be modular,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

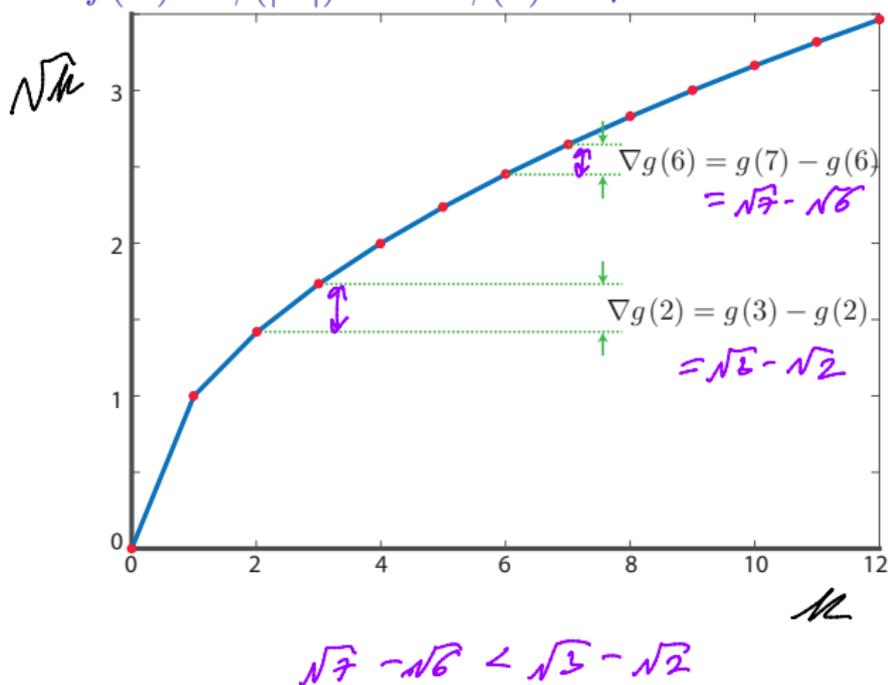


Submodularity's utility in ML

- 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.

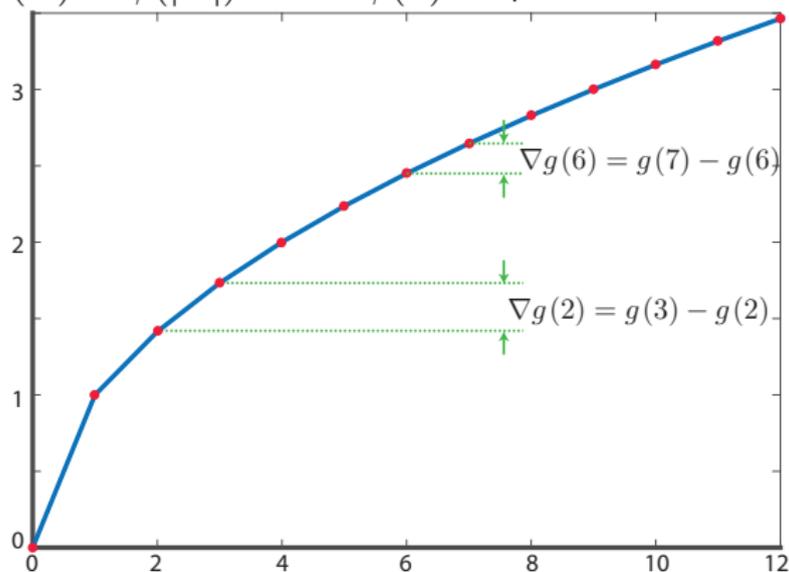
Square root of cardinality

- Consider $f(A) = \phi(|A|)$ where $\phi(k) = \sqrt{k}$



Square root of cardinality

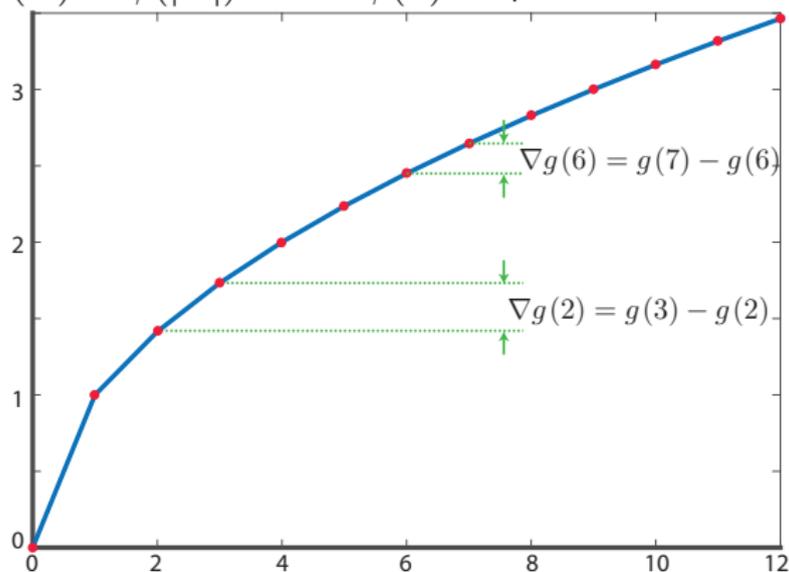
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- Hence, $f(v|A) = \sqrt{|A| + 1} - \sqrt{|A|} = \sqrt{k + 1} - \sqrt{k}$ when $|A| = k$ and is decreasing in k .

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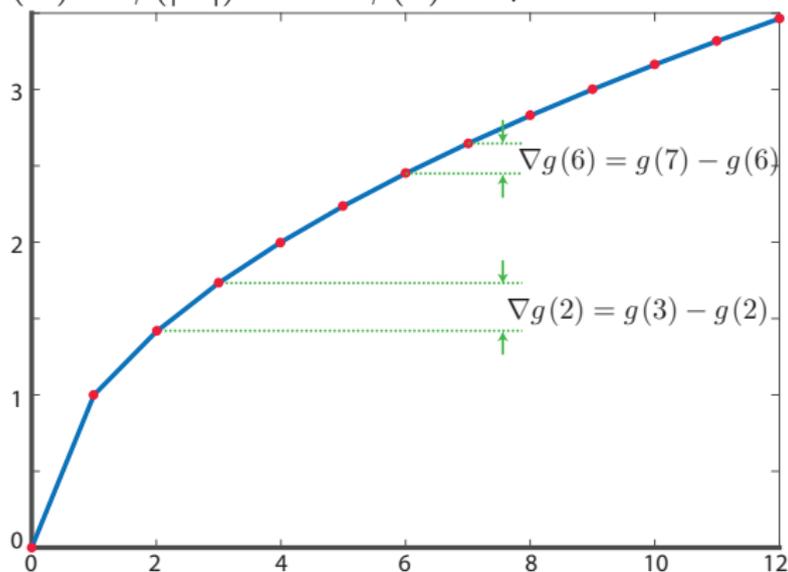
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- Hence f is submodular.

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- Hence f is submodular.
- Note that ϕ is a concave function.

Log of modular

$$m(\emptyset) = 0$$

- Given a non-negative normalized modular function

$$m(A) = \sum_{a \in A} m(a) \text{ where } m(a) \geq 0.$$

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

Log of modular

- Given a non-negative normalized modular function

$$m(A) = \sum_{a \in A} m(a) \text{ where } m(a) \geq 0.$$

- Consider $f(A) = \phi(m(A))$ where $\phi(x) = \log(1+x)$ for $x \in \mathbb{R}_+$.

$$\therefore f(\phi) = 0 \quad f(A) \geq 0 \quad \forall A.$$

Log of modular

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- Consider $f(A) = \phi(m(A))$ where $\phi(x) = \log(1 + x)$ for $x \in \mathbb{R}_+$.
- Then for $A \subseteq V$,

$$f(v|A) = \log(1 + m(v) + \sum_{a \in A} m(a)) - \log(1 + \sum_{a \in A} m(a)) \quad (2.1)$$

$$= \log\left(\frac{1 + m(v) + m(A)}{1 + m(A)}\right) \quad (2.2)$$

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- Since $f(v|A) \geq f(v|B)$, f is submodular.

Sums of concave composed with modular

- Let U be a set of indices.

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- Let ϕ_u be concave, then $f_u(X) = \phi_u(m_u(X))$ is a submodular function. \therefore we have 101 submodular functions.

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- Consider the following class of functions

$$f(X) = \sum_{u \in U} \alpha_u \phi_u(m_u(X)) \quad (2.3)$$

where ϕ_u is concave, and $\alpha_u \geq 0$ is a non-negative importance weight. It can be shown that f is submodular.

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- If all concave functions are non-negative monotone-nondecreasing, we can compose this with another concave function ϕ to reach:

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deep submodular functions.

Variable/Feature Selection in Classification/Regression

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

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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.

rather than
 $\Pr(y|x_V)$

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$$I(Y; X_A) = \sum_{y, x_A} \Pr(y, x_A) \log \frac{\Pr(y, x_A)}{\Pr(y) \Pr(x_A)} = \overset{\text{uncertainty about } Y}{H(Y)} - \overset{\text{residual uncertainty}}{H(Y|X_A)} \quad (2.5)$$

$$= H(X_A) - H(X_A|Y) = H(X_A) + H(Y) - H(X_A, Y) \quad (2.6)$$

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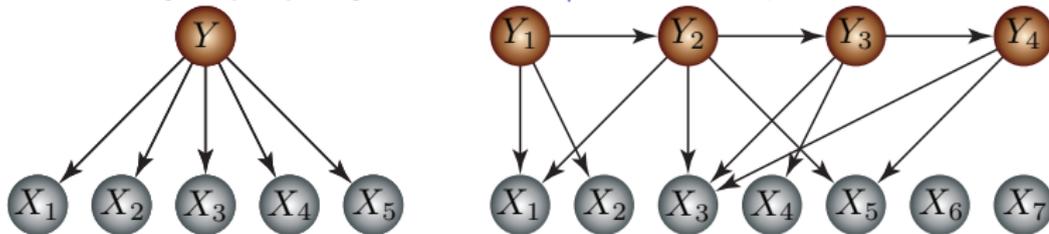
$$= H(X_A) - H(X_A|Y) = H(X_A) + H(Y) - H(X_A, Y) \quad (2.6)$$

- 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

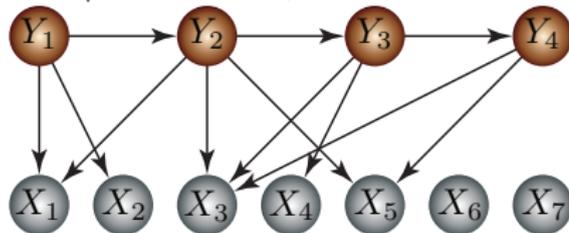
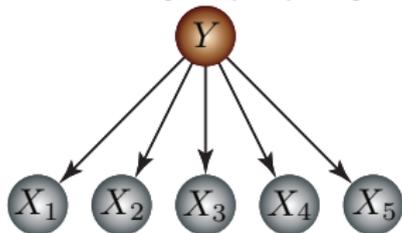
- Naïve Bayes property: $X_A \perp\!\!\!\perp X_B | Y$ for all A, B .



Information Gain and Feature Selection

in Pattern Classification: Naïve Bayes

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



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

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

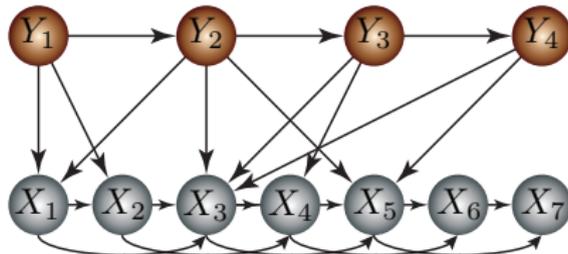
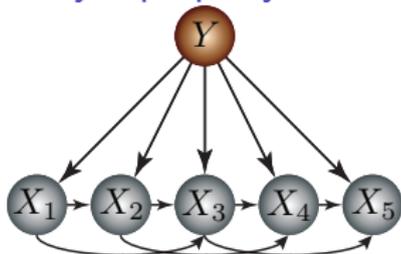
*Since $g(A) = H(X_A)$ is submodular
and $h(A) = \sum_{a \in A} H(X_a|Y)$ is modular,*

(2.7)

$f(A)$ is submodular (submodular minus modular).

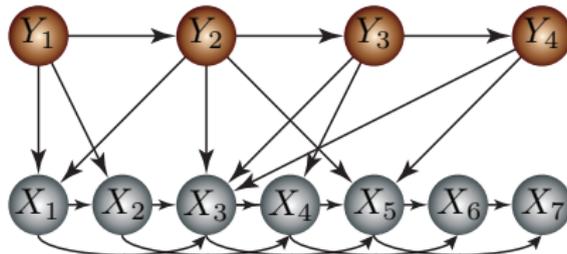
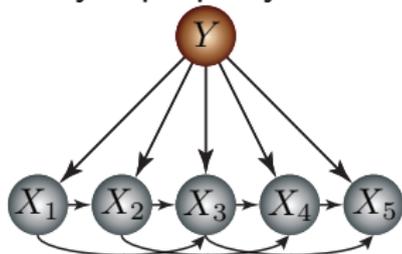
Variable Selection in Pattern Classification

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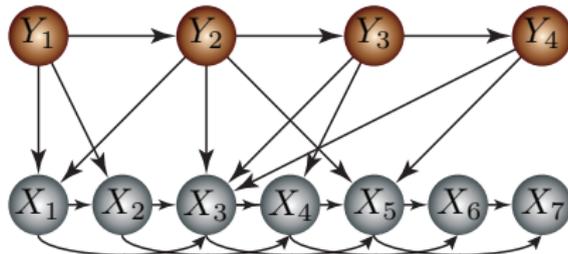
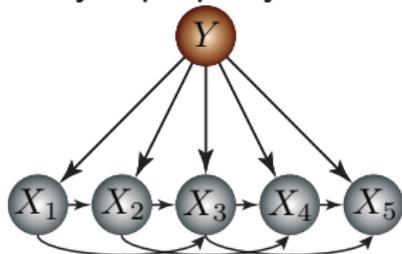
- $f(A)$ naturally expressed as a difference of two submodular functions

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which is a DS (difference of submodular) function.

Variable Selection in Pattern Classification

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which is a DS (difference of submodular) function.

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

$$f(A) = \sum_{a \in A} I(X_a; Y) - \lambda \sum_{a, a' \in A} I(X_a; X_{a'}|Y) \quad (2.9)$$

where $\lambda \geq 0$ is a tradeoff constant. *f(A) is also submodular.*

Variable Selection: Linear Regression Case

- Next, let Z be continuous. Predictor is linear $\tilde{Z}_A = \sum_{i \in A} \alpha_i X_i$.

Variable Selection: Linear Regression Case

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- Goodness measure is the squared multiple correlation, i.e.,

$$R_{Z,A}^2 = \frac{\overbrace{\text{Var}(Z) - E[(Z - \tilde{Z}_A)^2]}^{\text{reduction in variance}}}{\text{Var}(Z)} \quad (2.10)$$

\leftarrow normalizes.

we wish to find A of a given size that maximizes $R_{Z,A}^2$.

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we wish to find A of a given size that maximizes $R_{Z,A}^2$.

- $R_{Z,A}^2$'s maximizing parameters (i.e., under parameters for best linear predictor), for a given A , can be analytically computed.

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$$f(A) = b_A^\top \cdot b_A$$

Variable Selection: Linear Regression Case

- Next, let Z be continuous. Predictor is linear $\tilde{Z}_A = \sum_{i \in A} \alpha_i X_i$.
- Goodness measure is the squared multiple correlation, i.e.,

$$R_{Z,A}^2 = \frac{\text{Var}(Z) - E[(Z - \tilde{Z}_A)^2]}{\text{Var}(Z)} \quad (2.10)$$

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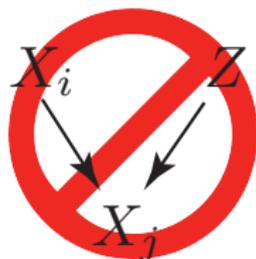
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- When \exists no “suppressor” variables (no v-structures that converge on X_j with parents X_i and Z), then

$$f(A) = R_{Z,A}^2 = b_A^\top (C_A^{-1})^\top b_A \quad (2.11)$$

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



Data/Feature 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, or coresets, or sketch).

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

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

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

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$$f(X) = \sum_{u \in U} \alpha_u \phi_u(m_u(X)) \quad (2.13)$$

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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 ϕ , 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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- 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: $\forall X \subseteq V,$

$$0 \leq \bar{m}_u(X) \triangleq \frac{m_u(X)}{\sum_{u' \in U} m_{u'}(X)} = \frac{m_u(X)}{m(X)} \leq 1 \quad (2.14)$$

where $m(X) \triangleq \sum_{u' \in U} m_{u'}(X)$.

$$m_v(X) = \sum_{a \in X} m_v(a)$$

$\bar{m}_v(X)$ is a set
of $2^{|V|}$ probability distributions
over V , one distribution
for each subset $X \subseteq V$.

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- Consider the KL-divergence between these two distributions:

$$D(p || \{\bar{m}_u(X)\}_{u \in U}) = \sum_{u \in U} p_u \log p_u - \sum_{u \in U} p_u \log(\bar{m}_u(X)) \quad (2.15)$$

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

$$= -H(p) + \log m(X) - \sum_{u \in U} p_u \log(m_u(X)) \quad (2.16)$$

Data Subset Selection, KL-divergence

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

$$D(p || \{\bar{m}_u(X)\}) = \text{const.} + \log m(X) - \sum_{u \in U} p_u \log(m_u(X)) \quad (2.17)$$

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- 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**.

$$\min_{X \subseteq V} D(p || \bar{m}_u(X)) \quad \text{subject to } m(X) = \alpha$$

$$\Rightarrow \max_{X \subseteq V} \sum_u p_u \log(m_u(X))$$

s. t. $m(X) = \alpha$

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- 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)

$$g(X) \triangleq \log m(X) - D(p||\{\bar{m}_u(X)\}) = \sum_{u \in U} p_u \log(m_u(X)) \quad (2.18)$$

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

Other examples as diversity models

- Sensor placement
- Social networks and influential nodes
- Viral marketing, information cascades, diffusion networks

Recall from lecture 1

- Next slide comes from lecture 1.

Sets, Characteristic Vectors, and pseudo-Boolean functions

- Any set $A \subseteq V$ can be represented as a binary vector $x \in \{0, 1\}^V$ (a “bit vector” representation of a set).
- The **characteristic vector** $\mathbf{1}_A \in \{0, 1\}^V$ of a set A is defined one where element $v \in V$ has value:

$$\mathbf{1}_A(v) = \begin{cases} 1 & \text{if } v \in A \\ 0 & \text{else} \end{cases} \quad (2.7)$$

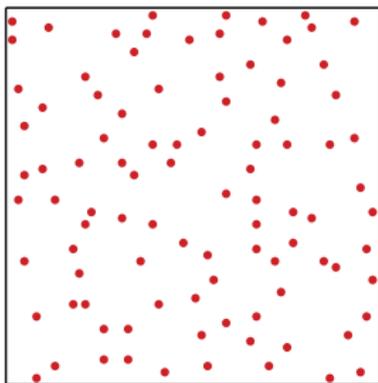
- Useful to be able to quickly map from set to binary vector, $\mathbf{1}_A$, and from vector to set, $A = V(\mathbf{1}_A)$.
- Given $x \in \{0, 1\}^V$, map to set via $V(x) \subseteq V$, where $v \in V(x)$ iff $x(v) = 1$.
- $f : \{0, 1\}^V \rightarrow \{0, 1\}$ are known as **Boolean function**.
- $f : \{0, 1\}^V \rightarrow \mathbb{R}$ is a **pseudo-Boolean function** (submodular functions are a special case).

Determinantal Point Processes (DPPs)

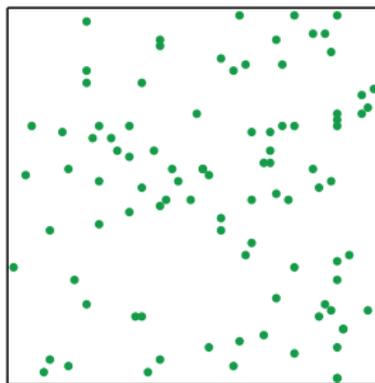
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DPP

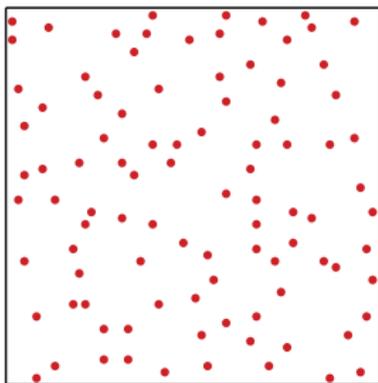


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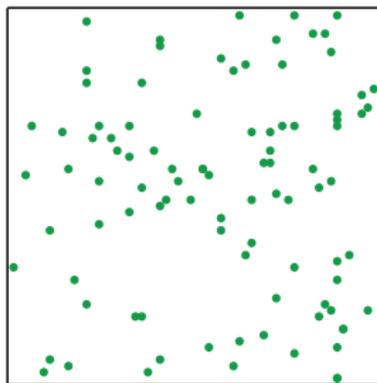
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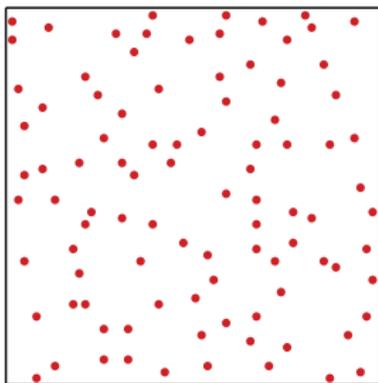
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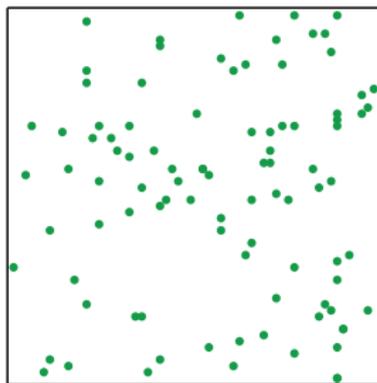
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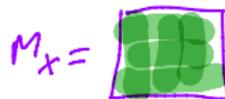
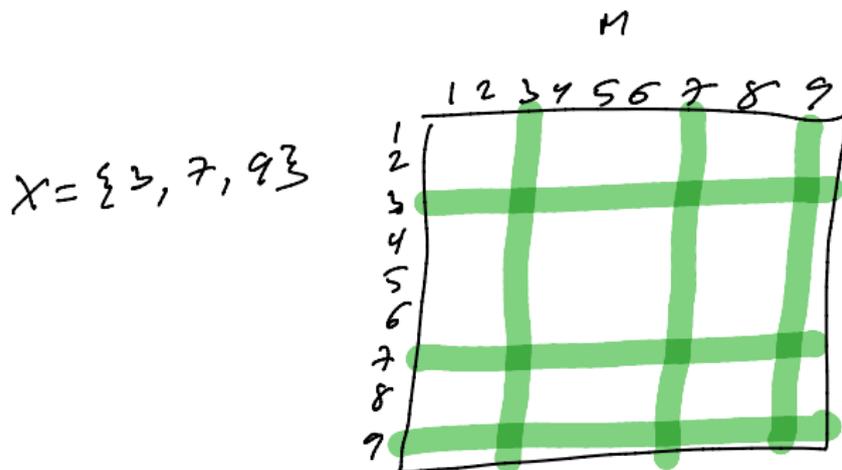
- A Determinantal point processes (DPPs) is a probability distribution over subsets A of V where the “energy” function is submodular.
- More “diverse” or “complex” samples are given higher probability.

DPPs and log-submodular probability distributions

- Given binary vectors $x, y \in \{0, 1\}^V$, $y \leq x$ if $y(v) \leq x(v), \forall v \in V$.

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$x \in \{0, 1\}^V$ $V = \{1, 2, 3, 4, 5\}$ $|V| = n = 5$
 $x = (0, 1, 1, 0, 1)$ $V(x) = \{2, 3, 5\} \subseteq V$ $V(x): \{0, 1, 3\} \rightarrow 2^V$

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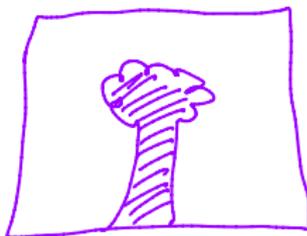
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- Therefore, a DPP is a log-submodular probability distribution.

Graphical Models and fast MAP Inference

- Distribution over $x \in \{0, 1\}^V$ that factors w.r.t. a graph:

$$p(x) = \frac{1}{Z} \exp(-E(x)) \quad (2.21)$$

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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- MAP inference problem is important in ML: compute

$$x^* \in \operatorname{argmax}_{x \in \{0,1\}^V} p(x) \quad (2.22)$$

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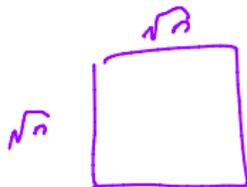
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$E_{i,j}(x_i, x_j)$
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- Many approximate inference strategies utilize additional factorization assumptions (e.g., mean-field, variational inference, expectation propagation, etc). *Suppose $E(x)$ is submodular.*
- Can we do exact MAP inference in polynomial time regardless of the tree-width, without even knowing the tree-width? **Yes!**

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- and two notions of “information amongst a collection of sets”:

$$I_f(S_1; S_2; \dots; S_k) = \sum_{i=1}^k f(S_i) - f(S_1 \cup S_2 \cup \dots \cup S_k) \quad (2.26)$$

$$I'_f(S_1; S_2; \dots; S_k) = \sum_{A \subseteq \{1, 2, \dots, k\}} (-1)^{|A|+1} f\left(\bigcup_{j \in A} S_j\right) \quad (2.27)$$

Submodular Parameterized Clustering

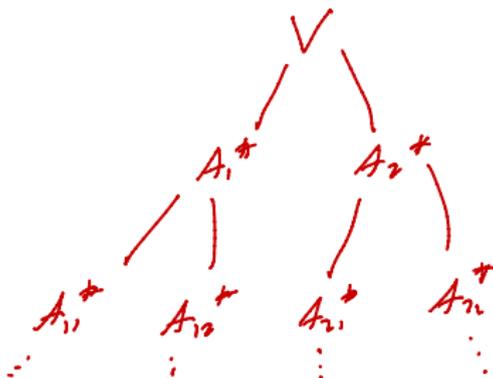
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- Hence, family of clustering algorithms parameterized by f .

Ground set: E or V ?

$$G = (V, E) \quad \curvearrowright$$

Submodular functions are functions defined on subsets of some finite set, called the **ground set**.

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- The terminology **ground set** comes from lattice theory, where V are the ground elements of a lattice (just above 0).

Notation \mathbb{R}^E , and modular functions as vectors

What does $x \in \mathbb{R}^E$ mean?

 \mathbb{R}^n
 $|E|$

$$\mathbb{R}^E = \{x = (x_j \in \mathbb{R} : j \in E)\} \quad (2.28)$$

and

$$\mathbb{R}_+^E = \{x = (x_j : j \in E) : x \geq 0\} \quad (2.29)$$

$$E = \{1, \dots, n\}$$

$$E = \{\text{apple}, \text{orange}\}$$



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Any vector $x \in \mathbb{R}^E$ can be treated as a normalized modular function, and vice versa. That is, for $A \subseteq E$,

$$x(A) = \sum_{a \in A} x_a \quad (2.30)$$

Note that x is said to be **normalized** since $x(\emptyset) = 0$.

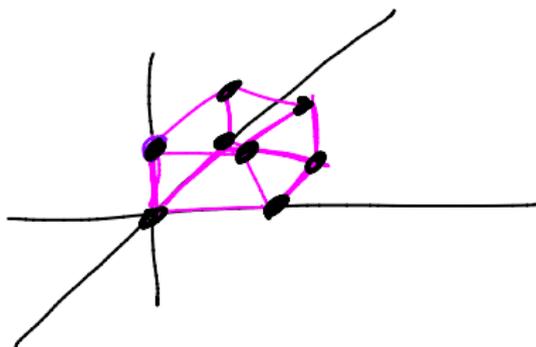
Characteristic vectors of sets & modular functions

- Given an $A \subseteq E$, define the incidence (or characteristic) vector $\mathbf{1}_A \in \{0, 1\}^E$ on the **unit hypercube** to be

$$\mathbf{1}_A(j) = \begin{cases} 1 & \text{if } j \in A; \\ 0 & \text{if } j \notin A \end{cases} \quad (2.31)$$

or equivalently,

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- Thus, given modular function $x \in \mathbb{R}^E$, we can write $x(A)$ in a variety of ways, i.e.,

$$x(A) = x^\top \cdot \mathbf{1}_A = \langle x, \mathbf{1}_A \rangle = \sum_{i \in A} x(i) \quad (2.33)$$

Other Notation: singletons and sets

When A is a set and k is a singleton (i.e., a single item), the union is properly written as $A \cup \{k\}$, but sometimes we will write just $A + k$.

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- What might 3^E mean?

Example Submodular: Entropy from Information Theory

$$A = \{a_1, a_2, \dots, a_{|A|}\}$$

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

$$f(A) = H(X_A) = - \sum_{x_A} p(x_A) \log p(x_A) \quad (2.34)$$

is submodular. $X_A = (X_{a_1}, X_{a_2}, \dots, X_{a_{|A|}})$

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

$$H(X_v | X_B) = H(X_{B+v}) - H(X_B) \quad (2.35)$$

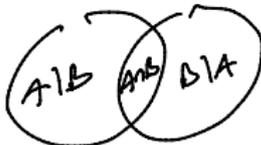
$$\leq H(X_{A+v}) - H(X_A) = H(X_v | X_A) \quad (2.36)$$

- We say "further" due to $B \setminus A$ not nec. empty.

$$H(X_v | X_B) = H(X_v | X_A, X_{B \setminus A}).$$

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:

$$\begin{aligned}
 I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B}) &= \sum_{x_{A \cup B}} p(x_{A \cup B}) \log \frac{p(x_{A \setminus B}, x_{B \setminus A} | x_{A \cap B})}{p(x_{A \setminus B} | x_{A \cap B}) p(x_{B \setminus A} | x_{A \cap B})} \\
 &= \sum_{x_{A \cup B}} p(x_{A \cup B}) \log \frac{p(x_{A \cup B}) p(x_{A \cap B})}{p(x_A) p(x_B)} \geq 0 \quad (2.37)
 \end{aligned}$$


then

$$\begin{aligned}
 I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B}) \\
 = H(X_A) + H(X_B) - H(X_{A \cup B}) - H(X_{A \cap B}) \geq 0 \quad (2.38)
 \end{aligned}$$

so entropy satisfies

$$H(X_A) + H(X_B) \geq H(X_{A \cup B}) + H(X_{A \cap B}) \quad (2.39)$$

Information Theory: Block Coding

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- 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.,

$$I(X_A; X_B) = H(X_A) + H(X_B) - H(X_A, X_B) \quad (2.40)$$

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.

Example Submodular: Mutual Information

- Also, symmetric mutual information is submodular,

$$f(A) = I(X_A; X_{V \setminus A}) = H(X_A) + H(X_{V \setminus A}) - H(X_V) \quad (2.41)$$

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).

Monge Matrices

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

$$c_{ij} + c_{rs} \leq c_{is} + c_{rj} \quad (2.42)$$

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

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$$c_{ij} + c_{rs} \leq c_{is} + c_{rj} \quad (2.42)$$

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

- Equivalently, for all $1 \leq i, r \leq m$, $1 \leq j, s \leq n$,

$$c_{\min(i,r),\min(j,s)} + c_{\max(i,r),\max(j,s)} \leq c_{is} + c_{rj} \quad (2.43)$$

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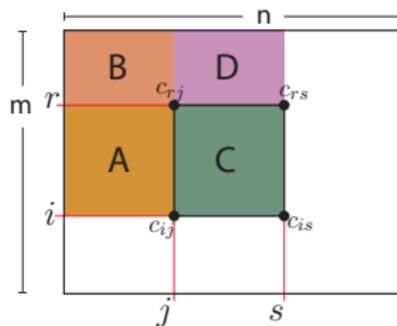
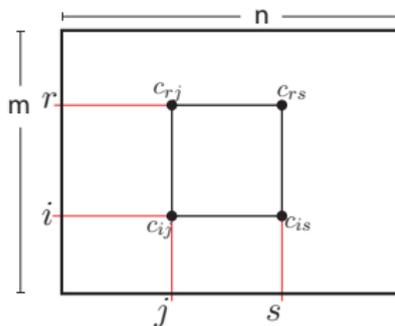
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- Consider four elements of the $m \times n$ matrix:



$$c_{ij} = A + B, \quad c_{rj} = B, \quad c_{rs} = B + D, \quad c_{is} = A + B + C + D.$$

Monge Matrices, where useful

- Useful for speeding up transportation, dynamic programming, flow, search, lot-sizing and many other problems.

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- Useful for speeding up transportation, dynamic programming, flow, search, lot-sizing and many other problems.
- Example, **Hitchcock transportation problem**: Given $m \times n$ cost matrix $C = [c_{ij}]_{ij}$, a non-negative supply vector $a \in \mathbb{R}_+^m$, a non-negative demand vector $b \in \mathbb{R}_+^n$ with $\sum_{i=1}^m a(i) = \sum_{j=1}^n b_j$, we wish to optimally solve the following linear program:

$$\begin{array}{ll} \text{minimize} & \sum_{i=1}^m \sum_{j=1}^n c_{ij} x_{ij} \\ X \in \mathbb{R}^{m \times n} & \end{array} \quad (2.44)$$

$$\text{subject to} \quad \sum_{i=1}^m x_{ij} = b_j \quad \forall j = 1, \dots, n \quad (2.45)$$

$$\sum_{j=1}^n x_{ij} = a_i \quad \forall i = 1, \dots, m \quad (2.46)$$

$$x_{i,j} \geq 0 \quad \forall i, j \quad (2.47)$$

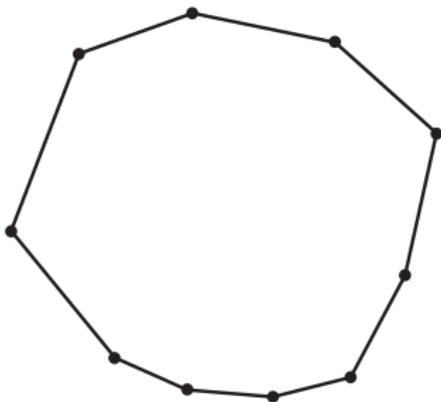
Monge Matrices, Hitchcock transportation

		C			
Producers, Sources, or Supply	a_1 2	0	1	3	3
	a_2 1	1	4	7	10
	a_3 5	0	4	9	14
		3	2	1	2
		b_1	b_2	b_3	b_4
		Consumers, Sinks, or Demand			

- Solving the linear program can be done easily and optimally using the “North-West Corner Rule” (a 2D greedy-like approach starting at top-left and moving down-right) in only $O(m + n)$ if the matrix C is Monge!

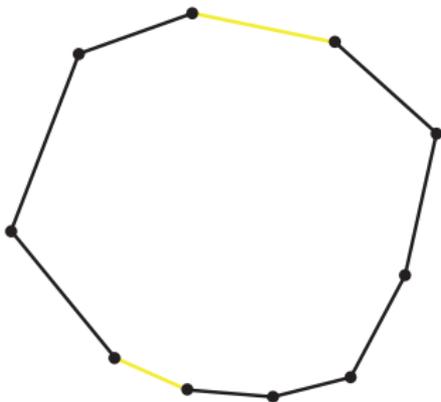
Monge Matrices and Convex Polygons

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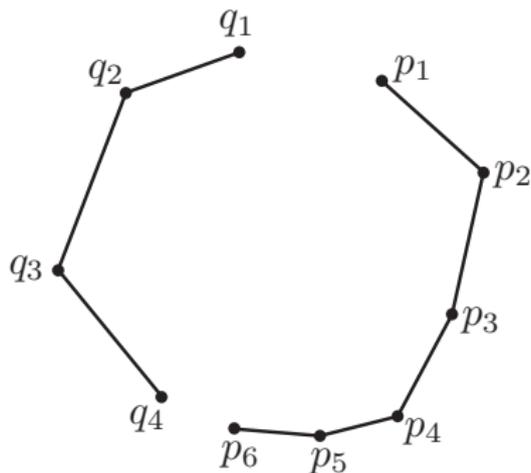
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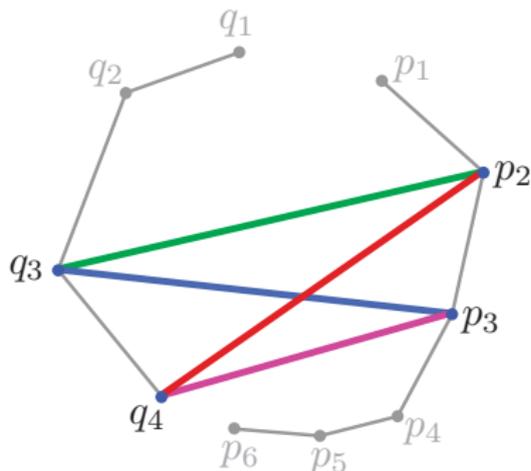
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- With $|V| = 2$, and $K + 1$ the side-dimension of the matrix, we get a Monge property (on square matrices).
- Non square: $f : \{0, 1, \dots, K_1\} \times \{0, 1, \dots, K_2\} \rightarrow \mathbb{R}$.

Two Equivalent Submodular Definitions

Definition 2.10.1 (submodular concave)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \quad (2.7)$$

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

Definition 2.10.2 (diminishing returns)

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

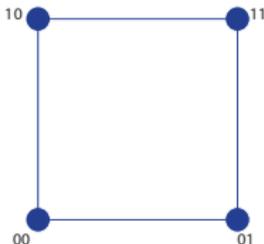
$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \quad (2.8)$$

- The incremental “value”, “gain”, or “cost” of v decreases (diminishes) as the context in which v is considered grows from A to B .
- Gain notation: Define $f(v|A) \triangleq f(A + v) - f(A)$. Then function f is submodular if $f(v|A) \geq f(v|B)$ for all $A \subseteq B \subseteq V \setminus \{v\}$, $v \in V$.

Submodular on Hypercube Vertices

We can test submodularity via values on vertices of hypercube.

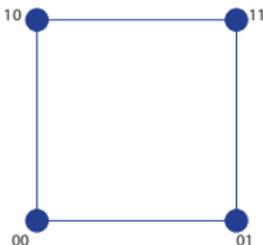
Example: with $|V| = n = 2$, this is easy:



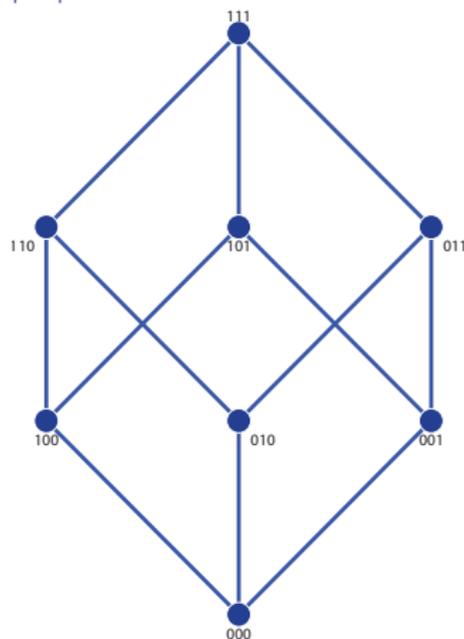
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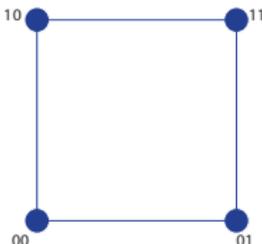
With $|V| = n = 3$, a bit harder.



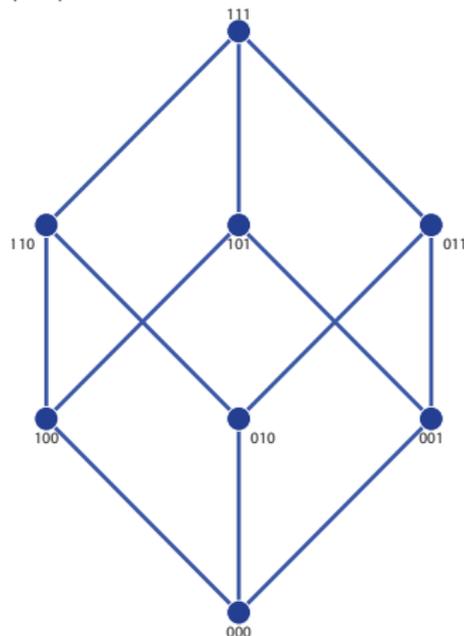
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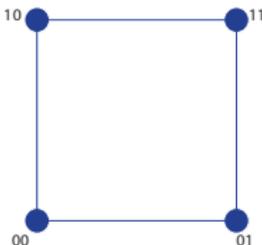


How many inequalities of form
 $f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$?

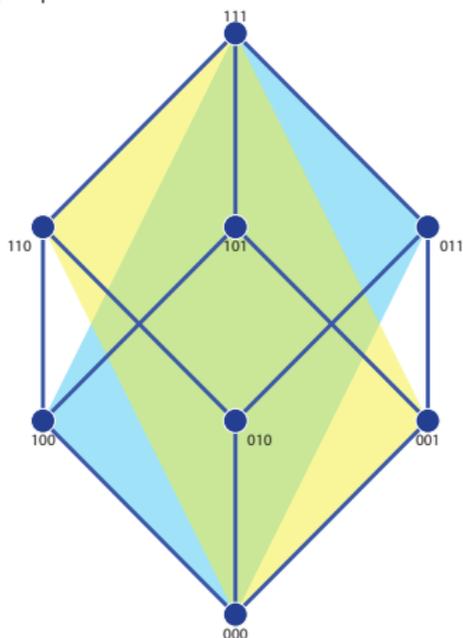
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Subadditive Definitions

Definition 2.10.1 (subadditive)

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

$$f(A) + f(B) \geq f(A \cup B) \quad (2.50)$$

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

Two Equivalent Supermodular Definitions

Definition 2.10.1 (supermodular)

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

$$f(A) + f(B) \leq f(A \cup B) + f(A \cap B) \quad (2.7)$$

Definition 2.10.2 (supermodular (improving returns))

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

$$f(A \cup \{v\}) - f(A) \leq f(B \cup \{v\}) - f(B) \quad (2.8)$$

- 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 $f(A) = c + \sum_{a \in A} \bar{f}(a)$ for some \bar{f} (often $c = 0$).

Superadditive Definitions

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

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- Ex: Let $0 < k < |V|$, and consider $f : 2^V \rightarrow \mathbb{R}_+$ where:

$$f(A) = \begin{cases} 1 & \text{if } |A| \leq k \\ 0 & \text{else} \end{cases} \quad (2.52)$$

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- This function is subadditive but not submodular.

Modular Definitions

Definition 2.10.3 (modular)

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

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

$$f(A) + f(B) = f(A \cap B) + f(A \cup B) \quad (2.53)$$

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

Proposition 2.10.4

If f is modular, it may be written as

$$f(A) = f(\emptyset) + \sum_{a \in A} \left(f(\{a\}) - f(\emptyset) \right) = c + \sum_{a \in A} f'(a) \quad (2.54)$$

which has only $|V| + 1$ parameters.

Modular Definitions

Proof.

We inductively construct the value for $A = \{a_1, a_2, \dots, a_k\}$.

For $k = 2$,

$$f(a_1) + f(a_2) = f(a_1, a_2) + f(\emptyset) \quad (2.55)$$

$$\text{implies } f(a_1, a_2) = f(a_1) - f(\emptyset) + f(a_2) - f(\emptyset) + f(\emptyset) \quad (2.56)$$

then for $k = 3$,

$$f(a_1, a_2) + f(a_3) = f(a_1, a_2, a_3) + f(\emptyset) \quad (2.57)$$

$$\text{implies } f(a_1, a_2, a_3) = f(a_1, a_2) - f(\emptyset) + f(a_3) - f(\emptyset) + f(\emptyset) \quad (2.58)$$

$$= f(\emptyset) + \sum_{i=1}^3 (f(a_i) - f(\emptyset)) \quad (2.59)$$

and so on ...



Complement function

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

Proposition 2.10.5

\bar{f} is submodular iff f is submodular.

Proof.

$$\bar{f}(A) + \bar{f}(B) \geq \bar{f}(A \cup B) + \bar{f}(A \cap B) \quad (2.60)$$

follows from

$$f(V \setminus A) + f(V \setminus B) \geq f(V \setminus (A \cup B)) + f(V \setminus (A \cap B)) \quad (2.61)$$

which is true because $V \setminus (A \cup B) = (V \setminus A) \cap (V \setminus B)$ and $V \setminus (A \cap B) = (V \setminus A) \cup (V \setminus B)$ (De Morgan's laws for sets). \square

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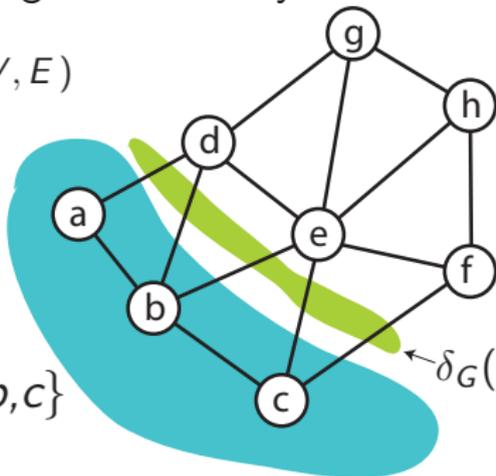
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$G = (V, E)$



$S = \{a, b, c\}$

$$\begin{aligned} \delta_G(S) &= \{\{u, v\} \in E : u \in S, v \in V \setminus S\}. \\ &= \{\{a, d\}, \{b, d\}, \{b, e\}, \{c, e\}, \{c, f\}\} \end{aligned}$$

Directed graphs, and cuts and flows

- If G is directed, define

$$E^+(X, Y) \triangleq \{(x, y) \in E(G) : x \in X \setminus Y, y \in Y \setminus X\} \quad (2.63)$$

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and edges entering X (**in-flow**) as

$$\delta^-(X) \triangleq E^+(V \setminus X, X) \quad (2.65)$$

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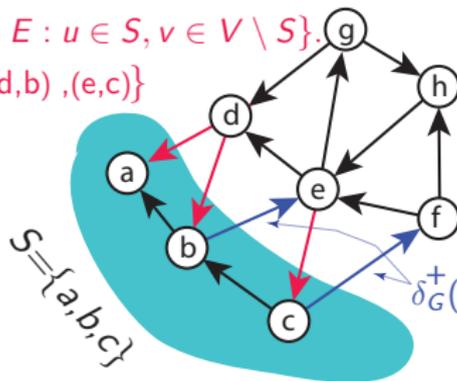
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$$\begin{aligned} \delta_G^-(S) &= \{(v, u) \in E : u \in S, v \in V \setminus S\} \\ &= \{(d, a), (d, b), (e, c)\} \end{aligned}$$



$$\begin{aligned} \delta_G^+(S) &= \{(u, v) \in E : u \in S, v \in V \setminus S\} \\ &= \{(b, e), (c, f)\} \end{aligned}$$

The Neighbor function in undirected graphs

- Given a set $X \subseteq V$, the neighbor function of X is defined as

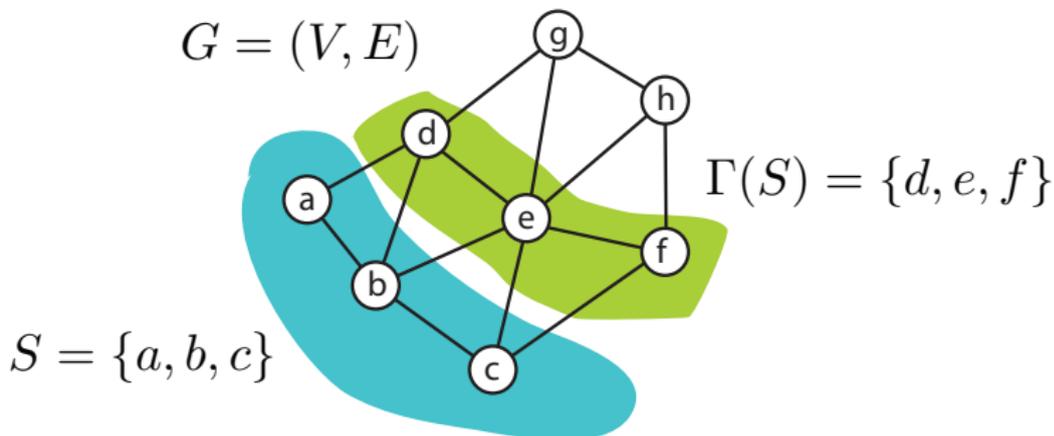
$$\Gamma(X) \triangleq \{v \in V(G) \setminus X : E(X, \{v\}) \neq \emptyset\} \quad (2.66)$$

The Neighbor function in undirected graphs

- Given a set $X \subseteq V$, the neighbor function of X is defined as

$$\Gamma(X) \triangleq \{v \in V(G) \setminus X : E(X, \{v\}) \neq \emptyset\} \quad (2.66)$$

- Example:



Directed Cut function: property

Lemma 2.11.1

For a digraph $G = (V, E)$ and any $X, Y \subseteq V$: we have

$$\begin{aligned} |\delta^+(X)| + |\delta^+(Y)| \\ = |\delta^+(X \cap Y)| + |\delta^+(X \cup Y)| + |E^+(X, Y)| + |E^+(Y, X)| \end{aligned} \quad (2.67)$$

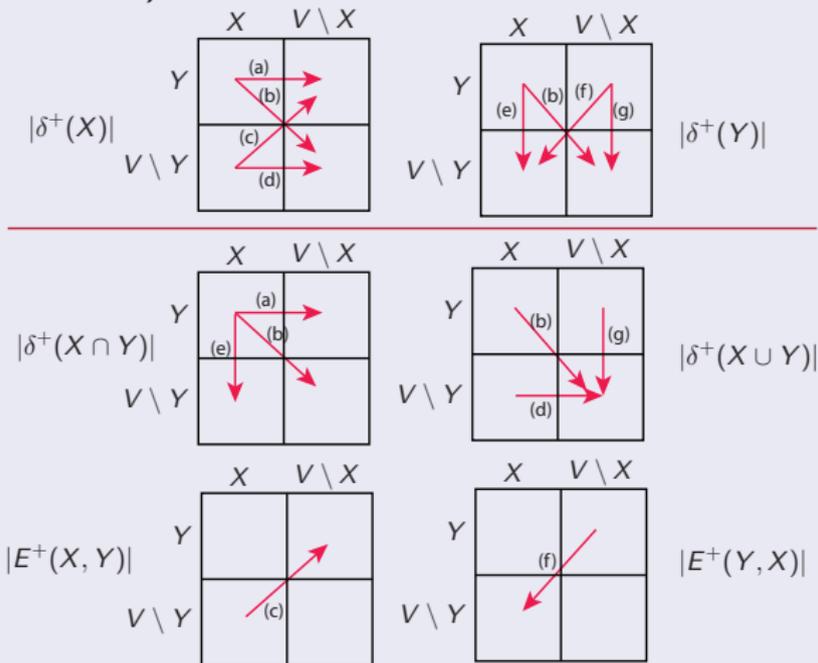
and

$$\begin{aligned} |\delta^-(X)| + |\delta^-(Y)| \\ = |\delta^-(X \cap Y)| + |\delta^-(X \cup Y)| + |E^-(X, Y)| + |E^-(Y, X)| \end{aligned} \quad (2.68)$$

Directed Cut function: proof of property

Proof.

We can prove Eq. (2.67) using a geometric counting argument (proof for $|\delta^-(X)|$ case is similar)



Q: Why is $(c) = |E^+(X, Y)|$?

Directed cut/flow functions: submodular

Lemma 2.11.2

For a digraph $G = (V, E)$ and any $X, Y \subseteq V$: both functions $|\delta^+(X)|$ and $|\delta^-(X)|$ are submodular.

Proof.

$|E^+(X, Y)| \geq 0$ and $|E^-(X, Y)| \geq 0$. □

More generally, in the non-negative weighted edge case, both in-flow and out-flow are submodular on subsets of the vertices.

Undirected Cut/Flow & the Neighbor function: submodular

Lemma 2.11.3

For an undirected graph $G = (V, E)$ and any $X, Y \subseteq V$: we have that both the undirected cut (or flow) function $|\delta(X)|$ and the neighbor function $|\Gamma(X)|$ are submodular. I.e.,

$$|\delta(X)| + |\delta(Y)| = |\delta(X \cap Y)| + |\delta(X \cup Y)| + 2|E(X, Y)| \quad (2.69)$$

and

$$|\Gamma(X)| + |\Gamma(Y)| \geq |\Gamma(X \cap Y)| + |\Gamma(X \cup Y)| \quad (2.70)$$

Proof.

- Eq. (2.69) follows from Eq. (2.67): we replace each undirected edge $\{u, v\}$ with two oppositely-directed directed edges (u, v) and (v, u) . Then we use same counting argument.

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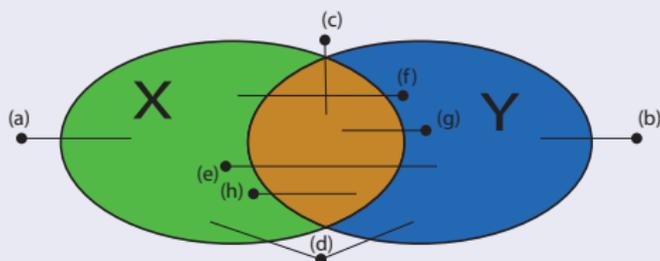
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- Eq. (2.70) follows as shown in the following page.

...

cont.



Graphically, we can count and see that

$$\Gamma(X) = (a) + (c) + (f) + (g) + (d) \quad (2.71)$$

$$\Gamma(Y) = (b) + (c) + (e) + (h) + (d) \quad (2.72)$$

$$\Gamma(X \cup Y) = (a) + (b) + (c) + (d) \quad (2.73)$$

$$\Gamma(X \cap Y) = (c) + (g) + (h) \quad (2.74)$$

so

$$\begin{aligned} |\Gamma(X)| + |\Gamma(Y)| &= (a) + (b) + 2(c) + 2(d) + (e) + (f) + (g) + (h) \\ &\geq (a) + (b) + 2(c) + (d) + (g) + (h) = |\Gamma(X \cup Y)| + |\Gamma(X \cap Y)| \end{aligned} \quad (2.75)$$

Undirected Neighbor functions

Therefore, the undirected cut function $|\delta(A)|$ and the neighbor function $|\Gamma(A)|$ of a graph G are both submodular.

Undirected cut/flow is submodular: alternate proof

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- Define a graph $G_{uv} = (\{u, v\}, \{e\}, w)$ with two nodes u, v and one edge $e = \{u, v\}$ with non-negative weight $w(e) \in \mathbb{R}_+$.

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- Define a graph $G_{uv} = (\{u, v\}, \{e\}, w)$ with two nodes u, v and one edge $e = \{u, v\}$ with non-negative weight $w(e) \in \mathbb{R}_+$.
- Weighted cut function over those two nodes: $w(\delta_{u,v}(\cdot))$ has valuation:

$$w(\delta_{u,v}(\emptyset)) = w(\delta_{u,v}(\{u, v\})) = 0 \quad (2.76)$$

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- General non-negative weighted graph $G = (V, E, w)$, define $w(\delta(\cdot))$:

$$f(X) = w(\delta(X)) = \sum_{(u,v) \in E(G)} w(\delta_{u,v}(X \cap \{u, v\})) \quad (2.79)$$

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- This is easily shown to be submodular using properties we will soon see (namely, submodularity closed under summation and restriction).

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- Let $V(X)$ be the vertices adjacent to some edge in $X \subseteq E(G)$, then $|V(X)|$ (the vertex function) is **submodular**.

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- Consider $f(A) = |\delta^+(A)| - |\delta^+(V \setminus A)|$. Guess, submodular, supermodular, modular, or neither? **Exercise: determine which one and prove it.**

Number of connected components in a graph via edges

- Recall, $f : 2^V \rightarrow \mathbb{R}$ is submodular, then so is $\bar{f} : 2^V \rightarrow \mathbb{R}$ defined as $\bar{f}(S) = f(V \setminus S)$.

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with $A \subseteq B \subseteq E \setminus \{a\}$.

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- Intuition: an edge is “more” (no less) able to bridge separate components (and reduce the number of connected components) when edge is added in a smaller context than when added in a larger context.

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- Intuition: an edge is “more” (no less) able to bridge separate components (and reduce the number of connected components) when edge is added in a smaller context than when added in a larger context.
- $\bar{c}(A) = c(E \setminus A)$ is number of connected components in G when we remove A ; supermodular monotone non-decreasing but not normalized.