Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 5 —

http://j.ee.washington.edu/~bilmes/classes/ee596b_spring_2014/

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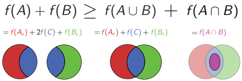

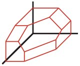

Cumulative Outstanding Reading

- Read chapter 1 from Fujishige's book.

Announcements, Assignments, and Reminders

- our room (Mueller Hall Room 154) is changed!
- Please do use our discussion board (`https://canvas.uw.edu/courses/895956/discussion_topics`) for all questions, comments, so that all will benefit from them being answered.
- Weekly Office Hours: Wednesdays, 5:00-5:50, or by skype or google hangout (email me).

Class Road Map - IT-I

- L1 (3/31): Motivation, Applications, & Basic Definitions
- L2: (4/2): Applications, Basic Definitions, Properties
- L3: More examples and properties (e.g., closure properties), and examples, spanning trees
- L4: proofs of equivalent definitions, independence, start matroids
- L5: matroids, basic definitions and examples
- L6: More on matroids, System of Distinct Reps, Transversals, Transversal Matroid, Matroid and representation
- L7: Dual Matroids, other matroid properties, Combinatorial Geometries
- L8: Combinatorial Geometries, matroids and greedy, Polyhedra, Matroid Polytopes,
- L9: From Matroid Polytopes to Polymatroids.
- L10: Polymatroids and Submodularity
- L11: More properties of polymatroids, SFM special cases
- L12: polymatroid properties, extreme points polymatroids,
- L13: sat, dep, supp, exchange capacity, examples
- L14: Lattice theory: partially ordered sets; lattices; distributive, modular, submodular, and boolean lattices; ideals and join irreducibles.
- L15: Supp, Base polytope, polymatroids and entropic Venn diagrams, exchange capacity,
- L16: proof that minimum norm point yields min of submodular function, and the lattice of minimizers of a submodular function, Lovasz extension
- L17: Lovasz extension, Choquet Integration, more properties/examples of Lovasz extension, convex minimization and SFM.
- L18: Lovasz extension examples and structured convex norms, The Min-Norm Point Algorithm detailed.
- L19: symmetric submodular function minimization, maximizing monotone submodular function w. card constraints.
- L20: maximizing monotone submodular function w. other constraints, non-monotone maximization.

Finals Week: June 9th-13th, 2014.

Many (Equivalent) Definitions of Submodularity

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V \tag{5.6}$$

$$f(j|S) \geq f(j|T), \ \forall S \subseteq T \subseteq V, \text{ with } j \in V \setminus T \tag{5.7}$$

$$f(C|S) \geq f(C|T), \forall S \subseteq T \subseteq V, \text{ with } C \subseteq V \setminus T \tag{5.8}$$

$$f(j|S) \geq f(j|S \cup \{k\}), \ \forall S \subseteq V \text{ with } j \in V \setminus (S \cup \{k\}) \tag{5.9}$$

$$f(A \cup B | A \cap B) \leq f(A|A \cap B) + f(B|A \cap B), \quad \forall A, B \subseteq V \tag{5.10}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S) - \sum_{j \in S \setminus T} f(j|S \cup T - \{j\}), \ \forall S, T \subseteq V \tag{5.11}$$

$$f(T) \leq f(S) + \sum_{j \in T \setminus S} f(j|S), \ \forall S \subseteq T \subseteq V \tag{5.12}$$

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

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- We saw several different "greedy" algorithms that proced optimal spanning trees (Borůvka's, Jarník/Prim/Dijkstra's, and Kruskal's).
- We wish to more formally connect the above, and generalize further.

From Matrix Rank → Matroid

- So V is set of column vector indices of a matrix.
- Let $\mathcal{I}$ be a set of all subsets of V such that for any $I \in \mathcal{I}$, the vectors indexed by I are linearly independent.
- Given a set $B \in \mathcal{I}$ of linearly independent vectors, then any subset $A \subseteq B$ is also linearly independent. Hence, $\mathcal{I}$ is down-closed or "subclusive", under subsets. In other words,

$$A \subseteq B \text{ and } B \in \mathcal{I} \Rightarrow A \in \mathcal{I} \tag{5.32}$$

- maxInd: Inclusionwise maximal independent subsets (or bases) of any set $B \subseteq V$.

$$\text{maxInd}(B) \triangleq \{A \subseteq B : A \in \mathcal{I} \text{ and } \forall v \in B \setminus A, A \cup \{v\} \notin \mathcal{I}\} \tag{5.33}$$

- 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 $B \subseteq V$,

$$\forall A_1, A_2 \in \text{maxInd}(B), \quad |A_1| = |A_2| \tag{5.34}$$

From Matrix Rank → Matroid

- Thus, for all $I \in \mathcal{I}$, the matrix rank function has the property

$$r(I) = |I| \tag{5.32}$$

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

$$r(B) = \max\{|A| : A \subseteq B \text{ and } A \in \mathcal{I}\} \leq |B| \tag{5.33}$$

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 5.2.4 (Matroid)

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

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

(I2) $\forall I \in \mathcal{I}, J \subset I \Rightarrow J \in \mathcal{I}$

(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)? Because without (I1) could have a non-matroid where $\mathcal{I} = \{\}$.

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- Crapo & Rota preferred the term "combinatorial geometry", or more specifically a "pregeometry" and said that pregeometries are "often described by the ineffably cacaphonic [sic] term 'matroid', which we prefer to avoid in favor of the term 'pregeometry'."

Matroid

Slight modification (non unit increment) that is equivalent.

Definition 5.3.1 (Matroid-II)

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

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

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

(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 $U \subseteq E$: For $U \subseteq E$, a subset $B \subseteq U$ is called a base of U if B is inclusionwise maximally independent subset of U. That is, $B \in \mathcal{I}$ and there is no $Z \in \mathcal{I}$ with $B \subset Z \subseteq U$.

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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).

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Proposition 5.3.2

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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).

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- $r(E) = r_{(E,\mathcal{I})}$ is the rank of the matroid, and is the common size of all the bases of the matroid.

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Definition 5.3.4 (matroid rank function)

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

$$r(A) = \max \{|X| : X \subseteq A, X \in \mathcal{I}\} = \max_{X \in \mathcal{I}} |A \cap X| \tag{5.1}$$

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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 5.3.5 (closed/flat/subspace)

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

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

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Definition 5.3.6 (closure)

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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Definition 5.3.7 (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 5.3.8 (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 5.3.9 (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 5.3.10 (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 $\mathcal{C}$;*
3. *if $C, C' \in \mathcal{C}$, and $x \in C \cap C'$, and $y \in C \setminus C'$, then $(C \cup C') \setminus \{x\}$ contains a set in $\mathcal{C}$ containing y;*

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Again, think about this for a moment in terms of linear spaces and matrices, and spanning trees.

Matroids by submodular functions

Theorem 5.3.11 (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:

$$\mathcal{C}(f) = \Big\{ C \subseteq E : C \text{ is non-empty, is inclusionwise-minimal, and has } f(C) < |C| \Big\} \tag{5.2}$$

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 5.3.7, the definition of a circuit.

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

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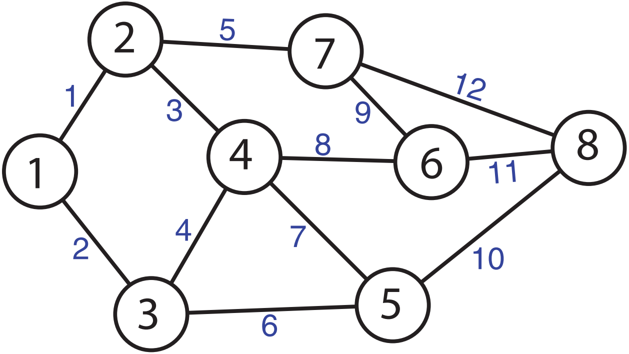
- Closure function adds all edges between the vertices adjacent to any edge in A. Closure of a spanning forest is G.

Example: graphic matroid

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



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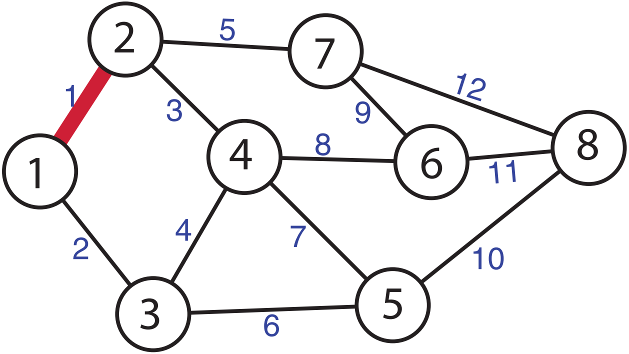

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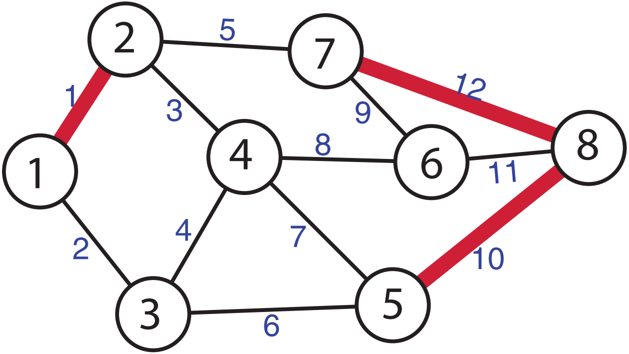

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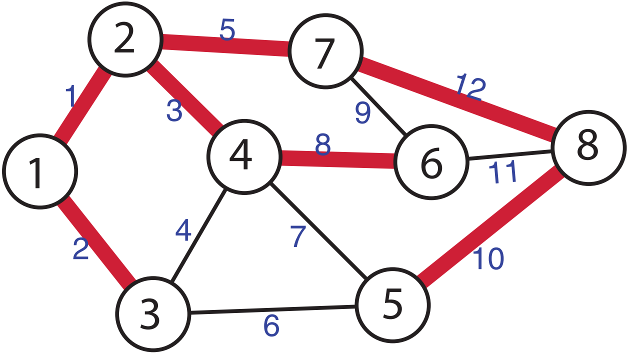

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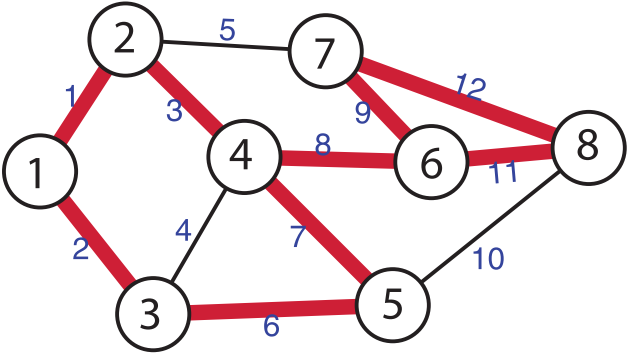

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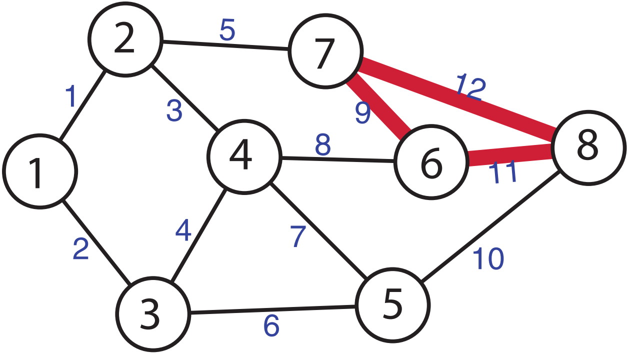

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$$\mathcal{I} = \{X \subseteq V : |X \cap V_i| \leq k_i \text{ for all } i = 1, \ldots, \ell\}. \tag{5.5}$$

where $k_1, \ldots, k_\ell$ are fixed parameters, $k_i \geq 0$. Then $M = (V, \mathcal{I})$ is a matroid.

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- Parameters associated with a partition matroid: ℓ and $k_1, k_2, \dots, k_\ell$ although often the k_i's are all the same.
- We'll show that property (I3') in Def 5.3.3 holds. 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, $V = \Big\{$

$\Big\}$

Partition Matroid

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

Partition Matroid

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

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

Lemma 5.5.1

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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$$\geq |X| + |Y| = r(A \cap B) + r(A \cup B) \tag{5.8}$$

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Matroids

In fact, we can use the rank of a matroid for its definition.

Theorem 5.5.2 (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)*

- So submodularity and non-negative monotone non-decreasing, and unit increase is necessary and sufficient to define the matroid.
- Given above, unit increment (if $r(A) = k$, then either $r(A \cup \{v\}) = k$ or $r(A \cup \{v\}) = k + 1$) holds.
- A matroid is sometimes given as (E, r) where E is ground set and r is rank function.

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- 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 $r(A \cup \{v\})$.

Matroids from rank

Proof of Theorem 5.5.2 (matroid from rank).

- Given a matroid $M = (E, \mathcal{I})$, we see its rank function as defined in Eq. 5.1 satisfies (R1), (R2), and, as we saw in Lemma 5.5.1, (R3) too.

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$$r(X) \geq r(Y) - r(Y \setminus X) \tag{5.9}$$

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- Next, assume we have (R1), (R2), and (R3). Define $\mathcal{I} = \{X \subseteq E : r(X) = |X|\}$. We will show that $(E, \mathcal{I})$ is a matroid.
- First, $\emptyset \in \mathcal{I}$.
- Also, if $Y \in \mathcal{I}$ and $X \subseteq Y$ then by submodularity,

$$r(X) \geq r(Y) - r(Y \setminus X) - r(\emptyset) \tag{5.9}$$

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

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Matroids from rank

Proof of Theorem 5.5.2 (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 $k \leq |B|$).

□

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- Suppose, to the contrary, that $\forall b \in B \setminus A$, $A + b \notin \mathcal{I}$, which means for all such b, $r(A + b) = r(A) = |A|$. Then

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$$r(B) \leq r(A \cup B) \tag{5.12}$$

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$$\leq r(A \cup (B \setminus \{b_1\})) + r(A \cup \{b_1\}) - r(A) \tag{5.13}$$

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&\leq r(A \cup (B \setminus \{b_1, b_2\})) + r(A \cup \{b_2\}) - r(A) && (5.15)
\end{aligned}
$$

$\square$

Matroids from rank

Proof of Theorem 5.5.2 (matroid from rank) cont.

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&= r(A \cup (B \setminus \{b_1, b_2\})) && (5.16)
\end{aligned}
$$

□

Matroids from rank

Proof of Theorem 5.5.2 (matroid from rank) cont.

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&\leq \dots \leq r(A) = |A| < |B| && (5.17)
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$$

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Matroids from rank

Proof of Theorem 5.5.2 (matroid from rank) cont.

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

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

Matroids from rank II

Another way of using function r to define a matroid.

Theorem 5.5.3 (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 $A \subseteq E$, 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* $r(X \cup \{x, y\}) = r(X)$.

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

- Independence (define the independent sets).
- Base axioms (exchangeability)
- Circuit axioms
- Closure axioms (we didn't see this, but it is possible)
- Rank axioms (normalized, monotone, cardinality bounded, submodular)

Maximization 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 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

- What is the partition matroid's rank function?

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- A partition matroids rank function:

$$r(A) = \sum_{i=1}^{\ell} \min(|A \cap V_i|, k_i) \tag{5.18}$$

which we also immediately see is submodular using properties we spoke about last week. That is:

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

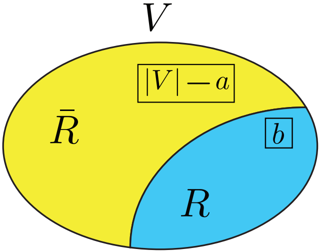
Matroid and Rank

- Thus, we can define a matroid as $M = (V, r)$ where r satisfies matroid rank axioms.
- Example: 2-partition matroid rank function: Given natural numbers $a, b \in \mathbb{Z}_+$ with $a > b$, and any set $R \subseteq V$ with $|R| = a$, two-block partition $V = (R, \bar{R})$, where $\bar{R} = V \setminus R$, define:

$$r(A) = \min(|A \cap R|, b) + \min(|A \cap \bar{R}|, |\bar{R}|) \quad (5.19)$$

$$= \min(|A \cap R|, b) + |A \cap \bar{R}| \quad (5.20)$$

- Partition matroid figure showing this:



$$b < |R| = a$$

Truncated Matroid Rank Function

- Can use this to define a truncated matroid rank function. With $r(A) = \min(|A \cap R|, b) + |A \cap \bar{R}|$, $b < a$, define:

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- Defines a matroid $M = (V, f_R) = (V, \mathcal{I})$ (Goemans et. al.) with

$$\mathcal{I} = \{I \subseteq V : |I| \leq a \text{ and } |I \cap R| \leq b\}, \tag{5.24}$$

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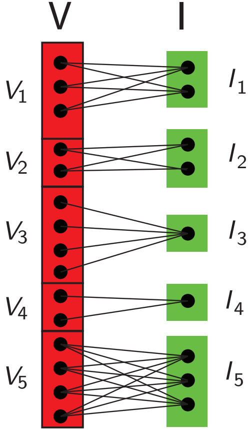
- For any B with $|B \cap R| = \ell$, with $b < \ell < a$, $f_R(B) = b + a - \ell$.
- R, the set with minimum valuation amongst size-a sets, is hidden within an exponentially larger set of size-a sets with larger valuation.

Partition Matroid, rank as matching

- A partition matroid can be viewed using a bipartite graph.
- Letting V denote the ground set, and $V_1, V_2, \ldots$ the partition, the 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.
- $I = (I_1, I_2, \ldots, I_\ell)$ 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.
- $(v, i) \in E(G)$ 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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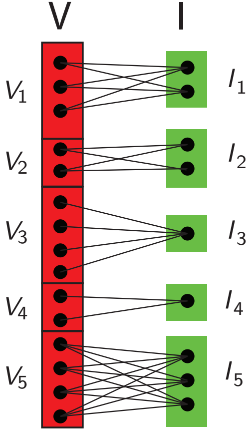

- Recall, $\Gamma : 2^V \to \mathbb{R}$ as the neighbor function in a bipartite graph, the neighbors of X is defined as $\Gamma(X) = \{v \in V(G) \setminus X : E(X, \{v\}) \neq \emptyset\}$, and recall that $|\Gamma(X)|$ is submodular.

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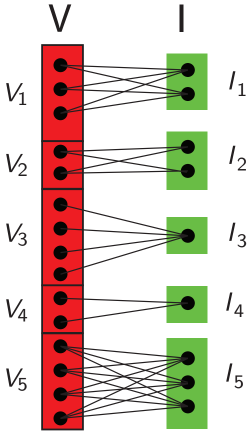

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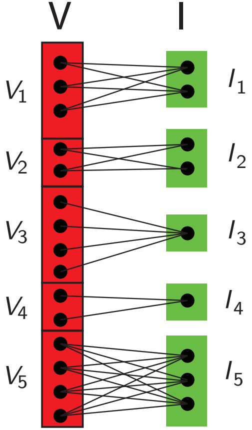
- Here, for $X \subseteq V$, we have $\Gamma(X) = \{i \in I : (v, i) \in E(G) \text{ and } v \in X\}$.

Partition Matroid, rank as matching

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



- 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.
- 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.

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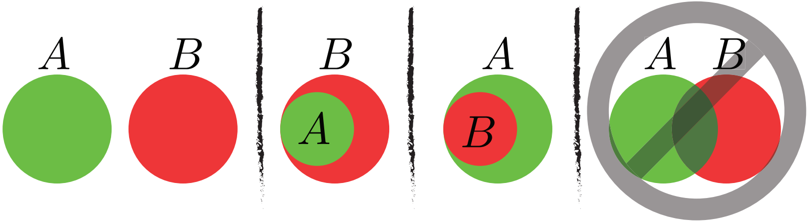

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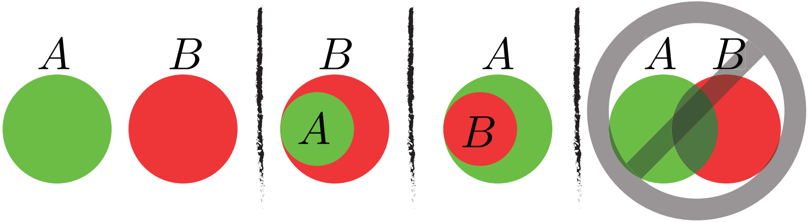

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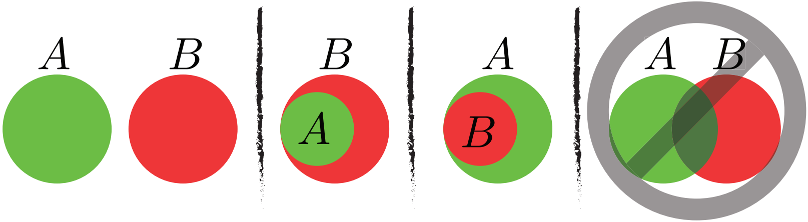

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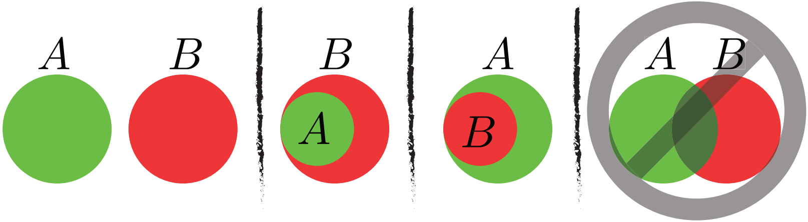

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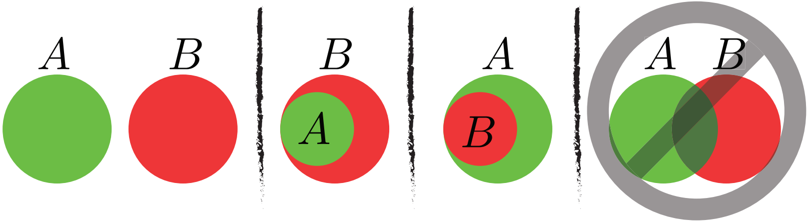

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- Exercise: what is the rank function here?