Submodular Functions, Optimization, and Applications to Machine Learning
— Fall Quarter, Lecture 5 —

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

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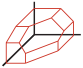
Oct 14th, 2020

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

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



Announcements, Assignments, and Reminders

Monday, 10/19/2020

- Homework 1 is out, due ~~Friday~~ at 11:59pm.

Class Road Map - EE563

- L1(9/30): Motivation, Applications, Definitions, Properties
- L2(10/5): Sums concave(modular), uses (diversity/costs, feature selection), information theory
- L3(10/7): Monge, More Definitions, Graph and Combinatorial Examples,
- L4(10/12): Graph & Combinatorial Examples, Matrix Rank, Properties, Other Defs, Independence
- L5(10/14): Independence, Matroids, Matroid Examples, Matroid Rank, More on Partition Matroid
- 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

Summary: Properties so far

- Cover functions $f(A) = w(\bigcup_{a \in A} U_a)$ are submodular.
- SCCM is submodular $f(A) = \sum_{u \in U} \phi_u(m_u(A))$ where m_u is a non-negative modular and ϕ_u is concave.
- max is submodular $f(A) = \max_{j \in A} c_j$, as is facility location $f(A) = \sum_{u \in U} \max_{a \in A} s_{a,u}$.
- Matrix rank function is submodular.
- Log determinant $f(A) = \log\det(\mathbf{\Sigma}_A)$ submodular for p.d. Σ.
- Matrix rank $r(A)$, dim. of space spanned by the vector set $\{x_a\}_{a \in A}$.
- Graph cut, set cover, and incidence functions,
- quadratics with non-positive off-diagonals $f(X) = m^\intercal \mathbf{1}_X + \frac{1}{2}\mathbf{1}_X^\intercal \mathbf{M} \mathbf{1}_X$.
- Number connected components in induced graph $c(A)$, and interior edge function $E(S)$, is supermodular.
- Submodular plus modular is submodular, $f(A) = f'(A) + m(A)$.
- Complementation: $f'(A) = f(V \setminus A)$ is submodular if f is submodular (same for supermodular, modular).
- Conix mixture: $\alpha_i \geq 0$, $f_i : 2^V \to \mathbb{R}$ submodular, then so is $\sum_i \alpha_i f_i$.
- Restrictions preserve submodularity: $f'(A) = f(A \cap S)$

Concave over non-negative modular

Let $m \in \mathbb{R}_+^E$ be a non-negative modular function, and ϕ a concave function over $\mathbb{R}$. Define $f : 2^E \to \mathbb{R}$ as

$$f(A) = \phi(m(A)) \tag{5.1}$$

then f is submodular.

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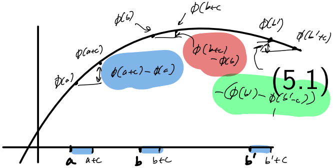

then f is submodular.

Proof.

Given $A \subseteq B \subseteq E \setminus v$, we have $0 \leq a = m(A) \leq b = m(B)$, and $0 \leq c = m(v)$. For g concave, we have $\phi(a + c) - \phi(a) \geq \phi(b + c) - \phi(b)$, and thus

$$\phi(m(A) + m(v)) - \phi(m(A)) \geq \phi(m(B) + m(v)) - \phi(m(B)) \tag{5.2}$$

$\square$

A form of converse is true as well.

Concave composed with non-negative modular

Theorem 5.3.1

Given a ground set V. The following two are equivalent:

1. *For all modular functions $m : 2^V \to \mathbb{R}_+$, then $f : 2^V \to \mathbb{R}$ defined as $f(A) = \phi(m(A))$ is submodular*
2. *$\phi : \mathbb{R}_+ \to \mathbb{R}$ is concave.*

- If ϕ is non-decreasing concave & $\phi(0) = 0$, then f is polymatroidal.

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- Sums of concave over modular functions are submodular

$$f(A) = \sum_{i=1}^{K} \alpha_i \, \phi_i(m_i(A)) \tag{5.3}$$

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- Very large class of functions, including graph cut, bipartite neighborhoods, set cover (Stobbe & Krause 2011), and "feature-based submodular functions" (Wei, Iyer, & Bilmes 2014).

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- Very large class of functions, including graph cut, bipartite neighborhoods, set cover (Stobbe & Krause 2011), and "feature-based submodular functions" (Wei, Iyer, & Bilmes 2014).
- However, Vondrak showed that a graphic matroid rank function over K_4 (we'll define this after we define matroids) are not members.

Monotonicity

Definition 5.3.2

A function $f : 2^V \to \mathbb{R}$ is monotone nondecreasing (resp. monotone increasing) if for all $A \subset B$, we have $f(A) \leq f(B)$ (resp. $f(A) < f(B)$).

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Definition 5.3.3

A function $f : 2^V \to \mathbb{R}$ is monotone nonincreasing (resp. monotone decreasing) if for all $A \subset B$, we have $f(A) \geq f(B)$ (resp. $f(A) > f(B)$).

Composition of non-decreasing submodular and non-decreasing concave

Theorem 5.3.4

Given two functions, one defined on sets

$$f : 2^V \to \mathbb{R} \tag{5.4}$$

and another continuous valued one:

$$\phi : \mathbb{R} \to \mathbb{R} \tag{5.5}$$

$\phi(x) = \min(x, \alpha)$

the composition formed as $h = \phi \circ f : 2^V \to \mathbb{R}$ (defined as $h(S) = \phi(f(S))$) is nondecreasing submodular, if ϕ is non-decreasing concave and f is nondecreasing submodular.

truncation

$f(A)$ polymatroid function

$h(A) = \min(f(A), \alpha)$ $\therefore$ h is polymatroid function too.

Monotone difference of two functions

Let f and g both be submodular functions on subsets of V and let $(f - g)(\cdot)$ be either monotone non-decreasing or monotone non-increasing Then $h : 2^V \to R$ defined by

$$h(A) = \min(f(A), g(A)) \tag{5.6}$$

is submodular.

Proof.

If h agrees with f on both X and Y (or g on both X and Y), and since

$$h(X) + h(Y) = f(X) + f(Y) \geq f(X \cup Y) + f(X \cap Y) \tag{5.7}$$

or

$$h(X) + h(Y) = g(X) + g(Y) \geq g(X \cup Y) + g(X \cap Y), \tag{5.8}$$

the result (Equation 5.6 being submodular) follows since

$$\begin{array}{c} f(X) + f(Y) \\ g(X) + g(Y) \end{array} \geq \min(f(X \cup Y), g(X \cup Y)) + \min(f(X \cap Y), g(X \cap Y))$$

$$= h(X \cup Y) + h(X \cap Y) \tag{5.9}$$

...

Monotone difference of two functions

...cont.

Otherwise, w.l.o.g., $h(X) = f(X)$ and $h(Y) = g(Y)$, giving

$$h(X) + h(Y) = f(X) + g(Y) \geq f(X \cup Y) + f(X \cap Y) + g(Y) - f(Y) \tag{5.10}$$

$f(X) + f(Y) \geq f(X \cup Y) + f(X \cap Y)$

$f(X) \geq f(X \cup Y) + f(X \cap Y) - f(Y)$

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$f(X \cup Y) - g(X \cup Y) \geq f(Y) - g(Y)$

Assume the case where $f - g$ is monotone non-decreasing. Hence, $f(X \cup Y) + g(Y) - f(Y) \geq g(X \cup Y)$ giving

$$h(X) + h(Y) \geq g(X \cup Y) + f(X \cap Y) \geq h(X \cup Y) + h(X \cap Y) \tag{5.11}$$

□

What is an easy way to prove the case where $f - g$ is monotone non-increasing?

Saturation via the $\min(\cdot)$ function

Let $f : 2^V \to \mathbb{R}$ be a monotone non-decreqasing or non-increasing submodular function and let α be a constant. Then the function $h : 2^V \to \mathbb{R}$ defined by

$$h(A) = \min(\alpha, f(A)) \tag{5.12}$$

is submodular.

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For constant k, we have that $(f - k)$ is non-decreasing (or non-increasing) so this follows from the previous result. □

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Note also, $g(a) = \min(k, a)$ for constant k is a non-decreasing concave function, so when f is monotone nondecreasing submodular, we can use the earlier result about composing a monotone concave function with a monotone submodular function to get a version of this.

More on Min - the saturate trick

- minimax facility location is similar to the following maximin function (a form of "robust facility location"): $h(A) = \min_{v \in V} \max_{a \in A} s(v, a)$ and the goal is to maximize this $\max_{A \subseteq V : |A| \leq k} h(A)$. h therefore is the min of a set of submodular functions.

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- However, when wishing to maximize two monotone non-decreasing submodular functions f, g, we can define function $h_\alpha : 2^V \to \mathbb{R}$ as

$$h_\alpha(A) = \frac{1}{2}\Big(\min(\alpha, f(A)) + \min(\alpha, g(A))\Big) \tag{5.13}$$

then h_α is submodular, and $h_\alpha(A) \geq \alpha$ if and only if both $f(A) \geq \alpha$ and $g(A) \geq \alpha$, for constant $\alpha \in \mathbb{R}$.

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- Useful in applications. Like DS functions, another instance of a submodular surrogate (where we take a non-submodular problem and find a submodular one that can tell us something about it).

Arbitrary functions: difference between submodular funcs.

Theorem 5.3.5

Given an arbitrary set function h, it can be expressed as a difference between two submodular functions (i.e., $\forall h \in 2^V \to \mathbb{R}$, $\exists f, g$ s.t. $\forall A, h(A) = f(A) - g(A)$ where both f and g are submodular).

Proof.

Let h be given and arbitrary, and define:

$$\alpha \triangleq \min_{X,Y : X \not\subseteq Y, Y \not\subseteq X} \Big(h(X) + h(Y) - h(X \cup Y) - h(X \cap Y) \Big) \tag{5.14}$$

$\geq \alpha \quad \geq 0$

If $\alpha \geq 0$ then h is submodular, so by assumption $\alpha < 0$.

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If $\alpha \geq 0$ then h is submodular, so by assumption $\alpha < 0$. Now let f be an arbitrary strict submodular function and define

$$\beta \triangleq \min_{X,Y : X \not\subseteq Y, Y \not\subseteq X} \Big(f(X) + f(Y) - f(X \cup Y) - f(X \cap Y) \Big). \tag{5.15}$$

Strict means that $\beta > 0$. $f(x) = \sqrt{|X|}$ ...

Arbitrary functions as difference between submodular funcs.

$\frac{f(A)}{\beta} = f'(A) \Rightarrow \beta' \leq 1$

...cont.

Define $h' : 2^V \to \mathbb{R}$ as

$$h'(A) = h(A) + \frac{|\alpha|}{\beta} f(A) \tag{5.16}$$

Then h' is submodular (why?), and $h = h'(A) - \frac{|\alpha|}{\beta} f(A)$, a difference between two submodular functions as desired. □

$I(X_A; X_B) = H(X_A) - H(X_A | X_B)$

$= f(A) - g(A)$

fixed B

$f - \lambda g$

Gain

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- This is called the gain and is used so often, there are equally as many ways to notate this. I.e., you might see:

$$f(A \cup \{j\}) - f(A) \triangleq \rho_j(A) \tag{5.17}$$
$$\triangleq \rho_A(j) \tag{5.18}$$
$$\triangleq \nabla_j f(A) \quad ✓ \tag{5.19}$$
$$\triangleq f(\{j\}|A) \tag{5.20}$$
$$\triangleq f(j|A) \quad ✓ \tag{5.21}$$

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(also $\nabla_j f(A)$)

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- We'll use $f(j|A)$.
- diminishing returns can be stated as saying that $f(j|A)$ is a monotone non-increasing function of A, since $f(j|A) \geq f(j|B)$ whenever $A \subseteq B$ (i.e., further conditioning reduces valuation).

Gain Notation

It will also be useful to extend this to sets.
Let A, B be any two sets. Then

$$f(A|B) \triangleq f(A \cup B) - f(B) \tag{5.22}$$

So when j is any singleton

$$f(j|B) = f(\{j\}|B) = f(\{j\} \cup B) - f(B) \tag{5.23}$$

$$f(A|A) = f(A \cup A) - f(A)$$
$$= f(A) - f(A) = 0$$

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Inspired from information theory notation and the notation used for conditional entropy $H(X_A|X_B) = H(X_A, X_B) - H(X_B)$.

Totally normalized functions

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$v \in V$

$$\bar{g}(v|A) = \underline{g(v|A)} + \alpha \geq 0 \quad \forall v, A$$

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- E.g., $g(A) = [g(A) + \alpha|A|] - \alpha|A|$, $\alpha \geq |\min_{v, A \subseteq V \setminus v} f(v|A)|$.
- More interestingly, given arbitrary normalized submodular $g : 2^V \to \mathbb{R}$, construct a function $\bar{g} : 2^V \to \mathbb{R}$ as follows:

$$\bar{g}(A) = g(A) - \sum_{a \in A} g(a|V \setminus \{a\}) = g(A) - m_g(A) \tag{5.24}$$

where $m_g(A) \triangleq \sum_{a \in A} g(a|V \setminus \{a\})$ is a modular function.

$$\boxed{m_g(a) = g(a \,/\, V \setminus a)}$$

$$g(a/A) \geq \underbrace{g(a/ V \setminus a)}_{\text{smallest possible gain of } a.}$$

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- $\bar{g}$ is normalized since $\bar{g}(\emptyset) = 0$.
- $\bar{g}$ is monotone non-decreasing since for $v \notin A \subseteq V$:

$$\bar{g}(v|A) = g(v|A) - g(v|V \setminus \{v\}) \geq 0 \tag{5.25}$$

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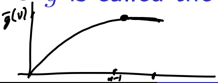
$$\bar{g}(v|A) = g(v|A) - g(v|V \setminus \{v\}) \geq 0 \tag{5.25}$$

- $\bar{g}$ is called the totally normalized version of g.



$\bar{g}(v|V\setminus v) = g(v|V\setminus v) - g(v|V\setminus v) = 0$

Totally normalized functions

- Any normalized submodular function g (even non-monotone) can be represented as a sum of a polymatroid (normalized monotone non-decreasing submodular) function $\bar{g}$ and a modular function m_g.
- E.g., $g(A) = [g(A) + \alpha|A|] - \alpha|A|$, $\alpha \geq |\min_{v, A \subseteq V \setminus v} f(v|A)|$.
- More interestingly, given arbitrary normalized submodular $g : 2^V \to \mathbb{R}$, construct a function $\bar{g} : 2^V \to \mathbb{R}$ as follows:

$$\bar{g}(A) = g(A) - \sum_{a \in A} g(a|V \setminus \{a\}) = g(A) - m_g(A) \tag{5.24}$$

  where $m_g(A) \triangleq \sum_{a \in A} g(a|V \setminus \{a\})$ is a modular function.
- $\bar{g}$ is normalized since $\bar{g}(\emptyset) = 0$.
- $\bar{g}$ is monotone non-decreasing since for $v \notin A \subseteq V$:

$$\bar{g}(v|A) = g(v|A) - g(v|V \setminus \{v\}) \geq 0 \tag{5.25}$$

- $\bar{g}$ is called the totally normalized version of g.
- Then $g(A) = \bar{g}(A) + m_g(A)$.

Arbitrary function as difference between two polymatroids

- Any normalized function h (i.e., $h(\emptyset) = 0$) can be represented as a difference not only between submodular, but between polymatroid (normalized monotone non-decreasing submodular) functions.

Arbitrary function as difference between two polymatroids

- Any normalized function h (i.e., $h(\emptyset) = 0$) can be represented as a difference not only between submodular, but between polymatroid (normalized monotone non-decreasing submodular) functions.
- Given submodular f and g, let $\bar{f}$ and $\bar{g}$ be them totally normalized.

Arbitrary function as difference between two polymatroids

- Any normalized function h (i.e., $h(\emptyset) = 0$) can be represented as a difference not only between submodular, but between polymatroid (normalized monotone non-decreasing submodular) functions.
- Given submodular f and g, let $\bar{f}$ and $\bar{g}$ be them totally normalized.
- Given arbitrary $h = f - g$ where f and g are normalized submodular,

$$h = f - g = \bar{f} + m_f - (\bar{g} + m_g) \tag{5.26}$$
$$= \bar{f} - \bar{g} + (m_f - m_g) \tag{5.27}$$
$$= \bar{f} - \bar{g} + m_{f-h} \tag{5.28}$$
$$= \bar{f} + m^+_{f-g} - (\bar{g} + (-m_{f-g})^+) \tag{5.29}$$

where m^+ is the positive part of modular function m. That is, $m^+(A) = \sum_{a \in A} m(a)\mathbf{1}(m(a) > 0)$.

$(-m)^+$

$m = m^+ - (-m)^+$

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- Both $\bar{f} + m^+_{f-g}$ and $\bar{g} + (-m_{f-g})^+$ are polymatroid functions!

Arbitrary function as difference between two polymatroids

- Any normalized function h (i.e., $h(\emptyset) = 0$) can be represented as a difference not only between submodular, but between polymatroid (normalized monotone non-decreasing submodular) functions.
- Given submodular f and g, let $\bar{f}$ and $\bar{g}$ be them totally normalized.
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  where m^+ is the positive part of modular function m. That is, $m^+(A) = \sum_{a \in A} m(a)\mathbf{1}(m(a) > 0)$.
- Both $\bar{f} + m^+_{f-g}$ and $\bar{g} + (-m_{f-g})^+$ are polymatroid functions!
- Thus, any function can be expressed as a difference between two, not only submodular (DS), but polymatroid functions.

Two Equivalent Submodular Definitions

Definition 5.4.1 (submodular concave)

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

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{5.7}$$

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

Definition 5.4.2 (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:

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \tag{5.8}$$

- 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 Definition: Group Diminishing Returns

An alternate and equivalent definition is:

Definition 5.4.1 (group diminishing returns)

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

$$f(A \cup C) - f(A) \geq f(B \cup C) - f(B) \tag{5.30}$$

This means that the incremental "value" or "gain" of set C decreases as the context in which C is considered grows from A to B (diminishing returns)

Submodular Definition Basic Equivalencies

We want to show that Submodular Concave (Definition 5.4.1), Diminishing Returns (Definition 5.4.2), and Group Diminishing Returns (Definition 5.4.1) are identical.

Submodular Definition Basic Equivalencies

We want to show that Submodular Concave (Definition 5.4.1), Diminishing Returns (Definition 5.4.2), and Group Diminishing Returns (Definition 5.4.1) are identical. We will show that:

- Submodular Concave $\Rightarrow$ Diminishing Returns
- Diminishing Returns $\Rightarrow$ Group Diminishing Returns
- Group Diminishing Returns $\Rightarrow$ Submodular Concave

Submodular Concave ⇒ Diminishing Returns

$f(S) + f(T) \geq f(S \cup T) + f(S \cap T) \Rightarrow f(v|A) \geq f(v|B), A \subseteq B \subseteq V \setminus v.$

- Assume Submodular concave, so $\forall S, T$ we have $f(S) + f(T) \geq f(S \cup T) + f(S \cap T)$.

$\square$

Submodular Concave $\Rightarrow$ Diminishing Returns

$f(S) + f(T) \geq f(S \cup T) + f(S \cap T) \Rightarrow f(v|A) \geq f(v|B), A \subseteq B \subseteq V \setminus v.$

- Assume Submodular concave, so $\forall S, T$ we have $f(S) + f(T) \geq f(S \cup T) + f(S \cap T)$.
- Given A, B and $v \in V$ such that: $A \subseteq B \subseteq V \setminus \{v\}$, we have from submodular concave that:

$$f(A + v) + f(B) \geq f(B + v) + f(A) \tag{5.31}$$

□

Submodular Concave ⇒ Diminishing Returns

$f(S) + f(T) \geq f(S \cup T) + f(S \cap T) \Rightarrow f(v|A) \geq f(v|B), A \subseteq B \subseteq V \setminus v.$

- Assume Submodular concave, so $\forall S, T$ we have $f(S) + f(T) \geq f(S \cup T) + f(S \cap T)$.
- Given A, B and $v \in V$ such that: $A \subseteq B \subseteq V \setminus \{v\}$, we have from submodular concave that:

$$f(A + v) + f(B) \geq f(B + v) + f(A) \tag{5.31}$$

- Rearranging, we have

$$f(A + v) - f(A) \geq f(B + v) - f(B) \tag{5.32}$$

□

Diminishing Returns ⇒ Group Diminishing Returns

$f(v|S) \geq f(v|T), S \subseteq T \subseteq V \setminus v \Rightarrow f(C|A) \geq f(C|B), A \subseteq B \subseteq V \setminus C.$

Let $C = \{c_1, c_2, \ldots, c_k\}$. Then diminishing returns implies

$$f(A \cup C) - f(A) \tag{5.33}$$

$$= f(A \cup C) - \sum_{i=1}^{k-1} \Big(f(A \cup \{c_1, \ldots, c_i\}) - f(A \cup \{c_1, \ldots, c_i\}) \Big) - f(A) \tag{5.34}$$

$$= \sum_{i=1}^{k} \Big(f(A \cup \{c_1 \ldots c_i\}) - f(A \cup \{c_1 \ldots c_{i-1}\}) \Big) = \sum_{i=1}^{k} f(c_i | A \cup \{c_1 \ldots c_{i-1}\}) \tag{5.35}$$

$$\geq \sum_{i=1}^{k} f(c_i | B \cup \{c_1 \ldots c_{i-1}\}) = \sum_{i=1}^{k} \Big(f(B \cup \{c_1 \ldots c_i\}) - f(B \cup \{c_1 \ldots c_{i-1}\}) \Big) \tag{5.36}$$

$$= f(B \cup C) - \sum_{i=1}^{k-1} \Big(f(B \cup \{c_1, \ldots, c_i\}) - f(B \cup \{c_1, \ldots, c_i\}) \Big) - f(B) \tag{5.37}$$

$$= f(B \cup C) - f(B) \tag{5.38}$$

□

Group Diminishing Returns ⇒ Submodular Concave

$f(U|S) \geq f(U|T), S \subseteq T \subseteq V \setminus U \Rightarrow f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$.

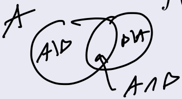
Assume group diminishing returns. Assume $A \neq B$ otherwise trivial. Define $A' = A \cap B$, $C = A \setminus B$, and $B' = B$. Then since $A' \subseteq B'$,

$$f(A' + C) - f(A') \geq f(B' + C) - f(B') \tag{5.39}$$

giving

$$f(A' + C) + f(B') \geq f(B' + C) + f(A') \tag{5.40}$$

or



$$f(A \cap B + A \setminus B) + f(B) \geq f(B + A \setminus B) + f(A \cap B) \tag{5.41}$$

which is the same as the submodular concave condition

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{5.42}$$

Submodular Definition: Four Points

Theorem 5.4.2 (“singleton”, or “four points”)

A function $f : 2^V \to \mathbb{R}$ is submodular iff for any $A \subset V$, and any $a, b \in V \setminus A$, we have that:

$$f(A \cup \{a\}) + f(A \cup \{b\}) \geq f(A \cup \{a, b\}) + f(A) \tag{5.43}$$

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

$2^n \times 2^n = 2^{2n}$

$\binom{n}{2} 2^{n-2} << 2^{2n}$

Submodular Definition: Four Points

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Only If: This follows immediately from diminishing returns.

Submodular Definition: Four Points

Theorem 5.4.2 (“singleton”, or “four points”)? ("Square")

A function $f : 2^V \to \mathbb{R}$ is submodular iff for any $A \subset V$, and any $a, b \in V \setminus A$, we have that:

$$f(A \cup \{a\}) + f(A \cup \{b\}) \geq f(A \cup \{a, b\}) + f(A) \tag{5.43}$$

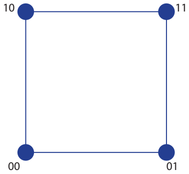
Only If: This follows immediately from diminishing returns. If: To achieve diminishing returns, assume $A \subset B$ with $B \setminus A = \{b_1, b_2, \ldots, b_k\}$. Then

$$\begin{aligned}
f(A + a) - f(A) &\geq f(A + b_1 + a) - f(A + b_1) && (5.44)\\
&\geq f(A + b_1 + b_2 + a) - f(A + b_1 + b_2) && (5.45)\\
&\geq \ldots && (5.46)\\
&\geq f(A + b_1 + \cdots + b_k + a) - f(A + b_1 + \cdots + b_k) && (5.47)\\
&= f(B + a) - f(B) && (5.48)
\end{aligned}$$

The Submodular Square, and Hypercube Vertices

We can test submodularity via values on vertices of hypercube.

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



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

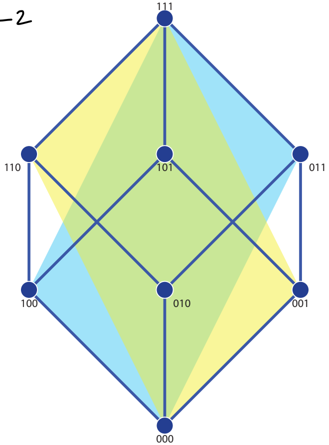
$|V| = 3$

$\binom{3}{2} \cdot 2^{3-2}$

$= 3 \cdot 2 = 6$

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

$\binom{n}{2} \cdot 2^{n-2}$



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

Submodular Concave ≡ Diminishing Returns, in one slide.

Theorem 5.4.3

Given function $f : 2^V \to \mathbb{R}$, *then*

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

if and only if

$$f(v|X) \geq f(v|Y) \text{ for all } X \subseteq Y \subseteq V \text{ and } v \notin Y \qquad \text{(DR)}$$

Proof.

(SC)⇒(DR): Set $A \leftarrow X \cup \{v\}$, $B \leftarrow Y$. Then $A \cup B = Y \cup \{v\}$ and $A \cap B = X$ and $f(A) - f(A \cap B) \geq f(A \cup B) - f(B)$ implies (DR).

(DR)⇒(SC): Order $A \setminus B = \{v_1, v_2, \ldots, v_r\}$ arbitrarily. For $i \in 1 : r$,

$$f(v_i|(A \cap B) \cup \{v_1, v_2, \ldots, v_{i-1}\}) \geq f(v_i|B \cup \{v_1, v_2, \ldots, v_{i-1}\}).$$

Applying telescoping summation to both sides, we get:

$$\sum_{i=1}^{r} f(v_i|(A \cap B) \cup \{v_1, v_2, \ldots, v_{i-1}\}) \geq \sum_{i=1}^{r} f(v_i|B \cup \{v_1, v_2, \ldots, v_{i-1}\})$$

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

Many (Equivalent) Definitions of Submodularity

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V \tag{5.54}$$

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$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \ \ \forall A, B \subseteq V \tag{5.54}$$

$$f(j|S) \geq f(j|T), \ \forall S \subseteq T \subseteq V, \text{ with } j \in V \setminus T \tag{5.55}$$

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$$f(j|S) \geq f(j|S \cup \{k\}), \; \forall S \subseteq V \text{ with } j \in V \setminus (S \cup \{k\}) \tag{5.57}$$

$f(S+j) - f(S) \geq f(S+k+j) - f(S+k)$

$f(S+j) + f(S+k) \geq f(S+k+j) - f(S)$

Many (Equivalent) Definitions of Submodularity

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V \tag{5.54}$$

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$$f(A \cup B|A \cap B) \leq f(A|A \cap B) + f(B|A \cap B), \quad \forall A, B \subseteq V \tag{5.58}$$

Conditional subadditivity.

Many (Equivalent) Definitions of Submodularity

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \;\; \forall A, B \subseteq V \tag{5.54}$$

$$f(j|S) \geq f(j|T), \; \forall S \subseteq T \subseteq V, \text{ with } j \in V \setminus T \tag{5.55}$$

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$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \; \forall S, T \subseteq V \tag{5.59}$$

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$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \; \forall S, T \subseteq V \tag{5.59}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S), \; \forall S \subseteq T \subseteq V \tag{5.60}$$

(5.59) => (5.60)

Many (Equivalent) Definitions of Submodularity

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \;\; \forall A, B \subseteq V \tag{5.54}$$

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Many (Equivalent) Definitions of Submodularity

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$$f(A \cup B|A \cap B) \leq f(A|A \cap B) + f(B|A \cap B), \quad \forall A, B \subseteq V \tag{5.58}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \; \forall S, T \subseteq V \tag{5.59}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S), \; \forall S \subseteq T \subseteq V \tag{5.60}$$

$$f(T) \leq f(S) - \sum_{j \in S \setminus T} f(j|S \setminus \{j\}) + \sum_{j \in T \setminus S} f(j|S \cap T) \; \forall S, T \subseteq V \tag{5.61}$$

$$f(T) \leq f(S) - \sum_{j \in S \setminus T} f(j|S \setminus \{j\}), \; \forall T \subseteq S \subseteq V \tag{5.62}$$

Equivalent Definitions of Submodularity

$f(A \cup B | A \cap B)$

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

$= f(A \cup B) - \cancel{f(A \cap B)}$

$\overset{?}{\le} f(A | A \cap B) = f(A) - f(A \cap B)$

$f(B | A \cap B) = f(B) - \cancel{f(A \cap B)}$

We've already seen that Eq. 5.54 ≡ Eq. 5.55 ≡ Eq. 5.56 ≡ Eq. 5.57 ≡ Eq. 5.58.

Many (Equivalent) Definitions of Submodularity

$$f(A) + f(B) \ge f(A \cup B) + f(A \cap B), \;\; \forall A, B \subseteq V \tag{5.54}$$

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$$f(A \cup B | A \cap B) \le f(A|A \cap B) + f(B|A \cap B), \;\; \forall A, B \subseteq V \tag{5.58}$$

$$f(T) \le f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \; \forall S, T \subseteq V \tag{5.59}$$

$$f(T) \le f(S) + \sum_{j \in T \setminus S} f(j|S), \; \forall S \subseteq T \subseteq V \tag{5.60}$$

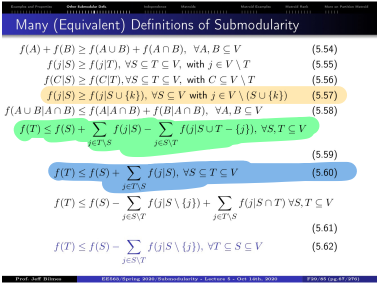
$$f(T) \le f(S) - \sum_{j \in S \setminus T} f(j|S \setminus \{j\}) + \sum_{j \in T \setminus S} f(j|S \cap T) \; \forall S, T \subseteq V \tag{5.61}$$

$$f(T) \le f(S) - \sum_{j \in S \setminus T} f(j|S \setminus \{j\}), \; \forall T \subseteq S \subseteq V \tag{5.62}$$

Equivalent Definitions of Submodularity

We've already seen that Eq. 5.54 $\equiv$ Eq. 5.55 $\equiv$ Eq. 5.56 $\equiv$ Eq. 5.57 $\equiv$ Eq. 5.58.

We next show that Eq. 5.57 $\Rightarrow$ Eq. 5.59 $\Rightarrow$ Eq. 5.60 $\Rightarrow$ Eq. 5.57.



Approach

To show these next results, we essentially first use:

$$f(S \cup T) = f(S) + f(T|S) \leq f(S) + \text{upper-bound} \tag{5.63}$$

and

$$f(T) + \text{lower-bound} \leq f(T) + f(S|T) = f(S \cup T) \tag{5.64}$$

$$f(C|S) \geq f(C|T), \forall S \subseteq T \subseteq V, \text{ with } C \subseteq V \setminus T \tag{5.56}$$

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$$f(A \cup B|A \cap B) \leq f(A|A \cap B) + f(B|A \cap B), \ \forall A, B \subseteq V \tag{5.58}$$

$$f(T) \leq f(S) + \underbrace{\sum_{j \in T \setminus S} f(j|S)}_{\text{upper}} - \underbrace{\sum_{j \in S \setminus T} f(j|S \cup T - \{j\})}_{\text{lower.}}, \forall S, T \subseteq V \tag{5.59}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S), \ \forall S \subseteq T \subseteq V \tag{5.60}$$

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$$f(S \cup T) = f(S) + f(T|S) \leq f(S) + \text{upper-bound} \tag{5.63}$$

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leading to

$$f(T) + \text{lower-bound} \leq f(S) + \text{upper-bound} \tag{5.65}$$

or

$$f(T) \leq f(S) + \text{upper-bound} - \text{lower-bound} \tag{5.66}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \ \forall S, T \subseteq V$$

Eq. 5.57 ⇒ Eq. 5.59

Let $T \setminus S = \{j_1, \ldots, j_r\}$ and $S \setminus T = \{k_1, \ldots, k_q\}$.
First, we upper bound the gain of T in the context of S:

$$f(S \cup T) - f(S) = \sum_{t=1}^{r} \Big(f(S \cup \{j_1, \ldots, j_t\}) - f(S \cup \{j_1, \ldots, j_{t-1}\}) \Big) \tag{5.67}$$

$$= \sum_{t=1}^{r} f(j_t | S \cup \{j_1, \ldots, j_{t-1}\}) \leq \sum_{t=1}^{r} f(j_t | S) \tag{5.68}$$

$$= \sum_{j \in T \setminus S} f(j|S) \tag{5.69}$$

or

$$f(T|S) \leq \sum_{j \in T \setminus S} f(j|S) \tag{5.70}$$

Eq. 5.57 ⇒ Eq. 5.59

Let $T \setminus S = \{j_1, \ldots, j_r\}$ and $S \setminus T = \{k_1, \ldots, k_q\}$.
Next, lower bound S in the context of T:

$$f(S \cup T) - f(T) = \sum_{t=1}^{q} [f(T \cup \{k_1, \ldots, k_t\}) - f(T \cup \{k_1, \ldots, k_{t-1}\})] \tag{5.71}$$

$$= \sum_{t=1}^{q} f(k_t | T \cup \{k_1, \ldots, k_t\} \setminus \{k_t\}) \geq \sum_{t=1}^{q} f(k_t | T \cup S \setminus \{k_t\}) \tag{5.72}$$

$$= \sum_{j \in S \setminus T} f(j | S \cup T \setminus \{j\}) \tag{5.73}$$

Eq. 5.57 ⇒ Eq. 5.59

Let $T \setminus S = \{j_1, \ldots, j_r\}$ and $S \setminus T = \{k_1, \ldots, k_q\}$.
So we have the upper bound

$$f(T|S) = f(S \cup T) - f(S) \leq \sum_{j \in T \setminus S} f(j|S) \tag{5.74}$$

and the lower bound

$$f(S|T) = f(S \cup T) - f(T) \geq \sum_{j \in S \setminus T} f(j|S \cup T \setminus \{j\}) \tag{5.75}$$

This gives upper and lower bounds of the form

$$f(T) + \text{lower bound} \leq f(S \cup T) \leq f(S) + \text{upper bound}, \tag{5.76}$$

and combining directly the left and right hand side gives the desired inequality.

Eq. 5.59 $\Rightarrow$ Eq. 5.60

This follows immediately since if $S \subseteq T$, then $S \setminus T = \emptyset$, and the last term of Eq. 5.59 vanishes.

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Eq. 5.60 $\Rightarrow$ Eq. 5.57

Here, we set $T = S \cup \{j,k\}$, $j \notin S \cup \{k\}$ into Eq. 5.60 to obtain

$$f(S \cup \{j,k\}) \leq f(S) + f(j|S) + f(k|S) \tag{5.77}$$

$$= f(S) + f(S+\{j\}) - f(S) + f(S+\{k\}) - f(S) \tag{5.78}$$

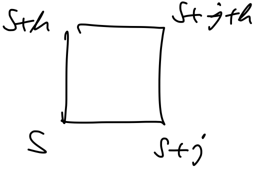
$$= f(S+\{j\}) + f(S+\{k\}) - f(S) \tag{5.79}$$

$$= f(j|S) + f(S+\{k\}) \tag{5.80}$$

giving

$$f(j|S \cup \{k\}) = f(S \cup \{j,k\}) - f(S \cup \{k\}) \tag{5.81}$$

$$\leq f(j|S) \tag{5.82}$$



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- Why do we call the $f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$ definition of submodularity, submodular concave?

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- Define a "discrete derivative" or difference operator defined on discrete functions $f : 2^V \to \mathbb{R}$ as follows:

$$(\nabla_B f)(A) \triangleq f(A \cup B) - f(A \setminus B) = f\big(B|(A \setminus B)\big) \tag{5.83}$$

read as: the derivative of f at A in the direction B.

$$(\nabla_{\{j\}} f)(A) = f(B | A \setminus B)$$

$$= f(j | A)$$

$j \notin A$

$$= f(A + j) - f(A)$$

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- Hence, if $A \cap B = \emptyset$, then $(\nabla_B f)(A) = f(B|A)$.
- Consider a form of second derivative or 2nd difference:

$$\begin{aligned}
(\nabla_B \nabla_C f)(A) &= \nabla_B[\,\overbrace{f(A \cup C) - f(A \setminus C)}^{(\nabla_C f)(A)}\,] && (5.84)\\
&= (\nabla_B f)(A \cup C) - (\nabla_B f)(A \setminus C) && (5.85)\\
&= f(A \cup B \cup C) - f((A \cup C) \setminus B) \\
&\quad - f((A \setminus C) \cup B) + f((A \setminus C) \setminus B) && (5.86)
\end{aligned}$$

Submodular Concave

- If the second difference operator everywhere nonpositive:

$$\begin{aligned} f(A \cup B \cup C) - f((A \cup C) \setminus B) \\ - f((A \setminus C) \cup B) + f(A \setminus C \setminus B) \leq 0 \end{aligned} \tag{5.87}$$

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- Define $A' = (A \cup C) \setminus B$ and $B' = (A \setminus C) \cup B$. Then the above implies:

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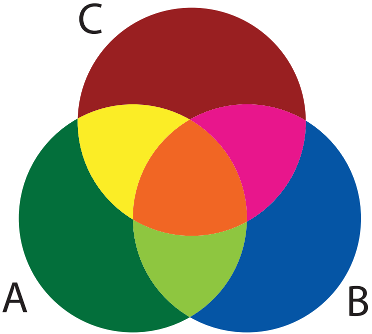
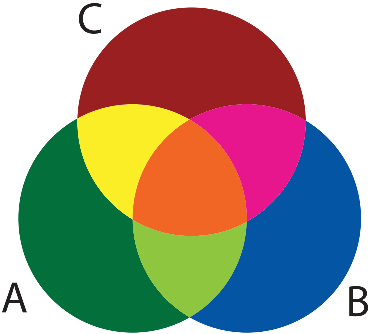
- One sense in which submodular functions are like concave functions.

Submodular Concave



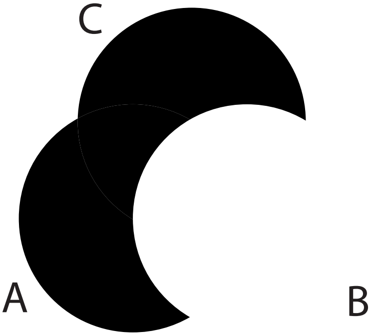
(a) $A' = (A \cup C) \setminus B$



(b) $B' = (A \setminus C) \cup B$

Figure: A figure showing $A' \cup B' = A \cup B \cup C$ and $A' \cap B' = A \setminus C \setminus B$.

Submodular Concave



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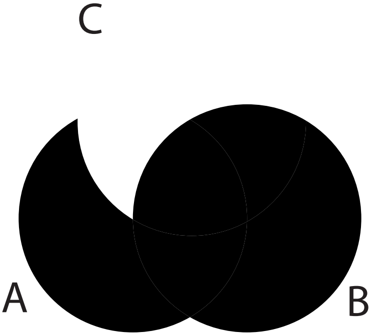

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- This gives us a simpler notion corresponding to concavity.
- Define gain as $\nabla_j(X) = f(X + j) - f(X)$, a form of discrete gradient.
- Trivially becomes a second-order condition, akin to concave functions: A function is submodular if for all $X \subseteq V$ and $j, k \in V$, we have:

$$\nabla_j \nabla_k f(X) \leq 0 \tag{5.91}$$

Example: Rank function of a matrix

Consider the following 4×8 matrix, so $V = \{1,2,3,4,5,6,7,8\}$.

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

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

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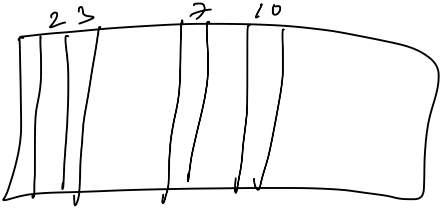
$A = \{2, 3, 7, 10\}$



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- If A, B are such that $\text{rank}(A) = |A|$ and $\text{rank}(B) = |B|$, with $|A| < |B|$, then the space spanned by B is greater, and we can find a vector in B that is linearly independent of the space spanned by vectors in A.

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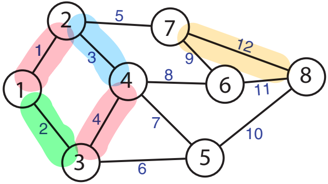
- To stress this point, note that the above condition is $|A| < |B|$, **not** $A \subseteq B$ which is sufficient (to be able to find an independent vector) but not required.
- In other words, given A, B with $\text{rank}(A) = |A|$ & $\text{rank}(B) = |B|$, then $|A| < |B| \Leftrightarrow \exists$ an $b \in B$ such that $\text{rank}(A \cup \{b\}) = |A| + 1$.

Spanning trees/forests

- We are given a graph $G = (V, E)$, and consider the edges $E = E(G)$ as an index set.
- Consider the $|V| \times |E|$ incidence matrix of undirected graph G, which is the matrix $\mathbf{X}_G = (x_{v,e})_{v \in V(G), e \in E(G)}$ where

$$x_{v,e} = \begin{cases} 1 & \text{if } v \in e \\ 0 & \text{if } v \notin e \end{cases} \tag{5.92}$$



$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array} \begin{array}{c} \begin{array}{cccccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \end{array} \\ \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix} \end{array} \tag{5.93}$$

Spanning trees/forests & incidence matrices

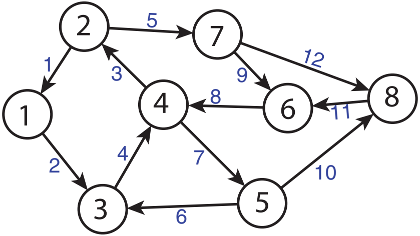
- We are given a graph $G = (V, E)$, we can arbitrarily orient the graph (make it directed) consider again the edges $E = E(G)$ as an index set.
- Consider instead the $|V| \times |E|$ incidence matrix of directed graph G, which is the matrix $\mathbf{X}_G = (x_{v,e})_{v \in V(G), e \in E(G)}$ where

$$x_{v,e} = \begin{cases} 1 & \text{if } v \in e^+ \\ -1 & \text{if } v \in e^- \\ 0 & \text{if } v \notin e \end{cases} \tag{5.94}$$

and where e^+ is the tail and e^- is the head of (now) directed edge e.

Spanning trees/forests & incidence matrices

- A directed version of the graph (right) and its adjacency matrix (below).
- Orientation can be arbitrary.
- Note, rank of this matrix is 7.



$$
\begin{array}{c}
 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8
\end{array}
\begin{array}{c}
\begin{array}{cccccccccccc}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12
\end{array} \\
\begin{pmatrix}
-1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\
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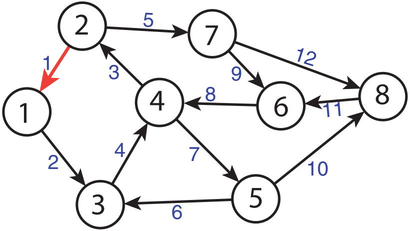
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1
\end{pmatrix}
\end{array}
$$

Spanning trees

- We can consider edge-induced subgraphs and the corresponding matrix columns.



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Here, $\text{rank}(\{x_1\}) = 1$.

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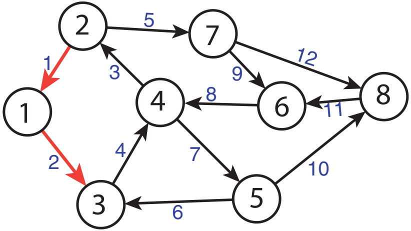

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Here, $\text{rank}(\{x_1, x_2\}) = 2$.

Spanning trees

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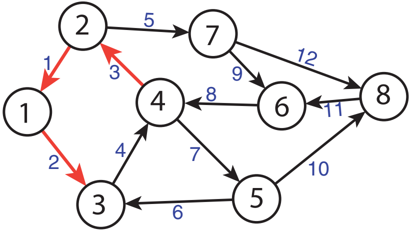

$$\begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{array}\begin{array}{c} \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{pmatrix} -1 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{array} \tag{5.95}$$

Here, $\text{rank}(\{x_1, x_2, x_3\}) = 3$.

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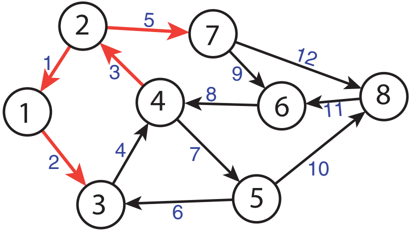

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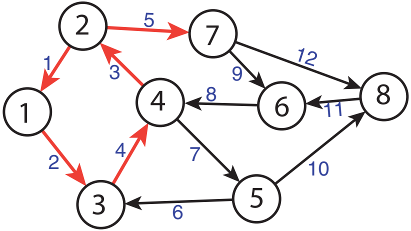

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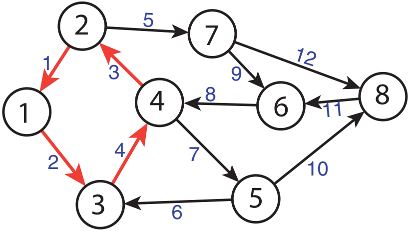

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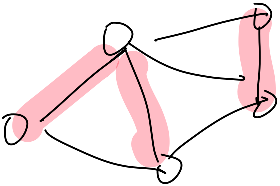

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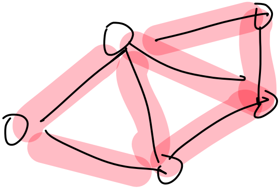

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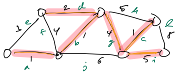
- We have rank$(A) = |V(G)| - k_G(A)$. $\therefore$ is submodular.

Spanning Tree Algorithms

- We are now given a positive edge-weighted connected graph $G = (V, E, w)$ where $w : E \to \mathbb{R}_+$ is a modular function the edges of the graph. The goal is to find the minimum spanning tree (MST) of the graph.
- Given a tree T, the cost of the tree is $\text{cost}(T) = \sum_{e \in T} w(e)$, the sum of the weights of the edges.



- There are several algorithms for MST:

Algorithm 1: Kruskal's Algorithm

Sort the edges so that $w(e_1) \leq w(e_2) \leq \cdots \leq w(e_m)$;
$T \leftarrow (V(G), \emptyset) = (V, \emptyset)$;
for $i = 1$ **to** m **do**
  if $E(T) \cup \{e_i\}$ *does not create a cycle in* T **then**
    $E(T) \leftarrow E(T) \cup \{e_i\}$;

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Algorithm 2: Jarník/Prim/Dijkstra Algorithm

1 $T \leftarrow \emptyset$;
2 **while** T *is not a spanning tree* **do**
3 $\quad T \leftarrow T \cup \{e\}$ for $e =$ the minimum weight edge extending the tree T to a not-yet connected vertex ;

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Algorithm 3: Borůvka's Algorithm

$F \leftarrow \emptyset$ /* We build up the edges of a forest in F */
while *$G(V, F)$ is disconnected* **do**
  forall *components C_i of F* **do**
    $F \leftarrow F \cup \{e_i\}$ for $e_i =$ the min weight-index edge in C_i;

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- The above are all examples of a matroid, which is the fundamental reason why the greedy algorithms work.

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- maxInd: Inclusionwise maximal independent subsets (i.e., the set of bases of) of any set $B \subseteq V$ defined as:

$$\text{maxInd}(B) \triangleq \{A \subseteq B : A \in \mathcal{I} \text{ and } \forall v \in B \setminus A, A \cup \{v\} \notin \mathcal{I}\} \tag{5.97}$$

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- Given any set $B \subset V$ of vectors, all maximal (by set inclusion) subsets of linearly independent vectors are the same size. That is, for all $B \subseteq V$,

$$\forall A_1, A_2 \in \text{maxInd}(B), \quad |A_1| = |A_2| = \text{rank}(B) \tag{5.98}$$

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- Let $\mathcal{I} = \{I_1, I_2, \ldots\}$ be the set of sets as described above.
- Thus, for all $I \in \mathcal{I}$, the matrix rank function has the property

$$r(I) = |I| \tag{5.99}$$

and for any $B \notin \mathcal{I}$,

$$r(B) = \max\{|A| : A \subseteq B \text{ and } A \in \mathcal{I}\} < |B| \tag{5.100}$$

Since all maximally independent subsets of a set are the same size, the rank function is well defined.

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- There are many definitions of matroids that are mathematically equivalent, we'll see some of them here.
- "If a theorem about graphs can be expressed in terms of edges and circuits only, it probably exemplifies a more general theorem about matroids." – Tutte

Independence System

Definition 5.6.1 (set system)

A (finite) ground set E and a set of subsets of E, $\emptyset \neq \mathcal{I} \subseteq 2^E$ is called a set system, notated $(E, \mathcal{I})$.

- Set systems can be arbitrarily complex since, as stated, there is no systematic method (besides exponential-cost exhaustive search) to determine if a given set $S \subseteq E$ has $S \in \mathcal{I}$.

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- One useful property is "heredity." Namely, a set system is a hereditary set system if for any $A \subset B \in \mathcal{I}$, we have that $A \in \mathcal{I}$.

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Definition 5.6.2 (independence (or hereditary) system)

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- Example: $E = \{1, 2, 3, 4\}$. With $\mathcal{I} = \{\emptyset, \{1\}, \{1, 2\}, \{1, 2, 4\}\}$.
- Then $(E, \mathcal{I})$ is a set system, but not an independence system since it is not down closed (e.g., we have $\{1, 2\} \in \mathcal{I}$ but not $\{2\} \in \mathcal{I}$).

Independence System

Definition 5.6.2 (independence (or hereditary) system)

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

$$\emptyset \in \mathcal{I} \quad \text{(emptyset containing)} \tag{I1}$$

and

$$\forall I \in \mathcal{I}, J \subset I \Rightarrow J \in \mathcal{I} \quad \text{(subclusive)} \tag{I2}$$

- Property (I2) called "down monotone," "down closed," or "subclusive"
- Example: $E = \{1, 2, 3, 4\}$. With $\mathcal{I} = \{\emptyset, \{1\}, \{1, 2\}, \{1, 2, 4\}\}$.
- Then $(E, \mathcal{I})$ is a set system, but not an independence system since it is not down closed (e.g., we have $\{1, 2\} \in \mathcal{I}$ but not $\{2\} \in \mathcal{I}$).
- With $\mathcal{I} = \{\emptyset, \{1\}, \{2\}, \{1, 2\}\}$, then $(E, \mathcal{I})$ is now an independence (hereditary) system.

Independence System

$$\begin{array}{c c} & \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \end{array} & \begin{pmatrix} 0 & 0 & 1 & 1 & 2 & 1 & 3 & 1 \\ 0 & 1 & 1 & 0 & 2 & 0 & 2 & 4 \\ 1 & 1 & 1 & 0 & 0 & 3 & 1 & 5 \end{pmatrix} \end{array} = \begin{array}{c} \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \end{array} \\ \begin{pmatrix} | & | & | & | & | & | & | & | \\ x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 \\ | & | & | & | & | & | & | & | \end{pmatrix} \end{array} \tag{5.101}$$

- Given any set of linearly independent vectors A, any subset $B \subset A$ will also be linearly independent.

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- Given any set of linearly independent vectors A, any subset $B \subset A$ will also be linearly independent.
- Given any forest G_f that is an edge-induced sub-graph of a graph G, any sub-graph of G_f is also a forest.
- So these both constitute independence systems.

Matroid

Independent set definition of a matroid is perhaps most natural. Note, if $J \in \mathcal{I}$, then J is said to be an independent set.

Definition 5.6.3 (Matroid)

A set system $(E, \mathcal{I})$ is a Matroid if

(I1) $\emptyset \in \mathcal{I}$

(I2) $\forall I \in \mathcal{I}, J \subset I \Rightarrow J \in \mathcal{I}$ (down-closed or subclusive)

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

Why is (I1) is not redundant given (I2)?

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Why is (I1) is not redundant given (I2)? Because without (I1) could have a non-matroid where $\mathcal{I} = \{\}$.

On Matroid History

- Abstract properties of linear dependence (Hassler Whitney, 1935), but already then found instances of objects with those properties not based on a matrix.

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- Matroid independent sets (i.e., A s.t. $r(A) = |A|$) are useful constraint set, and fast algorithms for submodular optimization subject to one (or more) matroid independence constraints exist.
- Crapo & Rota preferred the term "combinatorial geometry", or more specifically a "pregeometry" and said that pregeometries are "often described by the ineffably cacaphonic term 'matroid', which we prefer to avoid in favor of the term 'pregeometry'."

Matroid

Slight modification (non unit increment) that is equivalent.

Definition 5.6.4 (Matroid-II)

A set system $(E, \mathcal{I})$ is a Matroid if

(I1') $\emptyset \in \mathcal{I}$

(I2') $\forall I \in \mathcal{I}, J \subset I \Rightarrow J \in \mathcal{I}$ (down-closed or subclusive)

(I3') $\forall I, J \in \mathcal{I}$, with $|I| > |J|$, then there exists $x \in I \setminus J$ such that $J \cup \{x\} \in \mathcal{I}$

Note (I1)=(I1'), (I2)=(I2'), and we get (I3)≡(I3') using induction.

Matroids, independent sets, and bases

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- A base of a matroid: If $U = E$, then a "base of E" is just called a base of the matroid M (this corresponds to a basis in a linear space, or a spanning forest in a graph, or a spanning tree in a connected graph).

Matroids - important property

Proposition 5.6.5

In a matroid $M = (E, \mathcal{I})$, for any $U \subseteq E(M)$, any two bases of U have the same size.

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(I3') $\forall X \subseteq V$, and $I_1, I_2 \in \text{maxInd}(X)$, we have $|I_1| = |I_2|$ (all maximally independent subsets of X have the same size).

Matroids - rank

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Definition 5.6.7 (matroid rank function)

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

$$r(A) = \max \{|X| : X \subseteq A, X \in \mathcal{I}\} = \max_{X \in \mathcal{I}} |A \cap X| \tag{5.102}$$

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- From the above, we immediately see that $r(A) \leq |A|$.
- Moreover, if $r(A) = |A|$, then $A \in \mathcal{I}$, meaning A is independent (in this case, A is a self base).

Matroids, other definitions using matroid rank $r : 2^V \to \mathbb{Z}_+$

Definition 5.6.8 (closed/flat/subspace)

A subset $A \subseteq E$ is closed (equivalently, a flat or a subspace) of matroid M if for all $x \in E \setminus A$, $r(A \cup \{x\}) = r(A) + 1$.

Definition: A hyperplane is a flat of rank $r(M) - 1$.

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Given $A \subseteq E$, the closure (or span) of A, is defined by $\text{span}(A) = \{b \in E : r(A \cup \{b\}) = r(A)\}$.

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Therefore, a closed set A has $\text{span}(A) = A$.

Definition 5.6.10 (circuit)

A subset $A \subseteq E$ is circuit or a cycle if it is an inclusionwise-minimal dependent set (i.e., if $r(A) < |A|$ and for any $a \in A$, $r(A \setminus \{a\}) = |A| - 1$).

Matroids by bases

In general, besides independent sets and rank functions, there are other equivalent ways to characterize matroids.

Theorem 5.6.11 (Matroid (by bases))

Let E be a set and $\mathcal{B}$ be a nonempty collection of subsets of E. Then the following are equivalent.

1. *$\mathcal{B}$ is the collection of bases of a matroid;*
2. *if $B, B' \in \mathcal{B}$, and $x \in B' \setminus B$, then $B' - x + y \in \mathcal{B}$ for some $y \in B \setminus B'$.*
3. *If $B, B' \in \mathcal{B}$, and $x \in B' \setminus B$, then $B - y + x \in \mathcal{B}$ for some $y \in B \setminus B'$.*

Properties 2 and 3 are called "exchange properties."

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Properties 2 and 3 are called "exchange properties."
Proof here is omitted but think about this for a moment in terms of linear spaces and matrices, and (alternatively) spanning trees.

Matroids by circuits

A set is independent if and only if it contains no circuit. Therefore, it is not surprising that circuits can also characterize a matroid.

Theorem 5.6.12 (Matroid by circuits)

Let E be a set and $\mathcal{C}$ be a collection of subsets of E that satisfy the following three properties:

1. *(C1): $\emptyset \notin \mathcal{C}$*
2. *(C2): if $C_1, C_2 \in \mathcal{C}$ and $C_1 \subseteq C_2$, then $C_1 = C_2$.*
3. *(C3): if $C_1, C_2 \in \mathcal{C}$ with $C_1 \neq C_2$, and $e \in C_1 \cap C_2$, then there exists a $C_3 \in \mathcal{C}$ such that $C_3 \subseteq (C_1 \cup C_2) \setminus \{e\}$.*

Matroids by circuits

Several circuit definitions for matroids.

Theorem 5.6.13 (Matroid by circuits)

Let E be a set and $\mathcal{C}$ be a collection of nonempty subsets of E, such that no two sets in $\mathcal{C}$ are contained in each other. Then the following are equivalent.

1. *$\mathcal{C}$ is the collection of circuits of a matroid;*
2. *if $C, C' \in \mathcal{C}$, and $x \in C \cap C'$, then $(C \cup C') \setminus \{x\}$ contains a set in $\mathcal{C}$;*
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Again, think about this for a moment in terms of linear spaces and matrices, and spanning trees.

Uniform Matroid

- Given E, consider $\mathcal{I}$ to be all subsets of E that are at most size k. That is $\mathcal{I} = \{A \subseteq E : |A| \leq k\}$.

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- Note, if $I, J \in \mathcal{I}$, and $|I| < |J| \leq k$, and $j \in J$ such that $j \notin I$, then j is such that $|I + j| \leq k$ and so $I + j \in \mathcal{I}$.

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- Rank function

$$r(A) = \begin{cases} |A| & \text{if } |A| \leq k \\ k & \text{if } |A| > k \end{cases} \tag{5.103}$$

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$$r(A) = \begin{cases} |A| & \text{if } |A| \leq k \\ k & \text{if } |A| > k \end{cases} \tag{5.103}$$

- Note, this function is submodular. Not surprising since $r(A) = \min(|A|, k)$ which is a non-decreasing concave function applied to a modular function.

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- Rank function

$$r(A) = \begin{cases} |A| & \text{if } |A| \leq k \\ k & \text{if } |A| > k \end{cases} \tag{5.103}$$

- Note, this function is submodular. Not surprising since $r(A) = \min(|A|, k)$ which is a non-decreasing concave function applied to a modular function.
- Closure function

$$\text{span}(A) = \begin{cases} A & \text{if } |A| < k, \\ E & \text{if } |A| \geq k, \end{cases} \tag{5.104}$$

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- A "free" matroid sets $k = |E|$, so everything is independent.

Linear (or Matric) Matroid

- Let $\mathbf{X}$ be an $n \times m$ matrix and $E = \{1, \dots, m\}$
- Let $\mathcal{I}$ consists of subsets of E such that if $A \in \mathcal{I}$, and $A = \{a_1, a_2, \dots, a_k\}$ then the vectors $x_{a_1}, x_{a_2}, \dots, x_{a_k}$ are linearly independent.
- the rank function is just the rank of the space spanned by the corresponding set of vectors.
- rank is submodular, it is intuitive that it satisfies the diminishing returns property (a given vector can only become linearly dependent in a greater context, thereby no longer contributing to rank).
- Called both linear matroids and matric matroids.

Cycle Matroid of a graph: Graphic Matroids

- Let $G = (V, E)$ be a graph. Consider $(E, \mathcal{I})$ where the edges of the graph E are the ground set and $A \in \mathcal{I}$ if the edge-induced graph $G(V, A)$ by A does not contain any cycle.

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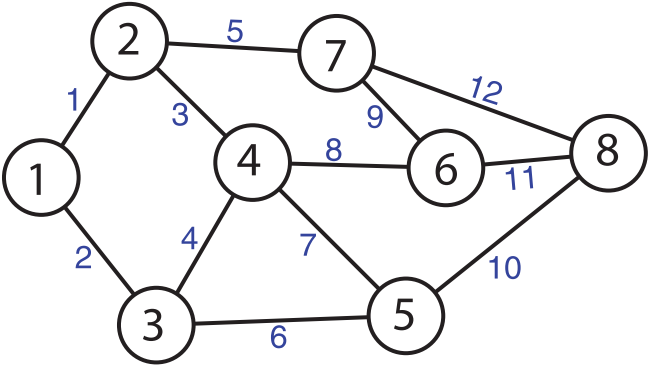
- Closure function adds all edges between the vertices adjacent to any edge in A. Closure of a spanning forest is G.

Example: graphic matroid

- A graph defines a matroid on edge sets, independent sets are those without a cycle.



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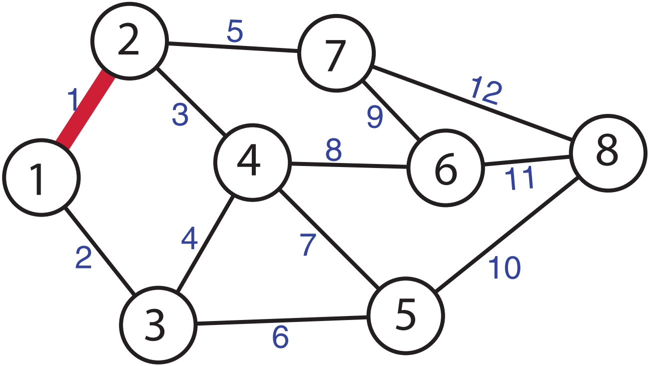

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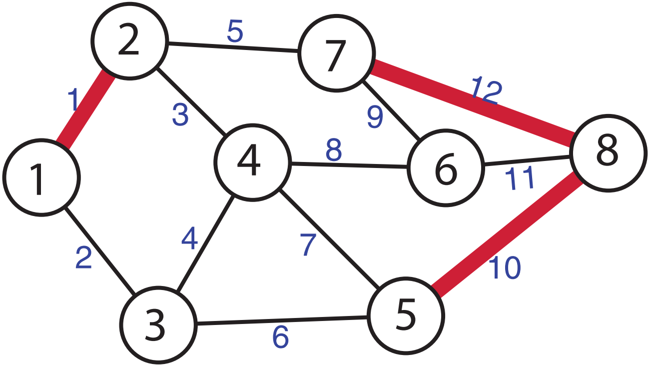

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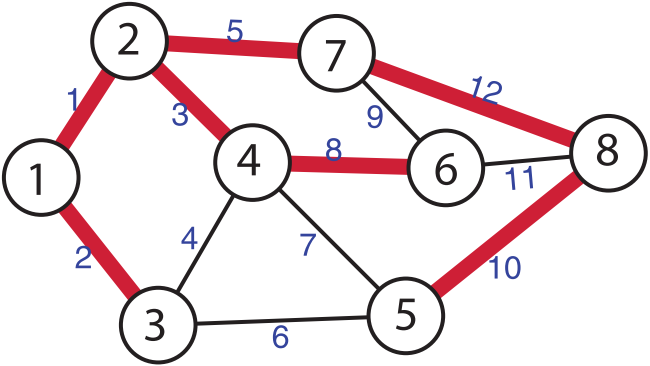

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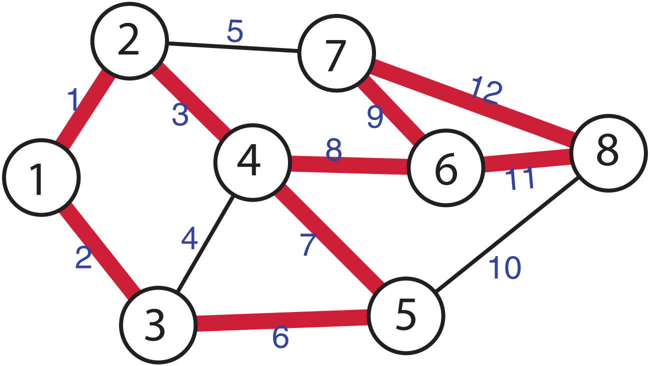

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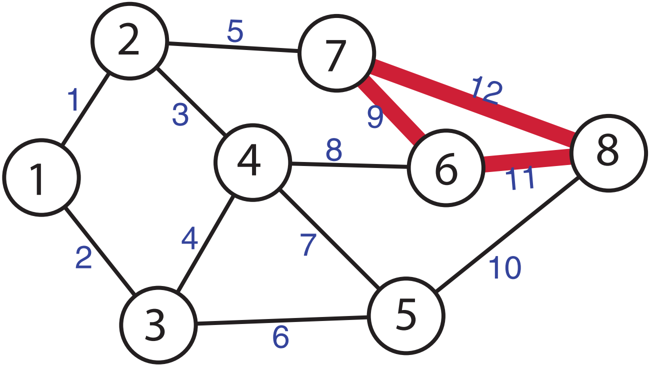

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- If $X, Y \in \mathcal{I}$ with $|Y| > |X|$, then there must be at least one i with $|Y \cap V_i| > |X \cap V_i|$. Therefore, adding one element $e \in V_i \cap (Y \setminus X)$ to X won't break independence.

Partition Matroid

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

$\Bigg\}$

Partition Matroid

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

Partition Matroid

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

Partition Matroid

Independent subset but not maximally independent.

Partition Matroid

Maximally independent subset, what is called a base.

Partition Matroid

Not independent since over limit in set six.

Matroids - rank function is submodular

Lemma 5.8.1

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

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$$\geq |X| + |Y| = r(A \cap B) + r(A \cup B) \tag{5.108}$$

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A matroid is defined from its rank function

Theorem 5.8.2 (Matroid from rank)

Let E be a set and let $r : 2^E \to \mathbb{Z}_+$ be a function. Then $r(\cdot)$ defines a matroid with r being its rank function if and only if for all $A, B \subseteq E$:

(R1) $\forall A \subseteq E \;\; 0 \leq r(A) \leq |A|$ *(non-negative cardinality bounded)*

(R2) $r(A) \leq r(B)$ *whenever* $A \subseteq B \subseteq E$ *(monotone non-decreasing)*

(R3) $r(A \cup B) + r(A \cap B) \leq r(A) + r(B)$ *for all* $A, B \subseteq E$ *(submodular)*

- From above, $r(\emptyset) = 0$. Let $v \notin A$, then by monotonicity and submodularity, $r(A) \leq r(A \cup \{v\}) \leq r(A) + r(\{v\})$ which gives only two possible values to $r(A \cup \{v\})$, namely $r(A)$ or $r(A) + 1$.

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- Can refer to matroid as (E, r), E is ground set, r is rank function.

Matroids from rank

Proof of Theorem 5.8.2 (matroid from rank).

- Given a matroid $M = (E, \mathcal{I})$, we see its rank function as defined in Eq. 5.102 satisfies (R1), (R2), and, as we saw in Lemma 5.8.1, (R3) too.

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- First, $\emptyset \in \mathcal{I}$.

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implying $r(X) = |X|$, and thus $X \in \mathcal{I}$.

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Matroids from rank

Proof of Theorem 5.8.2 (matroid from rank) cont.

- Let $A, B \in \mathcal{I}$, with $|A| < |B|$, so $r(A) = |A| < r(B) = |B|$. Let $B \setminus A = \{b_1, b_2, \ldots, b_k\}$ (note $1 \leq k \leq |B|$).

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$$\leq r(A \cup (B \setminus \{b_1\})) + r(A \cup \{b_1\}) - r(A) \tag{5.113}$$

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giving a contradiction since $B \in \mathcal{I}$. □

Matroids from rank II

Another way of using function r to define a matroid.

Theorem 5.8.3 (Matroid from rank II)

Let E be a finite set and let $r : 2^E \to \mathbb{Z}_+$ be a function. Then $r(\cdot)$ defines a matroid with r being its rank function if and only if for all $X \subseteq E$, and $x, y \in E$:

(R1') $r(\emptyset) = 0$;

(R2') $r(X) \leq r(X \cup \{y\}) \leq r(X) + 1$;

(R3') *If* $r(X \cup \{x\}) = r(X \cup \{y\}) = r(X)$, *then* $r(X \cup \{x, y\}) = r(X)$.

Matroids by submodular functions

Theorem 5.8.4 (Matroid by submodular functions)

Let $f : 2^E \to \mathbb{Z}$ be a integer valued monotone non-decreasing submodular function. Define a set of sets as follows:

$$\mathcal{C}(f) = \Big\{ C \subseteq E : C \text{ is non-empty, is inclusionwise-minimal, and has } f(C) < |C| \Big\} \tag{5.118}$$

Then $\mathcal{C}(f)$ is the collection of circuits of a matroid on E.

Inclusionwise-minimal in this case means that if $C \in \mathcal{C}(f)$, then there exists no $C' \subset C$ with $C' \in \mathcal{C}(f)$ (i.e., $C' \subset C$ would either be empty or have $f(C') \geq |C'|$). Also, recall inclusionwise-minimal in Definition 5.6.10, the definition of a circuit.

Summarizing: Many ways to define a Matroid

Summarizing what we've so far seen, we saw that it is possible to uniquely define a matroid based on any of:

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- Rank axioms (normalized, monotone, cardinality bounded, non-negative integral, submodular)
- Matroids by integral submodular functions.

Maximization problems for matroids

- Given a matroid $M = (E, \mathcal{I})$ and a modular value function $c : E \to \mathbb{R}$, the task is to find an $X \in \mathcal{I}$ such that $c(X) = \sum_{x \in X} c(x)$ is maximum.
- This seems remarkably similar to the max spanning tree problem.

Minimization problems for matroids

- Given a matroid $M = (E, \mathcal{I})$ and a modular cost function $c : E \to \mathbb{R}$, the task is to find a basis $B \in \mathcal{B}$ such that $c(B)$ is minimized.
- This sounds like a set cover problem (find the minimum cost covering set of sets).

Partition Matroid

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- $r(A)$ is also non-negative integral monotone non-decreasing, so it defines a matroid (the partition matroid).

From 2-partition matroid rank to truncated matroid rank

- Example: 2-partition matroid rank function: Given natural numbers $a, b \in \mathbb{Z}_+$ with $a < b$, and any set $R \subseteq V$ with $|R| = b$.

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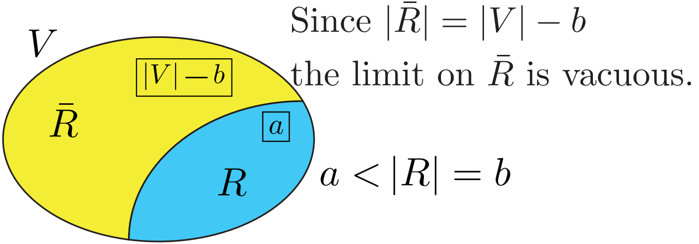
- Figure showing partition blocks and partition matroid limits.



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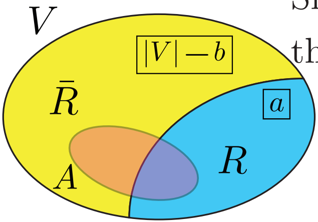

Since $|\bar{R}| = |V| - b$ the limit on $\bar{R}$ is vacuous.

$a < |R| = b$

Truncated Matroid Rank Function

- Define truncated matroid rank function. Start with 2-partition matroid rank $r(A) = \min(|A \cap R|, a) + \min(|A \cap \bar{R}|, |\bar{R}|)$, $a < b$. Define:

$$f_R(A) = \min\left\{ r(A), b \right\} \tag{5.124}$$

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Consider sets $B \subseteq V$ with $|B| = b$. Recall R fixed, and $|R| = b$.

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Truncated Matroid Rank Function

- Define truncated matroid rank function. Start with 2-partition matroid rank $r(A) = \min(|A \cap R|, a) + \min(|A \cap \bar{R}|, |\bar{R}|)$, $a < b$. Define:

$$f_R(A) = \min\left\{ r(A), b \right\} \tag{5.124}$$
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- Defines a matroid $M = (V, f_R) = (V, \mathcal{I})$ (Goemans et. al.) with

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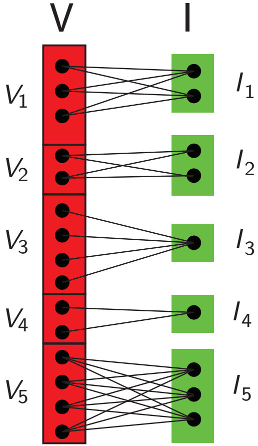
- R, the set with minimum valuation amongst size-b sets, is hidden within an exponentially larger set of size-b sets with larger valuation.

Partition Matroid, rank as matching

- A partition matroid can be viewed using a bipartite graph.
- Letting V denote the ground set, and $V_1, V_2, \dots$ the partition, the bipartite graph is $G = (V, I, E)$ where V is the ground set, I is a set of "indices", and E is the set of edges.
- $I = (I_1, I_2, \dots, I_\ell)$ is a set of $k = \sum_{i=1}^{\ell} k_i$ nodes, grouped into ℓ clusters, where there are k_i nodes in the i^{th} group I_i, and $|I_i| = k_i$.
- $(v, i) \in E(G)$ iff $v \in V_j$ and $i \in I_j$.

Partition Matroid, rank as matching

- Example where $\ell = 5$, $(k_1, k_2, k_3, k_4, k_5) = (2, 2, 1, 1, 3)$.



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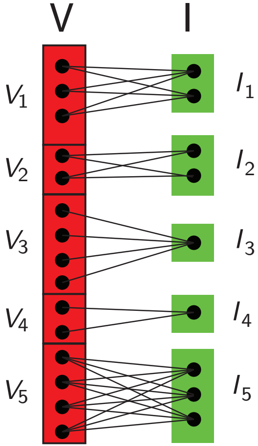

- Recall, $\Gamma : 2^V \to \mathbb{R}$ as the neighbor function in a bipartite graph, the neighbors of X is defined as $\Gamma(X) = \{v \in V(G) \setminus X : E(X, \{v\}) \neq \emptyset\}$, and recall that $|\Gamma(X)|$ is submodular.

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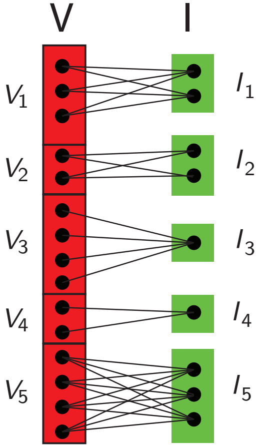

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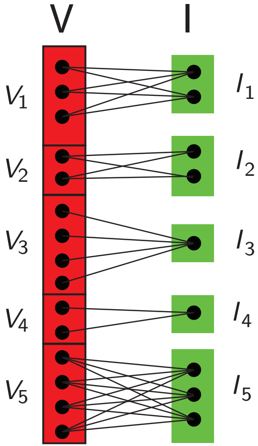

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- Here, for $X \subseteq V$, we have $\Gamma(X) = \{i \in I : (v, i) \in E(G) \text{ and } v \in X\}$.
- For such a constructed bipartite graph, the rank function of a partition matroid is $r(X) = \sum_{i=1}^{\ell} \min(|X \cap V_i|, k_i) =$ the maximum matching involving X.