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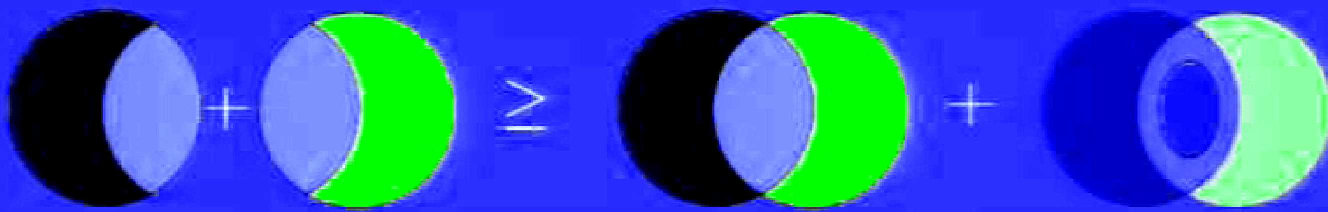

Deep Mathematical Properties of Submodularity with Applications to Machine Learning

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Thursday, December 5th, 2013

Outline

1. Introduction

Where to get these slides

- Where to get these slides right now:

  http://goo.gl/PSzuPv

- QR Code:

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A Dedication

This tutorial dedicated to Ben Taskar, and his family. RIP Ben.

Goals of the Tutorial

- Get an intuitive sense for submodular functions, should be able to apply them.
- Learn to recognize submodularity, or recognize when it might be useful.
- Learn to realize why submodularity can be useful in machine learning. Why is it worth your time to study it.
- Learn to realize when submodularity is inapplicable.

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Submodularity

- Definition: given a finite ground set V, a function $f : 2^V \to \mathbb{R}$ is said to be submodular if

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B), \quad \forall A, B \subseteq V \tag{1}$$

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- Goals of tutorial: will be very simple, an attempt to cover some important parts of the iceberg in 2 hours.
- The tutorial itself is the tip of the iceberg!
- One last goal: Let A be a set of tutorials on submodularity, and $f(A)$ the information provided by tutorials A. Our goal is to be a member of:

$$\operatorname*{argmax}_{v \in V \setminus B} f(B \cup \{v\}) \tag{2}$$

where B is the set of previous tutorials given on submodularity.

Outline

2 Basics

Sets and set functions

We are given a finite "ground" set of objects:

$$V = \left\{ \right.$$  $$\left. \right\}$$

Also given a set function $f : 2^V \to \mathbb{R}$ that valuates subsets $A \subseteq V$.
Ex: $f(V) = 6$

Sets and set functions

Subset $A \subseteq V$ of objects:

$A = \{$  $\}$

Also given a set function $f : 2^V \to \mathbb{R}$ that valuates subsets $A \subseteq V$.
Ex: $f(A) = 1$

Set functions are pseudo-Boolean functions

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- It is sometimes useful to go back and forth between X and $x(X) \triangleq \mathbf{1}_X$.
- $f(x) : \{0, 1\}^V \to \mathbb{R}$ is a pseudo-Boolean function, and submodular functions are a special case.

Two equivalent basic definitions

Definition (submodular)

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Definition (submodular (diminishing returns))

A function $f : 2^V \to \mathbb{R}$ is submodular if for any $A \subseteq B \subset V$, and $v \in V \setminus B$, we have that:

$$f(A \cup \{v\}) - f(A) \geq f(B \cup \{v\}) - f(B) \tag{5}$$

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Example: Rank function of a matrix

- Given an $n \times m$ matrix, thought of as m column vectors:

$$\mathbf{X} = \begin{pmatrix} & 1 & 2 & 3 & 4 & & m \\ & | & | & | & | & & | \\ & x_1 & x_2 & x_3 & x_4 & \dots & x_m \\ & | & | & | & | & & | \end{pmatrix} \tag{6}$$

- Let set $V = \{1, 2, \dots, m\}$ be the set of column vector indices.
- For any subset of column vector indices $A \subseteq V$, let $r(A)$ be the rank of the column vectors indexed by A.
- Hence $r : 2^V \rightarrow \mathbb{Z}_+$ and $r(A)$ is the dimensionality of the vector space spanned by the set of vectors $\{x_a\}_{a \in A}$.
- Intuitively, $r(A)$ is the size of the largest set of independent vectors contained within the set of vectors indexed by A.

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Example: Rank function of a matrix

Consider the following 4×8 matrix, so $V = \{1, 2, 3, 4, 5, 6, 7, 8\}$.

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3	0	0	0	0	3	0	0	5
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- Given any set $B \subseteq V$ of vectors, all maximal (by set inclusion) subsets of linearly independent vectors are the same size. That is, for all $B \subseteq V$,

$$\forall A_1, A_2 \in \text{maxInd}(B), \quad |A_1| = |A_2| \tag{9}$$

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

$$r(I) = |I| \tag{10}$$

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

$$r(B) = \max\{|A| : A \subseteq B \text{ and } A \in \mathcal{I}\} \leq |B| \tag{11}$$

Independence System

Definition (set system)

A (finite) ground set V and a set of subsets of V, $\emptyset \neq \mathcal{I} \subseteq 2^V$ is called a set system, notated $(V, \mathcal{I})$.

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A set system $(V, \mathcal{I})$ is an independence system if

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- If $\mathcal{I} = \{\emptyset, \{1\}, \{2\}, \{1, 2\}\}$, then $(V, \mathcal{I})$ is independence system.

Matroids, many equivalent definitions

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

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Linear (or Matric) Matroid

- Let $\mathbf{X}$ be an $n \times m$ matrix and $V = \{1, \dots, m\}$
- Let $\mathcal{I}$ consists of subsets of V such that if $A \in \mathcal{I}$, and $A = \{a_1, a_2, \dots, a_k\}$ then the vectors $x_{a_1}, x_{a_2}, \dots, x_{a_k}$ are linearly independent.
- The rank function is just the rank of the space spanned by the corresponding set of vectors.
- A base of a matroid is maximally independent set. So a base of this matroid is a set of rank V independent vectors.

Cycle Matroid of a graph, or Graphic Matroids

- Let $G = (V, E)$ be a graph. Consider $(E, \mathcal{I})$ where the edges of the graph E are the ground set and $A \in \mathcal{I}$ if the edge-induced graph $G(V, A)$ by A does not contain any cycle.
- Then $M = (E, \mathcal{I})$ is a matroid.
- $\mathcal{I}$ contains all forests and trees.
- Bases are spanning forests (spanning trees if G is connected).
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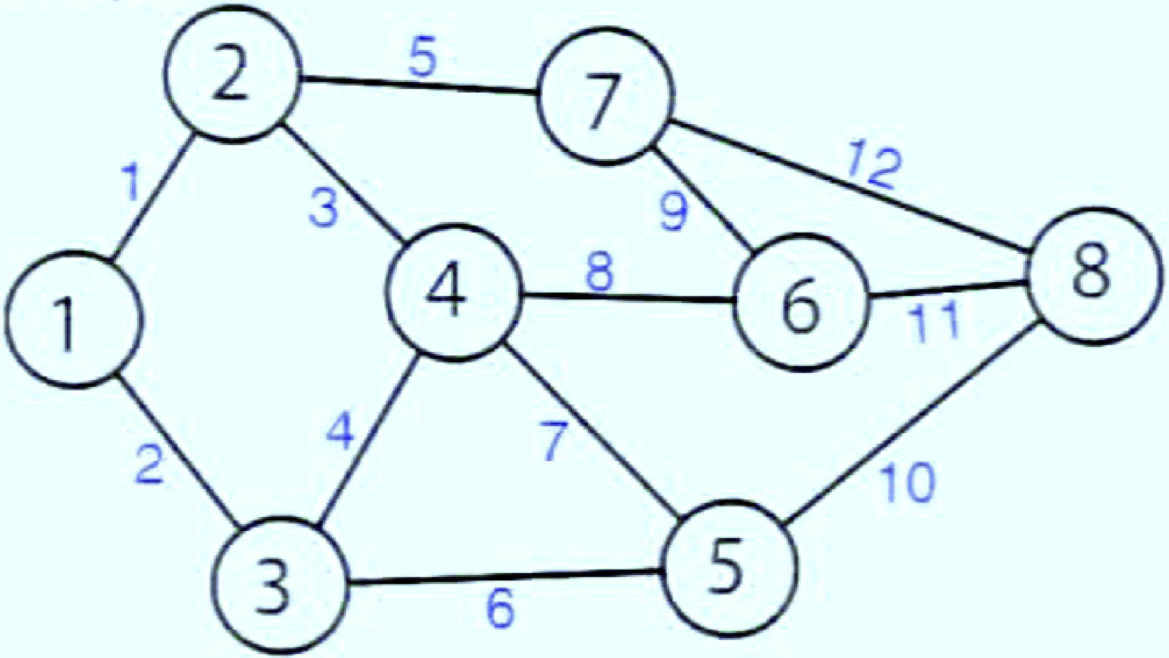
Example: graphic matroid

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



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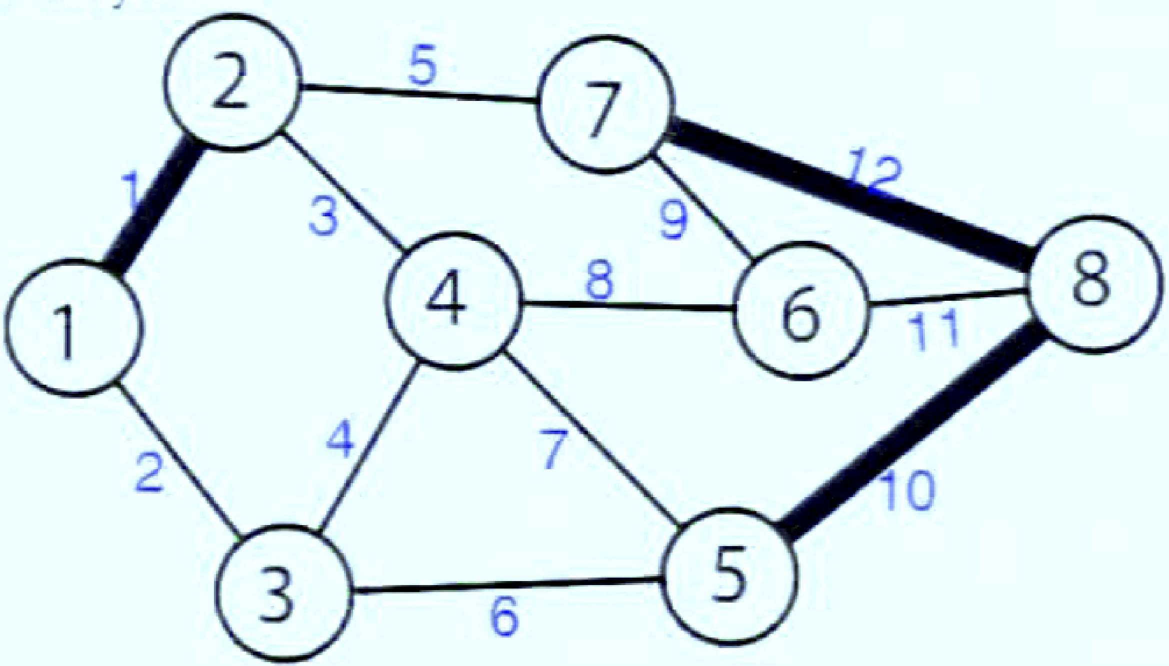

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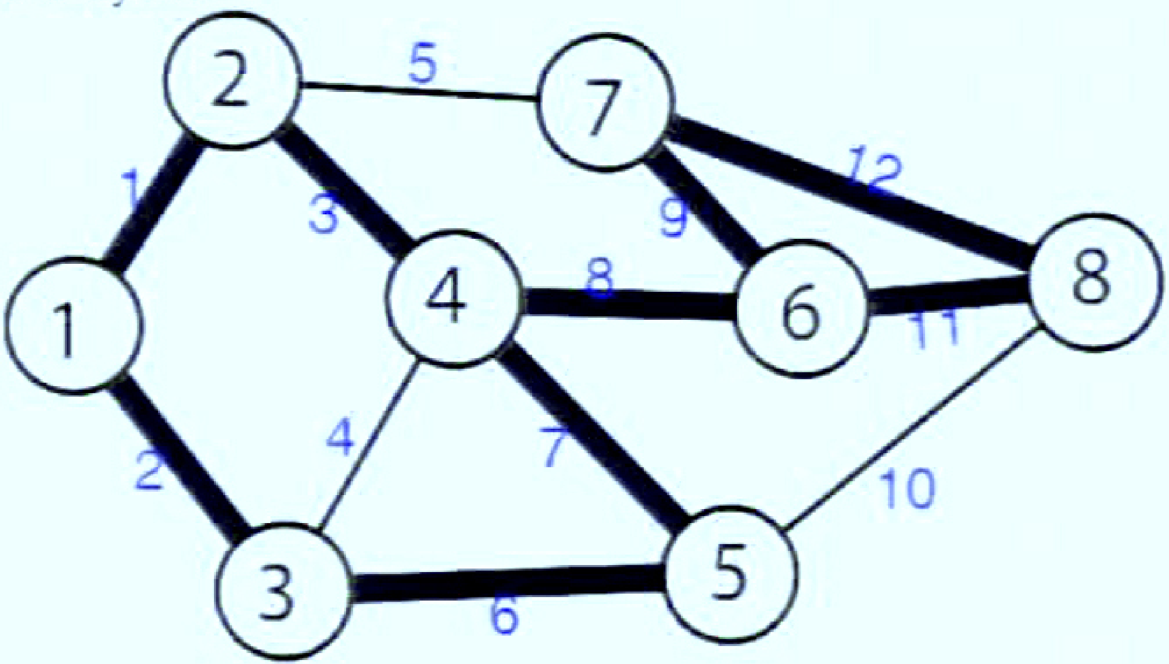


Partition Matroid

Ground set of objects, $V = \Big\{$

$\Big\}$

Partition Matroid

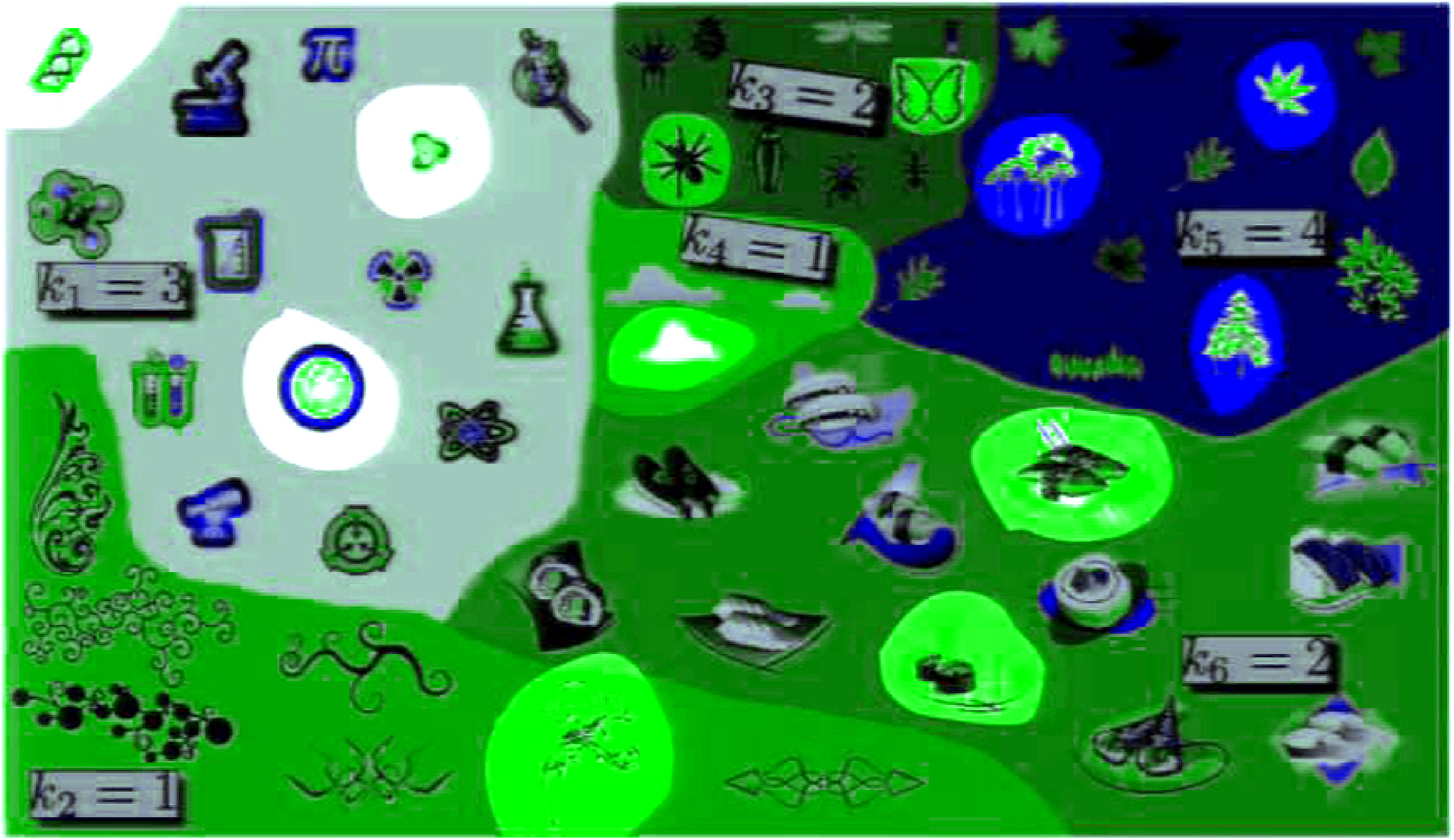
Partition of V into six blocks, $V_1, V_2, \dots, V_6$

Partition Matroid

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

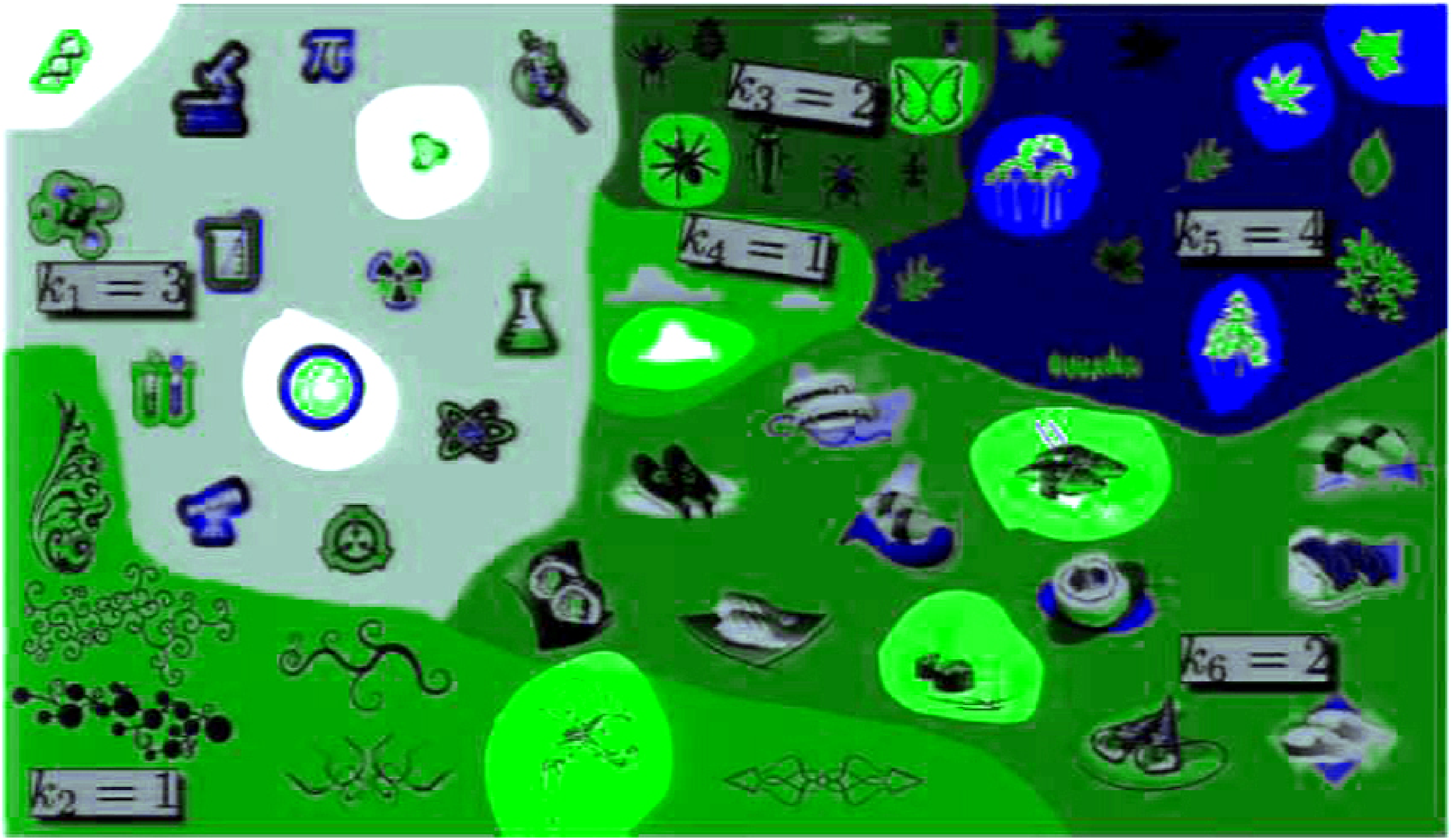
Partition Matroid

Independent subset but not maximally independent.



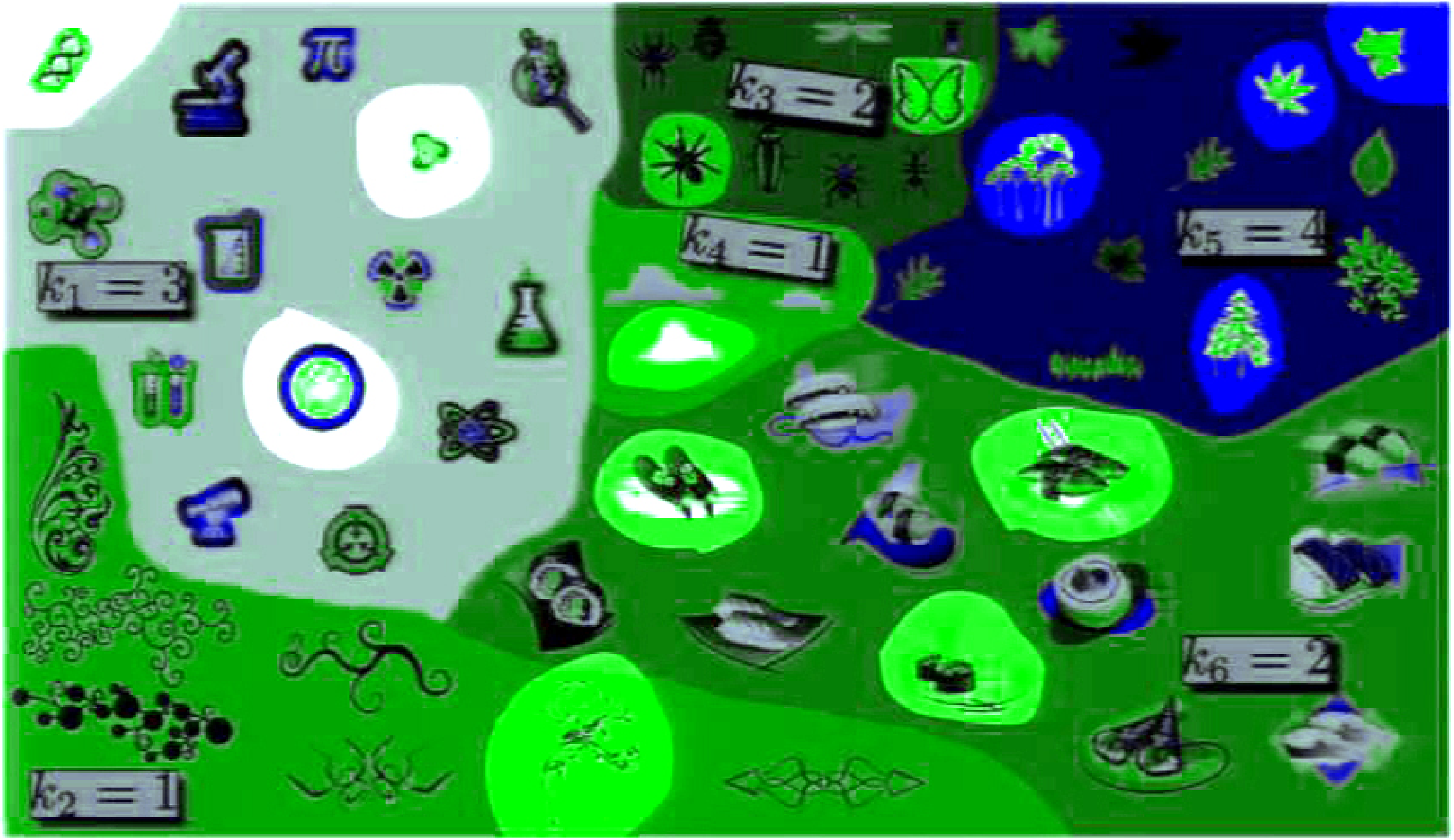
Partition Matroid

Maximally independent subset, what is called a base.



Partition Matroid

Not independent since over limit in set six.



Partition Matroid

- Let $V = V_1 \cup V_2 \cup \dots \cup V_\ell$ be a partition of V into disjoint sets (disjoint union). Define a set of subsets of V as

$$\mathcal{I} = \{X \subseteq V : |X \cap V_i| \leq k_i \text{ for all } i = 1, \dots, \ell\}. \tag{12}$$

  where $k_1, \dots, k_\ell$ are fixed parameters, $k_i \geq 0$. Then $M = (V, \mathcal{I})$ is a matroid.
- A partition matroids rank function is:

$$r(A) = \sum_{i=1}^{\ell} \min(|A \cap V_i|, k_i) \tag{13}$$

Matroids - rank and submodularity

We can a bit more formally define the rank function this way.

Definition

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

$$r(A) = \max\{|X| : X \subseteq A, X \in \mathcal{I}\} = \max_{X \in \mathcal{I}} |A \cap X| \quad (14)$$

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Lemma

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

Matroids via rank

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

Theorem (Matroid from rank)

Let V be a set and let $r : 2^V \to \mathbb{Z}_+$ be a function. Then $r(\cdot)$ defines a matroid with r being its rank function if and only if for all $A, B \subseteq V$:

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- Unit increment (if $r(A) = k$, then either $r(A \cup \{v\}) = k$ or $r(A \cup \{v\}) = k + 1$) follows from the above.
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- Hence, the characteristic vector $\mathbf{1}_A$ of a set is modular.

Matroid and the greedy algorithm

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- Same as sorting items by decreasing weight w, and then choosing items in that order that retain independence.

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Given an independence system, matroids are defined equivalently by any of the following:

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Maximal points in a set

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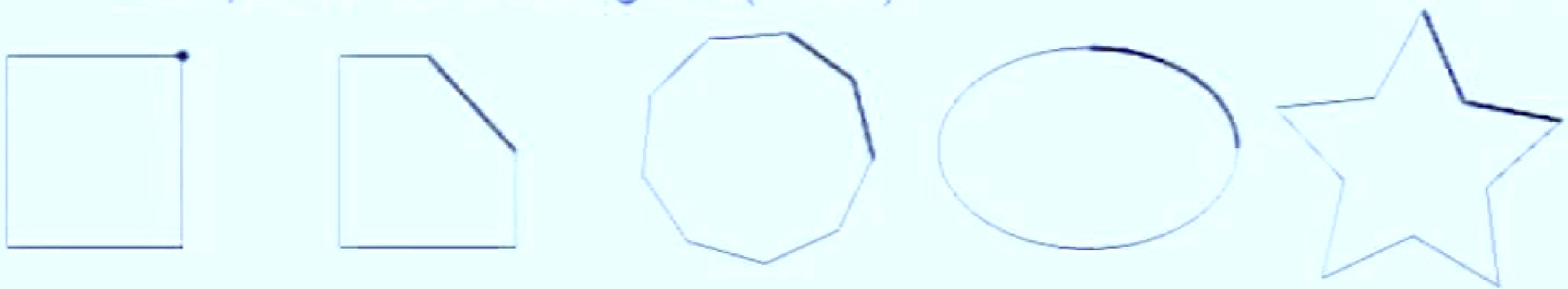

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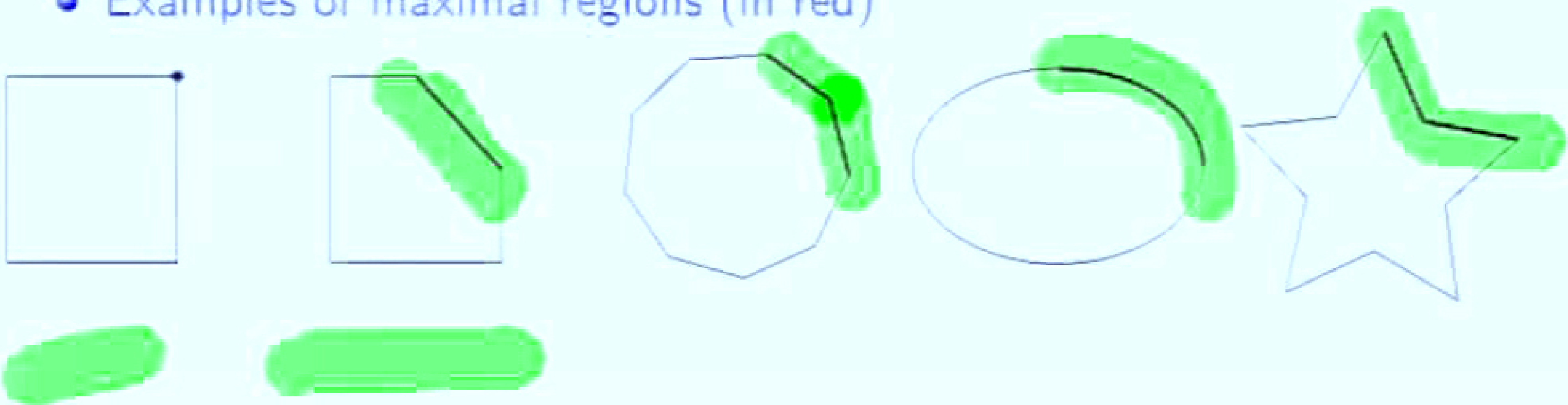

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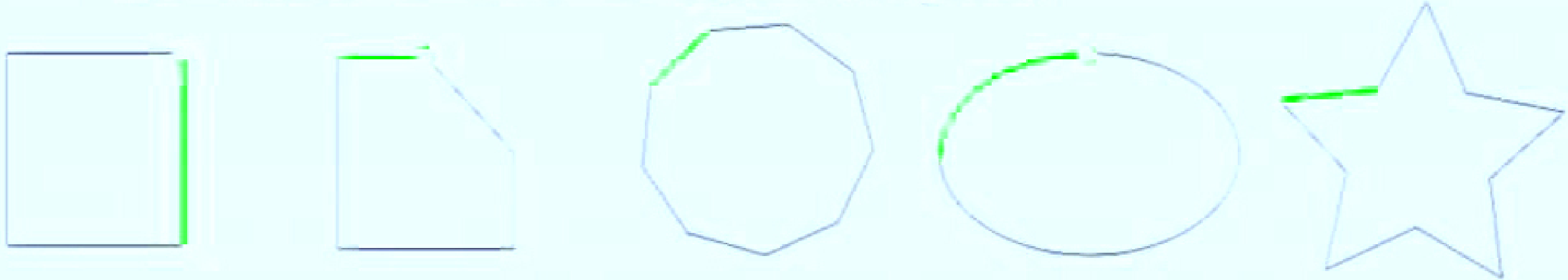
- Given any set $P \subseteq \mathbb{R}^V$, we say that a vector x is maximal within P if it is the case that for any $\epsilon > 0$, and for all $v \in V$, we have that

$$x + \epsilon \mathbf{1}_v \notin P \tag{16}$$

- Examples of non-maximal regions (in green)



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

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

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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 $z \geq y + \epsilon \mathbf{1}_v$ for some $v \in V$ and $\epsilon > 0$) having the properties of y (the properties of y being: in P, and a subvector of x).

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The "rank" of a vector

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

$$\text{rank}(A) = \max\{|I| : I \subseteq A, I \in \mathcal{I}\} \tag{17}$$

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$$\text{rank}(x) = \max(y(V) : y \leq x, y \in P) \quad (18)$$

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

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- 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 (polymatroid)

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- Condition 3 restated (again): For every vector $x \in \mathbb{R}_+^V$, every maximal independent subvector y of x has the same component sum $y(V) = \text{rank}(x)$.
- Condition 3 restated (yet again): All P-bases of x have the same component sum.

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- 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, than $\text{rank}(x) = y(V)$ for any $y \in \mathcal{B}_x$.

Matroid and Polymatroid: side-by-side

A Matroid is:

A Polymatroid is:

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A Matroid is:

1. a set system $(V, \mathcal{I})$
2. empty-set containing $\emptyset \in \mathcal{I}$

A Polymatroid is:

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3. subclusive, 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 $|I|$).

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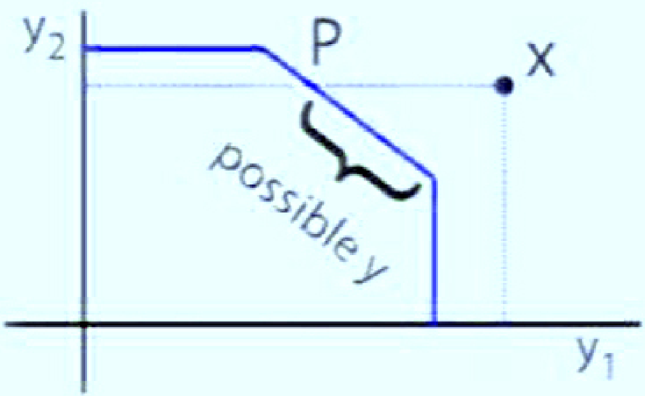
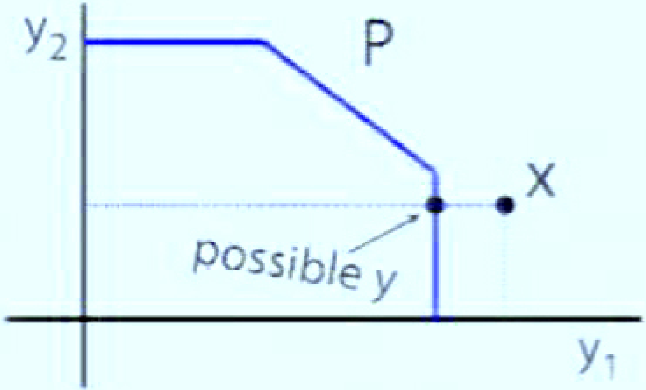
Polymatroidal polyhedron (or a "polymatroid")





Left: $\exists$ multiple maximal $y \leq x$ Right: $\exists$ only one maximal $y \leq x$,

- Polymatroid condition here: $\forall$ maximal $y \in P$, with $y \leq x$ (which here means componentwise $y_1 \leq x_1$ and $y_2 \leq x_2$), we just have $y(V) = y_1 + y_2 = \text{const}$.

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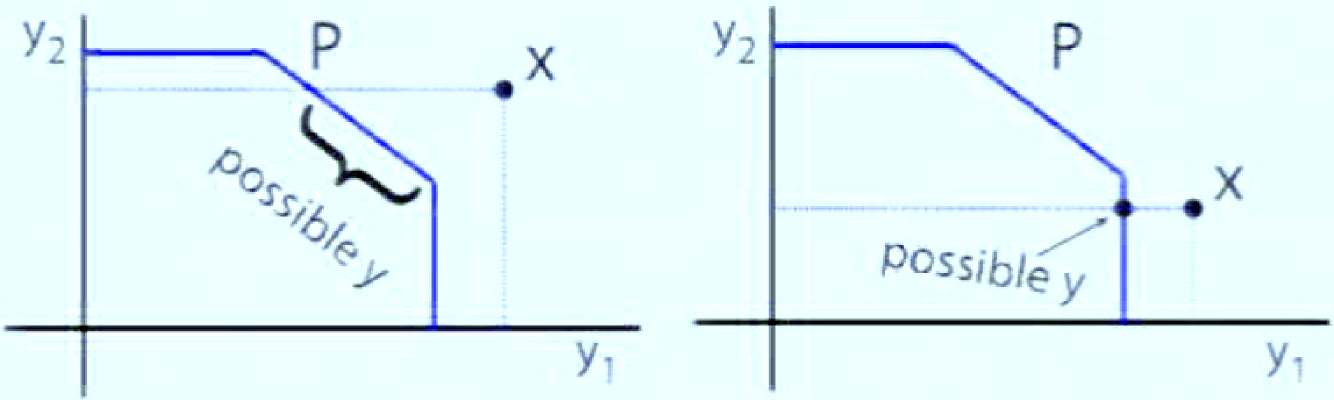

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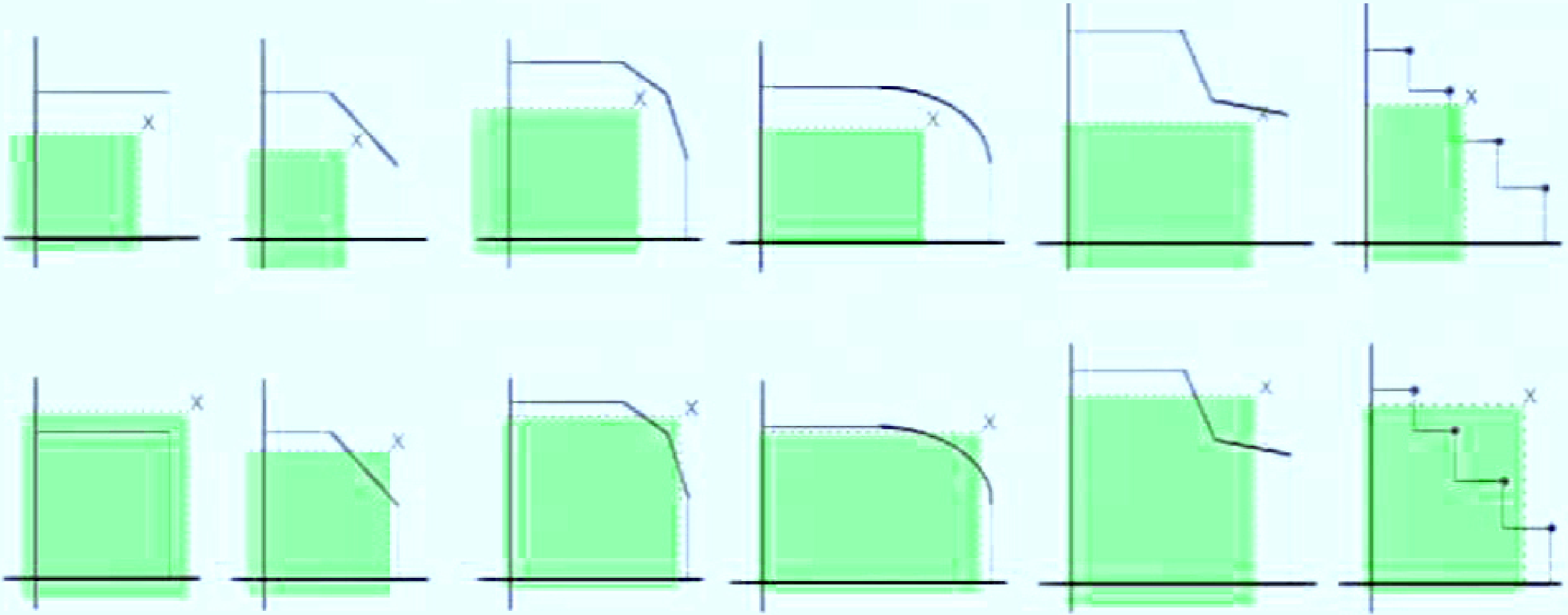
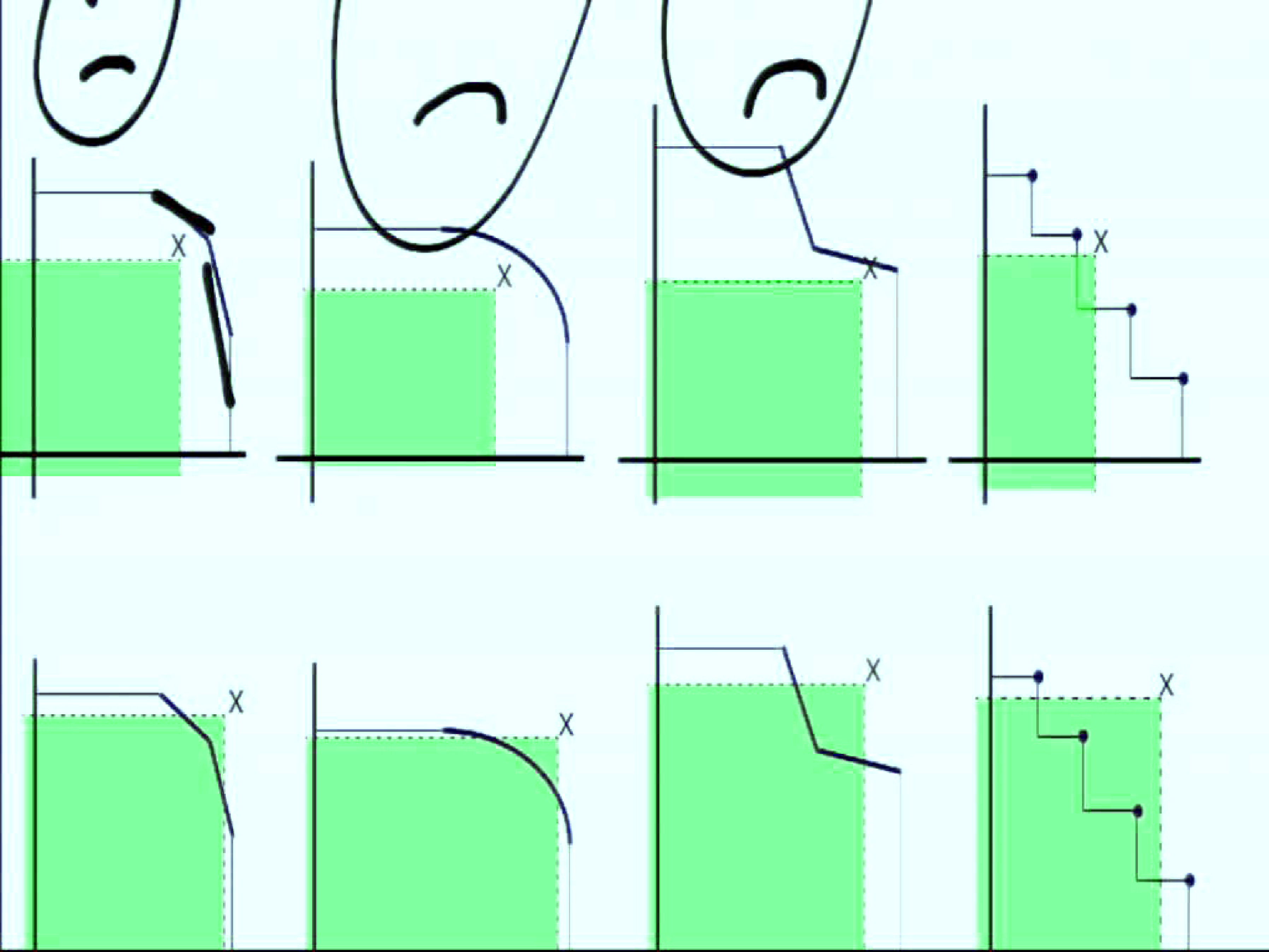
- On the left, we see there are multiple possible maximal $y \in P$ such that $y \leq x$. Each such y must have the same value $y(V)$.
- On the right, there is only one maximal $y \in P$. Since there is only one, the condition on the same value of $y(V)$, $\forall y$ is vacuous.

Other examples: Polymatroid or not?

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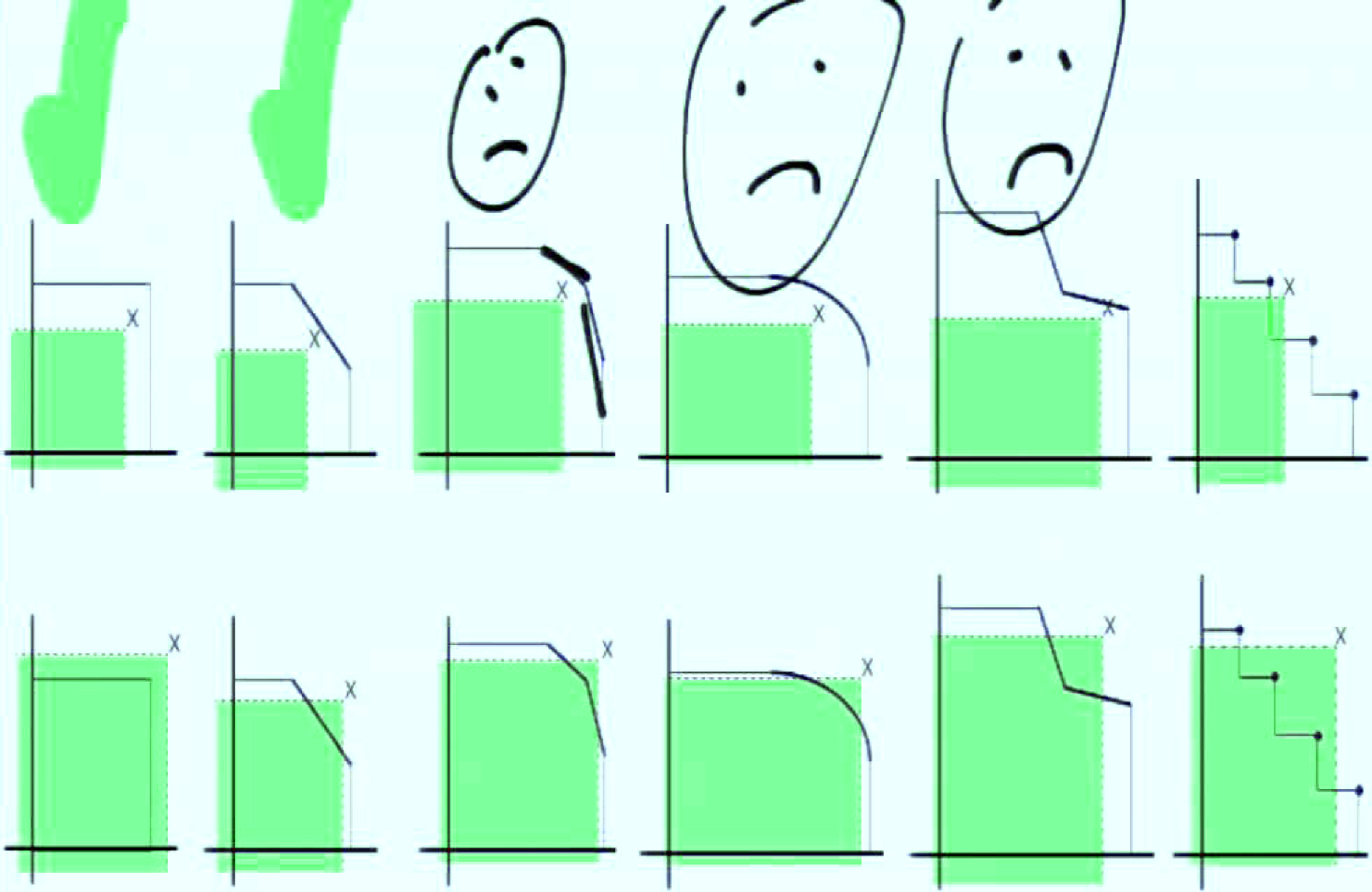
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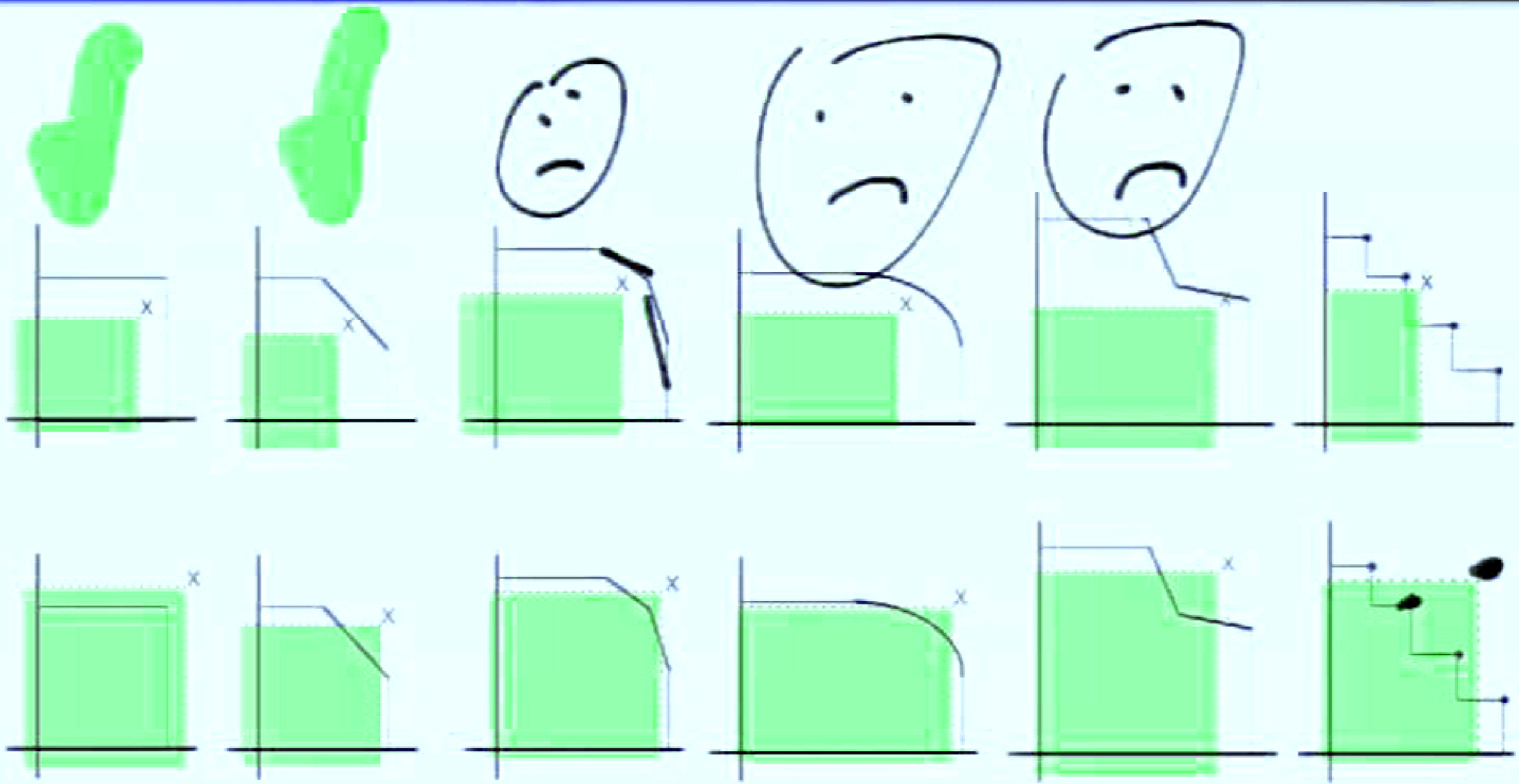
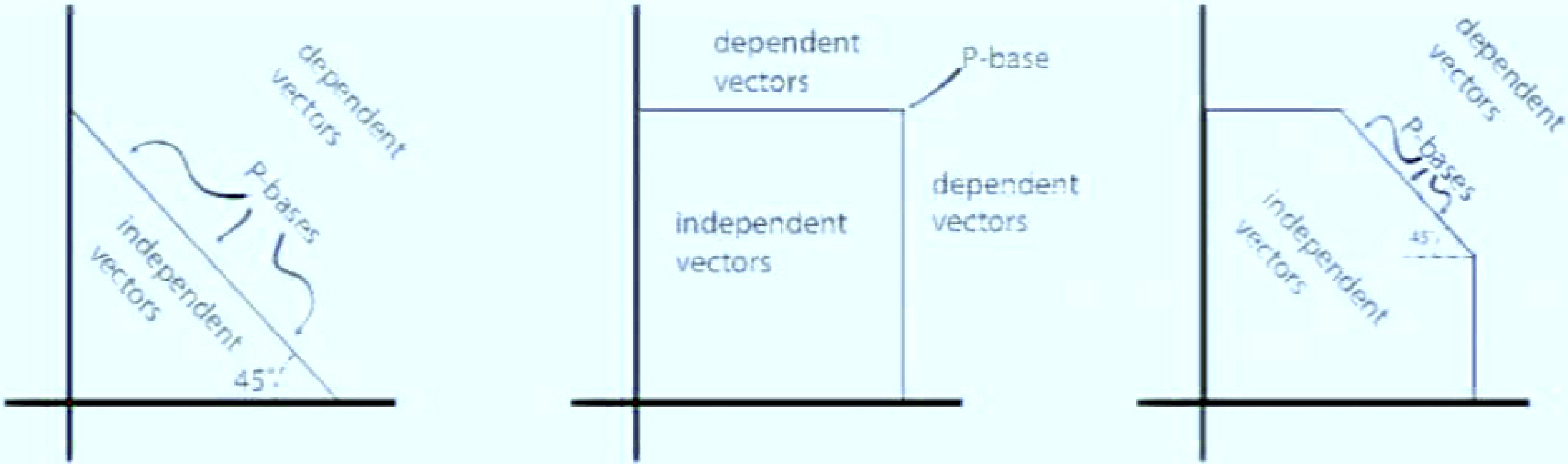


Some possible polymatroid forms in 2D



It appears that we have three possible forms of polymatroid in 2D, when neither of the elements $\{v_1, v_2\}$ are self-dependent.

1. On the left: full dependence between v_1 and v_2
2. In the middle: full independence between v_1 and v_2
3. On the right: partial independence between v_1 and v_2

- The P-bases (or single P-base in the middle case) are as indicated.
- Independent vectors are those within or on the boundary of the polytope. Dependent vectors are exterior to the polytope.
- The set of P-bases for a polytope is called the base polytope.

Polymatroid function and its polyhedron.

Definition

A polymatroid function is a real-valued function f defined on subsets of V which is normalized, non-decreasing, and submodular. That is:

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

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

$$P_f^+ = \left\{ y \in \mathbb{R}_+^V : y(A) \leq f(A) \text{ for all } A \subseteq V \right\} \quad (19)$$

$$= \left\{ y \in \mathbb{R}^V : y \geq 0, y(A) \leq f(A) \text{ for all } A \subseteq V \right\} \quad (20)$$

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A polymatroid function's polyhedron is a polymatroid.

Theorem (Edmonds, 1970)

Let f be a polymatroid function defined on subsets of V. For any $x \in \mathbb{R}_+^V$, and any P_f^+-basis $y^x \in \mathbb{R}_+^V$ of x, the component sum of y^x is

$$y^x(V) = rank(x) = \max\left(y(V) : y \leq x, y \in P_f^+\right) = \min\left(x(A) + f(V \setminus A) : A \subseteq V\right) \quad (21)$$

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With an appropriate choice of x, we can define/recover the submodular function from the polymatroid polyhedron via the following:

$$f(A) = \max\left\{y(A) : y \in P_f^+\right\} \qquad (22)$$

There are many important consequences of this theorem (other than just P_f^+ is a polymatroid), regarding submodular function minimization.

A polymatroid is a polymatroid function's polytope

Thus, 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 $P = P_f^+$?

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

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Polymatroid from polymatroid function

- Recall, a matroid may be given as (V, r) where r is the rank function.
- We mention also that the term "polymatroid" is sometimes not used for the polytope itself, but instead but for the pair (V, f).
- Since (V, f) is equivalent to a polymatroid polytope, this is sensible.

Polymatroidal polyhedron and greedy

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- Can we also characterize a polymatroid in this way?
- That is, if we consider $\max(wx : x \in P_f^+)$ where P_f^+ represents the "independent vectors", is it the case that P_f^+ is a polymatroid iff greedy works for this maximization?

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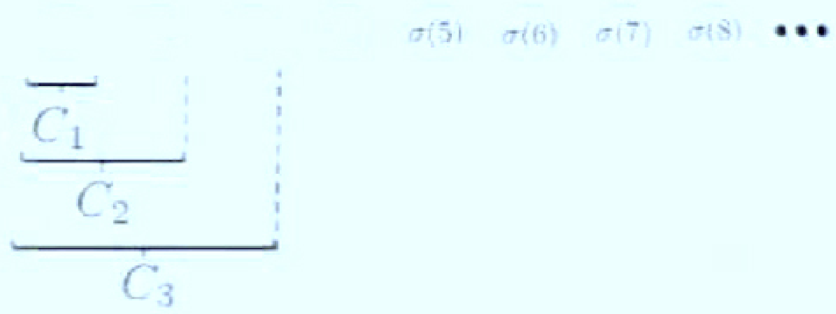

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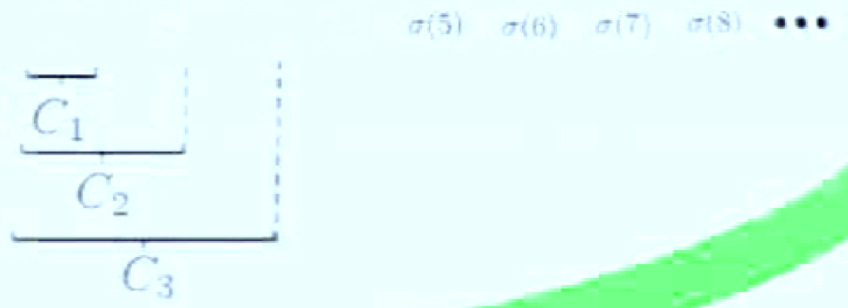

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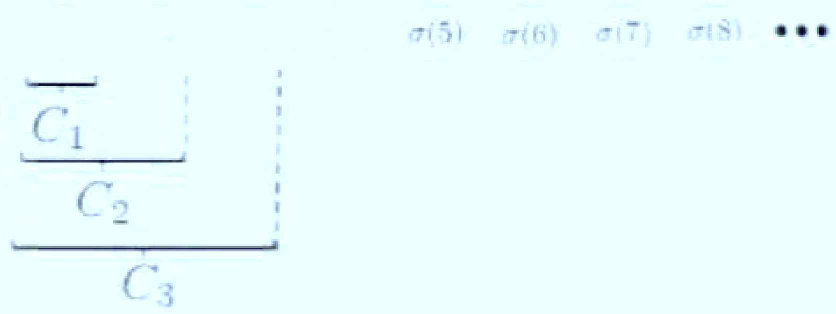

- Can also form a chain from a vector $w \in \mathbb{R}^V$ sorted in descending order. Choose σ so that $w(\sigma_1) \geq w(\sigma_2) \geq \dots \geq w(\sigma_n)$.

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$$f(A \cup \{j\}) - f(A) \triangleq \rho_j(A) \quad (25)$$
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- Submodularity's diminishing returns definition can be stated as saying that $f(j|A)$ is a monotone non-increasing function of A, since $f(j|A) \geq f(j|B)$ whenever $A \subseteq B$ (conditioning reduces valuation).

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- Next, form chain of sets based on w sorted descended, giving:

$$V_i \stackrel{\text{def}}{=} \{v_1, v_2, \dots, v_i\} \tag{30}$$

for $i = 0 \dots m$. Note $V_0 = \emptyset$, and $f(V_0) = 0$.

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Polymatroid extreme points

Greedy does more than this. In fact, we have:

Theorem

For a given ordering $V = (v_1, \dots, v_m)$ of V and a given V_i and x generated by V_i using the greedy procedure, then x is an extreme point of P_f

Corollary

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

Intuition: why greedy works with polymatroids

- Given w, the goal is to find $x = (x(e_1), x(e_2))$ that maximizes $x^\top w = x(e_1)w(e_1) + x(e_2)w(e_2)$.
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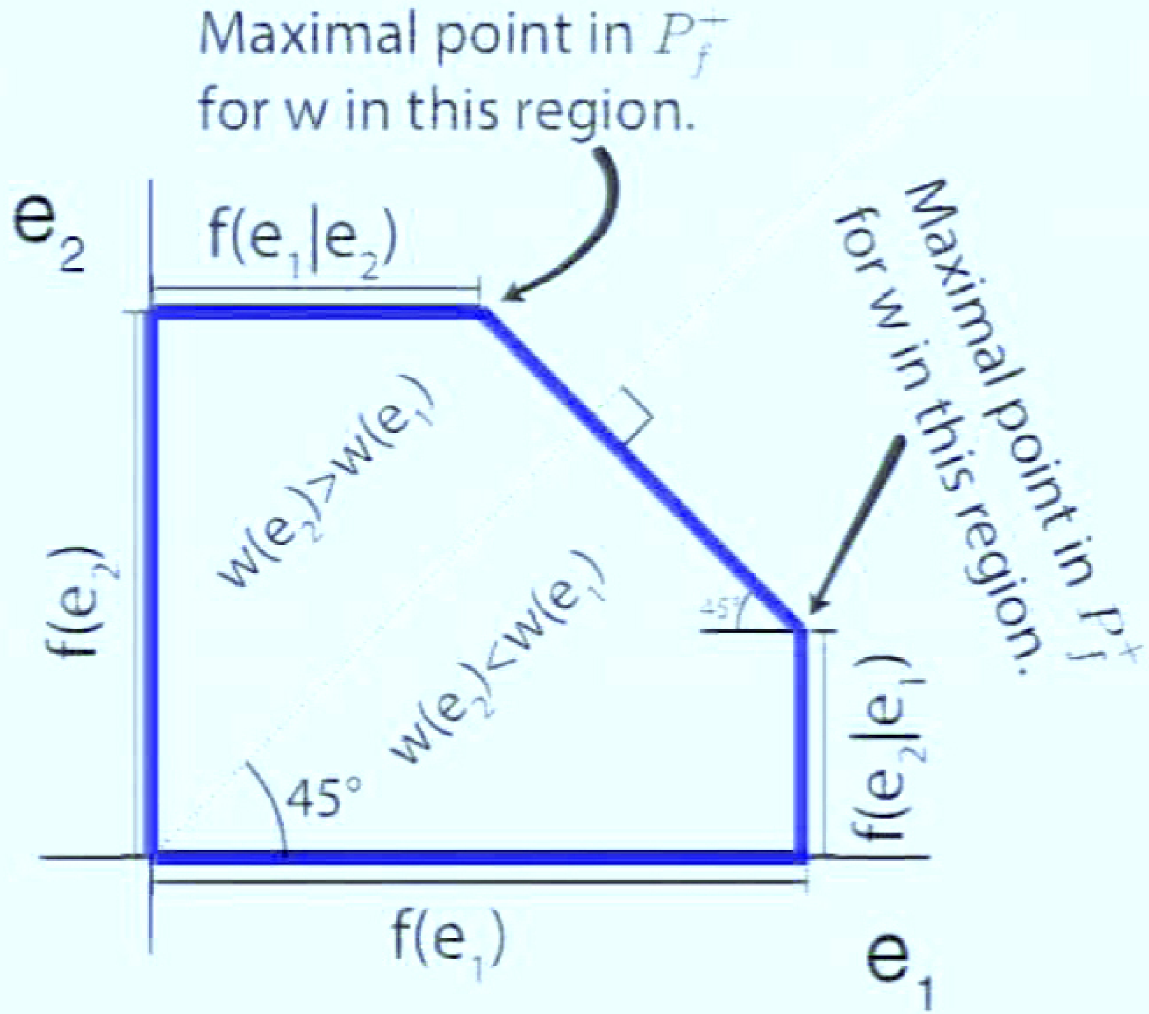

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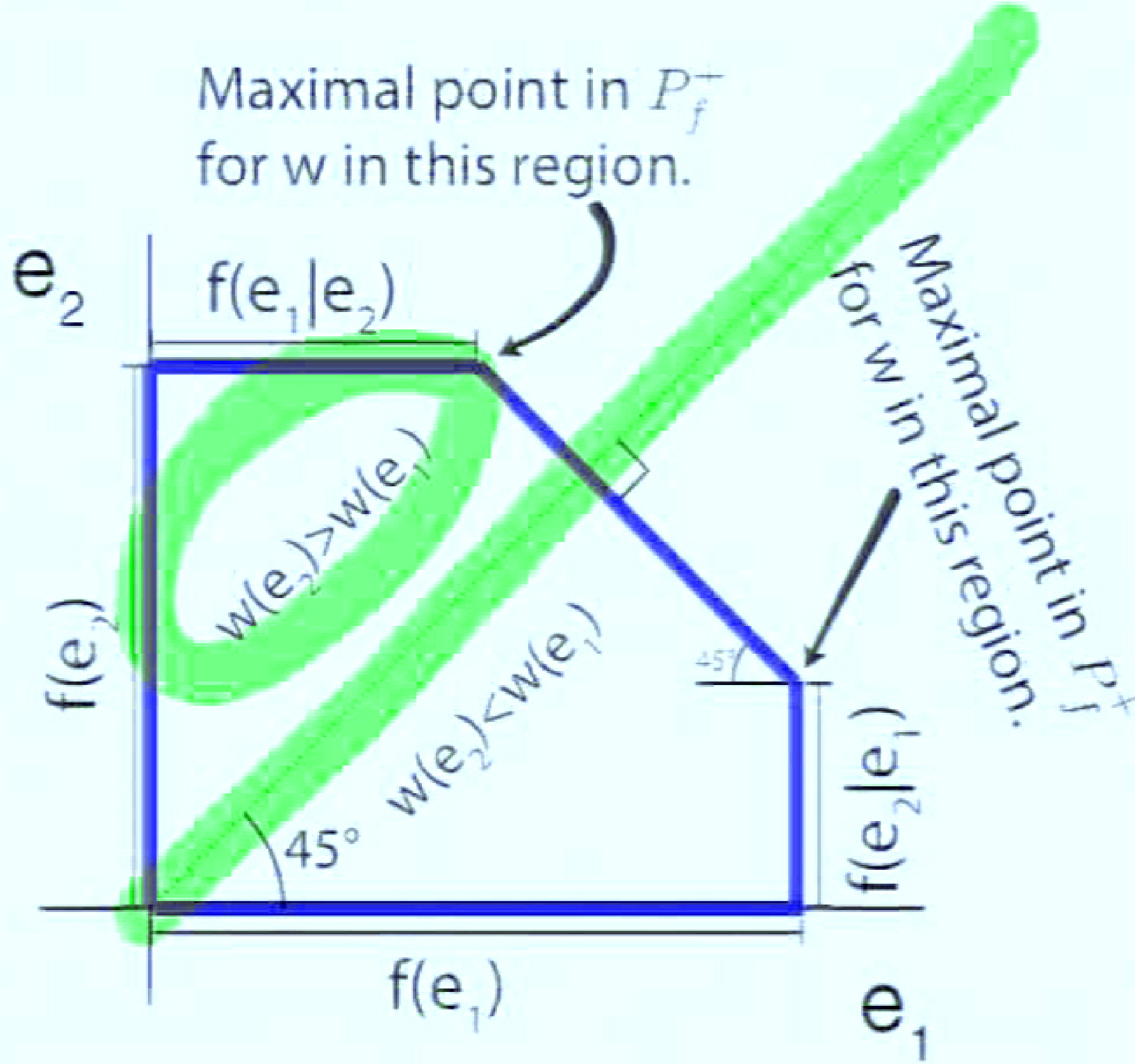

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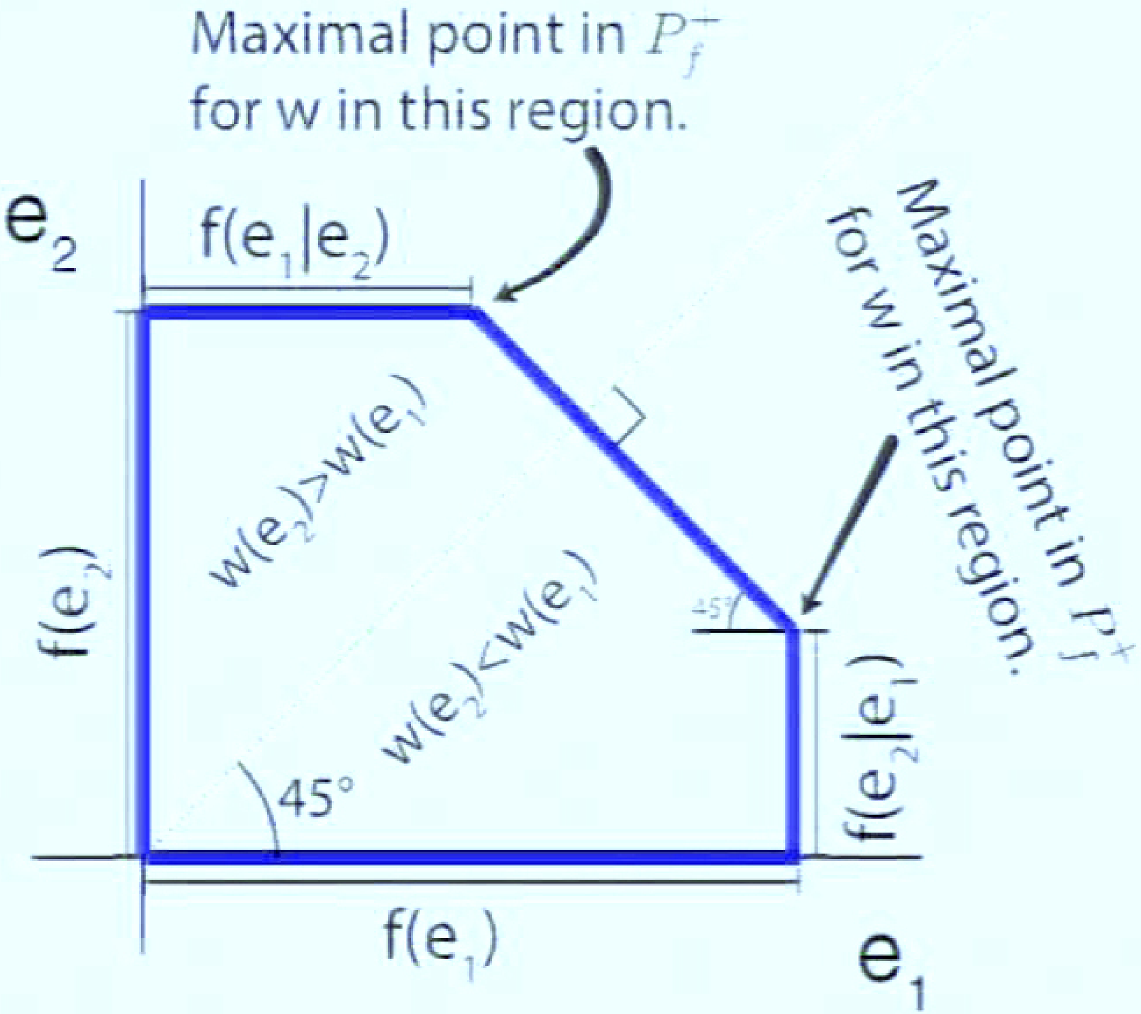

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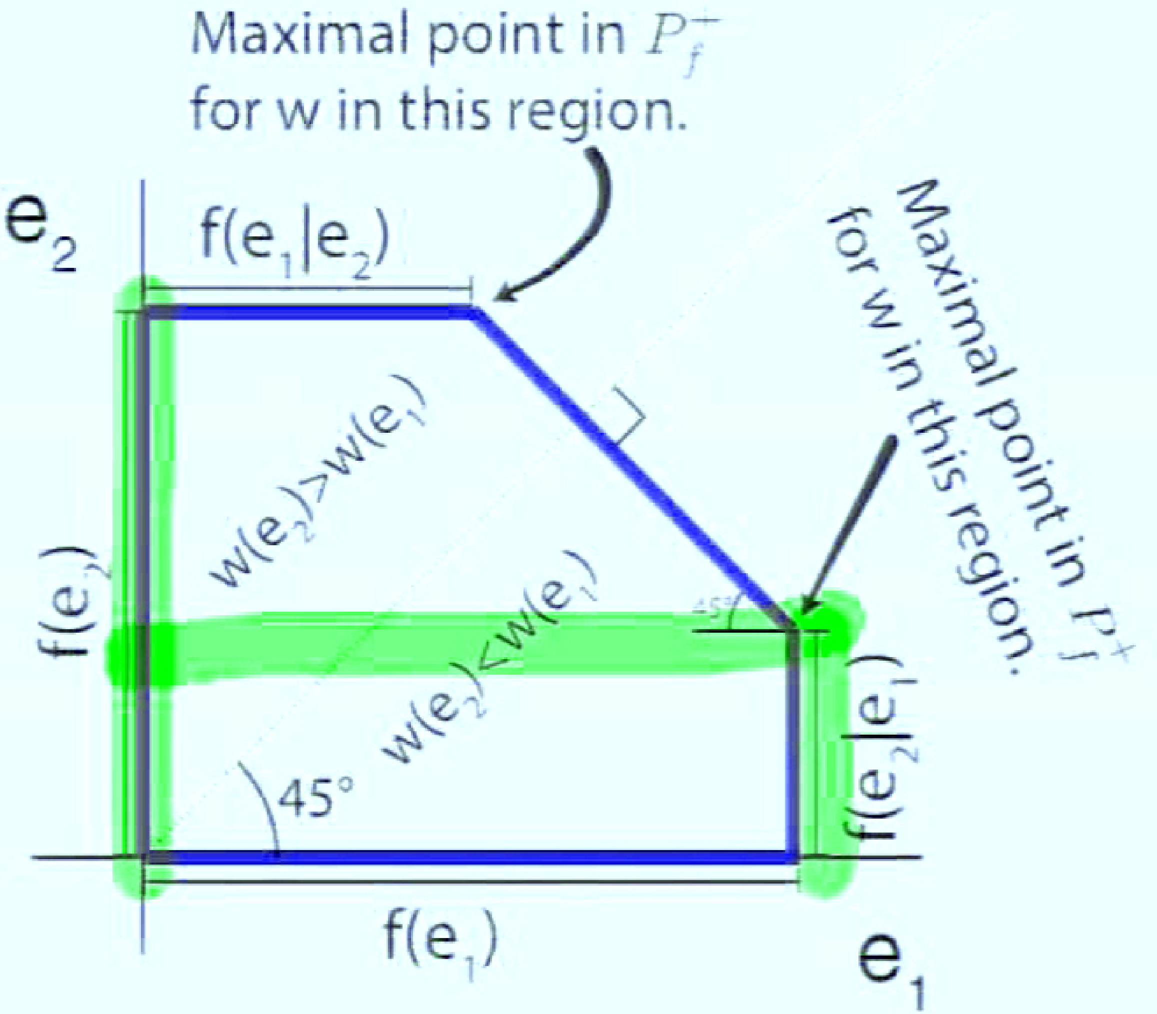

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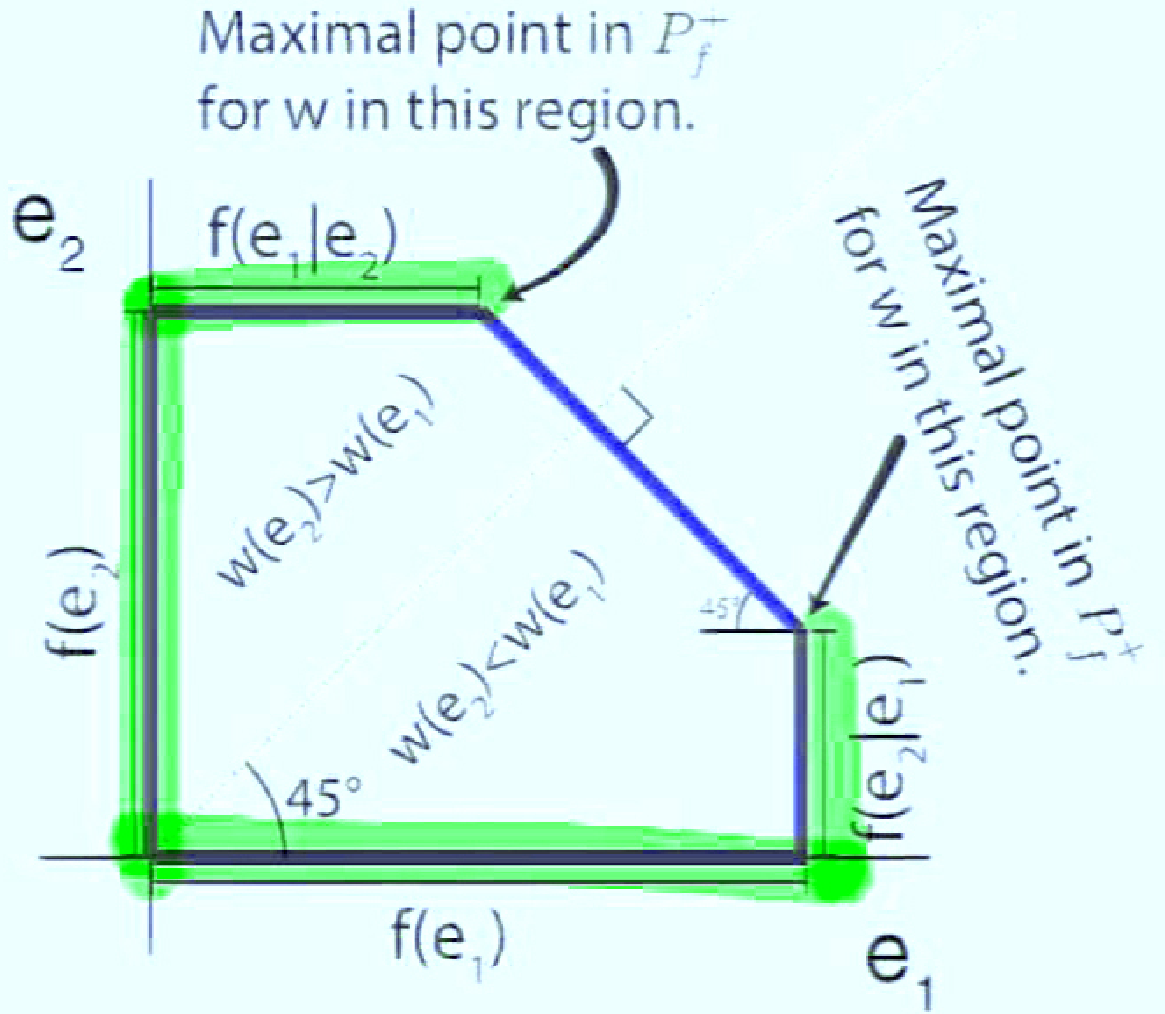
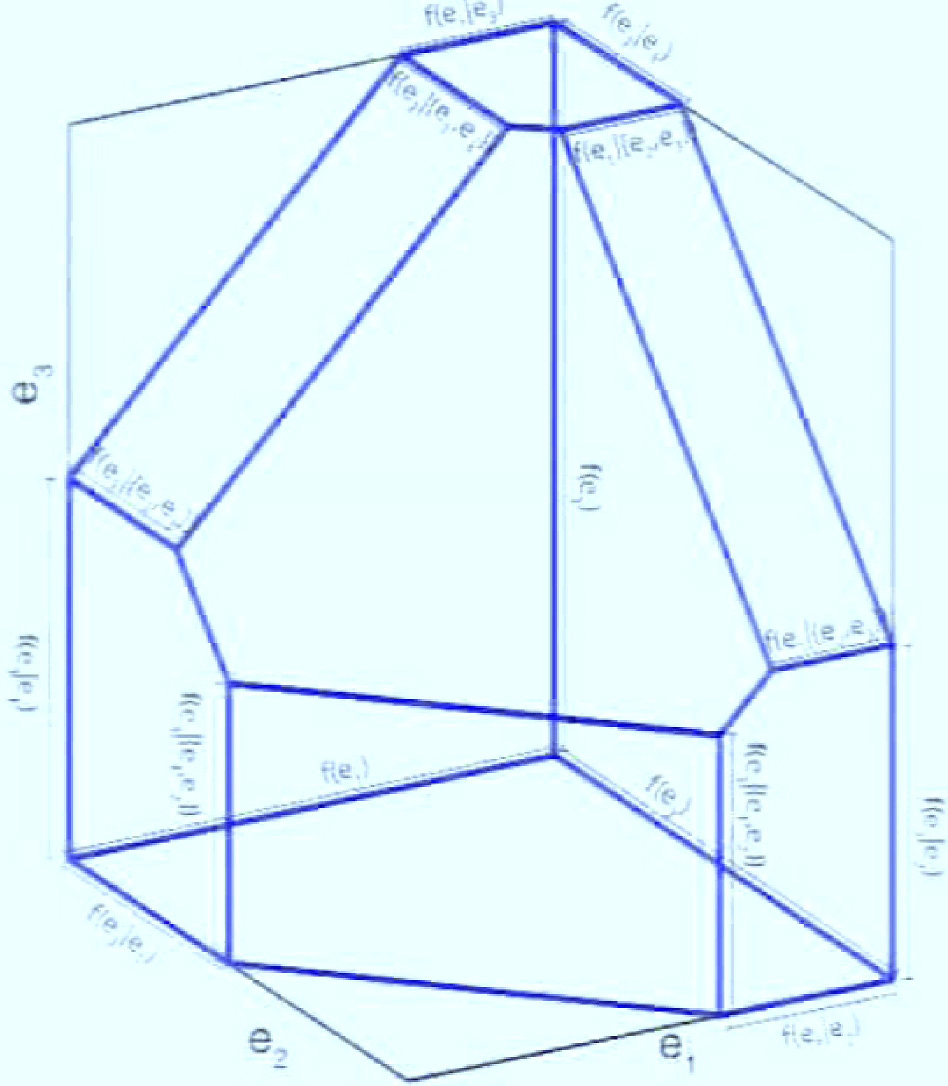
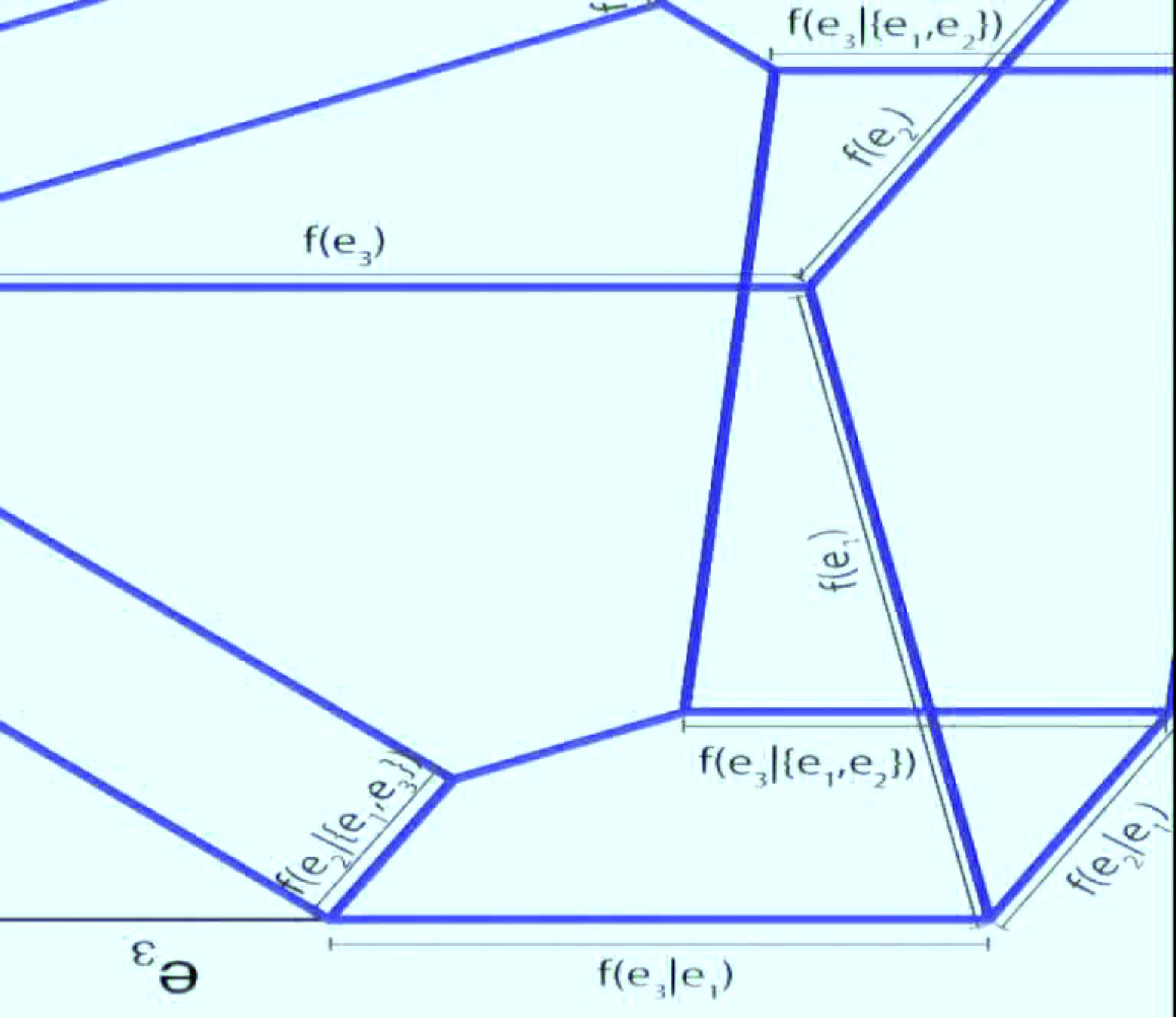


Polymatroid with labeled edge lengths





f(e3|{e1,e2})
f(e2)
f(e3)
f(e1)
f(e3|{e1,e2})
f(e2|{e1,e3})
f(e2|e1)
e3
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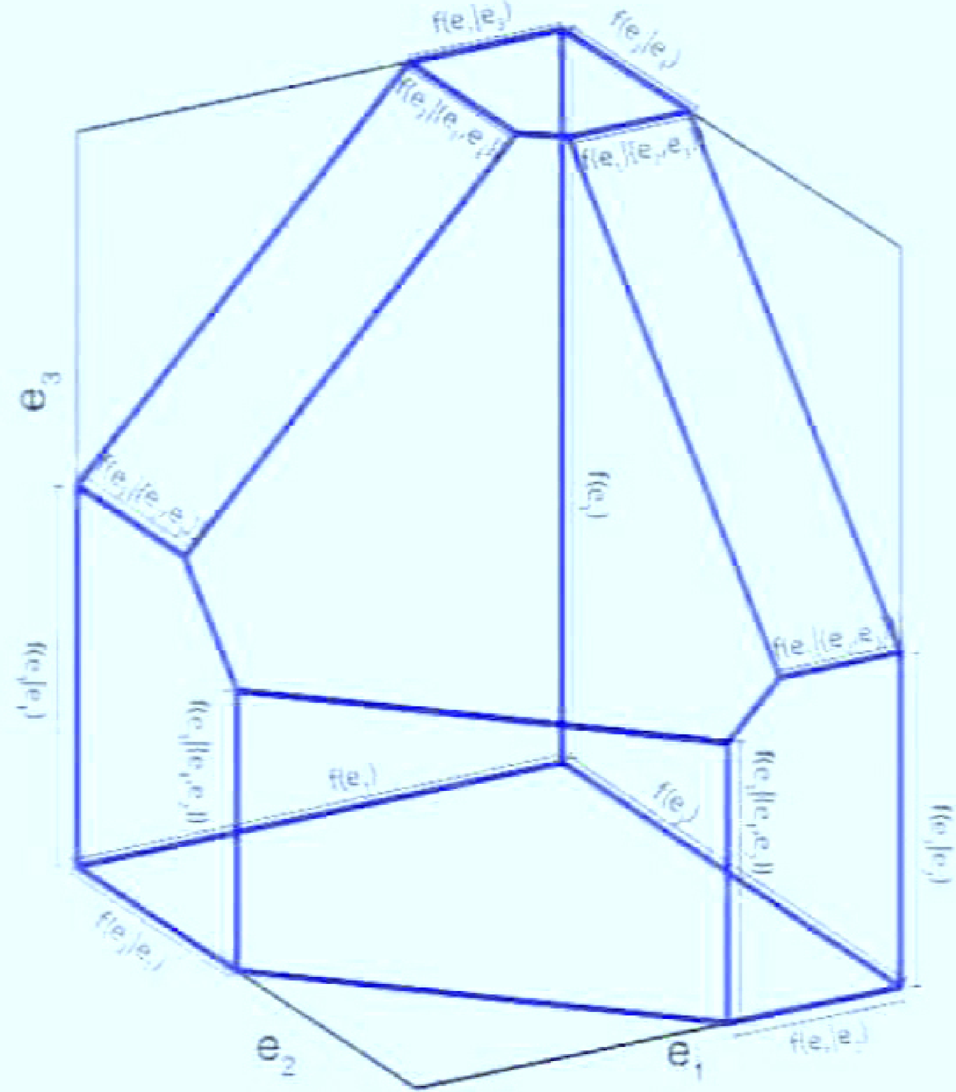

A polymatroid function's polyhedron vs. a polymatroid.

- Given these results, 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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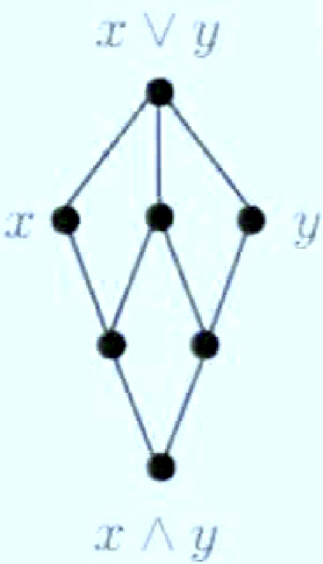
Outline

4. Submodular Definitions, Examples, and Properties

Submodular (or Upper-SemiModular) Lattices

The name "Submodular" comes from lattice theory, and refers to a property of the "height" function of an upper-semimodular lattice. Ex: consider the following lattice over 7 elements.



height
3
2
1
0

submodularity

$h(x)+h(y) > h(x \vee y) + h(x \wedge y)$

$2+2>3+0$

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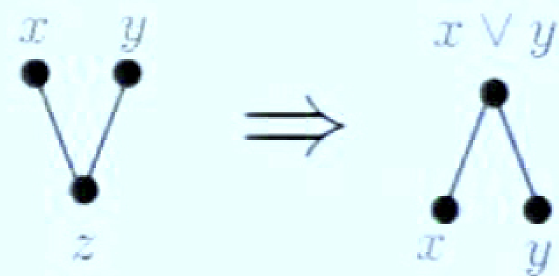

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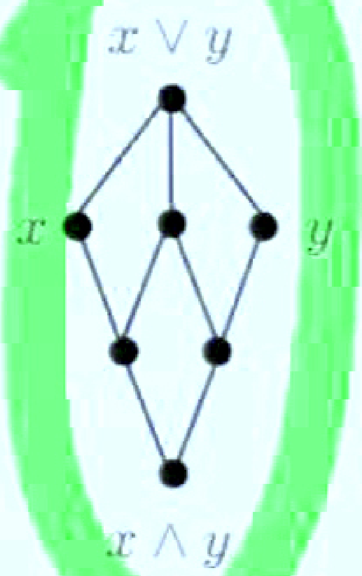
Submodular (or Upper-SemiModular) Lattices

The name "Submodular" comes from lattice theory, and refers to a property of the "height" function of an upper-semimodular lattice. Ex: consider the following lattice over 7 elements.



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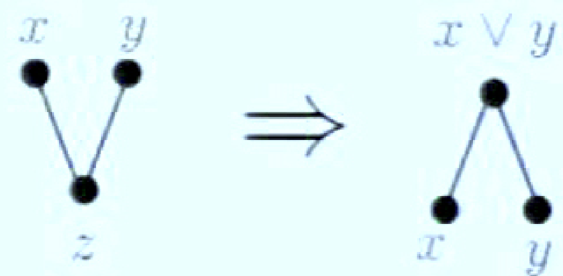

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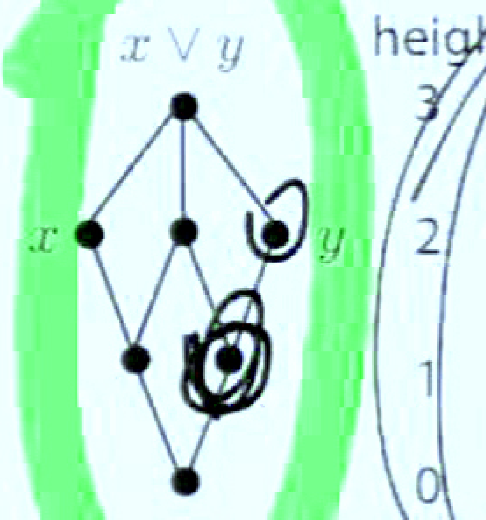

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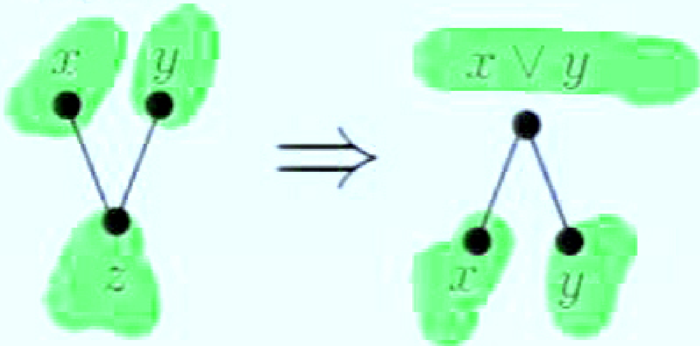

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Submodular Definitions

Definition (submodular)

A function $f : 2^V \to \mathbb{R}$ is submodular if for any $A, B \subseteq V$, we have that:

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \tag{32}$$

- General submodular function, f need not be monotone, non-negative, nor normalized (i.e., $f(\emptyset)$ need not be $= 0$).

Normalized Submodular Function

- Given any submodular function $f : 2^V \to \mathbb{R}$, form a normalized variant $f' : 2^V \to \mathbb{R}$, with

$$f'(A) = f(A) - f(\emptyset) \tag{33}$$

- Then $f'(\emptyset) = 0$.
- This operation does not affect submodularity, or any minima or maxima
- We will assume that all functions in this tutorial are so normalized.

Submodular Polymatroidal Decomposition

- Given any arbitrary submodular function $f : 2^V \to \mathbb{R}$, consider the identity

$$f(A) = \underbrace{f(A) - m(A)}_{\bar{f}(A)} + m(A) = \bar{f}(A) + m(A) \tag{34}$$

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- m is like a unary score, $\bar{f}$ is where things interact . All of the real structure is in $\bar{f}$
- Hence, any submodular function is a sum of polymatroid and modular.

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- Then the telescoping summation property of the gains is as follows:

$$\sum_{i=1}^{r-1} f(A_{i+1}|A_i) = \sum_{i=2}^{r} f(A_i) - \sum_{i=1}^{r-1} f(A_i) = f(A_r) - f(A_1) \quad (39)$$

Submodular Definitions

Theorem

Given function $f : 2^V \to \mathbb{R}$, *then*

$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B) \text{ for all } A, B \subseteq V \qquad \text{(SC)}$$

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Proof.

(SC)⇒(DR): Set $A \leftarrow X \cup \{v\}$, $B \leftarrow Y$. Then $A \cup B = B \cup \{v\}$ and $A \cap B = X$ and $f(A) - f(A \cap B) \geq f(A \cup B) - f(B)$ implies (DR).

(DR)⇒(SC): Order $A \setminus B = \{v_1, v_2, \dots, v_r\}$ arbitrarily. Then $f(v_i|A \cap B \cup \{v_1, v_2, \dots, v_{i-1}\}) \geq f(v_1|B \cup \{v_1, v_2, \dots, v_{i-1}\})$, $i \in [r-1]$ Applying telescoping summation to both sides, we get:

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

□

Many (Equivalent) Definitions of Submodularity

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

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

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

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

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Basic ops: Sums, Restrictions, Conditioning

- Given submodular $f_1, f_2, \ldots, f_k$ each $\in 2^V \to \mathbb{R}$, then conic combinations are submodular. I.e.,

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  where $\alpha_i \geq 0$.
- Restrictions: $f(A) = g(A \cap C)$ is submodular whenever g is, for all C.
- Conditioning: $f(A) = g(A \cup C) - f(C) = f(A|C)$ is submodular whenever g is for all C.

The "or" of two polymatroid functions

- Given two polymatroid functions f and g, suppose feasible A are defined as $\{A : f(A) \geq \alpha_f \text{ or } g(A) \geq \alpha_g\}$ for real α_f, α_g.

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- Therefore, h can be used as a submodular surrogate for the "or" of multiple submodular functions.

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- However, we have a number of forms of composition results that preserve submodularity, which we turn to next:

Grouping elements, set cover, and bipartite neighborhoods

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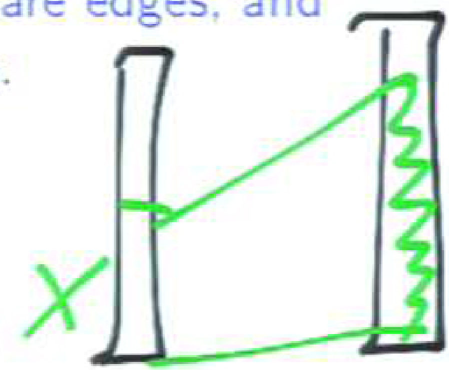

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Given functions $f : 2^V \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$, the composition $h = f \circ g : 2^V \to \mathbb{R}$ (i.e., $h(S) = g(f(S))$) is nondecreasing submodular, if g is non-decreasing concave and f is nondecreasing submodular.

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Given a ground set V. The following two are equivalent:

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- However, Vondrak showed that a graphic matroid rank function over K_4 can't be represented in this fashion.

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- Submodularity is a natural property of an "information" or "complexity" function over subsets of objects.
- All submodular functions express a form of "abstract independence" or "generalized complexity"

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- and a notion of "conditional mutual information"

$$I_f(A; B|C) \triangleq f(A \cup C) + f(B \cup C) - f(A \cup B \cup C) - f(C) \geq 0$$

- and two notions of "information amongst a collection of sets":

$$I_f(S_1; S_2; \ldots; S_k) = \sum_{i=1}^{k} f(S_k) - f(S_1 \cup S_2 \cup \cdots \cup S_k) \tag{54}$$

$$I'_f(S_1; S_2; \ldots; S_k) = \sum_{A \subseteq \{1,2,\ldots,k\}} (-1)^{|A|+1} f(\bigcup_{j \in A} S_j) \tag{55}$$

Submodular Separation and Symmetric Submodular Minimization

- Subsets A and B are separable if $f(A \cup B) = f(A) + f(B)$
- Hence, separability is the same as statistical independence when f is the entropy function.
- Partitioning V into separable blocks can be performed using symmetric SFM.
- Given any polymatroid f, symmetrize it as follows:

Gaussian entropy, and the log-determinant function

Definition (differential entropy $h(X)$)

$$h(X) = -\int_S f(x) \log f(x) dx \tag{59}$$

- When $x \sim \mathcal{N}(\mu, \Sigma)$ is multivariate Gaussian, the (differential) entropy of the r.v. X is given by

$$h(X) = \log \sqrt{|2\pi e \mathbf{\Sigma}|} = \log \sqrt{(2\pi e)^n |\mathbf{\Sigma}|} \tag{60}$$

  and in particular, for a variable subset A and a constant γ,

$$f(A) = h(X_A) = \log \sqrt{(2\pi e)^{|A|} |\mathbf{\Sigma}_A|} = \gamma |A| + \frac{1}{2} \log |\mathbf{\Sigma}_A| \tag{61}$$

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- Application of Jensen's inequality shows that $I(X_{A \setminus B}; X_{B \setminus A} | X_{A \cap B}) = h(X_A) + h(X_B) - h(X_{A \cup B}) - h(X_{A \cap B}) \geq 0$. Hence differential entropy is submodular, and thus so is the logdet function.

Are all polymatroid functions entropy functions?

- No, entropy functions must also satisfy the following:

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Theorem (Yeung)

For any four discrete random variables $\{X, Y, Z, U\}$, then

$$I(X;Y) = I(X;Y|Z) = 0 \tag{62}$$

implies that

$$I(X;Y|Z,U) \leq I(Z;U|X,Y) + I(X;Y|U) \tag{63}$$

where $I(\cdot;\cdot|\cdot)$ is the standard Shannon mutual information function.

Containment, Gaussian Entropy, and DPPs

- Submodular functions $\supset$ Polymatroid functions $\supset$ Entropy functions $\supset$ Gaussian Entropy functions = DPPs.

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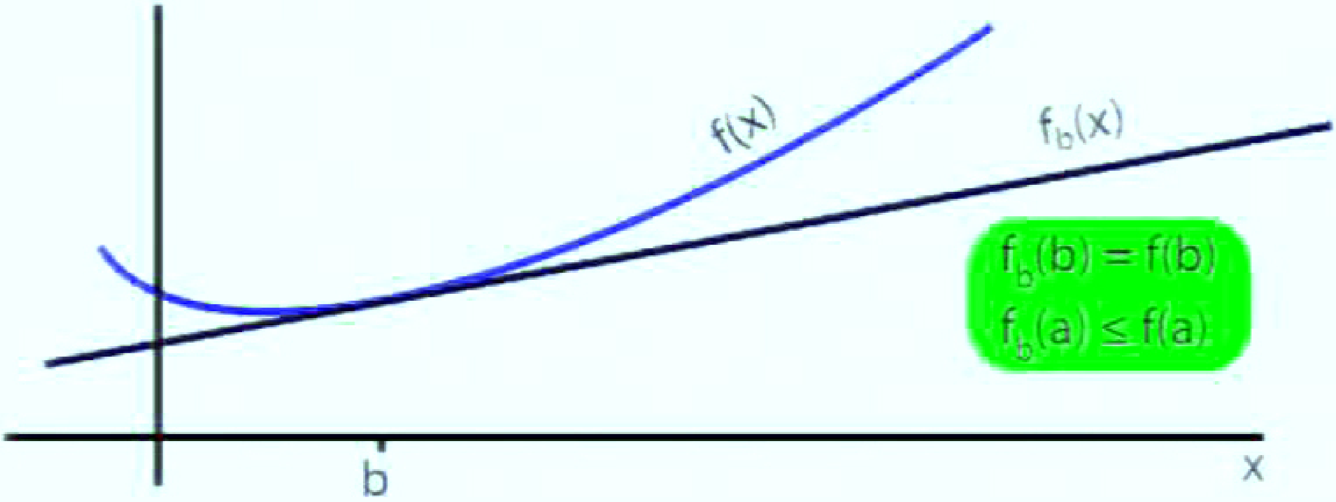
- Submodular functions $\supset$ Polymatroid functions $\supset$ Entropy functions $\supset$ Gaussian Entropy functions = DPPs.
- DPP is a point process where $\Pr(\mathbf{Y} = Y) \propto \det(L_Y)$ for some positive-definite matrix L, so DPPs are log-submodular.

Outline

5. Discrete Semimodular Semigradients

Convex Functions and Tight Subgradients



- A convex function f has a subgradient at any in-domain point b, namely there exists f_b such that

$$f(x) - f(b) \ge \langle f_b, x - b \rangle, \forall x. \tag{64}$$

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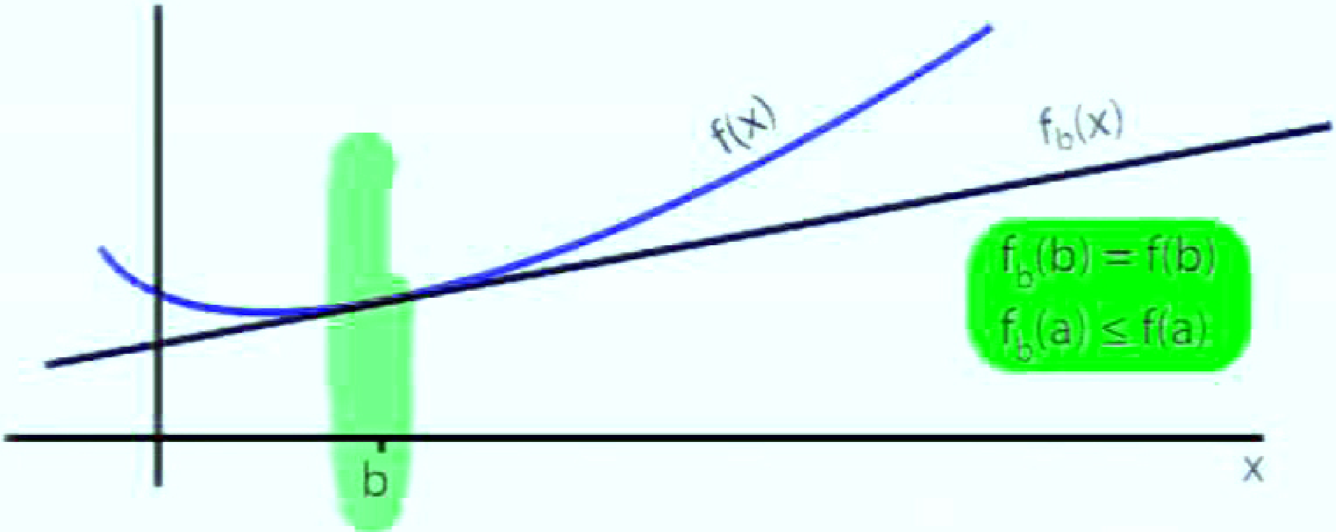

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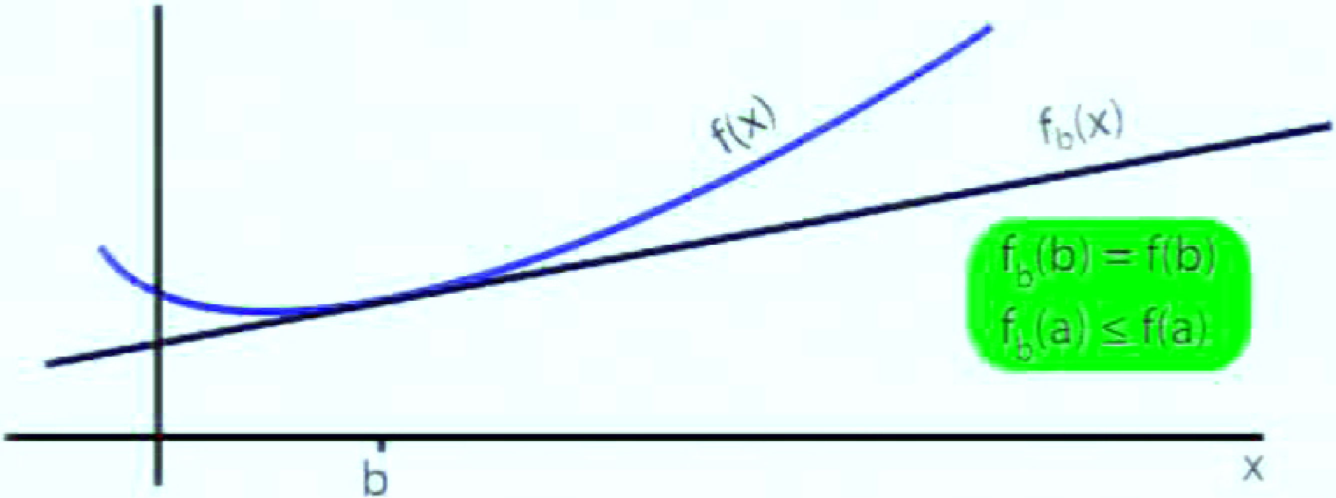

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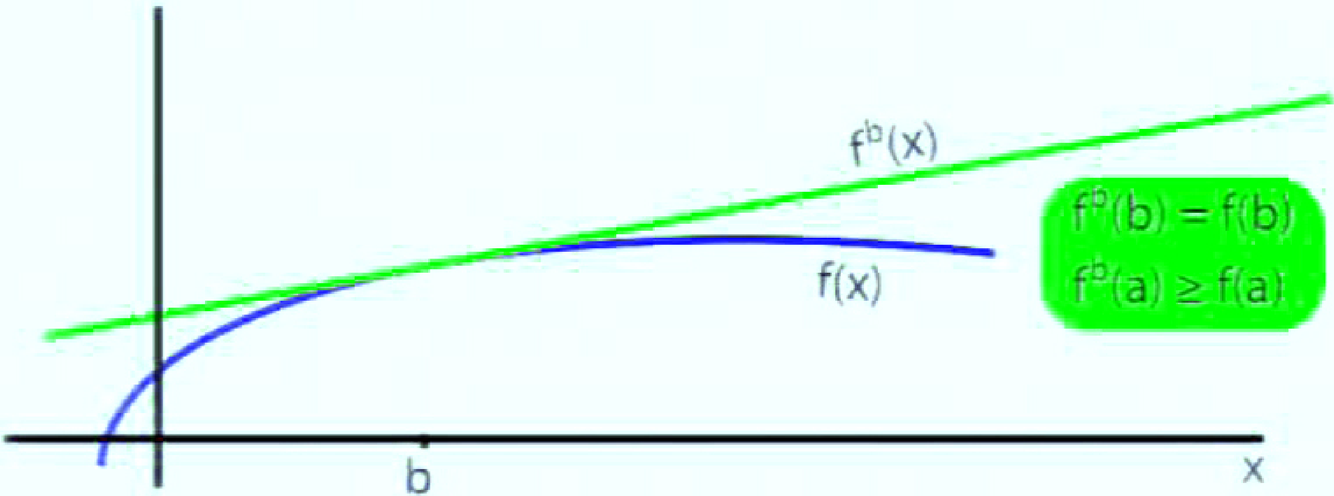
$$f(x) - f(b) \geq \langle f_b, x - b \rangle, \forall x. \quad (64)$$

- We have that $f(x)$ is convex, $f_b(x)$ is affine, and is a tight subgradient (tight at b, affine lower bound on $f(x)$).

Convex Functions and Tight Subgradients



- A concave f has a supergradient at any in-domain point b, namely there exists f^b such that

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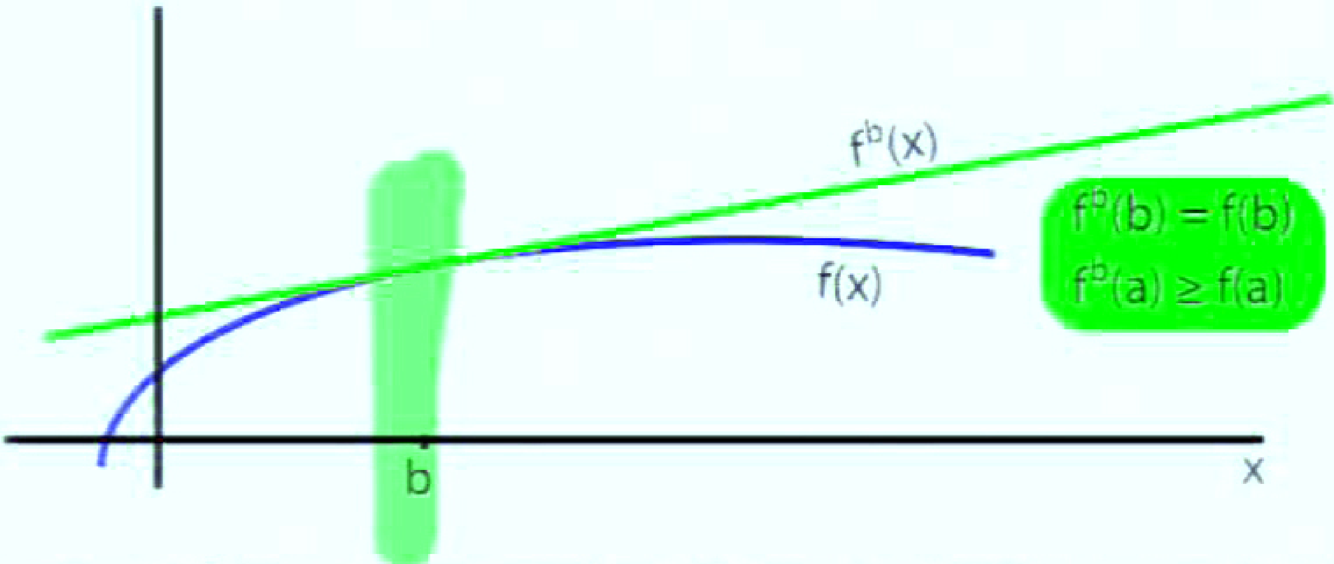

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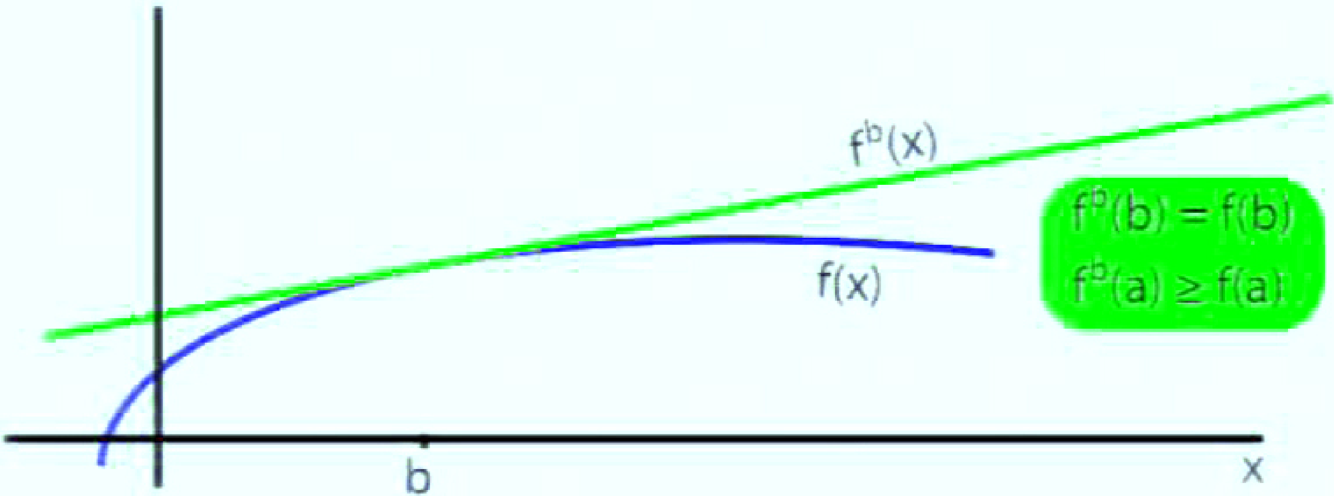

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Trivial additive upper/lower bounds

- Any submodular function has trivial additive upper and lower bounds. That is for all $A \subseteq V$,

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where

$$m^f(A) = \sum_{a \in A} f(a) \tag{67}$$

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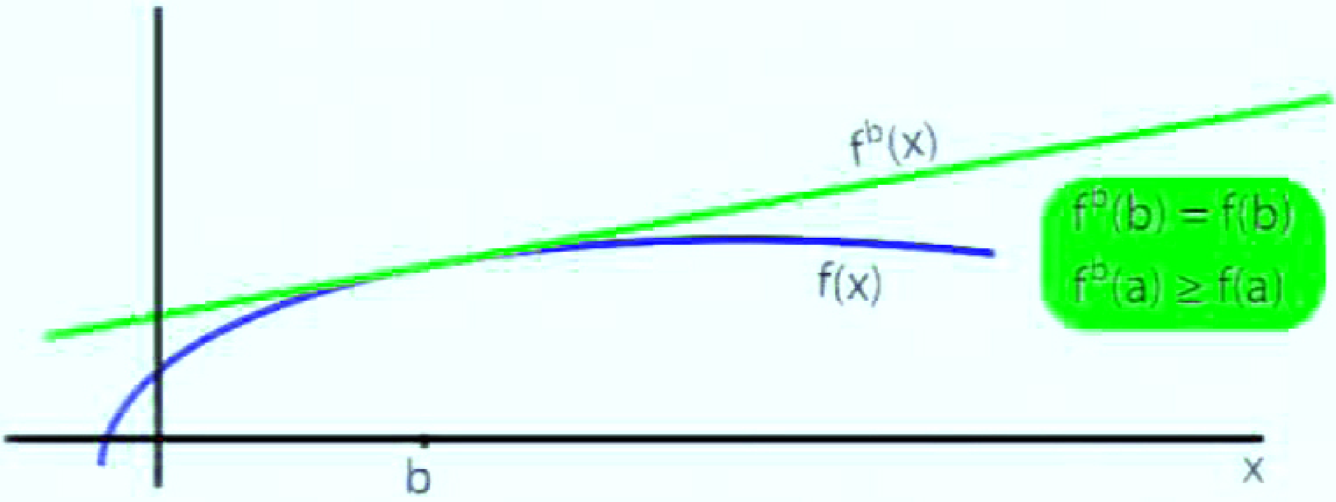

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- $m^f \in \mathbb{R}^V$ and $m_f \in \mathbb{R}^V$ are both modular (or additive) functions.
- A "semigradient" is customized, and at least at one point is tight.

Submodular Subgradients

- For submodular function f, the subdifferential (all subgradients tight at $X \subseteq V$) can be defined as:

$$\partial f(X) = \{x \in \mathbb{R}^V : \forall Y \subseteq V, x(Y) - x(X) \leq f(Y) - f(X)\} \quad (69)$$

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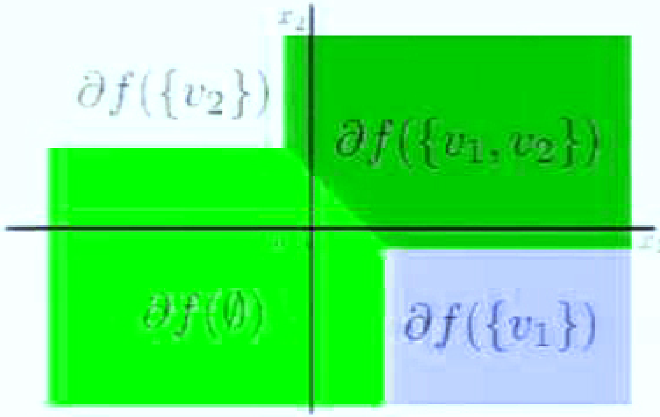

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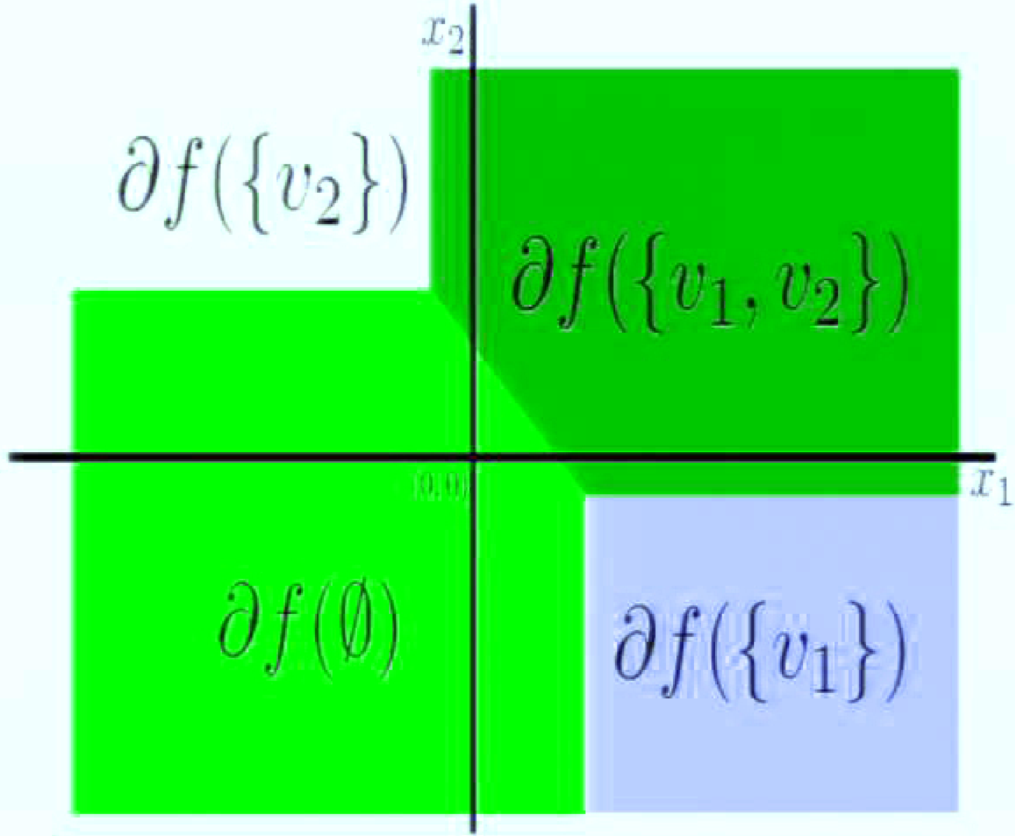

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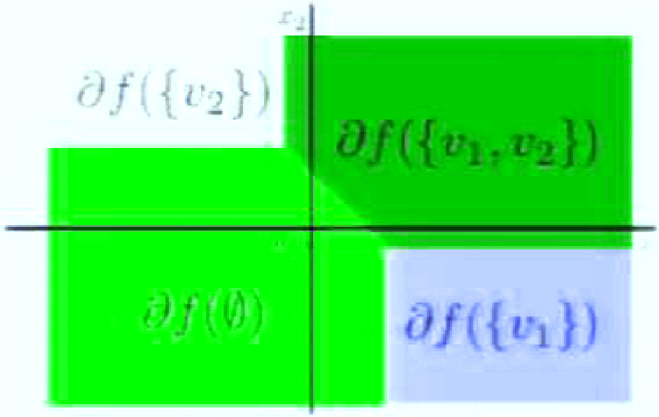

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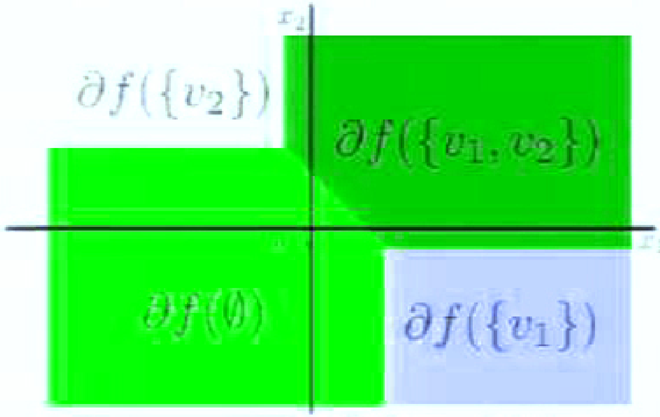

- Extreme points are easy to get via Edmonds's greedy algorithm:

Theorem (Fujishige 2005, Theorem 6.11)

A point $y \in \mathbb{R}^V$ is an extreme point of $\partial f(X)$, iff there exists a maximal chain $\emptyset = S_0 \subset S_1 \subset \cdots \subset S_n$ with $X = S_j$ for some j, such that $y(S_i \setminus S_{i-1}) = y(S_i) - y(S_{i-1}) = f(S_i) - f(S_{i-1})$.

The Submodular Subgradients (Fujishige 2005)

- For an arbitrary $Y \subseteq V$
- Let σ be a permutation of V and define $S_i^\sigma = \{\sigma(1), \sigma(2), \dots, \sigma(i)\}$ as σ's chain where $S_k^\sigma = Y$ where $|Y| = k$.
- We can define a subgradient h_Y^f corresponding to f as:

$$h^f_{Y,\sigma}(\sigma(i)) = \begin{cases} f(S_1^\sigma) & \text{if } i = 1 \\ f(S_i^\sigma) - f(S_{i-1}^\sigma) & \text{otherwise} \end{cases}.$$

- We get a tight modular lower bound of f as follows:

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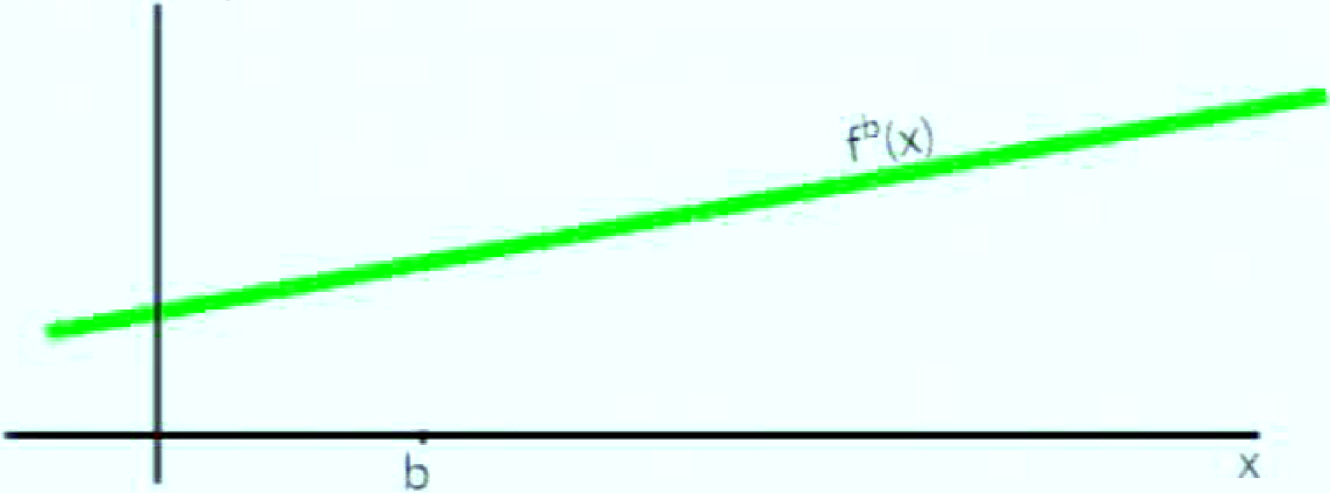

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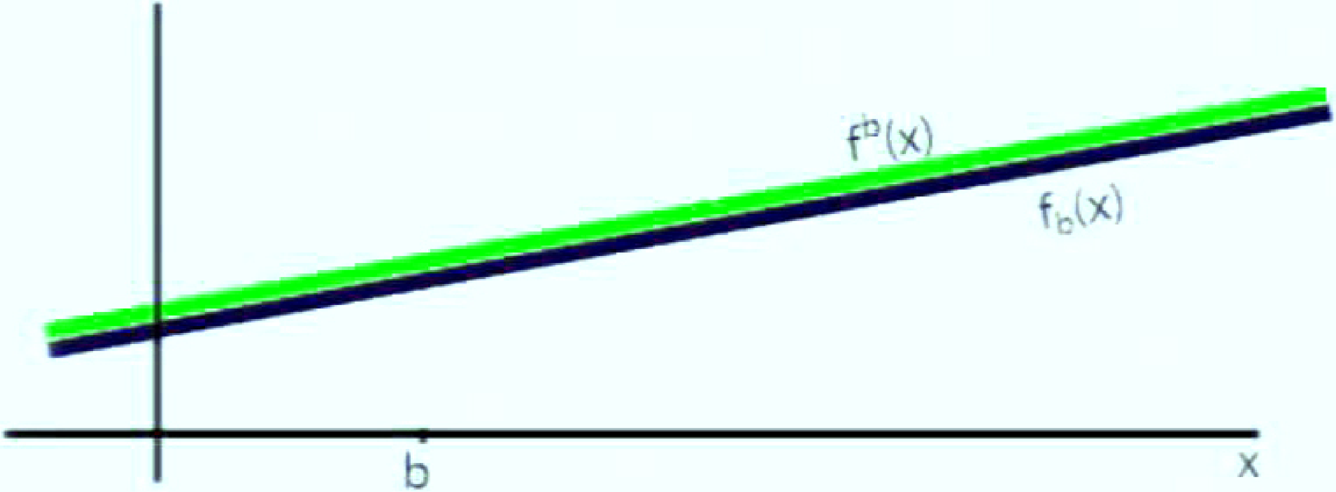

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- Can a submodular function also have a supergradient? We saw that in the continuous case, simultaneous sub/super gradients meant linear.
- (Nemhauser, Wolsey, & Fisher 1978) established the following iff conditions for submodularity (if either hold, f is submodular):

$$f(Y) \leq f(X) - \sum_{j \in X \setminus Y} f(j|X \setminus j) + \sum_{j \in Y \setminus X} f(j|X \cap Y),$$

$$f(Y) \leq f(X) - \sum_{j \in X \setminus Y} f(j|(X \cup Y) \setminus j) + \sum_{j \in Y \setminus X} f(j|X)$$

Recall that $f(A|B) \triangleq f(A \cup B) - f(B)$ is the gain of adding A in the context of B.

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Submodular and Supergradients

- Using submodularity further, these can be relaxed to produce two tight modular upper bounds (Jegelka & Bilmes, 2011, Iyer & Bilmes 2013):

$$f(Y) \leq m^f_{X,1}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j|X \setminus j) + \sum_{j \in Y \setminus X} f(j|\emptyset),$$

$$f(Y) \leq m^f_{X,2}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j|V \setminus j) + \sum_{j \in Y \setminus X} f(j|X).$$

Hence, this yields three tight (at set X) modular upper bounds $m^f_{X,1}, m^f_{X,2}$ for any submodular function f.

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Hence, this yields three tight (at set X) modular upper bounds $m^f_{X,1}, m^f_{X,2}$ for any submodular function f.

Why is $m^f_{X,2}$ Modular?

- $m : 2^V \to \mathbb{R}$ is modular if $m(X) + m(Y) = m(X \cup Y) + m(X \cap Y)$, or equivalently if it can be expressed as, for any $X \subseteq V$:

$$m(X) = c + \sum_{j \in X} m(j) \tag{70}$$

where c is a constant. I.e., $m \in \mathbb{R}^V$.

- For example, the function

$$m^f_{X,2}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j|V \setminus j) + \sum_{j \in Y \setminus X} f(j|X) \tag{71}$$

is modular in Y as Equation (70) with

$$m^f_{X,2}(Y) \triangleq \Big[f(X) - \sum_{j \in X} f(j|V \setminus j)\Big] + \sum_{j \in (X \cap Y)} f(j|V \setminus j) \tag{72}$$

$$+ \sum_{j \in Y \setminus X} f(j|X) \tag{73}$$

Submodular Supergradients (Iyer et al, 2013)

- These three supergradients (which we call grow, shrink, and bar) are easy to obtain.

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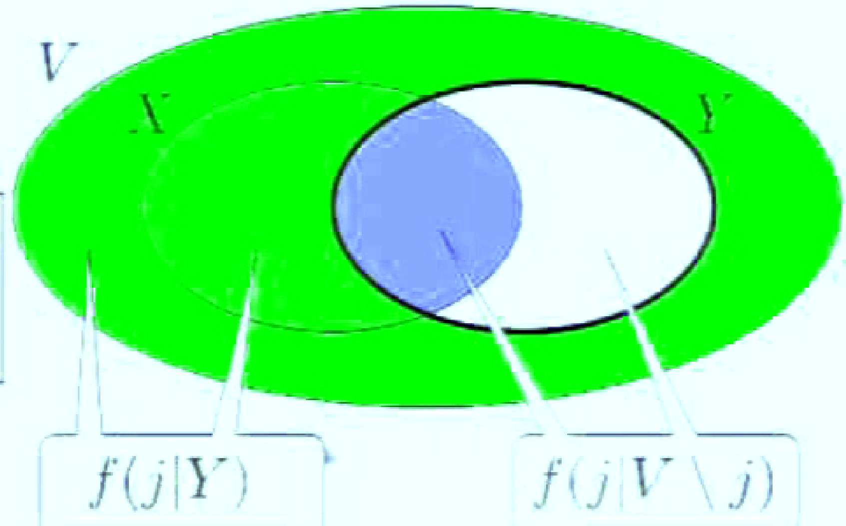
Grow:

$$\hat{g}_Y(j) = \begin{cases} f(j|Y) & \text{for } j \notin Y \\ f(j|V \setminus \{j\}) & \text{for } j \in Y \end{cases}$$



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Shrink:

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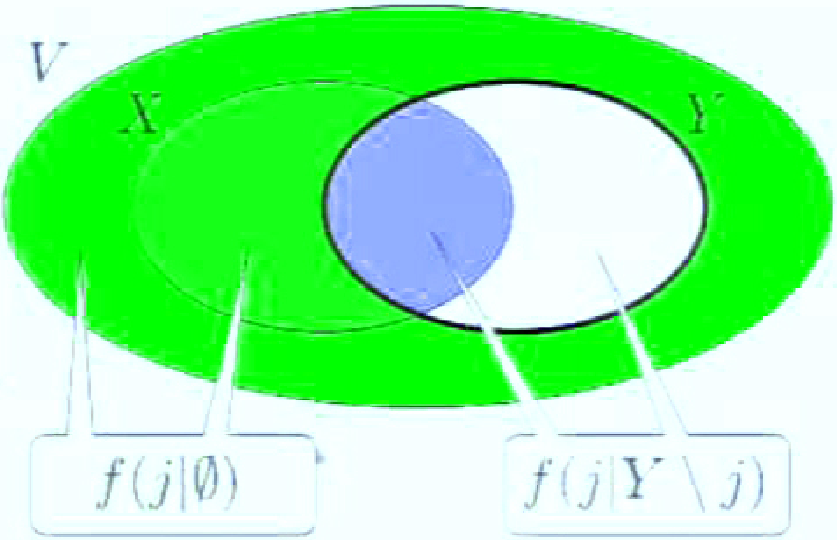

Submodular Supergradients (Iyer et al, 2013)

- These three supergradients (which we call grow, shrink, and bar) are easy to obtain.

Bar:

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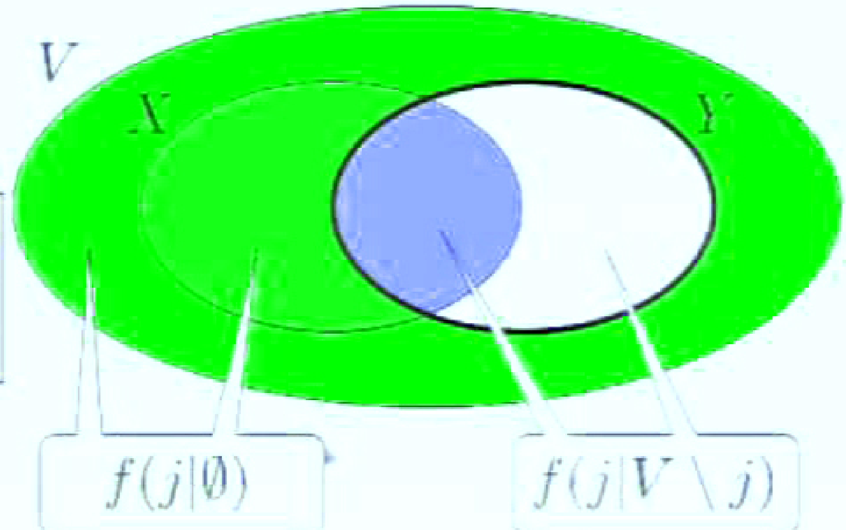

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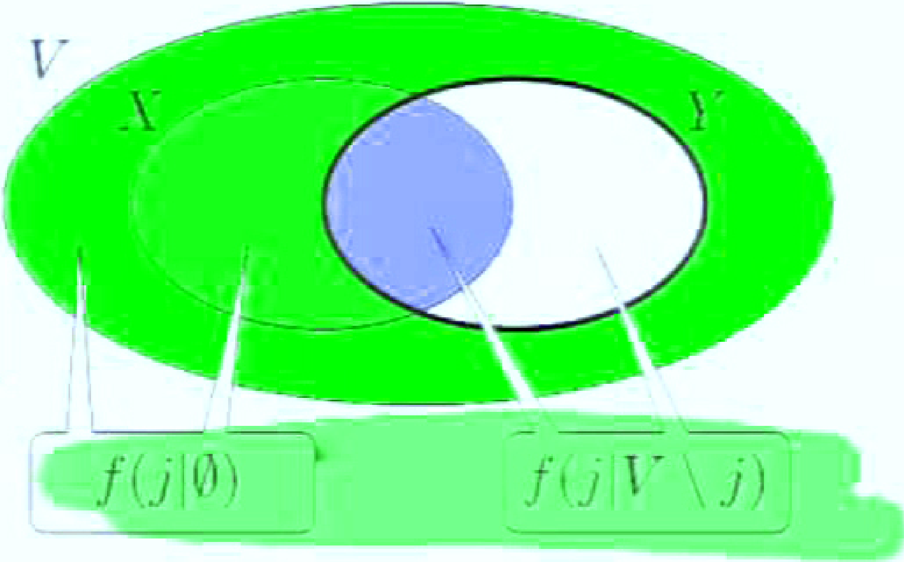

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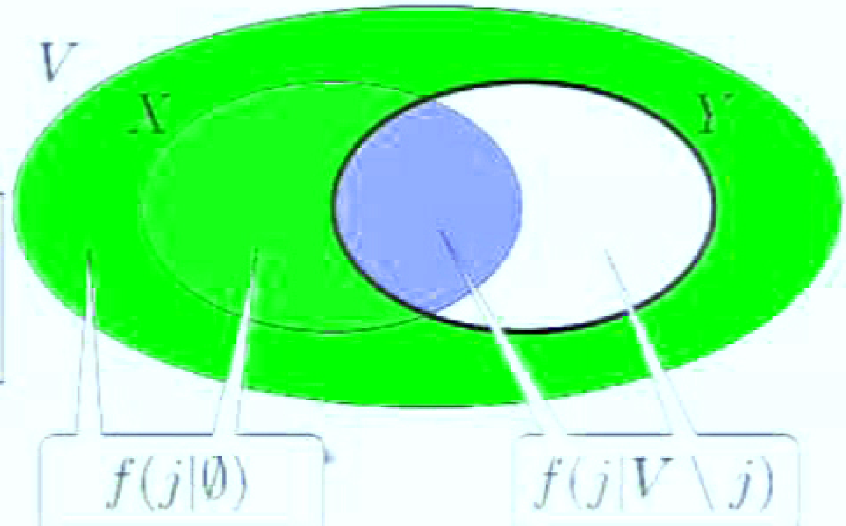

- Modular upper bound: $m^{g_Y}(X) = f(Y) + g_Y(X) - g_Y(Y) \leq f(X)$.

Arbitrary functions as difference between submodular funcs.

Theorem

Given an arbitrary set function f, it can be expressed as a difference $f = g - h$ between two polymatroid functions, where both g and h are polymatroidal.

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- The semi-gradients above offer a majorization/maximization framework to minimize any function that is naturally expressed as such a difference.
- E.g., to minimize $f = g - h$, starting with a candidate solution X, repeatedly choose a modular supergradient for g and modular subgradient for h, and perform modular minimization (easy). (see Iyer & Bilmes, 2012).

Applications

- Sensor placement with submodular costs. I.e., let V be a set of possible sensor locations. $f(A) = I(X_A; X_{V \setminus A})$ measures the quality of a subset A of placed sensors, and $c(A)$ the submodular cost. We have $\min_A f(A) - \lambda c(A)$.
- Discriminatively structured graphical models, EAR measure $I(X_A; X_{V \setminus A}) - I(X_A; X_{V \setminus A} | C)$, and synergy in neuroscience.
- Feature selection: a problem of maximizing $I(X_A; C) - \lambda c(A) = H(X_A) - [H(X_A|C) + \lambda c(A)]$, the difference between two submodular functions, where H is the entropy and c is a feature cost function.
- Graphical Model Inference. Finding x that maximizes $p(x) \propto \exp(-v(x))$ where $x \in \{0, 1\}^n$ and v is a pseudo-Boolean function. When v is non-submodular, it can be represented as a difference between submodular functions.

Outline

6. Continuous Extensions

Continuous Extensions of Discrete Set Functions

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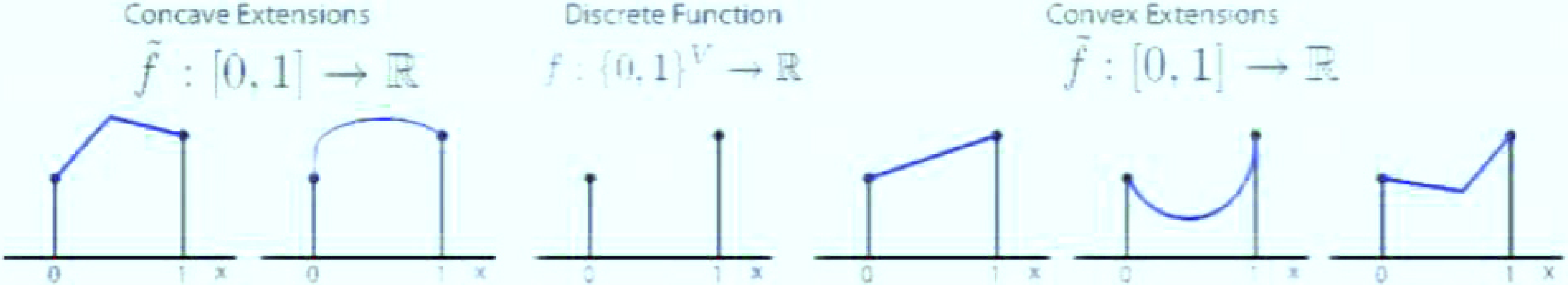

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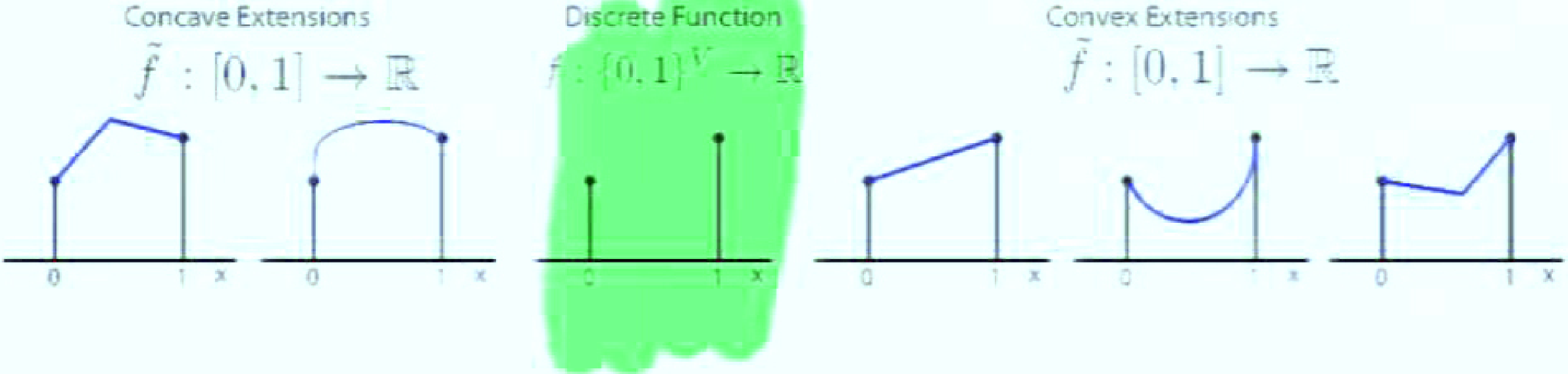

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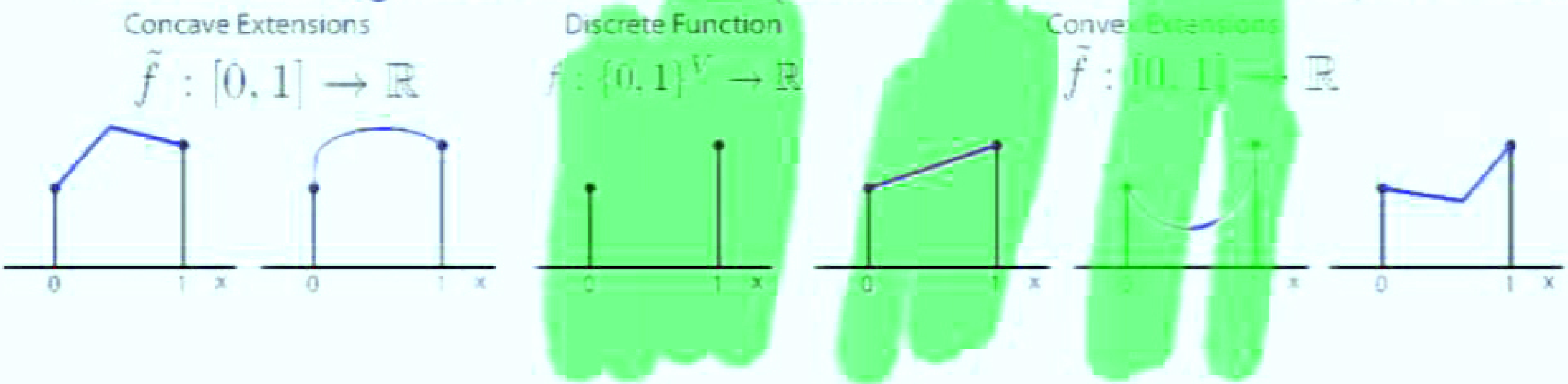

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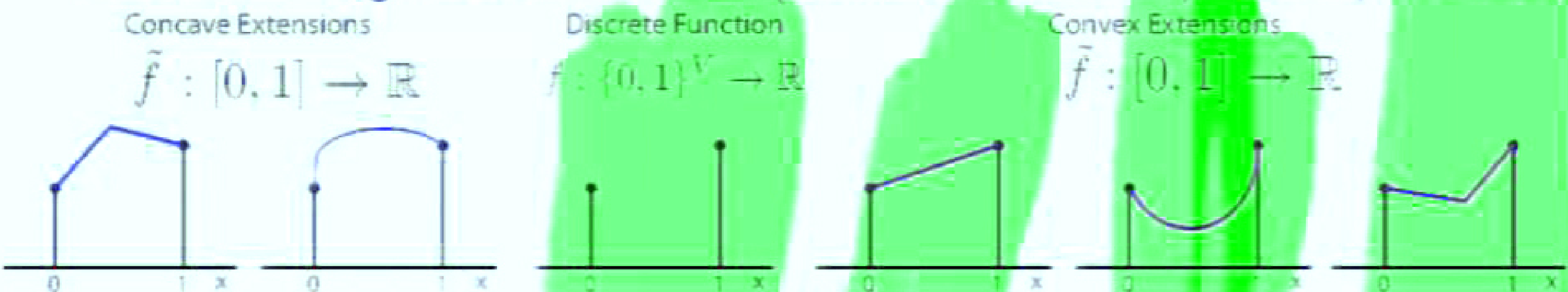

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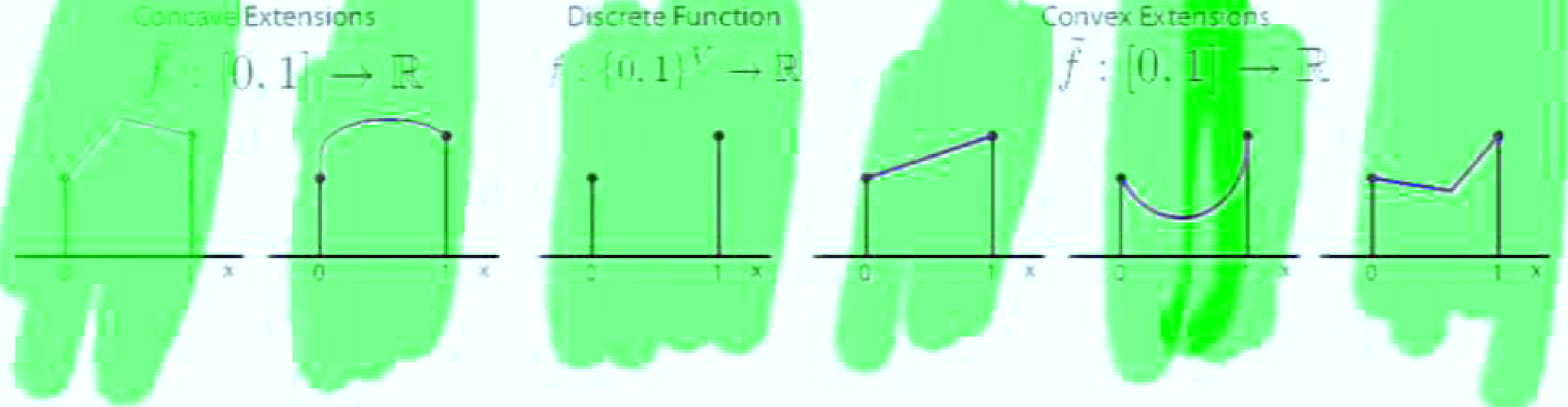

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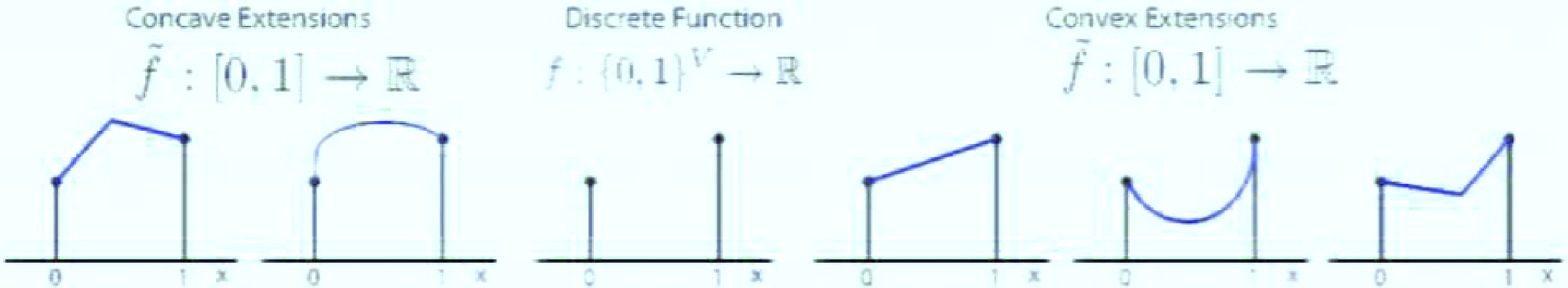

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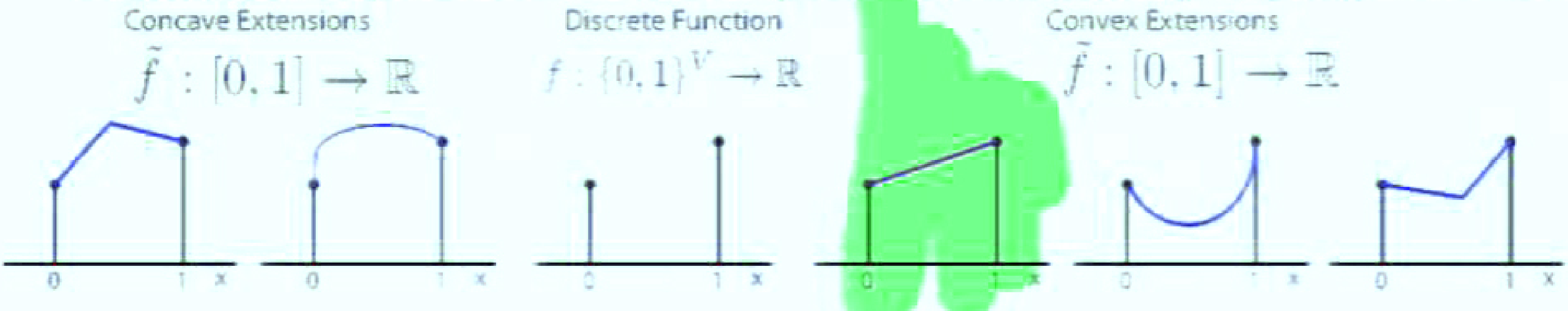

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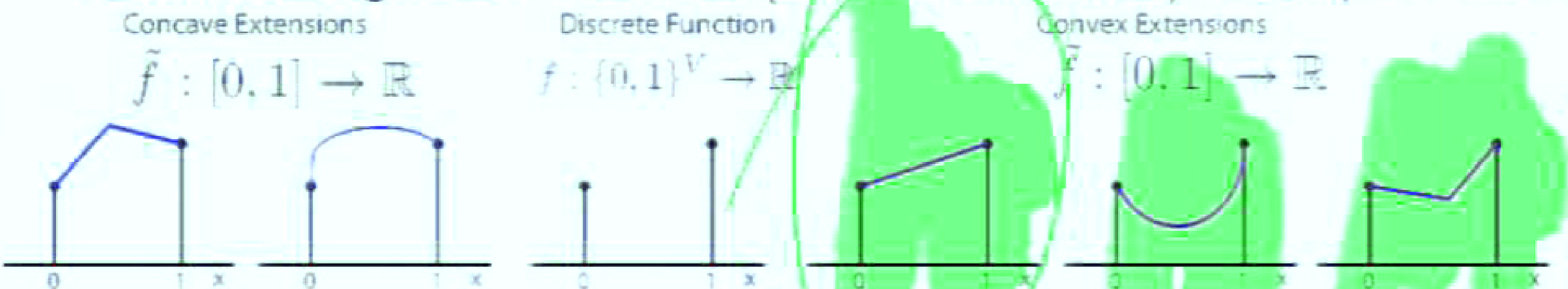

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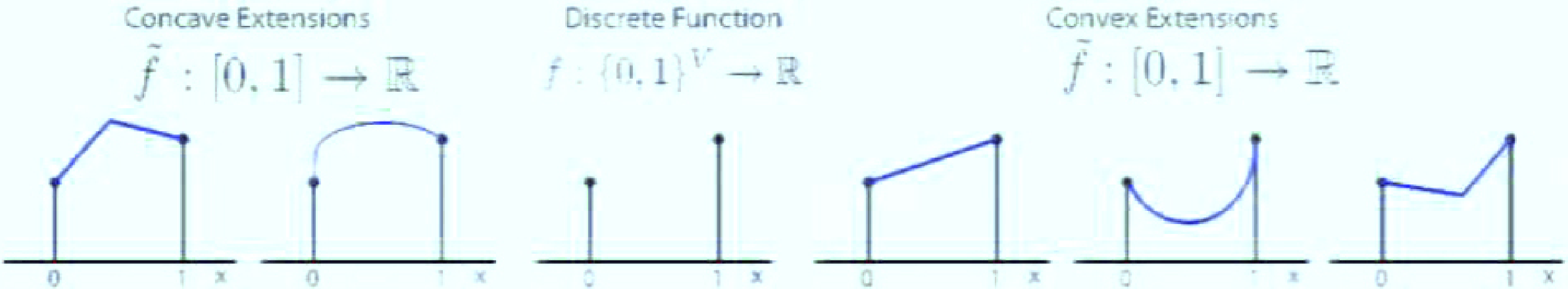

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  3. When are they useful for something practical?

A continuous extension of f

- Given a submodular function f, a $w \in \mathbb{R}^V$, define chain $V_i = \{v_1, v_2, \ldots, v_i\}$ based on w sorted in decreasing order. Then Edmonds's greedy algorithm gives us:

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- Then we can show that, for each i s.t. $\lambda_i > 0$,

$$f(V_i^*) = f(A^*) \tag{86}$$

So such $\{V_i^*\}$ are also minimizers.

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Theorem

Let f be a submodular function defined on subsets of V. For any $x \in \mathbb{R}^V$, we have:

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If we take x to be zero, we get:

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Duality of convex minimization of Lovász extension and min-norm point algorithm

- Let f be a submodular function with $\tilde{f}$ it's Lovász extension. Then the following two problems are duals:

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- Often has to be approximated.

Outline

- Discrete Semimodular Semigradients
- Continuous Extensions
- 7 Like Concave or Convex?
- Optimization
- Parameterization and Applications
- Reading

Submodular: Concave? Convex? Neither? Both?

- Are submodular functions more like convex or more like concave functions?

Submodular is like Concave

- **Convex 1:** Like convex functions, submodular functions can be minimized efficiently (polynomial time).

Submodular is like Concave

- **Convex 3:** Frank's discrete separation theorem: Let $f : 2^V \to \mathbb{R}$ be a submodular function and $g : 2^V \to \mathbb{R}$ be a supermodular function such that for all $A \subseteq V$,

$$g(A) \leq f(A) \quad (91)$$

Then there exists modular function $x \in \mathbb{R}^V$ such that for all $A \subseteq V$:

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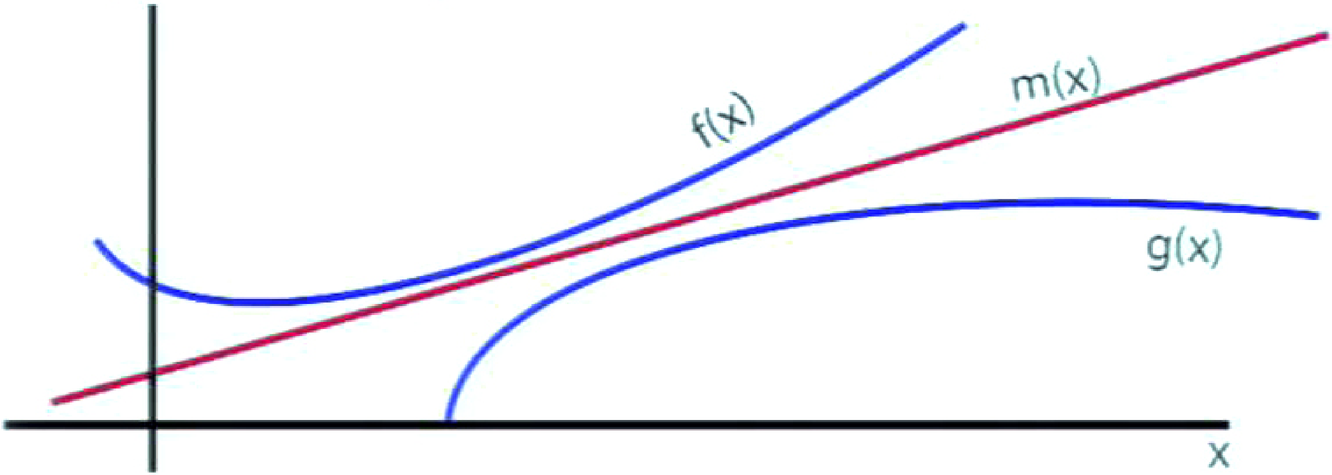
- Compare to convex/concave case.



Submodular is like Concave

- **Convex 4:** Set of minimizers of a convex function is a convex set. Set of minimizers of a submodular function is a lattice. I.e., if $A, B \in \text{argmin}_{A \subseteq V} f(A)$ then $A \cup B \in \text{argmin}_{A \subseteq V} f(A)$ and $A \cap B \in \text{argmin}_{A \subseteq V} f(A)$

Submodularity and Concave

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$$f(X + j) + f(X + k) \geq f(X + j + k) + f(X) \tag{93}$$

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- **Neither 5:** Convex functions have local optimality conditions of the form $\nabla_x f(x) = 0$. Analogous submodular function semi-gradient condition $m(X) = 0$ offers no such guarantee (for neither maximization nor minimization).

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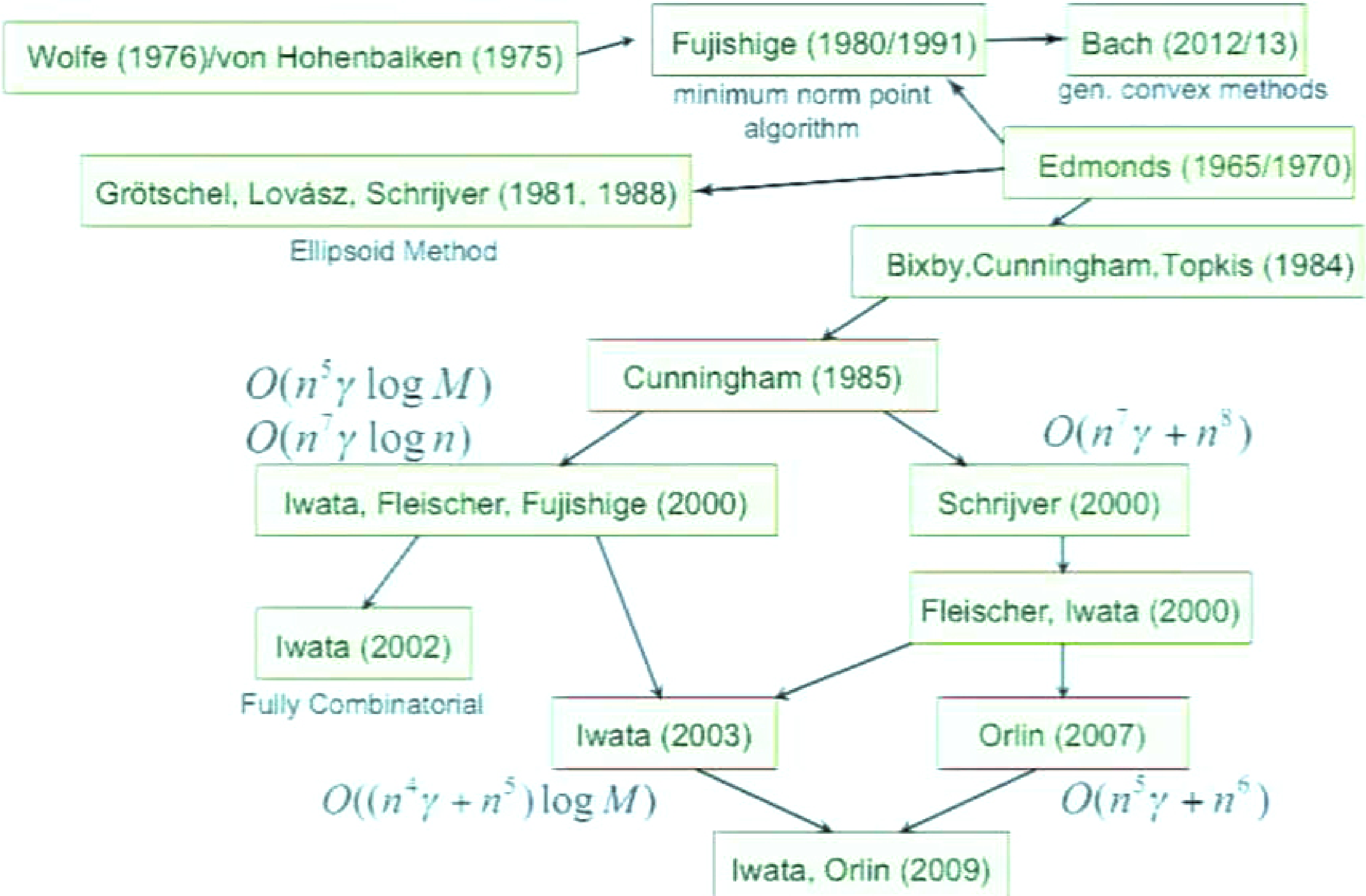
8 Optimization

SFM Summary (modified from S. Iwata's slides)

General Submodular Function Minimization



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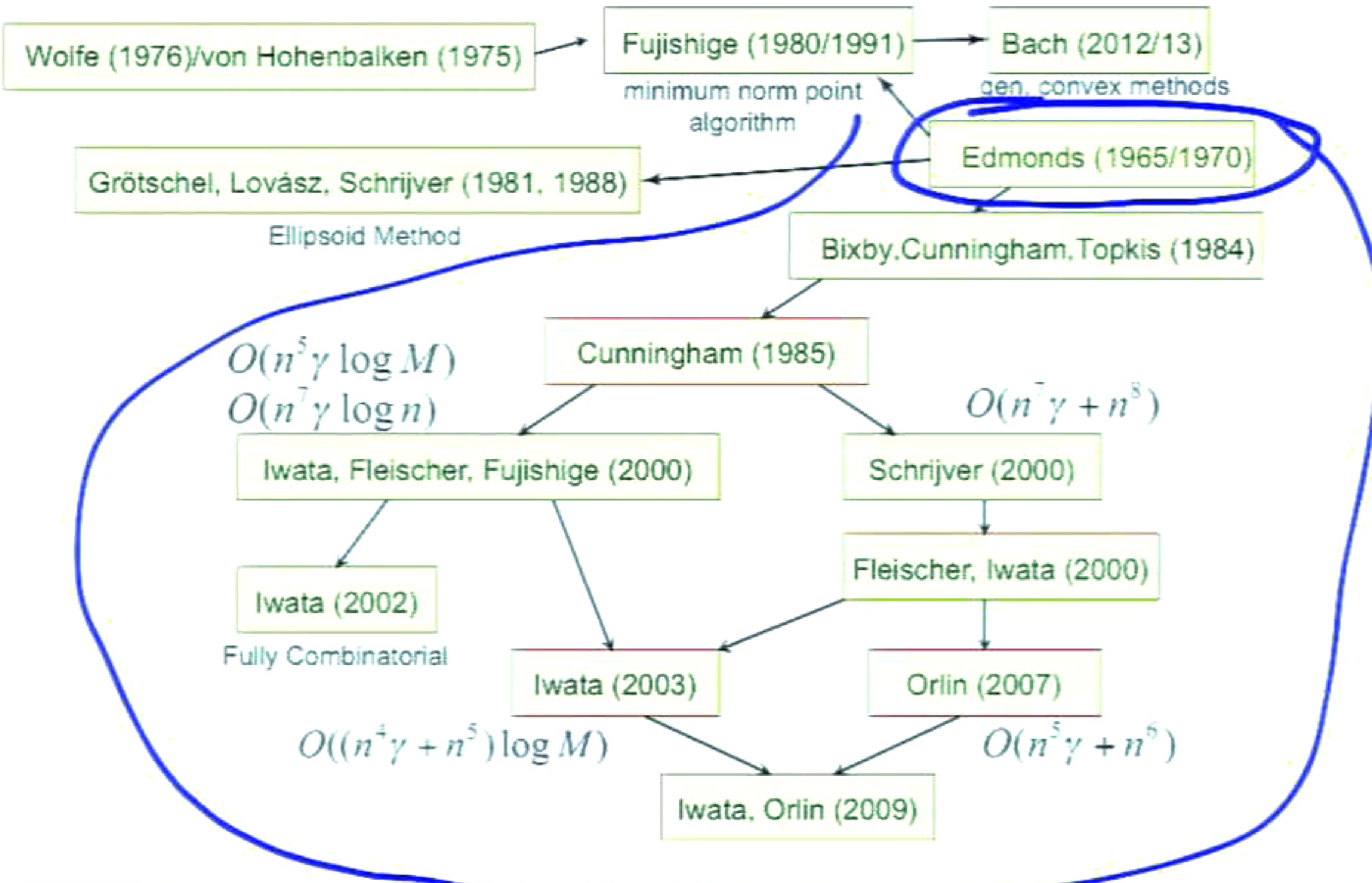

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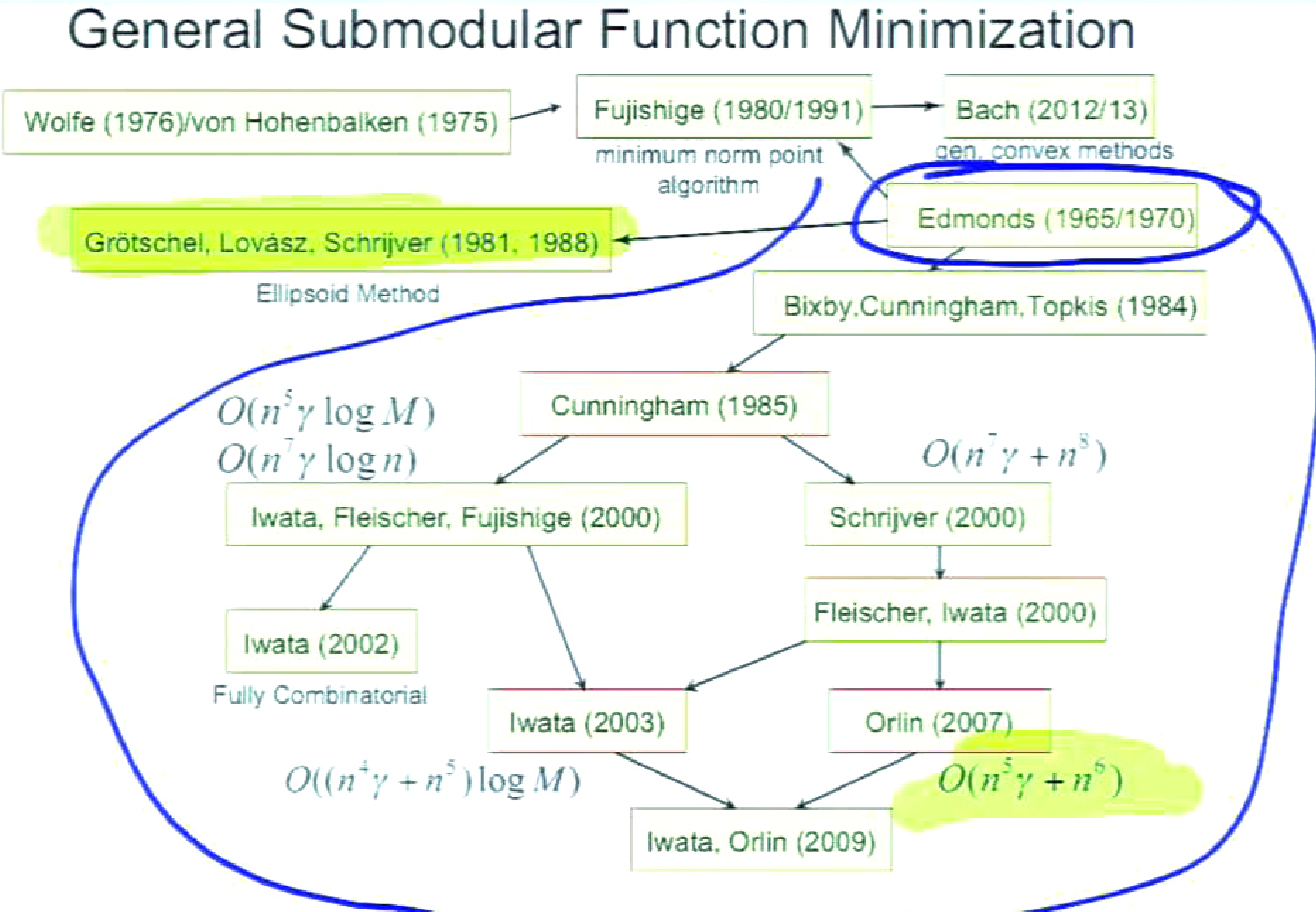

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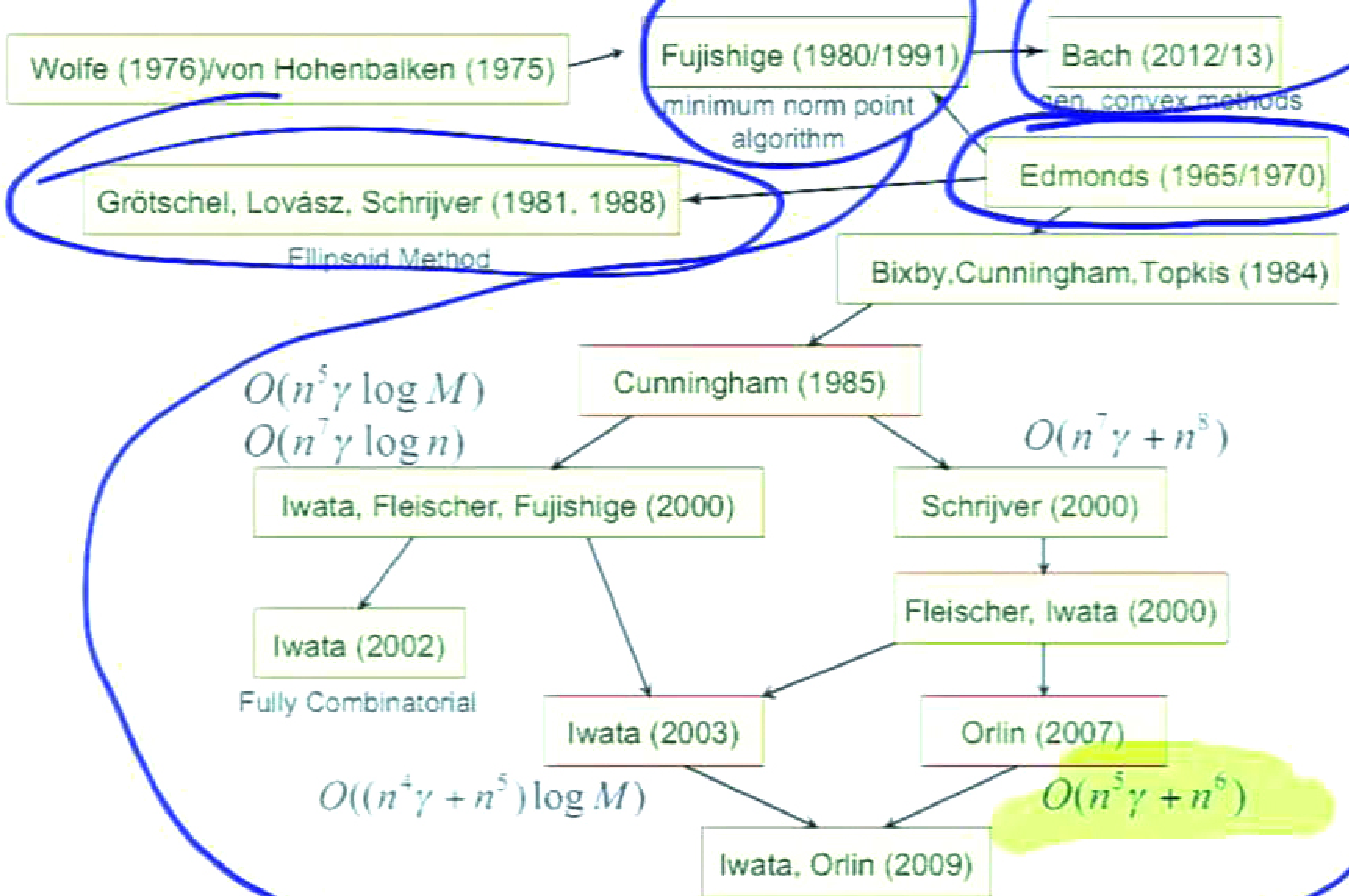

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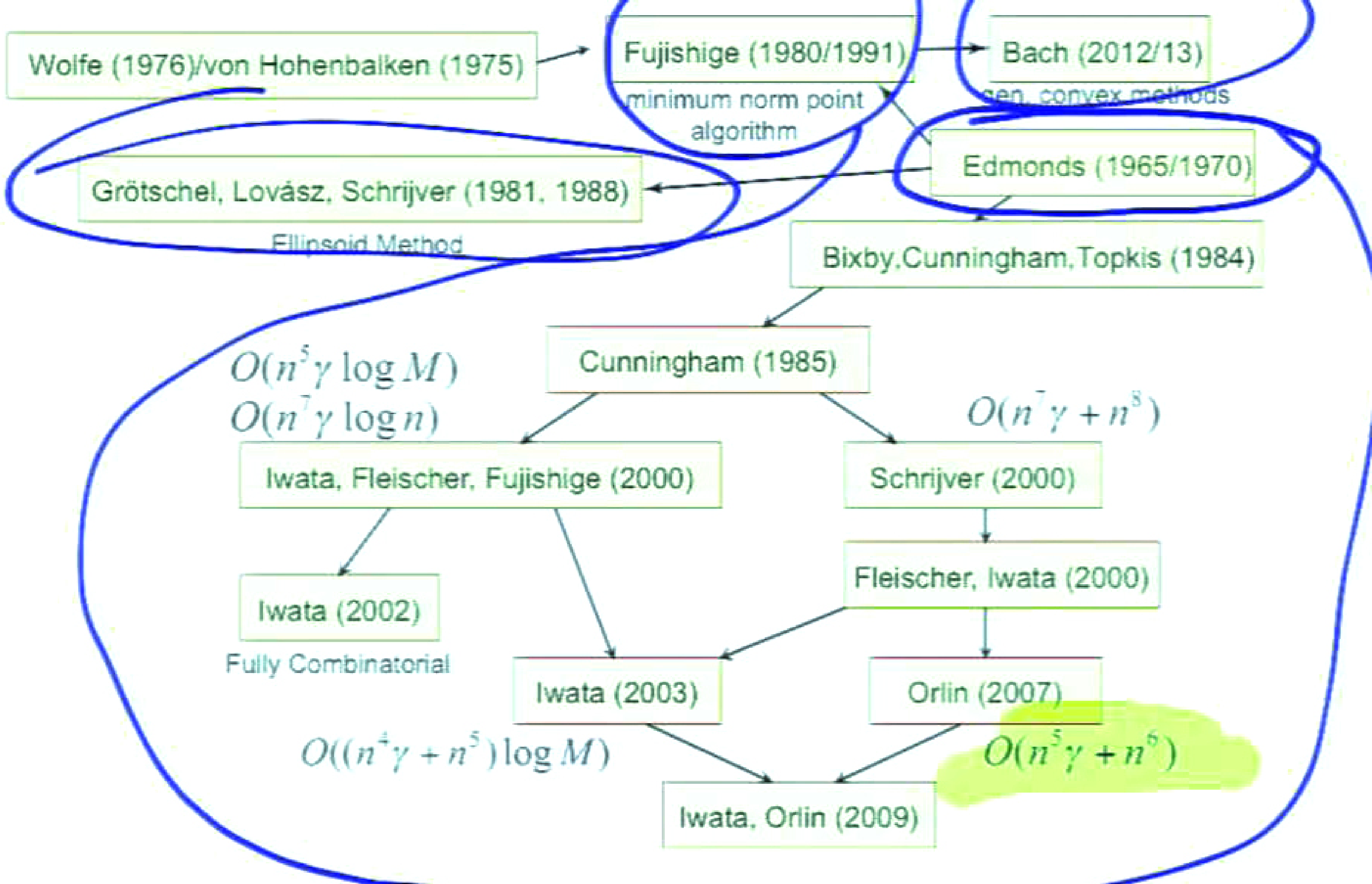

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- $\mathcal{C}$ can be paths, matchings, or spanning trees (Goel et. al.), cover constraints (Iwata & Nagano), cuts (Jegelka & Bilmes), or cardinality lower bounds (Svitkina & Fleischer).
- Some cardinality constraints can be obtained via the min-norm algorithm (Nagano & Kawahara, 2013).
- Other forms of constraints are "easy" (e.g., certain lattices, odd/even sets (see McCormick's SFM tutorial paper).
- In general, many constraints make the problem NP-hard although approximation guarantees are possible (although often hardness is things like $\Omega(n)$ or $\Omega(n^{2/3})$).
- Other forms of constraints: $\mathcal{C} = \{A \subseteq V : g(A) \geq \alpha\}$ for some other submodular function g. This is studied for the first time here at NIPS-2013 (see Saturday talk, Iyer & Bilmes, NIPS 2013).

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Submodular Maximization: Unconstrained

- In general, NP-hard.
- The greedy algorithm for monotone submodular maximization:

Algorithm 2: The Greedy Algorithm

Set $S_0 \leftarrow \emptyset$;
for $i \leftarrow 0 \ldots |V| - 1$ **do**
  Choose v_i as follows: $v_i = \left\{ \text{argmax}_{v \in V \setminus S_i} f(S_i \cup \{v\}) \right\}$;
  Set $S_{i+1} \leftarrow S_i \cup \{v_i\}$;

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- In some cases, it may be useful to view a submodular function $f : 2^V \to \mathbb{R}$ as a input "parameter" to a machine learning algorithm.
- Hence, it is imperative in the ML community to develop ways to learn or approximately learn such submodular parameterizations.
- Ex: Structured sparsity-encouraging convex norm (Bach): i.e., a submodular function f, via its Lovász extension $\tilde{f}$, gives us a norm

$$\|w\|_f = \tilde{f}(|w|) \tag{96}$$

- So finding a desirable norm is equivalent to finding a desirable submodular function.

Graphical Models vs. log-supermodular distributions

- Consider family of distributions $p : \{0.1\}^V \to [0.1]$ of the form:

$$p(x) = \frac{1}{Z} \exp(f(x)) \tag{97}$$

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- If $-f$ is supermodular, MAP assignment is a submodular minimization problem. Typical example:

$$p(x) = \frac{1}{Z}\exp(-f(x) + m(x)) \tag{98}$$

  where f is submodular "energy" (often a graph-cut problem) and m is modular (unaries). Common in computer vision.
- Complexity is polynomial regardless of the tree-width of f — submodularity is anti-graphical.
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- Hence $p(x)$ is a determinantal point process.

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Classic References

- Jack Edmonds's paper "Submodular Functions, Matroids, and Certain Polyhedra" from 1970.
- Nemhauser, Wolsey, Fisher, "A Analysis of Approximations for Maximizing Submodular Set Functions-I", 1978
- Lovász's paper, "Submodular functions and convexity", from 1983.

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- Stefanie Jegelka and Andreas Krause's ICML 2013 tutorial http://techtalks.tv/talks/submodularity-in-machine-learning-new-directions-part-i/58125/
- Francis Bach's updated 2013 text. http://hal.archives-ouvertes.fr/docs/00/87/06/09/PDF/submodular_fot_revised_hal.pdf
- Tom McCormick's overview paper on submodular minimization http://people.commerce.ubc.ca/faculty/mccormick/sfmchap8a.pdf
- Georgia Tech's 2012 workshop on submodularity: http://www.arc.gatech.edu/events/arc-submodularity-workshop

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- Francis Bach's updated 2013 text. http://hal.archives-ouvertes.fr/docs/00/87/06/09/PDF/submodular_fot_revised_hal.pdf
- Tom McCormick's overview paper on submodular minimization http://people.commerce.ubc.ca/faculty/mccormick/sfmchap8a.pdf
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- Francis Bach's updated 2013 text. http://hal.archives-ouvertes.fr/docs/00/87/06/09/PDF/submodular_fot_revised_hal.pdf
- Tom McCormick's overview paper on submodular minimization http://people.commerce.ubc.ca/faculty/mccormick/sfmchap8a.pdf
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