Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 13 —

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

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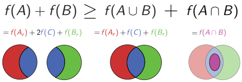
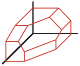




Cumulative Outstanding Reading

- Good references for today: Schrijver-2003, Oxley-1992/2011, Welsh-1973, Goemans-2010, Cunningham-1984, Edmonds-1969.
- Read Tom McCormick's overview paper on SFM http://people.commerce.ubc.ca/faculty/mccormick/sfmchap8a.pdf
- Read chapters 1 - 4 from Fujishige book.
- Matroid properties http://www-math.mit.edu/~goemans/18433S09/matroid-notes.pdf

Announcements, Assignments, and Reminders

- 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, exchange capacity, minimum norm point algorithm and the lattice of minimizers of a submodular function, Lovasz extension
- L16:
- L17:
- L18:
- L19:
- L20:

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

Tight sets $\mathcal{D}(y)$ are closed, and max tight set $\text{sat}(y)$

Recall the definition of the set of tight sets at $y \in P_f^+$:

$$\mathcal{D}(y) \triangleq \{A : A \subseteq E, \; y(A) = f(A)\} \tag{13.18}$$

Theorem 13.2.1

For any $y \in P_f^+$, with f a polymatroid function, then $\mathcal{D}(y)$ is closed under union and intersection.

Proof.

We have already proven this as part of Theorem **??** □

Also recall the definition of $\text{sat}(y)$, the maximal set of tight elements relative to $y \in \mathbb{R}_+^E$.

$$\text{sat}(y) \stackrel{\text{def}}{=} \bigcup \{T : T \in \mathcal{D}(y)\} \tag{13.19}$$

Fundamental circuits in matroids

Lemma 13.2.3

Let $I \in \mathcal{I}(M)$, and $e \in E$, then $I \cup \{e\}$ contains at most one circuit in M.

Proof.

- Suppose, to the contrary, that there are two distinct circuits C_1, C_2 such that $C_1 \cup C_2 \subseteq I \cup \{e\}$.
- Then $e \in C_1 \cap C_2$, and by (C2), there is a circuit C_3 of M s.t. $C_3 \subseteq (C_1 \cup C_2) \setminus \{e\} \subseteq I$
- This contradicts the independence of I.

$\square$

In general, let $C(I, e)$ be the unique circuit associated with $I \cup \{e\}$ (commonly called the fundamental circuit in M w.r.t. I and e).

Matroid Partition Problem

Theorem 13.2.1

Let M_i be a collection of k matroids as described. Then, a set $S \subseteq E$ can be partitioned into k subsets $I_i, i = 1 \dots k$ where $I_i \in \mathcal{I}_i$ is independent in matroid i, if and only if, for all $A \subseteq S$

$$|A| \leq \sum_{i=1}^{k} r_i(A) \tag{13.1}$$

where r_i is the rank function of M_i.

- Now, if all matroids are the same $M_i = M$ for all i, we get condition

$$|A| \leq kr(A) \;\; \forall A \subseteq E \tag{13.2}$$

- But considering vector of all ones $\mathbf{1} \in \mathbb{R}_+^E$, this is the same as

$$\frac{1}{k}|A| = \frac{1}{k}\mathbf{1}(A) \leq r(A) \;\; \forall A \subseteq E \tag{13.3}$$

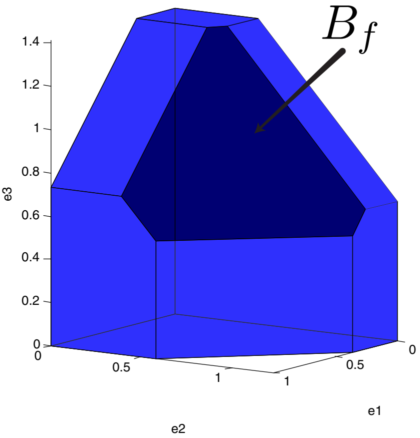
Polymatroidal polyhedron and greedy

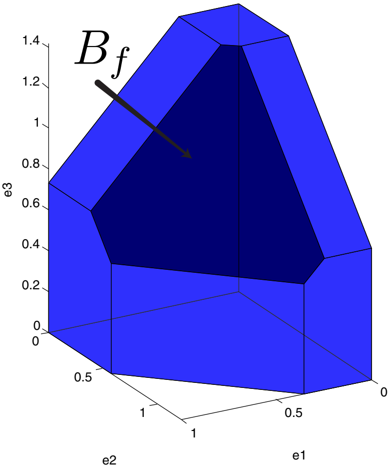
- Thus, restating the above results into a single complete theorem, we have a result very similar to what we saw for matroids (i.e., Theorem **??**)

Theorem 13.2.1

If $f : 2^E \to \mathbb{R}_+$ *is given, and* P *is a polytope in* $\mathbb{R}_+^E$ *of the form* $P = \left\{x \in \mathbb{R}_+^E : x(A) \leq f(A), \forall A \subseteq E\right\}$*, then the greedy solution to the problem* $\max(wx : x \in P)$ *is* $\forall w$ *optimum iff* f *is monotone non-decreasing submodular (i.e., iff* P *is a polymatroid).*

Base Polytope in 3D





$$P_f = \left\{x \in \mathbb{R}^E : x(S) \le f(S), \forall S \subseteq E\right\} \tag{13.5}$$

$$B_f = P_f \cap \left\{x \in \mathbb{R}^E : x(E) = f(E)\right\} \tag{13.6}$$

Polymatroid extreme points

Theorem 13.2.1

For a given ordering $E = (e_1, \dots, e_m)$ of E and a given $E_i = (e_1, \dots, e_i)$ and x generated by E_i using the greedy procedure ($x(e_i) = f(e_i|E_{i-1})$), then x is an extreme point of P_f

Proof.

- We already saw that $x \in P_f$ (Theorem **??**).
- To show that x is an extreme point of P_f, note that it is the unique solution of the following system of equations

$$x(E_j) = f(E_j) \text{ for } 1 \leq j \leq i \leq m \tag{13.9}$$

$$x(e) = 0 \text{ for } e \in E \setminus E_i \tag{13.10}$$

There are $i \leq m$ equations and $i \leq m$ unknowns, and simple Gaussian elimination gives us back the x constructed via the Greedy algorithm!!

Polymatroid extreme points

- Moreover, we have (and will ultimately prove)

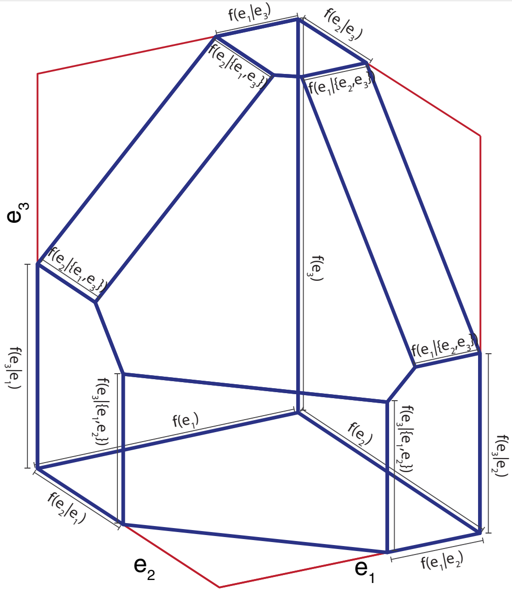
Corollary 13.2.2

If x is an extreme point of P_f and $B \subseteq E$ is given such that $\text{supp}(x) = \{e \in E : x(e) \neq 0\} \subseteq B \subseteq \cup(A : x(A) = f(A)) = \text{sat}(x)$, then x is generated using greedy by some ordering of B.

- Note, $\text{sat}(x) = \text{cl}(x) = \cup(A : x(A) = f(A))$ is also called the closure of x (recall that sets A such that $x(A) = f(A)$ are called tight, and such sets are closed under union and intersection, as seen in Lecture 8, Theorem **??**)
- Thus, $\text{cl}(x)$ is a tight set.
- Also, $\text{supp}(x) = \{e \in E : x(e) \neq 0\}$ is called the support of x.
- For arbitrary x, $\text{supp}(x)$ is not necessarily tight, but for an extreme point, $\text{supp}(x)$ is.

Polymatroid with labeled edge lengths

- Recall $f(e|A) = f(A+e) - f(A)$
- Notice how submodularity, $f(e|B) \leq f(e|A)$ for $A \subseteq B$, defines the shape of the polytope.
- In fact, we have strictness here $f(e|B) < f(e|A)$ for $A \subset B$.
- Also, consider how the greedy algorithm proceeds along the edges of the polytope.



Minimizers of a Submodular Function form a lattice

Theorem 13.2.2

For arbitrary submodular f, the minimizers are closed under union and intersection. That is, let $\mathcal{M} = \operatorname{argmin}_{X \subseteq E} f(X)$ be the set of minimizers of f. Let $A, B \in \mathcal{M}$. Then $A \cup B \in \mathcal{M}$ and $A \cap B \in \mathcal{M}$.

Proof.

Since A and B are minimizers, we have $f(A) = f(B) \leq f(A \cap B)$ and $f(A) = f(B) \leq f(A \cup B)$.
By submodularity, we have

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{13.8}$$

Hence, we must have $f(A) = f(B) = f(A \cup B) = f(A \cap B)$. □

Thus, the minimizers of a submodular function form a lattice, and there is a maximal and a minimal minimizer of every submodular function.

The sat function = Polymatroid Closure

- Matroid closure is generalized by the unique maximal element in $\mathcal{D}(x)$, also called the polymatroid closure or sat (saturation function).
- For some $x \in P_f$, we have defined:

$$\mathsf{cl}(x) \stackrel{\text{def}}{=} \mathrm{sat}(x) \stackrel{\text{def}}{=} \bigcup \{A : A \in \mathcal{D}(x)\} \tag{13.8}$$

$$= \bigcup \{A : A \subseteq E, x(A) = f(A)\} \tag{13.9}$$

$$= \{e : e \in E, \forall \alpha > 0, x + \alpha \mathbf{1}_e \notin P_f\} \tag{13.10}$$

- Hence, $\mathrm{sat}(x)$ is the maximal (zero-valued) minimizer of the submodular function $f_x(A) \triangleq f(A) - x(A)$.
- Eq. (**??**) says that sat consists of any point x that is P_f saturated (any additional positive movement, in that dimension, leaves P_f). We'll revisit this in a few slides.
- First, we see how sat generalizes matroid closure.

The sat function = Polymatroid Closure

- Consider matroid $(E, \mathcal{I}) = (E, r)$, some $I \in \mathcal{I}$. Then $\mathbf{1}_I \in P_r$ and

$$\mathcal{D}(\mathbf{1}_I) = \{A : \mathbf{1}_I(A) = r(A)\} \tag{13.1}$$

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and

$$\mathrm{sat}(\mathbf{1}_I)$$

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$$= \bigcup \{A : A \subseteq E, |I \cap A| = r(A)\} \tag{13.4}$$

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- Notice that $\mathbf{1}_I(A) = |I \cap A| \leq |I|$.

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- Notice that $\mathbf{1}_I(A) = |I \cap A| \leq |I|$.
- Intuitively, consider an $A \supset I \in \mathcal{I}$ that doesn't increase rank, meaning $r(A) = r(I)$. If $r(A) = |I \cap A| = r(I \cap A)$, as in Eqn. (13.4), then A is in I's span, so should get $\mathrm{sat}(\mathbf{1}_I) = \mathrm{span}(I)$.

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- We formalize this next.

The sat function = Polymatroid Closure

Lemma 13.3.1 (Matroid $\mathrm{sat} : \mathbb{R}_+^E \to 2^E$ is the same as closure.)

For $I \in \mathcal{I}$, we have $$\mathrm{sat}(\mathbf{1}_I) = \mathrm{span}(I) \tag{13.5}$$

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Proof.

- For $\mathbf{1}_I(I) = |I| = r(I)$, so $I \in \mathcal{D}(\mathbf{1}_I)$ and $I \subseteq \text{sat}(\mathbf{1}_I)$. Also, $I \subseteq \text{span}(I)$.

...

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- Consider some $b \in \text{span}(I) \setminus I$.

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- Consider some $b \in \mathrm{span}(I) \setminus I$.
- Then $I \cup \{b\} \in \mathcal{D}(\mathbf{1}_I)$ since $\mathbf{1}_I(I \cup \{b\}) = |I| = r(I \cup \{b\}) = r(I)$.

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Lemma 13.3.1 (Matroid $\text{sat} : \mathbb{R}_+^E \to 2^E$ is the same as closure.)

For $I \in \mathcal{I}$, we have $\text{sat}(\mathbf{1}_I) = \text{span}(I)$ (13.5)

Proof.

- For $\mathbf{1}_I(I) = |I| = r(I)$, so $I \in \mathcal{D}(\mathbf{1}_I)$ and $I \subseteq \text{sat}(\mathbf{1}_I)$. Also, $I \subseteq \text{span}(I)$.
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- Thus, $b \in \text{sat}(\mathbf{1}_I)$.
- Therefore, $\text{sat}(\mathbf{1}_I) \supseteq \text{span}(I)$.

...

The sat function = Polymatroid Closure

. . . proof continued.

- Now, consider $b \in \text{sat}(\mathbf{1}_I) \setminus I$.

$\square$

The sat function = Polymatroid Closure

. . . proof continued.

- Now, consider $b \in \text{sat}(\mathbf{1}_I) \setminus I$.
- Choose any $A \in \mathcal{D}(\mathbf{1}_I)$ with $b \in A$, thus $b \in A \setminus I$.

□

The sat function = Polymatroid Closure

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- Now, consider $b \in \text{sat}(\mathbf{1}_I) \setminus I$.
- Choose any $A \in \mathcal{D}(\mathbf{1}_I)$ with $b \in A$, thus $b \in A \setminus I$.
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- Now $r(A) = |A \cap I| \leq |I| = r(I)$.

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- Now $r(A) = |A \cap I| \leq |I| = r(I)$.
- Also, $r(A \cap I) = |A \cap I|$ since $A \cap I \in \mathcal{I}$.

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- Also, $r(A \cap I) = |A \cap I|$ since $A \cap I \in \mathcal{I}$.
- Hence, $r(A \cap I) = r(A) = r((A \cap I) \cup (A \setminus I))$ meaning $(A \setminus I) \subseteq \text{span}(A \cap I) \subseteq \text{span}(I)$.

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- Since $b \in A \setminus I$, we get $b \in \text{span}(I)$.

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The sat function = Polymatroid Closure

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- Since $b \in A \setminus I$, we get $b \in \text{span}(I)$.
- Thus, $\text{sat}(\mathbf{1}_I) \subseteq \text{span}(I)$.

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- Since $b \in A \setminus I$, we get $b \in \text{span}(I)$.
- Thus, $\boxed{\text{sat}(\mathbf{1}_I) \subseteq \text{span}(I)}$.
- Hence $\boxed{\text{sat}(\mathbf{1}_I) = \text{span}(I)}$

$\square$

The sat function = Polymatroid Closure

- Now, consider a matroid (E, r) and some $C \subseteq E$ with $C \notin \mathcal{I}$, and consider $\mathbf{1}_C$.

The sat function = Polymatroid Closure

- Now, consider a matroid (E, r) and some $C \subseteq E$ with $C \notin \mathcal{I}$, and consider $\mathbf{1}_C$. Is $\mathbf{1}_C \in P_r$?

The sat function = Polymatroid Closure

- Now, consider a matroid (E, r) and some $C \subseteq E$ with $C \notin \mathcal{I}$, and consider $\mathbf{1}_C$. Is $\mathbf{1}_C \in P_r$? No, it might not be a vertex, or even a member, of P_r.

The sat function = Polymatroid Closure

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$$\mathrm{sat}(\mathbf{1}_C) \triangleq \mathrm{sat}(\mathbf{1}_B) \text{ for } B \in \mathcal{B}(C) \tag{13.6}$$

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Exercise: is $\text{span}(C) = \text{sat}(\mathbf{1}_C)$? Prove or disprove it.

The sat function, span, and submodular function minimization

- Thus, for a matroid, $\mathrm{sat}(\mathbf{1}_I)$ is exactly the closure (or span) of I in the matroid. I.e., for matroid (E, r), we have $\mathrm{span}(I) = \mathrm{sat}(\mathbf{1}_B)$.

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- Recall, for $x \in P_f$ and polymatroidal f, $\text{sat}(x)$ is the maximal (by inclusion) minimizer of $f(A) - x(A)$, and thus in a matroid, span(I) is the maximal minimizer of the submodular function formed by $r(A) - \mathbf{1}_I(A)$.

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- Submodular function minimization can solve "span" queries in a matroid or "sat" queries in a polymatroid.

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- We next show more formally that these are the same.

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- So now, if A is any set such that $x(A) = f(A)$, then we clearly have

$$\forall e \in A, e \in \operatorname{sat}(x), \text{ and therefore that } \operatorname{sat}(x) \supseteq A \tag{13.16}$$

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- . . . and therefore, with sat as defined in Eq. (**??**),

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- On the other hand, for any $e \in \text{sat}(x)$ defined as in Eq. (13.15), since e is itself a member of a tight set, there is a set $A \ni e$ such that $x(A) = f(A)$, giving

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- Therefore, the two definitions of sat are identical.

Saturation Capacity

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Saturation Capacity

- The max is achieved when

$$\alpha = \hat{c}(x;e) \stackrel{\text{def}}{=} \min\{f(A) - x(A), \forall A \supseteq \{e\}\} \tag{13.23}$$

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- Note that any α with $0 \leq \alpha \leq \hat{c}(x;e)$ we have $x + \alpha \mathbf{1}_e \in P_f$.

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- $\hat{c}(x;e)$ is known as the saturation capacity associated with $x \in P_f$ and e.
- Thus we have for $x \in P_f$,
$$\hat{c}(x;e) \stackrel{\text{def}}{=} \min\{f(A) - x(A), \forall A \ni e\} \tag{13.24}$$
$$= \max\{\alpha : \alpha \in \mathbb{R}, x + \alpha \mathbf{1}_e \in P_f\} \tag{13.25}$$
- We immediately see that for $e \in E \setminus \text{sat}(x)$, we have that $\hat{c}(x;e) > 0$.
- Also, for $e \in \text{sat}(x)$, we have that $\hat{c}(x;e) = 0$.
- Note that any α with $0 \leq \alpha \leq \hat{c}(x;e)$ we have $x + \alpha \mathbf{1}_e \in P_f$.
- We also see that computing $\hat{c}(x;e)$ is a form of submodular function minimization.

Dependence Function

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$$\mathcal{D}(x,e) = \{A : e \in A \subseteq E, x(A) = f(A)\} \tag{13.26}$$

$$= \mathcal{D}(x) \cap \{A : A \subseteq E, e \in A\} \tag{13.27}$$

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- Therefore, we can define a unique minimal element of $\mathcal{D}(x, e)$ denoted as follows:

$$\text{dep}(x, e) = \begin{cases} \bigcap \{A : e \in A \subseteq E, x(A) = f(A)\} & \text{if } e \in \text{sat}(x) \\ \emptyset & \text{else} \end{cases} \tag{13.28}$$

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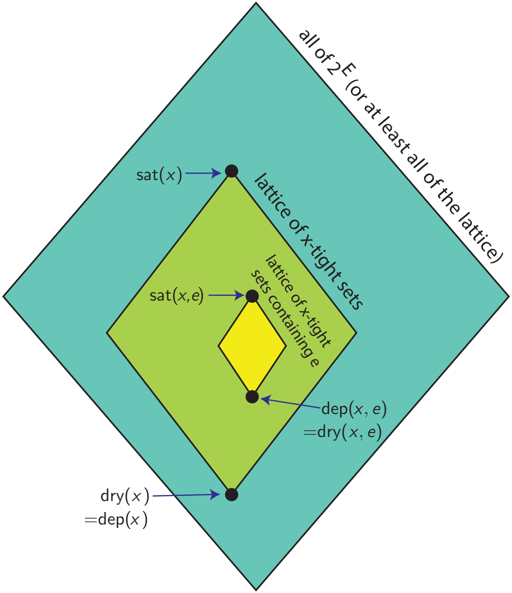
- I.e., $\text{dep}(x,e)$ is the minimal element in $\mathcal{D}(x)$ that contains e (the minimal x-tight set containing e).

dep and sat in a lattice

- Given some $x \in P_f$,
- The picture on the right summarizes the relationships between the lattices and sublattices.
- Note, $\bigcap_e \text{dep}(x, e) = \text{dep}(x)$.



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- Note that dry need not be the empty set. Exercise: give example.

An alternate expression for $\text{dep} = \text{dry}$

- Now, given $x \in P_f$, and $e \in \text{sat}(x)$, recall distributive sub-lattice of e-containing tight sets $\mathcal{D}(x, e) = \{A : e \in A, x(A) = f(A)\}$

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- This can be read as, for any $e' \in \text{dry}(x, e)$, any e-containing set that does not contain e' is not tight for x.
- But actually, $\text{dry}(x, e) = \text{dep}(x, e)$, so we have derived another expression for $\text{dep}(x, e)$ in Eq. (13.30).

Dependence Function and Fundamental Matroid Circuit

- Now, let $(E, \mathcal{I}) = (E, r)$ be a matroid, and let $I \in \mathcal{I}$ giving $\mathbf{1}_I \in P_r$. We have $\text{sat}(\mathbf{1}_I) = \text{span}(I) = \text{closure}(I)$.

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- By SFM lattice, $\exists$ a unique minimal $A \ni e$ with $|I \cap A| = r(A)$.
- Thus, $\text{dep}(\mathbf{1}_I, e)$ must be a circuit since if it included more than a circuit, it would not be minimal in this sense.

Dependence Function and Fundamental Matroid Circuit

- Therefore, when $e \in \text{sat}(\mathbf{1}_I) \setminus I$, then $\text{dep}(\mathbf{1}_I, e) = C(I, e)$ where $C(I, e)$ is the unique circuit contained in $I + e$ in a matroid (the fundamental circuit of e and I that we encountered before).

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- We are thus free to take subsets of I as A, all of which must contain e, but all of which have rank equal to size.
- Also note: in general for $x \in P_f$ and $e \in \text{sat}(x)$, we have $\text{dep}(x, e)$ is tight by definition.

Summary of sat, and dep

- For $x \in P_f$, $\text{sat}(x)$ (span, closure) is the maximal saturated (x-tight) set w.r.t. x. I.e., $\text{sat}(x) = \{e : e \in E, \forall \alpha > 0, x + \alpha \mathbf{1}_e \notin P_f\}$. That is,

$$\text{cl}(x) \stackrel{\text{def}}{=} \text{sat}(x) \triangleq \bigcup \{A : A \in \mathcal{D}(x)\} \tag{13.34}$$

$$= \bigcup \{A : A \subseteq E, x(A) = f(A)\} \tag{13.35}$$

$$= \{e : e \in E, \forall \alpha > 0, x + \alpha \mathbf{1}_e \notin P_f\} \tag{13.36}$$

- For $e \in \text{sat}(x)$, we have $\text{dep}(x, e)$ (fundamental circuit) is the minimal (common) saturated (x-tight) set w.r.t. x containing e. That is,

$$\text{dep}(x, e) = \begin{cases} \bigcap \{A : e \in A \subseteq E, x(A) = f(A)\} & \text{if } e \in \text{sat}(x) \\ \emptyset & \text{else} \end{cases}$$

$$= \left\{e' : \exists \alpha > 0, \text{ s.t. } x + \alpha(\mathbf{1}_e - \mathbf{1}_{e'}) \in P_f\right\} \tag{13.37}$$

Dependence Function and exchange

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- Analogously, for $e \in \text{sat}(x)$, any $x + \alpha \mathbf{1}_e \notin P_f$ for $\alpha > 0$. This is a vector increase restriction property.
- Recall, we have $C(I, e) \setminus e' \in \mathcal{I}$ for $e' \in C(I, e)$. I.e., $C(I, e)$ consists of elements that when removed recover independence.

Dependence Function and exchange

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- Analogously, for $e \in \text{sat}(x)$, any $x + \alpha \mathbf{1}_e \notin P_f$ for $\alpha > 0$. This is a vector increase restriction property.
- Recall, we have $C(I, e) \setminus e' \in \mathcal{I}$ for $e' \in C(I, e)$. I.e., $C(I, e)$ consists of elements that when removed recover independence.
- In other words, for $e \in \text{span}(I) \setminus I$, we have that

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- But, analogous to the circuit case, is there an exchange property for $\text{dep}(x, e)$ in the form of vector movement restriction?
- We might expect the vector $\text{dep}(x, e)$ property to take the form: a positive move in the e-direction stays within P_f^+ only if we simultaneously take a negative move in one of the $\text{dep}(x, e)$ directions.

Dependence Function and exchange in 2D

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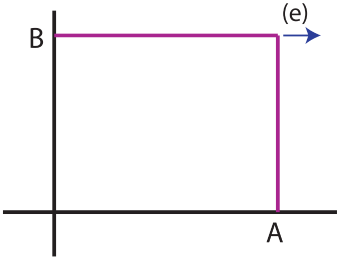
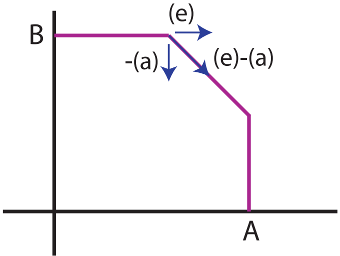
- Viewable in 2D, we have for $A, B \subseteq E$, $A \cap B = \emptyset$:



Left: $A \cap \mathrm{dep}(x, e) = \emptyset$, and we can't move further in (e) direction, and moving in any negative $a \in A$ direction doesn't change that. Notice no dependence between (e) and any element in A.



Right: $A \subseteq \mathrm{dep}(x, e)$, and we can't move further in the (e) direction, but we can move further in (e) direction by moving in some $a \in A$ negative direction. Notice dependence between (e) and elements in A.

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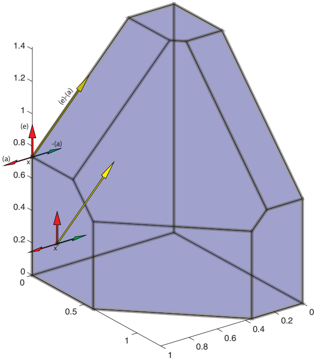

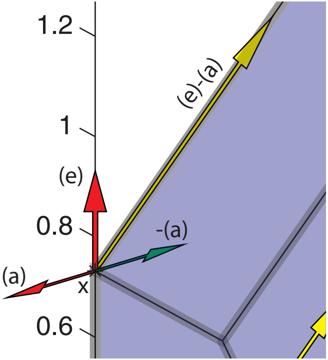

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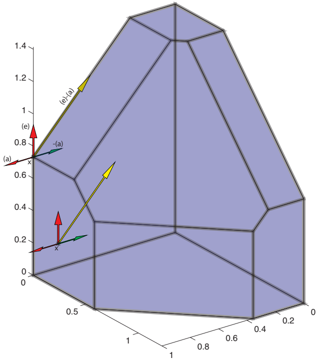

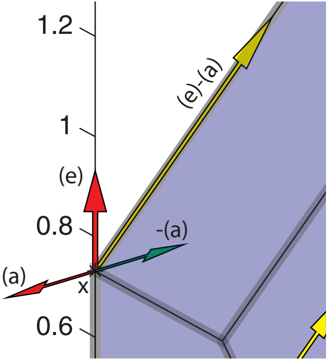

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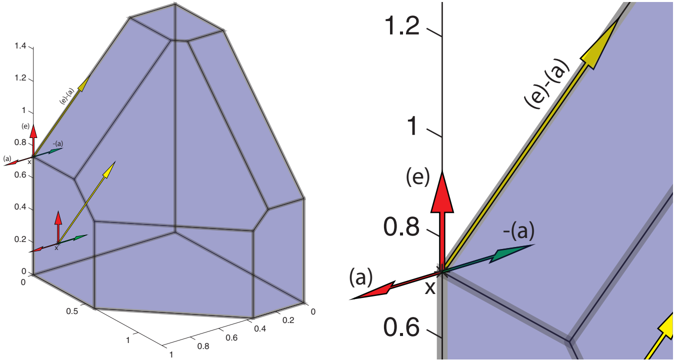

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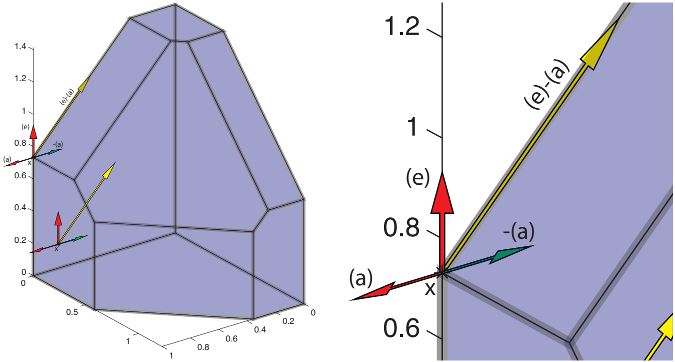

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- We next show this formally . . .

dep and exchange derived

- The derivation for $\mathrm{dep}(x, e)$ involves turning a strict inequality into a non-strict one with a strict explicit slack variable α:

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- Now, $1_e(A) - \mathbf{1}_{e'}(A) = 0$ if either $\{e, e'\} \subseteq A$, or $\{e, e'\} \cap A = \emptyset$.
- Also, if $e' \in A$ but $e \notin A$, then $x(A) + \alpha(\mathbf{1}_e(A) - \mathbf{1}_{e'}(A)) = x(A) - \alpha \leq f(A)$ since $x \in P_f$.

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- thus, we get the same in the above if we remove the constraint $A \not\ni e', e \in A$, that is we get

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- Compare with original, the minimal element of $\mathcal{D}(x, e)$, with $e \in \text{sat}(x)$:

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