Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 6 —

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

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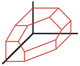
$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$$

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



Cumulative Outstanding Reading

- Read chapters 1 and 2, and sections 3.1-3.2 from Fujishige's book.

Announcements, Assignments, and Reminders

- Homework 1 is out, due Wednesday April 23rd, 11:45pm, electronically via our assignment dropbox (`https://canvas.uw.edu/courses/895956/assignments`).
- All homeworks must be done electronically, only PDF file format accepted.
- 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.

Matroid

Slight modification (non unit increment) that is equivalent.

Definition 6.2.1 (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)$\equiv$(I3') using induction.

Matroids - important property

Proposition 6.2.1

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 6.2.2 (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 $I_1, I_2 \in \text{maxInd}(X)$, we have $|I_1| = |I_2|$ (all maximally independent subsets of X have the same size).

Matroids - rank

- Thus, in any matroid $M = (E, \mathcal{I})$, $\forall U \subseteq E(M)$, any two bases of U have the same size.
- The common size of all the bases of U is called the rank of U, denoted $r_M(U)$ or just $r(U)$ when the matroid in equation is unambiguous.
- $r(E) = r_{(E,\mathcal{I})}$ is the rank of the matroid, and is the common size of all the bases of the matroid.
- We can a bit more formally define the rank function this way.

Definition 6.2.1 (matroid rank function)

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

$$r(A) = \max\{|X| : X \subseteq A, X \in \mathcal{I}\} = \max_{X \in \mathcal{I}} |A \cap X| \qquad (6.1)$$

- 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 - rank

Lemma 6.2.1

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

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

$$r(A) + r(B) \geq |Y \cap A| + |Y \cap B| \tag{6.3}$$
$$= |Y \cap (A \cap B)| + |Y \cap (A \cup B)| \tag{6.4}$$
$$\geq |X| + |Y| = r(A \cap B) + r(A \cup B) \tag{6.5}$$

□

Partition Matroid

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

$$\mathcal{I} = \{X \subseteq V : |X \cap V_i| \leq k_i \text{ for all } i = 1, \ldots, \ell\}. \tag{6.3}$$

  where $k_1, \ldots, k_\ell$ are fixed 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 $k_1, k_2, \ldots, k_\ell$ although often the k_i's are all the same.
- We'll show that property (I3') in Def **??** 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

- What is the partition matroid's rank function?
- A partition matroids rank function:

$$r(A) = \sum_{i=1}^{\ell} \min(|A \cap V_i|, k_i) \tag{6.12}$$

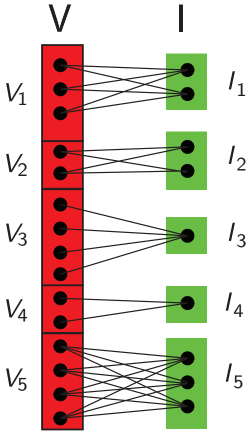
which we also immediately see is submodular using properties we spoke about last week. That is:

1. $|A \cap V_i|$ is submodular (in fact modular) in A
2. $\min(\text{submodular}(A), k_i)$ is submodular in A since $|A \cap V_i|$ is monotone.
3. sums of submodular functions are submodular.

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

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.

System of Representatives

- Let $(V, \mathcal{V})$ be a set system (i.e., $\mathcal{V} = (V_i : i \in I)$ where $\emptyset \subset V_i \subseteq V$ for all i), and I is an index set. Hence, $|I| = |\mathcal{V}|$.

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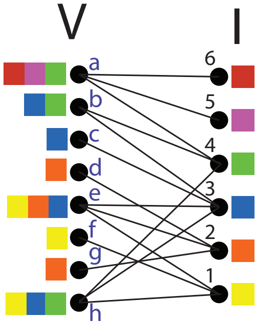
- Here, $\ell = 6$ groups, with $\mathcal{V} = (V_1, V_2, \dots, V_6)$ $= (\{e, f, h\}, \{d, e, g\}, \{b, c, e, h\}, \{a, b, h\}, \{a\}, \{a\})$.



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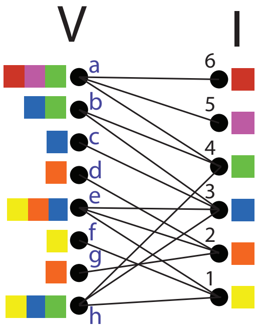

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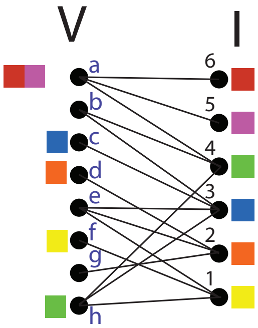

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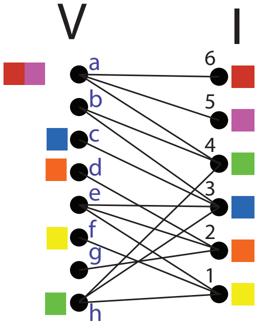

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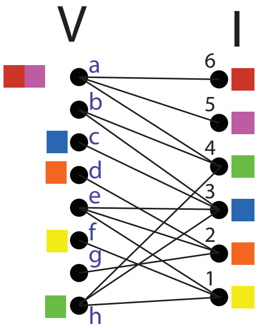

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- The representatives $(\{a, c, d, f, h\})$ are shown as colors on the left.
- Here, the set of representatives is not distinct. Why? In fact, due to the red and pink group, a distinct group of representatives is impossible (since there is only one common choice to represent both color groups).

System of Distinct Representatives

- Let $(V, \mathcal{V})$ be a set system (i.e., $\mathcal{V} = (V_k : i \in I)$ where $V_i \subseteq V$ for all i), and I is an index set. Hence, $|I| = |\mathcal{V}|$.

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Definition 6.3.1 (transversal)

Given a set system $(V, \mathcal{V})$ 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

$$x \in V_{\pi(x)} \text{ for all } x \in T \tag{6.1}$$

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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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- Therefore, for any transversal T, any subset $T' \subseteq T$ is a partial transversal.
- 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

$$V(J) = \cup_{j \in J} V_j \tag{6.2}$$

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- We have

Theorem 6.4.1 (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 $J \subseteq I$

$$|V(J)| \geq |J| \tag{6.3}$$

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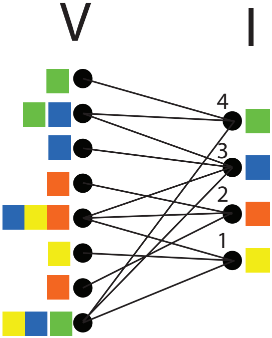

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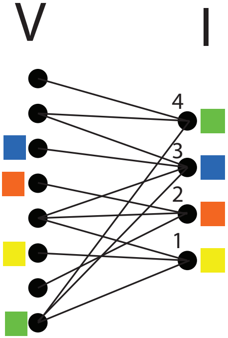

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$$V(J) = \cup_{j \in J} V_j \tag{6.2}$$

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

- Moreover, we have

Theorem 6.4.2 (Rado's theorem (1942))

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 6.4.3 (Polymatroid transversal theorem)

If $\mathcal{V} = (V_i : i \in I)$ is a finite family of non-empty subsets of V, and $f : 2^V \to \mathbb{Z}_+$ 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

$$f(\cup_{i \in J}\{v_i\}) \geq |J| \text{ for all } J \subseteq I \tag{6.5}$$

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- Given Theorem 6.4.3, we immediately get Theorem 6.4.1 by taking $f(S) = |S|$ for $S \subseteq V$. *In which case, Eq. 6.5 requires the system of representatives to be distinct.*

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- We get Theorem 6.4.2 by taking $f(S) = r(S)$ for $S \subseteq V$, the rank function of the matroid. *where, Eq. 6.5 insists the system of representatives is independent in M.*

Submodular Composition with Set-to-Set functions

- Note the condition in Theorem 6.4.3 is $f(V(J)) \geq |J|$ for all $J \subseteq I$, where $f : 2^V \to \mathbb{Z}_+$ 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 verse!

More general conditions for existence of transversals

first part proof of Theorem 6.4.3.

- Suppose $\mathcal{V}$ has a system of representatives $(v_i : i \in I)$ such that Eq. 6.5 is true.

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first part proof of Theorem 6.4.3.

- Suppose $\mathcal{V}$ has a system of representatives $(v_i : i \in I)$ such that Eq. 6.5 is true.
- 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. 6.6 immediately follows.

...

More general conditions for existence of transversals

Lemma 6.4.5 (contraction lemma)

Suppose Eq. 6.6 ($f(V(J)) \geq |J|, \forall J \subseteq I$) 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 $(V_1 \setminus \{\bar{v}\}, V_2, \ldots, V_{|I|})$ also satisfies Eq 6.6.

Proof.

- When Eq. 6.6 holds, this means that for any subsets $J_1, J_2 \subseteq I \setminus \{1\}$, we have that, for $J \in \{J_1, J_2\}$,

$$f(V(J \cup \{1\})) \geq |J \cup \{1\}| \tag{6.8}$$

and hence

$$f(V_1 \cup V(J_1)) \geq |J_1| + 1 \tag{6.9}$$
$$f(V_1 \cup V(J_2)) \geq |J_2| + 1 \tag{6.10}$$

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- Suppose, to the contrary, the consequent is false. Then we may take any $\bar{v}_1, \bar{v}_2 \in V_1$ as two distinct elements in V_1 ...

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Proof.

- Suppose, to the contrary, the consequent is false. Then we may take any $\bar{v}_1, \bar{v}_2 \in V_1$ as two distinct elements in V_1 ...
- ...and there must exist subsets J_1, J_2 of $I \setminus \{1\}$ such that

$$f((V_1 \setminus \{\bar{v}_1\}) \cup V(J_1)) < |J_1| + 1, \tag{6.11}$$

$$f((V_1 \setminus \{\bar{v}_2\}) \cup V(J_2)) < |J_2| + 1, \tag{6.12}$$

(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:

$$X \cup Y = V_1 \cup V(J_1 \cup J_2), \tag{6.13}$$

$$X \cap Y \supseteq V(J_1 \cap J_2), \tag{6.14}$$

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- since f submodular monotone non-decreasing, & Eqs 6.13-6.15,

$$|J_1| + |J_2| \geq f(V_1 \cup V(J_1 \cup J_2)) + f(V(J_1 \cap J_2)) \tag{6.16}$$

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- Since $\mathcal{V}$ satisfies Eq. 6.6, $1 \notin J_1 \cup J_2$, & Eqs 6.9-6.10, this gives

$$|J_1| + |J_2| \geq |J_1 \cup J_2| + 1 + |J_1 \cap J_2| \tag{6.17}$$

which is a contradiction since cardinality is modular.

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- W.l.o.g., let $|V_1| \geq 2$, then by Lemma 6.4.5, the family of subsets $(V_1 \setminus \{\bar{v}\}, V_2, \ldots, V_{|I|})$ also satisfies Eq 6.6 for the right $\bar{v}$.

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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 6.5.1

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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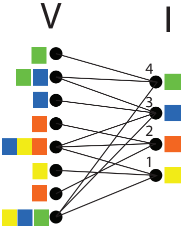
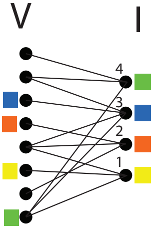
- A matching in this graph is a set of edges no two of which that have a common endpoint.





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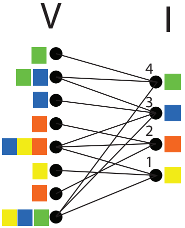

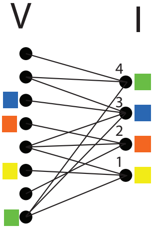

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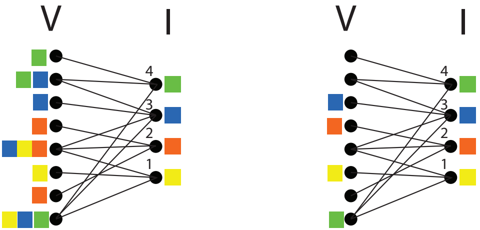
- A matching in this graph is a set of edges no two of which that have a common endpoint. In fact, we easily have:

Lemma 6.5.2

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).



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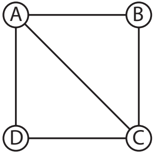

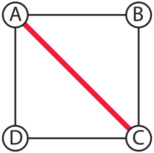

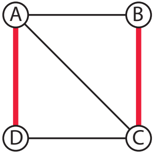

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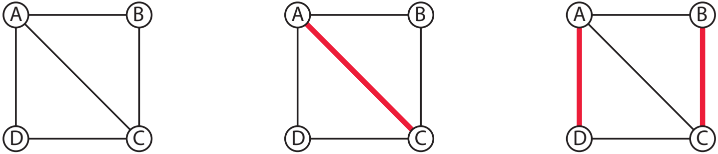
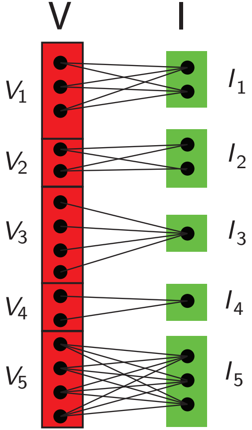


- $\{AC\}$ is a maximum matching, as is $\{AD, BC\}$, but they are not the same size.

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.

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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- We start with partition matroid rank function in the subsequent equations.

$$r(A) = \sum_{i=1}^{\ell} \min(|A \cap V_i|, k_i) \tag{6.18}$$

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- 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, $V(J) = \cup_{j \in J} V_j$).
- We start with partition matroid rank function in the subsequent equations.

$$r(A) = \sum_{i=1}^{\ell} \min(|A \cap V_i|, k_i) \tag{6.18}$$

$$= \sum_{i=1}^{\ell} \min(|A \cap V(I_i)|, |I_i|) \tag{6.19}$$

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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 6.5.3

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.

$\square$

Transversal Matroid Rank

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- Therefore, this function is submodular.
- Note that it is a minimum over a set of modular functions. Is this true in general? Exercise:

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 matric (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 6.6.1 (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 $\pi : V_1 \to V_2$ 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 GF(p) where p is prime (such as GF(2)). Succinctly: A field is a set with $+$, $*$, closure, associativity, commutativity, and additive and multiplictaive identities and inverses.

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Definition 6.6.2 (linear matroids on a field)

Let $\mathbf{X}$ be an $n \times m$ matrix and $E = \{1, \ldots, m\}$, 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 6.6.3 (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 6.6.4

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 6.6.5

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.

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

Definition 6.7.1 (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 $r(M) - 1$.

Definition 6.7.2 (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 6.7.3 (circuit)

A subset $A \subseteq E$ is circuit or a cycle if it is an <u>inclusionwise-minimal dependent set</u> (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

- Given a matroid $M = (V, \mathcal{I})$, a dual matroid $M^* = (V, \mathcal{I}^*)$ can be defined on the same ground set V, but using a very different set of independent sets $\mathcal{I}^*$.

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- Dual of the dual: Note, we have that $(M^*)^* = M$.