

Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 7 —

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

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April 16th, 2018



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

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



Cumulative Outstanding Reading

- Read chapter 1 from Fujishige's book.
- Read chapter 2 from Fujishige's book.

Announcements, Assignments, and Reminders

- If you have any questions about anything, please ask them via our discussion board (https://canvas.uw.edu/courses/1216339/discussion_topics).

Class Road Map - EE563

- L1(3/26): Motivation, Applications, & Basic Definitions,
- L2(3/28): Machine Learning Apps (diversity, complexity, parameter, learning target, surrogate).
- L3(4/2): Info theory exs, more apps, definitions, graph/combinatorial examples
- L4(4/4): Graph and Combinatorial Examples, Matrix Rank, Examples and Properties, visualizations
- L5(4/9): More Examples/Properties/ Other Submodular Defs., Independence,
- L6(4/11): Matroids, Matroid Examples, Matroid Rank, Partition/Laminar Matroids
- L7(4/16): Laminar Matroids, System of Distinct Reprs, Transversals, Transversal Matroid, Matroid Representation, Dual Matroids
- L8(4/18):
- L9(4/23):
- L10(4/25):
- L11(4/30):
- L12(5/2):
- L13(5/7):
- L14(5/9):
- L15(5/14):
- L16(5/16):
- L17(5/21):
- L18(5/23):
- L-(5/28): Memorial Day (holiday)
- L19(5/30):
- L21(6/4): Final Presentations maximization.

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

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

Matroids - important property

Proposition 7.2.3

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

- In matrix terms, given a set of vectors U , all sets of independent vectors that span the space spanned by U have the same size.
- In fact, under (I1),(I2), this condition is equivalent to (I3). **Exercise: show the following is equivalent to the above.**

Definition 7.2.4 (Matroid)

A set system (V, \mathcal{I}) is a **Matroid** if

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

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

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

Partition Matroid

- Let V be our ground set.
- Let $V = V_1 \cup V_2 \cup \dots \cup V_\ell$ be a partition of V into ℓ blocks (i.e., disjoint sets). Define a set of subsets of V as

$$\mathcal{I} = \{X \subseteq V : |X \cap V_i| \leq k_i \text{ for all } i = 1, \dots, \ell\}. \quad (7.4)$$

where k_1, \dots, k_ℓ are fixed “limit” parameters, $k_i \geq 0$. Then $M = (V, \mathcal{I})$ is a matroid.

- Note that a k -uniform matroid is a trivial example of a partition matroid with $\ell = 1$, $V_1 = V$, and $k_1 = k$.
- Parameters associated with a partition matroid: ℓ and k_1, k_2, \dots, k_ℓ although often the k_i 's are all the same.
- We'll show that property (I3') in Def ?? holds. First note, for any $X \subseteq V$, $|X| = \sum_{i=1}^{\ell} |X \cap V_i|$ since $\{V_1, V_2, \dots, V_\ell\}$ is a partition.
- 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.

Matroids - rank function is submodular

Lemma 7.2.3

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

Proof.

- 1 Let $X \in \mathcal{I}$ be an inclusionwise maximal set with $X \subseteq A \cap B$
- 2 Let $Y \in \mathcal{I}$ be inclusionwise maximal set with $X \subseteq Y \subseteq A \cup B$.
- 3 Since M is a matroid, we know that $r(A \cap B) = r(X) = |X|$, and $r(A \cup B) = r(Y) = |Y|$. Also, for any $U \in \mathcal{I}$, $r(A) \geq |A \cap U|$.
- 4 Then we have (since $X \subseteq A \cap B$, $X \subseteq Y$, and $Y \subseteq A \cup B$),

$$r(A) + r(B) \geq |Y \cap A| + |Y \cap B| \quad (7.4)$$

$$= |Y \cap (A \cap B)| + |Y \cap (A \cup B)| \quad (7.5)$$

$$\geq |X| + |Y| = r(A \cap B) + r(A \cup B) \quad (7.6)$$



A matroid is defined from its rank function

Theorem 7.2.3 (Matroid from rank)

Let E be a set and let $r : 2^E \rightarrow \mathbb{Z}_+$ 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) $\forall A \subseteq E \quad 0 \leq r(A) \leq |A|$ (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)

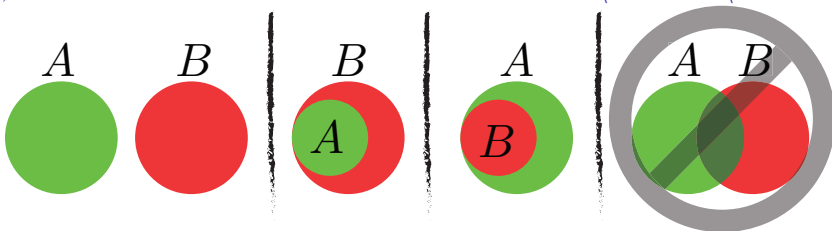
- From above, $r(\emptyset) = 0$. Let $v \notin A$, then by monotonicity and submodularity, $r(A) \leq r(A \cup \{v\}) \leq r(A) + r(\{v\})$ which gives only two possible values to $r(A \cup \{v\})$, namely $r(A)$ or $r(A) + 1$.
- Hence, unit increment (if $r(A) = k$, then either $r(A \cup \{v\}) = k$ or $r(A \cup \{v\}) = k + 1$) holds.
- Thus, **submodularity**, **non-negative monotone non-decreasing**, and **unit increment** of rank is necessary and sufficient to define a matroid.
- Can refer to matroid as (E, r) , E is ground set, r is rank function.

Laminar Family and Laminar Matroid

- We can define a matroid with structures richer than just partitions.

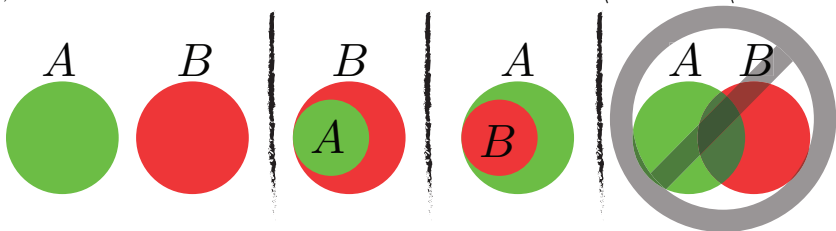
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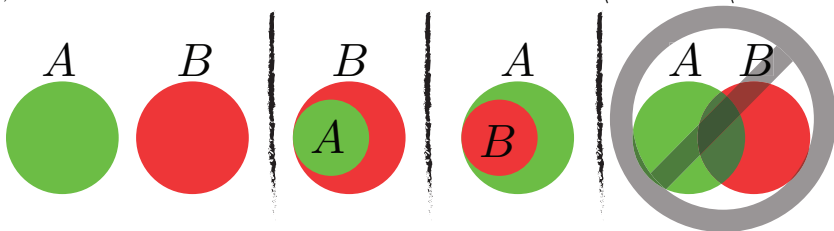
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- Family is laminar \exists no two properly intersecting members: $\forall A, B \in \mathcal{F}$, either A, B disjoint ($A \cap B = \emptyset$) or comparable ($A \subseteq B$ or $B \subseteq A$).

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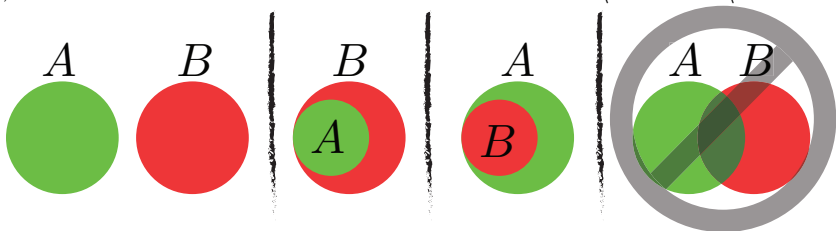
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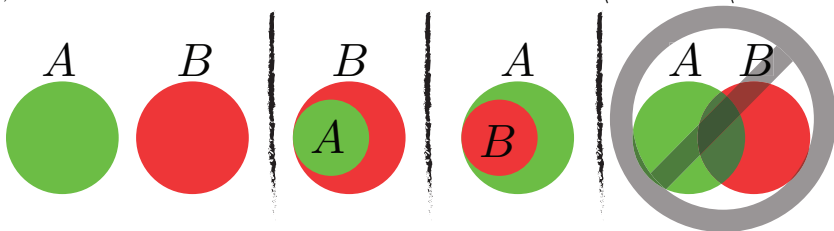


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- **Exercise:** what is the rank function here?

System of Representatives

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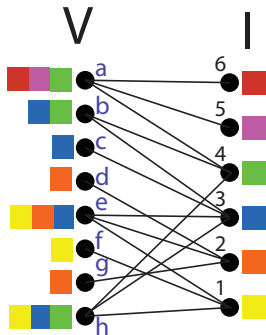
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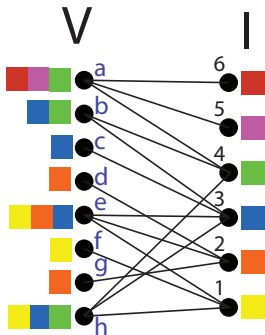
System of Representatives

- We can view this as a bipartite graph. The groups of V are marked by color tags on the left, and also via right neighbors in the graph.
- Here, $\ell = 6$ groups, with $\mathcal{V} = (V_1, V_2, \dots, V_6)$
 $= \left(\{e, f, h\}, \{d, e, g\}, \{b, c, e, h\}, \{a, b, h\}, \{a\}, \{a\} \right)$.



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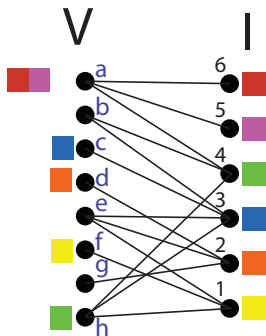
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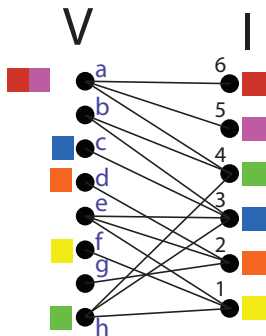
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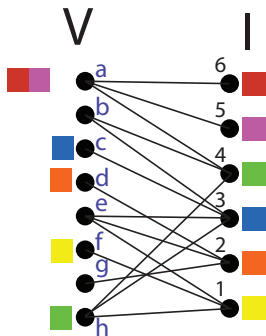
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- Here, the set of representatives is not distinct. Why? In fact, due to the red and pink group, a distinct group of representatives is impossible (since there is only one common choice to represent both color groups).

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Given a set system (V, \mathcal{V}) and index set I for \mathcal{V} as defined above, a set $T \subseteq V$ is a **transversal** of \mathcal{V} if there is a bijection $\pi : T \leftrightarrow I$ such that

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- Note that due to $\pi : T \leftrightarrow I$ being a bijection, all of I and T are “covered” (so this makes things distinct automatically).

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- Thus, transversals are down closed (subclusive).

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- Given a set system (V, \mathcal{V}) with $\mathcal{V} = (V_i : i \in I)$, and $V_i \subseteq V$ for all i . Then, for any $J \subseteq I$, let

$$V(J) = \cup_{j \in J} V_j \quad (7.3)$$

so $|V(J)| : 2^I \rightarrow \mathbb{Z}_+$ is the set cover func. (we know is submodular).

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$$V(J) = \cup_{j \in J} V_j \quad (7.3)$$

so $|V(J)| : 2^I \rightarrow \mathbb{Z}_+$ is the set cover func. (we know is submodular).

- We have

Theorem 7.5.1 (Hall's theorem)

Given a set system (V, \mathcal{V}) , the family of subsets $\mathcal{V} = (V_i : i \in I)$ has a transversal $(v_i : i \in I)$ iff for all $J \subseteq I$

$$|V(J)| \geq |J| \quad (7.4)$$

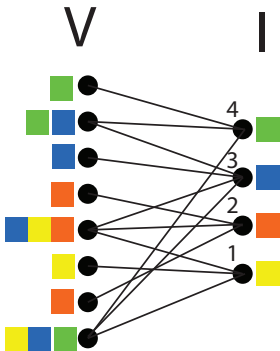
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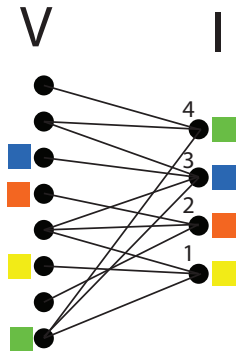
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If $M = (V, r)$ is a matroid on V with rank function r , then the family of subsets $(V_i : i \in I)$ of V has a transversal $(v_i : i \in I)$ that is independent in M iff for all $J \subseteq I$

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- Note, a transversal T independent in M means that $r(T) = |T|$.

More general conditions for existence of transversals

Theorem 7.5.3 (Polymatroid transversal theorem)

If $\mathcal{V} = (V_i : i \in I)$ is a finite family of non-empty subsets of V , and $f : 2^V \rightarrow \mathbb{Z}_+$ is a non-negative, integral, monotone non-decreasing, and submodular function, then \mathcal{V} has a system of representatives $(v_i : i \in I)$ such that

$$f(\cup_{i \in J} \{v_i\}) \geq |J| \text{ for all } J \subseteq I \quad (7.6)$$

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Submodular Composition with Set-to-Set functions

- Note the condition in Theorem 7.5.3 is $f(V(J)) \geq |J|$ for all $J \subseteq I$, where $f : 2^V \rightarrow \mathbb{Z}_+$ is non-negative, integral, monotone non-decreasing and submodular, and $V(J) = \cup_{j \in J} V_j$ with $V_i \subseteq V$.

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- Hence, the condition for existence can be solved by (a special case of) submodular function minimization, or vice versa!

More general conditions for existence of transversals

first part proof of Theorem 7.5.3.

- Suppose \mathcal{V} has a system of representatives $(v_i : i \in I)$ such that Eq. 7.6 (i.e., $f(\cup_{i \in J} \{v_i\}) \geq |J|$ for all $J \subseteq I$) is true.

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- Then since f is monotone, and since $V(J) \supseteq \cup_{i \in J} \{v_i\}$ when $(v_i : i \in I)$ is a system of representatives, then Eq. 7.7 (i.e., $f(V(J)) \geq |J|$ for all $J \subseteq I$) immediately follows.

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Lemma 7.5.5 (contraction lemma)

Suppose Eq. 7.7 ($f(V(J)) \geq |J|, \forall J \subseteq I$) is true for $\mathcal{V} = (V_i : i \in I)$, and there exists an i such that $|V_i| \geq 2$ (w.l.o.g., say $i = 1$). Then there exists $\bar{v} \in V_1$ such that the family of subsets $(V_1 \setminus \{\bar{v}\}, V_2, \dots, V_{|I|})$ also satisfies Eq 7.7.

Proof.

- When Eq. 7.7 holds, this means that for any subsets $J_1, J_2 \subseteq I \setminus \{1\}$, we have that, for $J \in \{J_1, J_2\}$,

$$f(V(J \cup \{1\})) \geq |J \cup \{1\}| \quad (7.9)$$

and hence

$$f(V_1 \cup V(J_1)) \geq |J_1| + 1 \quad (7.10)$$

$$f(V_1 \cup V(J_2)) \geq |J_2| + 1 \quad (7.11)$$

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- \dots and there must exist subsets J_1, J_2 of $I \setminus \{1\}$ such that

$$f((V_1 \setminus \{\bar{v}_1\}) \cup V(J_1)) < |J_1| + 1, \quad (7.12)$$

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(note that either one or both of J_1, J_2 could be empty).

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Proof.

- Taking $X = (V_1 \setminus \{\bar{v}_1\}) \cup V(J_1)$ and $Y = (V_1 \setminus \{\bar{v}_2\}) \cup V(J_2)$, we have $f(X) \leq |J_1|$, $f(Y) \leq |J_2|$, and that:

$$X \cup Y = V_1 \cup V(J_1 \cup J_2), \quad (7.14)$$

$$X \cap Y \supseteq V(J_1 \cap J_2), \quad (7.15)$$

and

$$\begin{aligned} |J_1| + |J_2| &\geq f(X) + f(Y) \\ &\geq f(X \cup Y) + f(X \cap Y) \end{aligned} \quad (7.16)$$

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- since f submodular monotone non-decreasing, & Eqs 7.14-7.16,

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- Since \mathcal{V} satisfies Eq. 7.7, $1 \notin J_1 \cup J_2$, & Eqs 7.10-7.11, this gives

$$|J_1| + |J_2| \geq |J_1 \cup J_2| + 1 + |J_1 \cap J_2| \quad (7.18)$$

which is a contradiction since cardinality is modular. □

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This theorem can be used to produce a variety of other results quite easily, and shows how submodularity is the key ingredient in its truth.

Transversal Matroid

Transversals, themselves, define a matroid.

Theorem 7.6.1

If \mathcal{V} is a family of finite subsets of a ground set V , then the collection of partial transversals of \mathcal{V} is the set of independent sets of a matroid $M = (V, \mathcal{V})$ on V .

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- This means that the transversals of \mathcal{V} are the bases of matroid M .
- Therefore, all maximal partial transversals of \mathcal{V} have the same cardinality!

Transversals and Bipartite Matchings

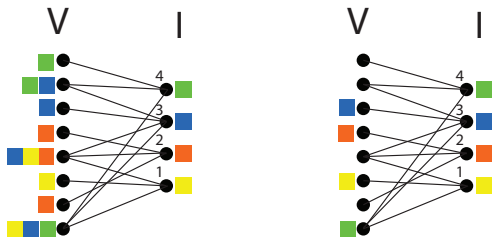
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- Given a set system (V, \mathcal{V}) , with $\mathcal{V} = (V_i : i \in I)$, we can define a bipartite graph $G = (V, I, E)$ associated with \mathcal{V} that has edge set $\{(v, i) : v \in V, i \in I, v \in V_i\}$.

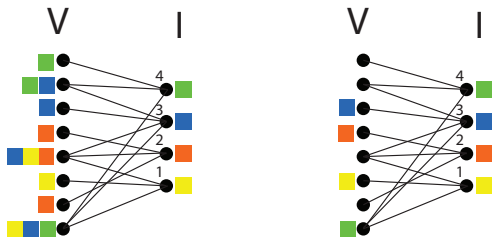
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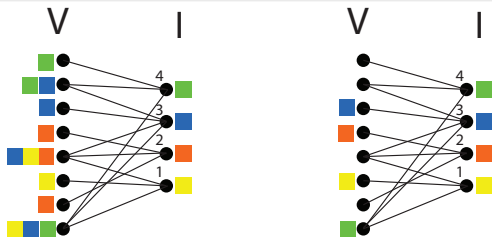


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Lemma 7.6.2

A subset $T \subseteq V$ is a partial transversal of \mathcal{V} iff there is a matching in (V, I, E) in which every edge has one endpoint in T (T matched into I).

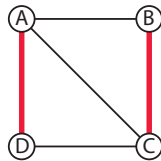
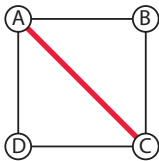
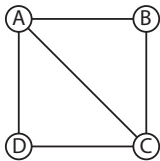


Arbitrary Matchings and Matroids?

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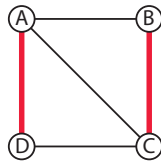
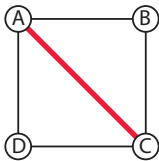
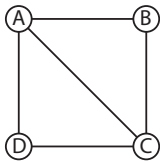
Arbitrary Matchings and Matroids?

- Are arbitrary matchings matroids?
- Consider the following graph (left), and two max-matchings (two right instances)



Arbitrary Matchings and Matroids?

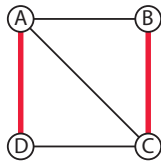
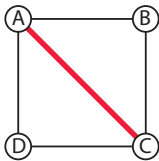
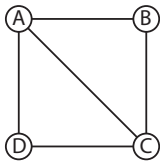
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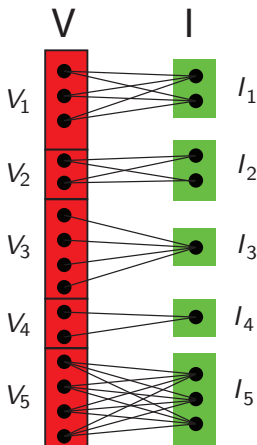
- $\{AC\}$ is a maximum matching, as is $\{AD, BC\}$, but they are not the same size.
- Let \mathcal{M} be the set of matchings in an arbitrary graph $G = (V, E)$. Hence, (E, \mathcal{M}) is a set system. I1 holds since $\emptyset \in \mathcal{M}$. I2 also holds since if $M \in \mathcal{M}$ is a matching, then so is any $M' \subseteq M$. I3 doesn't hold (as seen above). **Exercise:** fully characterize the problem of finding the largest subset $\mathcal{M}' \subset \mathcal{M}$ of matchings so that (E, \mathcal{M}') also satisfies I3?

Review from Lecture 7

The next frame comes from lecture 7.

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, $\Gamma : 2^V \rightarrow \mathbb{R}$ 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 .

Morphing Partition Matroid Rank

- Recall the partition matroid rank function. Note, $k_i = |I_i|$ in the bipartite graph representation, and since a matroid, w.l.o.g., $|V_i| \geq k_i$ (also, recall, $V(J) = \cup_{j \in J} V_j$).

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- Start with partition matroid rank function in the subsequent equations.

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- In fact, this bottom (more general) expression is the expression for the rank of a transversal matroid.

Partial Transversals Are Independent Sets in a Matroid

In fact, we have

Theorem 7.6.3

Let (V, \mathcal{V}) where $\mathcal{V} = (V_1, V_2, \dots, V_\ell)$ be a subset system. Let $I = \{1, \dots, \ell\}$. Let \mathcal{I} be the set of partial transversals of \mathcal{V} . Then (V, \mathcal{I}) is a matroid.

Proof.



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- Suppose that T_1 and T_2 are partial transversals of \mathcal{V} such that $|T_1| < |T_2|$. **Exercise: show that (I3') holds.**



Transversal Matroid Rank

- Transversal matroid has rank

$$r(A) = \min_{J \subseteq I} (|V(J) \cap A| - |J| + |I|) \quad (7.28)$$

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- Note that it is a minimum over a set of modular functions in I . Is this true in general? **Exercise:**
- **Exercise:** Can you identify a set of sufficient properties over a set of modular functions $m_i : V \rightarrow \mathbb{R}_+$ so that $f(A) = \min_i m_i(A)$ is submodular? Can you identify both necessary and sufficient conditions?

Matroid loops

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

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- In a matrix (i.e., linear) matroid, the only such loop is the value $\mathbf{0}$, as all non-zero vectors have rank 1. The $\mathbf{0}$ can appear > 1 time with different indices, as can a self loop in a graph appear on different nodes.

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- Note, we also say that two elements s, t are said to be **parallel** if $\{s, t\}$ is a circuit.

Representable

Definition 7.7.1 (Matroid isomorphism)

Two matroids M_1 and M_2 respectively on ground sets V_1 and V_2 are **isomorphic** if there is a bijection $\pi : V_1 \rightarrow V_2$ which preserves independence (equivalently, rank, circuits, and so on).

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- Let \mathbb{F} be any field (such as \mathbb{R} , \mathbb{Q} , or some finite field \mathbb{F} , such as a Galois field $\text{GF}(p)$ where p is prime (such as $\text{GF}(2)$), but not \mathbb{Z} . Succinctly: A field is a set with $+$, $*$, closure, associativity, commutativity, and additive and multiplicative identities and inverses.

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Definition 7.7.2 (linear matroids on a field)

Let \mathbf{X} be an $n \times m$ matrix and $E = \{1, \dots, m\}$, where $\mathbf{X}_{ij} \in \mathbb{F}$ for some field, and let \mathcal{I} be the set of subsets of E such that the columns of \mathbf{X} are linearly independent over \mathbb{F} .

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- We can more generally define matroids on a field.

Definition 7.7.3 (representable (as a linear matroid))

Any matroid isomorphic to a linear matroid on a field is called **representable over \mathbb{F}**

Representability of Transversal Matroids

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- In particular:

Theorem 7.7.4

Transversal matroids are representable over all finite fields of sufficiently large cardinality, and are representable over any infinite field.

Converse: Representability of Transversal Matroids

The converse is not true, however.

Example 7.7.5

Let $V = \{1, 2, 3, 4, 5, 6\}$ be a ground set and let $M = (V, \mathcal{I})$ be a set system where \mathcal{I} is all subsets of V of cardinality ≤ 2 except for the pairs $\{1, 2\}$, $\{3, 4\}$, $\{5, 6\}$.

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- It can be shown that this is a matroid and is representable.
- However, this matroid is not isomorphic to any transversal matroid.

Review from Lecture 6

The next frame comes from lecture 6.

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

Definition 7.8.3 (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 $r(M) - 1$.

Definition 7.8.4 (closure)

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

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

Definition 7.8.5 (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 $a \in A$, $r(A \setminus \{a\}) = |A| - 1$).

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- A base of a matroid is a minimal spanning set (and it is independent) but supersets of a base are also spanning.
- V is always trivially spanning.
- Consider the terminology: “spanning tree in a graph”, comes from spanning in a matroid sense.

Dual of a Matroid

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Theorem 7.8.3 (Dual matroid bases)

Let $M = (V, \mathcal{I})$ be a matroid and $\mathcal{B}(M)$ be the set of bases of M . Then define

$$\mathcal{B}^*(M) = \{V \setminus B : B \in \mathcal{B}(M)\}. \quad (7.33)$$

Then $\mathcal{B}^*(M)$ is the set of basis of M^* (that is, $\mathcal{B}^*(M) = \mathcal{B}(M^*)$).

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- All dependent sets in a cocycle matroid are cuts (i.e., a dependent set is a minimal cut or contains one).

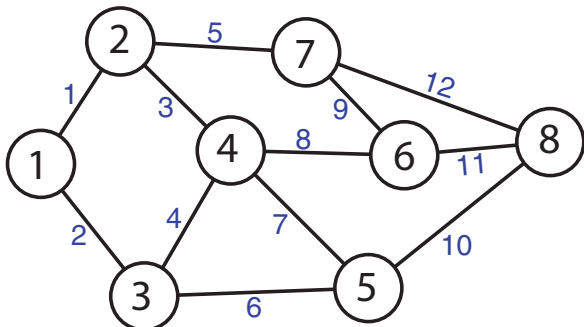
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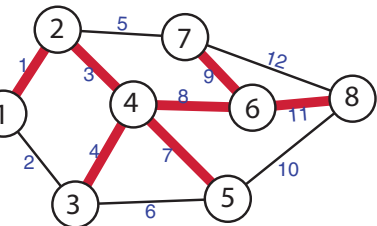
A graph G



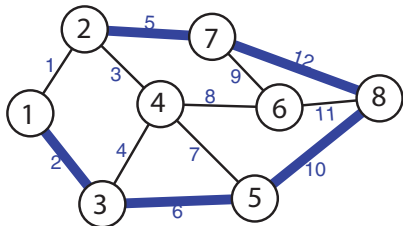
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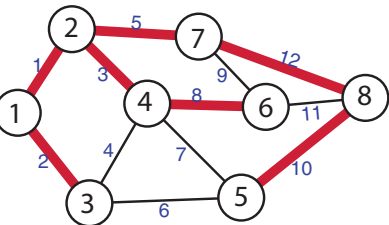
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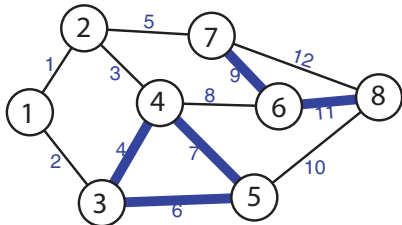
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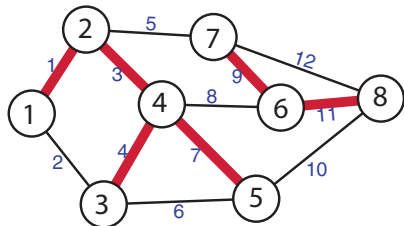
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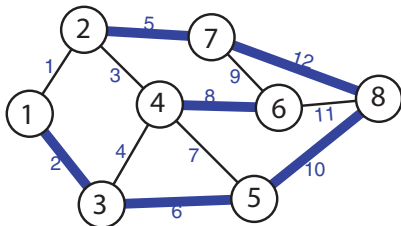
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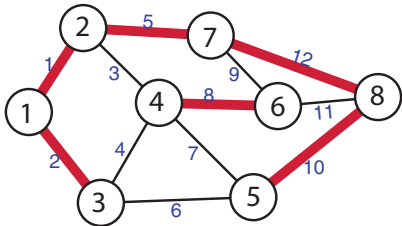
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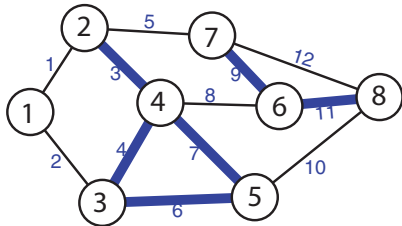
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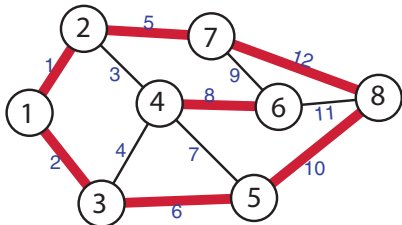
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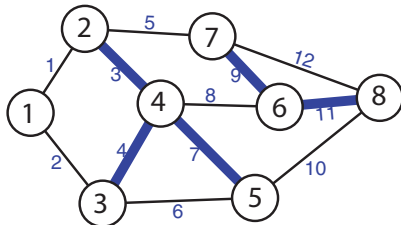
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A hyperplane in M , dependent but not spanning in M



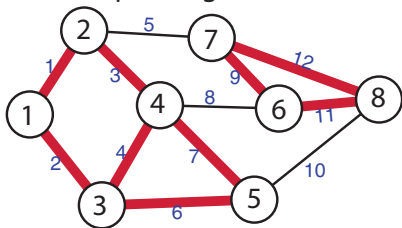
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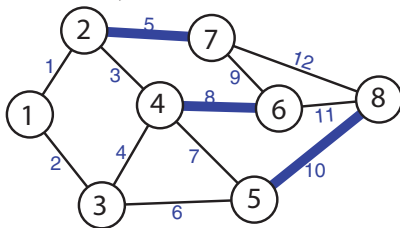
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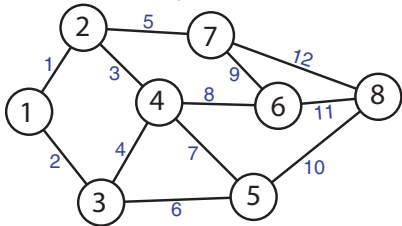
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Cycle Matroid - independent sets have no cycles.



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