

Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 10 —

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

Prof. Jeff Bilmes

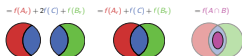
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May 5th, 2014



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



Cumulative Outstanding Reading

- Read chapters 1 and 2, and sections 3.1-3.2 from Fujishige's book.
- Good references for today: Schrijver-2003, Oxley-1992/2011, Welsh-1973, Goemans-2010, Cunningham-1984, Edmonds-1969.

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:
- L13:
- L14:
- L15:
- L16:
- L17:
- L18:
- L19:
- L20:

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

Maximum weight independent set via greedy weighted rank

Theorem 10.2.6

Let $M = (V, \mathcal{I})$ be a matroid, with rank function r , then for any weight function $w \in \mathbb{R}_+^V$, there exists a chain of sets $U_1 \subset U_2 \subset \cdots \subset U_n \subseteq V$ such that

$$\max \{w(I) | I \in \mathcal{I}\} = \sum_{i=1}^n \lambda_i r(U_i) \quad (10.19)$$

where $\lambda_i \geq 0$ satisfy

$$w = \sum_{i=1}^n \lambda_i \mathbf{1}_{U_i} \quad (10.20)$$

Polytope Equivalence (Summarizing the above)

- For each $I \in \mathcal{I}$ of a matroid $M = (E, \mathcal{I})$, we can form the incidence vector $\mathbf{1}_I$.
- Taking the convex hull, we get the **independent set polytope**, that is

$$P_{\text{ind. set}} = \text{conv} \{ \cup_{I \in \mathcal{I}} \{ \mathbf{1}_I \} \} \quad (10.12)$$

- Now take the rank function r of M , and define the following polyhedron:

$$P_r^+ = \{ x \in \mathbb{R}^E : x \geq 0, x(A) \leq r(A), \forall A \subseteq E \} \quad (10.13)$$

Theorem 10.2.2

$$P_r^+ = P_{\text{ind. set}} \quad (10.14)$$

P -basis of x given compact set $P \subseteq \mathbb{R}_+^E$

Definition 10.2.4 (subvector)

y is a subvector of x if $y \leq x$ (meaning $y(e) \leq x(e)$ for all $e \in E$).

Definition 10.2.5 (P -basis)

Given a compact set $P \subseteq \mathbb{R}_+^E$, for any $x \in \mathbb{R}_+^E$, a subvector y of x is called a **P -basis** of x if y maximal in P .

In other words, y is a P -basis of x if y is a maximal P -contained subvector of x .

Here, by y being “maximal”, we mean that there exists no $z > y$ (more precisely, no $z \geq y + \epsilon \mathbf{1}_e$ for some $e \in E$ and $\epsilon > 0$) having the properties of y (the properties of y being: in P , and a subvector of x).

In still other words: y is a P -basis of x if:

- ① $y \leq x$ (y is a subvector of x); and
- ② $y \in P$ and $y + \epsilon \mathbf{1}_e \notin P$ for all $e \in E$ where $y(e) < x(e)$ and $\forall \epsilon > 0$ (y is maximal P -contained).

A vector form of rank

- Recall the definition of rank from a matroid $M = (E, \mathcal{I})$.

$$\text{rank}(A) = \max \{|I| : I \subseteq A, I \in \mathcal{I}\} \quad (10.25)$$

- vector rank:** Given a compact set $P \subseteq \mathcal{R}_+^E$, we can define a form of “vector rank” relative to this P in the following way: Given an $x \in \mathbb{R}^E$, we define the vector rank, relative to P , as:

$$\text{rank}(x) = \max \{y(E) : y \leq x, y \in P\} \quad (10.26)$$

where $y \leq x$ is componentwise inequality ($y_i \leq x_i, \forall i$).

- If \mathcal{B}_x is the set of P -bases of x , then $\text{rank}(x) = \max_{y \in \mathcal{B}_x} y(E)$.
- If $x \in P$, then $\text{rank}(x) = x(E)$ (x is its own unique self P -basis).
- In general, this might be hard to compute and/or have ill-defined properties. We next look at an object that restrains and cultivates this form of rank.

Polymatroidal polyhedron (or a “polymatroid”)

Definition 10.2.4 (polymatroid)

A **polymatroid** is a compact set $P \subseteq \mathbb{R}_+^E$ satisfying

- ① $0 \in P$
 - ② If $y \leq x \in P$ then $y \in P$ (called **down monotone**).
 - ③ For every $x \in \mathbb{R}_+^E$, any maximal vector $y \in P$ with $y \leq x$ (i.e., any P -basis of x), has the same component sum $y(E)$
- Vectors within P (i.e., any $y \in P$) are called **independent**, and any vector outside of P is called **dependent**.
 - Since all P -bases of x have the same component sum, if \mathcal{B}_x is the set of P -bases of x , then $\text{rank}(x) = y(E)$ for any $y \in \mathcal{B}_x$.

Matroid and Polymatroid: side-by-side

A Matroid is:

- 1 a set system (E, \mathcal{I})
- 2 empty-set containing $\emptyset \in \mathcal{I}$
- 3 down closed, $\emptyset \subseteq I' \subseteq I \in \mathcal{I} \Rightarrow I' \in \mathcal{I}$.
- 4 any maximal set I in \mathcal{I} , bounded by another set A , has the same matroid rank (any maximal independent subset $I \subseteq A$ has same size $|I|$).

A Polymatroid is:

- 1 a compact set $P \subseteq \mathbb{R}_+^E$
- 2 zero containing, $\mathbf{0} \in P$
- 3 down monotone, $0 \leq y \leq x \in P \Rightarrow y \in P$
- 4 any maximal vector y in P , bounded by another vector x , has the same vector rank (any maximal independent subvector $y \leq x$ has same sum $y(E)$).

Polymatroid function and its polyhedron.

Definition 10.2.4

A **polymatroid function** is a real-valued function f defined on subsets of E which is normalized, non-decreasing, and submodular. That is we have

- ① $f(\emptyset) = 0$ (normalized)
- ② $f(A) \leq f(B)$ for any $A \subseteq B \subseteq E$ (monotone non-decreasing)
- ③ $f(A \cup B) + f(A \cap B) \leq f(A) + f(B)$ for any $A, B \subseteq E$
(submodular)

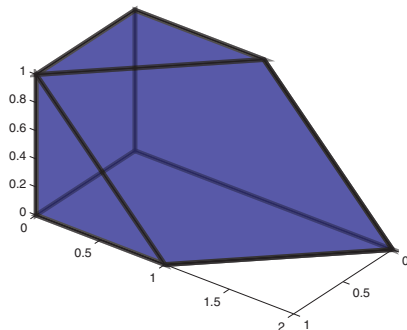
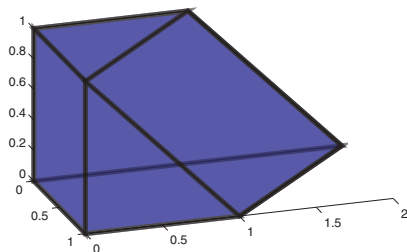
We can define the polyhedron P_f^+ associated with a polymatroid function as follows

$$P_f^+ = \{y \in \mathbb{R}_+^E : y(A) \leq f(A) \text{ for all } A \subseteq E\} \quad (10.25)$$

$$= \{y \in \mathbb{R}^E : y \geq 0, y(A) \leq f(A) \text{ for all } A \subseteq E\} \quad (10.26)$$

Associated polyhedron with a polymatroid function

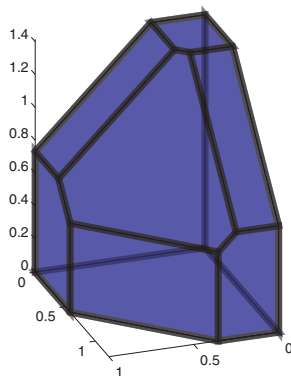
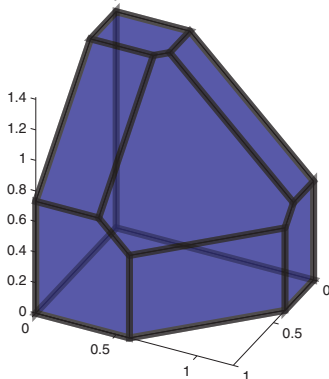
- Consider the asymmetric graph cut function on the simple chain graph $v_1 - v_2 - v_3$. That is, $f(S) = |\{(v, s) \in E(G) : v \in V, s \in S\}|$ is count of any edges within S or between S and $V \setminus S$, so that $\delta(S) = f(S) + f(V \setminus S) - f(V)$ is the standard graph cut.
- Observe: P_f^+ (at two views):



- which axis is which?

Associated polyhedron with a polymatroid function

- Consider modular function $w : V \rightarrow \mathbb{R}_+$ as $w = (1, 1.5, 2)^\top$, and then the submodular function $f(S) = \sqrt{w(S)}$.
- Observe: P_f^+ (at two views):



- which axis is which?

A polymatroid vs. a polymatroid function's polyhedron

- Summarizing the above, we have:
 - Given a **polymatroid function** f , its associated polytope is given as

$$P_f^+ = \{y \in \mathbb{R}_+^E : y(A) \leq f(A) \text{ for all } A \subseteq E\} \quad (10.34)$$

- We also have the definition of a **polymatroidal polytope** P (compact subset, zero containing, down-monotone, and $\forall x$ any maximal independent subvector $y \leq x$ has same component sum $y(E)$).
- Is there any relationship between these two polytopes?
- In the next theorem, we show that any P_f^+ -basis has the same component sum, when f is a polymatroid function, and P_f^+ satisfies the other properties so that P_f^+ is a polymatroid.

Proof.

- • •

Proof.

- Clearly $0 \in P_f^+$ since f is non-negative.
- Also, for any $y \in P_f^+$ then any $x \leq y$ is also such that $x \in P_f^+$.
So, P_f^+ is down-monotone.

...

A polymatroid function's polyhedron is a polymatroid.

Proof.

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So, P_f^+ is down-monotone.
- Now suppose that we are given an $x \in \mathbb{R}_+^E$, and maximal $y^x \in P_f^+$ with $y^x \leq x$ (i.e., y^x is a P_f^+ -basis of x).

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- Goal is to show that any such y^x has $y^x(E) = \text{const}$, dependent only on x and also f (which defines the polytope) but not dependent on y^x , the particular P -basis.

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Proof.

- Clearly $0 \in P_f^+$ since f is non-negative.
- Also, for any $y \in P_f^+$ then any $x \leq y$ is also such that $x \in P_f^+$. So, P_f^+ is down-monotone.
- Now suppose that we are given an $x \in \mathbb{R}_+^E$, and maximal $y^x \in P_f^+$ with $y^x \leq x$ (i.e., y^x is a P_f^+ -basis of x).
- Goal is to show that any such y^x has $y^x(E) = \text{const}$, dependent only on x and also f (which defines the polytope) but not dependent on y^x , the particular P -basis.
- Doing so will thus establish that P_f^+ is a polymatroid.

...

Downloaded from <http://ajph.org/> at University of California, San Diego on June 11, 2015

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... proof continued.

- 2nd trivial case: when $x(A) > f(A), \forall A \subseteq E$ (i.e., $x \notin P_f^+$ strictly),

... proof continued.

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- Then for any order (a_1, a_2, \dots) of the elements and $A_i \triangleq (a_1, a_2, \dots, a_i)$, we have $x(a_i) \geq f(a_i) \geq f(a_i|A_{i-1})$, the second inequality by submodularity.

... proof continued.

- $$= x(E) + f(E) - x(E) = f(E) \quad (10.9)$$

A polymatroid function's polyhedron is a polymatroid.

... proof continued.

- Assume neither trivial case. Because $y^x \in P_f^+$, we have that $y^x(A) \leq f(A)$ for all $A \subseteq E$.

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A polymatroid function's polyhedron is a polymatroid.

... proof continued.

- Assume neither trivial case. Because $y^x \in P_f^+$, we have that $y^x(A) \leq f(A)$ for all $A \subseteq E$.
- We show that the constant is given by

$$y^x(E) = \min (x(A) + f(E \setminus A) : A \subseteq E) \quad (10.10)$$

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$$y^x(E) = \min (x(A) + f(E \setminus A) : A \subseteq E) \quad (10.10)$$

- For any P_f^+ -basis y^x of x , and any $A \subseteq E$, we have that

$$y^x(E) = y^x(A) + y^x(E \setminus A) \quad (10.11)$$

$$\leq x(A) + f(E \setminus A). \quad (10.12)$$

This follows since $y^x \leq x$ and since $y^x \in P_f^+$.

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$$\leq x(A) + f(E \setminus A). \quad (10.12)$$

This follows since $y^x \leq x$ and since $y^x \in P_f^+$.

- Given one A where equality holds, the above min result follows.

...

A polymatroid function's polyhedron is a polymatroid.

... proof continued.

- For any $y \in P_f^+$, call a set $B \subseteq E$ **tight** if $y(B) = f(B)$. The union (and intersection) of tight sets B, C is again tight, since

$$f(B) + f(C)$$

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$$\leq f(B \cap C) + f(B \cup C) \quad (10.15)$$

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which requires equality everywhere above.

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- Because $y(B) \leq f(B), \forall B$, this means $y(B \cap C) = f(B \cap C)$ and $y(B \cup C) = f(B \cup C)$, so both also are tight.

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- Because $y(B) \leq f(B), \forall B$, this means $y(B \cap C) = f(B \cap C)$ and $y(B \cup C) = f(B \cup C)$, so both also are tight.
- For $y \in P_f^+$, it will be ultimately useful to define this lattice family of tight sets: $\mathcal{D}(y) \triangleq \{A : A \subseteq E, y(A) = f(A)\}$.

...

A polymatroid function's polyhedron is a polymatroid.

... proof continued.

- Also, define $\text{sat}(y) \stackrel{\text{def}}{=} \bigcup \{T : T \in \mathcal{D}(y)\}$



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- Consider again a P_f^+ -basis y^x (so maximal).



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- Consider again a P_f^+ -basis y^x (so maximal).
- Given a $e \in E$, either $y^x(e)$ is cut off due to x (so $y^x(e) = x(e)$) or e is saturated by f , meaning it is an element of some tight set and $e \in \text{sat}(y^x)$.



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- Let $E \setminus A = \text{sat}(y^x)$ be the union of all such tight sets (which is also tight, so $y^x(E \setminus A) = f(E \setminus A)$).
- Hence, we have

$$y^x(E) = y^x(A) + y^x(E \setminus A) = x(A) + f(E \setminus A) \quad (10.17)$$



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- Given a $e \in E$, either $y^x(e)$ is cut off due to x (so $y^x(e) = x(e)$) or e is saturated by f , meaning it is an element of some tight set and $e \in \text{sat}(y^x)$.
- Let $E \setminus A = \text{sat}(y^x)$ be the union of all such tight sets (which is also tight, so $y^x(E \setminus A) = f(E \setminus A)$).
- Hence, we have

$$y^x(E) = y^x(A) + y^x(E \setminus A) = x(A) + f(E \setminus A) \quad (10.17)$$

- So we identified the A to be the elements that are non-tight, and achieved the min, as desired.



A polymatroid is a polymatroid function's polytope

- So, when f is a polymatroid function, P_f^+ is a polymatroid.

A polymatroid is a polymatroid function's polytope

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- Is it the case that, conversely, for any polymatroid P , there is an associated polymatroidal function f such that $P = P_f^+$?

A polymatroid is a polymatroid function's polytope

- So, when f is a polymatroid function, P_f^+ is a polymatroid.
- Is it the case that, conversely, for any polymatroid P , there is an associated polymatroidal function f such that $P = P_f^+$?

Theorem 10.3.1

For any polymatroid P (compact subset of \mathbb{R}_+^E , zero containing, down-monotone, and $\forall x \in \mathbb{R}_+^E$ any maximal independent subvector $y \leq x$ has same component sum $y(E) = \text{rank}(x)$), there is a polymatroid function $f : 2^E \rightarrow \mathbb{R}$ (normalized, monotone non-decreasing, submodular) such that $P = P_f^+$ where $P_f^+ = \{x \in \mathbb{R}^E : x \geq 0, x(A) \leq f(A), \forall A \subseteq E\}$.

First, a bit on $\mathcal{D}(y)$

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

$$\mathcal{D}(y) \triangleq \{A : A \subseteq E, y(A) = f(A)\} \quad (10.18)$$

Theorem 10.3.2

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

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Proof.

We have already proven this as part of Theorem 9.4.5 □

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

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Theorem 10.3.2

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 9.4.5 □

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

$$\text{sat}(y) \stackrel{\text{def}}{=} \bigcup \{T : T \in \mathcal{D}(y)\} \quad (10.19)$$

Join \vee and meet \wedge for $x, y \in \mathbb{R}_+^E$

- For $x, y \in \mathbb{R}_+^E$, define vectors $x \wedge y \in \mathbb{R}_+^E$ and $x \vee y \in \mathbb{R}_+^E$ such that, for all $e \in E$

$$(x \vee y)(e) = \max(x(e), y(e)) \quad (10.20)$$

$$(x \wedge y)(e) = \min(x(e), y(e)) \quad (10.21)$$

Hence,

$$x \vee y \triangleq \left(\max(x(e_1), y(e_1)), \max(x(e_2), y(e_2)), \dots, \max(x(e_n), y(e_n)) \right)$$

and similarly

$$x \wedge y \triangleq \left(\min(x(e_1), y(e_1)), \min(x(e_2), y(e_2)), \dots, \min(x(e_n), y(e_n)) \right)$$

Join \vee and meet \wedge for $x, y \in \mathbb{R}_+^E$

- For $x, y \in \mathbb{R}_+^E$, define vectors $x \wedge y \in \mathbb{R}_+^E$ and $x \vee y \in \mathbb{R}_+^E$ such that, for all $e \in E$

$$(x \vee y)(e) = \max(x(e), y(e)) \quad (10.20)$$

$$(x \wedge y)(e) = \min(x(e), y(e)) \quad (10.21)$$

Hence,

$$x \vee y \triangleq \left(\max(x(e_1), y(e_1)), \max(x(e_2), y(e_2)), \dots, \max(x(e_n), y(e_n)) \right)$$

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- From this, we can define things like an lattices, and other constructs.

Vector rank, $\text{rank}(x)$, is submodular

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Theorem 10.3.3 (vector rank and submodularity)

Let P be a polymatroid polytope. The vector rank function $\text{rank} : \mathbb{R}_+^E \rightarrow \mathbb{R}$ with $\text{rank}(x) = \max(y(E) : y \leq x, y \in P)$ satisfies, for all $u, v \in \mathbb{R}_+^E$

$$\text{rank}(u) + \text{rank}(v) \geq \text{rank}(u \vee v) + \text{rank}(u \wedge v) \quad (10.22)$$

Vector rank $\text{rank}(x)$ is submodular, proof

Proof of Theorem 10.3.3.

- Let a be a P -basis of $u \wedge v$, so $\text{rank}(u \wedge v) = a(E)$.

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- Let a be a P -basis of $u \wedge v$, so $\text{rank}(u \wedge v) = a(E)$.
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- Given $e \in E$, if $a(e)$ is maximal due to P , then then
 $a(e) = b(e) \leq \min(u(e), v(e))$.

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- Since $a = b \wedge (u \wedge v)$ and since $b \leq u \vee v$, we get

$$a + b \tag{10.23}$$

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To see this, consider each case where either b is the minimum, or u is minimum with $b \leq v$, or v is minimum with $b \leq u$.

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$$\leq \text{rank}(u) + \text{rank}(v) \quad (10.26)$$



A polymatroid function's polyhedron vs. a polymatroid.

- Note the remarkable similarity between the proof of Theorem 10.3.3 and the proof of Theorem ?? that the standard matroid rank function is submodular.

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- Next, we prove Theorem 10.3.1, that any polymatroid polytope P has a polymatroid function f such that $P = P_f^+$.
- Given this result, we can conclude that a polymatroid is really an extremely natural polyhedral generalization of a matroid. This was all realized by Jack Edmonds in the mid 1960s (and published in 1969 in his landmark paper “Submodular Functions, Matroids, and Certain Polyhedra”).

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- Define a function $f : 2^V \rightarrow \mathbb{R}$ as, for any $A \subseteq E$,

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- Hence, $P \subseteq P_f^+$.
- We will next show that $P_f^+ \subseteq P$ to complete the proof.

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- Hence, $\text{rank}(x) = \text{rank}(w)$, and the set of P -bases of w are also P -bases of x .

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- For any $A \subseteq E$, define $x_A \in \mathbb{R}_+^E$ as

$$x_A(e) = \begin{cases} x(e) & \text{if } e \in A \\ 0 & \text{else} \end{cases} \quad (10.35)$$

note this is an analogous definition to $\mathbf{1}_A$ but for a non-unity vector.

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$$x_A(e) = \begin{cases} x(e) & \text{if } e \in A \\ 0 & \text{else} \end{cases} \quad (10.35)$$

note this is an analogous definition to $\mathbf{1}_A$ but for a non-unity vector.

- Now, we have

$$y(N(y)) < w(N(y)) \leq f(N(y)) = \text{rank}(\alpha_{\max} \mathbf{1}_{N(y)}) \quad (10.36)$$

the last inequality follows since $w \leq x \in P_f^+$, and $y \leq w$.

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- Thus, $y \wedge x_{N(y)}$ is not a P -basis of $w \wedge x_{N(y)}$ since, over $N(y)$, it is neither tight at w nor tight at the rank (i.e., not a maximal independent subvector on $N(y)$).

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- Thus, \hat{y} is a base of x , which violates the maximality of $|N(y)|$.
- This contradiction means that we must have had $x \in P$.
- Therefore, $P_f^+ = P$.



More on polymatroids

Theorem 10.3.4

A polymatroid can equivalently be defined as a pair (E, P) where E is a finite ground set and $P \subseteq R_+^E$ is a compact non-empty set of independent vectors such that

- ① *every subvector of an independent vector is independent (if $x \in P$ and $y \leq x$ then $y \in P$, i.e., down closed)*

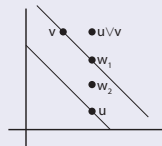
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- ② If $u, v \in P$ (i.e., are independent) and $u(E) < v(E)$, then there exists a vector $w \in P$ such that

$$u < w \leq u \vee v \quad (10.37)$$



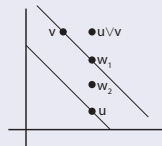
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Corollary 10.3.5

The independent vectors of a polymatroid form a convex polyhedron in \mathbb{R}_+^E .

Review

- The next slide comes from lecture 5.

Matroids by bases

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

Theorem 10.3.1 (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.”

Proof here is omitted but think about this for a moment in terms of linear spaces and matrices, and (alternatively) spanning trees.

More on polymatroids

For any compact set P , b is **a base of P** if it is a maximal subvector within P . Recall the bases of matroids. In fact, we can define a polymatroid via vector bases (analogous to how a matroid can be defined via matroid bases).

Theorem 10.3.6

A polymatroid can equivalently be defined as a pair (E, P) where E is a finite ground set and $P \subseteq R_+^E$ is a compact non-empty set of independent vectors such that

- ① *every subvector of an independent vector is independent (if $x \in P$ and $y \leq x$ then $y \in P$, i.e., down closed)*
- ② *if b, c are bases of P and d is such that $b \wedge c < d < b$, then there exists an f , with $d \wedge c < f \leq c$ such that $d \vee f$ is a base of P*
- ③ *All of the bases of P have the same rank.*

Note, all three of the above are required for a polymatroid (a matroid analogy would require the equivalent of only the first two).