# Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 18 —

http://www.ee.washington.edu/people/faculty/bilmes/classes/ee596b\_spring\_2016/

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$$f(A) + f(B) \ge f(A \cup B) + f(A \cap B)$$
  
 $-f(A_i) + 2f(C) + f(B_i) - f(A_i) + f(C) + f(B_i) - f(A \cap B)$ 









# Cumulative Outstanding Reading

- Read chapters 2 and 3, 4, and 5 from Fujishige's book.
- Read chapter 1 from Fujishige's book.

## Announcements, Assignments, and Reminders

- Final Project description, available at our assignment dropbox (https://canvas.uw.edu/courses/1039754/assignments), due (electronically) Wednesday (6/8) at 1:00pm.
- Homework 4, available at our assignment dropbox (https://canvas.uw.edu/courses/1039754/assignments), due (electronically) Wednesday (5/25) at 11:55pm.
- Homework 3, available at our assignment dropbox (https://canvas.uw.edu/courses/1039754/assignments), due (electronically) Monday (5/2) at 11:55pm.
- Homework 2, available at our assignment dropbox (https://canvas.uw.edu/courses/1039754/assignments), due (electronically) Monday (4/18) at 11:55pm.
- Homework 1, available at our assignment dropbox (https://canvas.uw.edu/courses/1039754/assignments), due (electronically) Friday (4/8) at 11:55pm.
- Weekly Office Hours: Mondays, 3:30-4:30, or by skype or google

Logistics

# Class Road Map - IT-I

- L1(3/28): Motivation, Applications, & Basic Definitions
- L2(3/30): Machine Learning Apps (diversity, complexity, parameter, learning target, surrogate).
- L3(4/4): Info theory exs, more apps, definitions, graph/combinatorial examples, matrix rank example, visualization
- L4(4/6): Graph and Combinatorial Examples, matrix rank, Venn diagrams, examples of proofs of submodularity, some useful properties
- L5(4/11): Examples & Properties, Other Defs., Independence
- L6(4/13): Independence, Matroids, Matroid Examples, matroid rank is submodular
- L7(4/18): Matroid Rank, More on Partition Matroid, System of Distinct Reps, Transversals, Transversal Matroid,
- L8(4/20): Transversals, Matroid and representation, Dual Matroids,
- L9(4/25): Dual Matroids, Properties, Combinatorial Geometries, Matroid and Greedy
- L10(4/27): Matroid and Greedy, Polyhedra, Matroid Polytopes,

- L11(5/2): From Matroids to Polymatroids. Polymatroids
- L12(5/4): Polymatroids, Polymatroids and Greedy
- L13(5/9): Polymatroids and Greedy; Possible Polytopes; Extreme Points; Polymatroids, Greedy, and Cardinality Constrained Maximization
- L14(5/11): Cardinality Constrained Maximization; Curvature; Submodular Max w. Other Constraints
- L15(5/16): Submodular Max w. Other Constraints, Most Violated ≤, Matroids cont., Closure/Sat,
- L16(5/18): Closure/Sat, Fund. Circuit/Dep,
- L17(5/23): Min-Norm Point and SFM, Min-Norm Point Algorithm,
- L18(5/25): Proof that min-norm gives optimal, Lovász extension.
- L19(6/1):
- L20(6/6): Final Presentations maximization.

Finals Week: June 6th-10th, 2016.

#### Min-Norm Point: Definition

Consider the optimization:

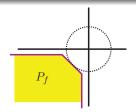
$$minimize ||x||_2^2 (18.1a)$$

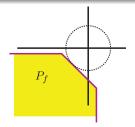
subject to 
$$x \in B_f$$
 (18.1b)

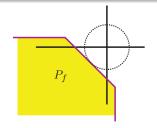
where  $B_f$  is the base polytope of submodular f, and  $\|x\|_2^2 = \sum_{e \in E} x(e)^2$  is the squared 2-norm. Let  $x^*$  be the optimal solution.

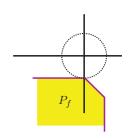
- Note, x\* is the unique optimal solution since we have a strictly convex objective over a set of convex constraints.
- $x^*$  is called the minimum norm point of the base polytope.

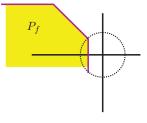
# Min-Norm Point: Examples

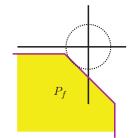












#### Min-Norm Point and Submodular Function Minimization

• Given optimal solution  $x^*$  to the above, consider the quantities

$$y^* = x^* \land 0 = (\min(x^*(e), 0) | e \in E)$$
(18.1)

$$A_{-} = \{e : x^{*}(e) < 0\}$$
(18.2)

$$A_0 = \{e : x^*(e) \le 0\} \tag{18.3}$$

• Thus, we immediately have that:

$$A_{-} \subseteq A_0 \tag{18.4}$$

and that

$$x^*(A_-) = x^*(A_0) = y^*(A_-) = y^*(A_0)$$
(18.5)

- It turns out, these quantities will solve the submodular function minimization problem, as we now show.
- The proof is nice since it uses the tools we've been recently developing.

# A polymatroid function's polyhedron is a polymatroid.

#### Theorem 18.2.1

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

$$\mathit{rank}(x) = \max{(y(E): y \leq x, y \in \textcolor{red}{P_f})} = \min{(x(A) + f(E \setminus A): A \subseteq E)} \tag{18.1}$$

Essentially the same theorem as Theorem ??, but note  $P_f$  rather than  $P_f^+$ . Taking x=0 we get:

#### Corollary 18.2.2

Let f be a submodular function defined on subsets of E. We have:

$$rank(0) = \max(y(E) : y \le 0, y \in P_f) = \min(f(A) : A \subseteq E)$$
 (18.2)

# Summary of supp, sat, and dep

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

$$\operatorname{cl}(x) \stackrel{\text{def}}{=} \operatorname{sat}(x) \triangleq \bigcup \{A : A \in \mathcal{D}(x)\}$$
 (18.25)

$$= \bigcup \left\{ A : A \subseteq E, x(A) = f(A) \right\} \tag{18.26}$$

$$= \{e : e \in E, \forall \alpha > 0, x + \alpha \mathbf{1}_e \notin P_f\}$$
 (18.27)

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

$$dep(x, e) = \begin{cases} \bigcap \{A : e \in A \subseteq E, x(A) = f(A)\} & \text{if } e \in sat(x) \\ \emptyset & \text{else} \end{cases}$$
$$= \{e' : \exists \alpha > 0, \text{ s.t. } x + \alpha(\mathbf{1}_e - \mathbf{1}_{e'}) \in P_f \}$$
(18.28)

Note, if  $x + \alpha(\mathbf{1}_e - \mathbf{1}_{e'}) \in P_f$ , then  $x + \alpha'(\mathbf{1}_e - \mathbf{1}_{e'}) \in P_f$  for any  $0 \le \alpha' < \alpha$ .

# Summary important definitions so far: tight, dep, & sat

- x-tight sets: For  $x \in P_f$ ,  $\mathcal{D}(x) \triangleq \{A \subseteq E : x(A) = f(A)\}.$
- Polymatroid closure/maximal x-tight set: For  $x \in P_f$ ,  $\operatorname{sat}(x) \triangleq \bigcup \{A : A \in \mathcal{D}(x)\} = \{e : e \in E, \forall \alpha > 0, x + \alpha \mathbf{1}_e \notin P_f\}.$
- $\min \{ f(A) x(A) | \forall A \ni e \} = \max \{ \alpha : \alpha \in \mathbb{R}, x + \alpha \mathbf{1}_e \in P_f \}$
- Recall:  $sat(x) = \{e : \hat{c}(x; e) = 0\}$  and  $E \setminus sat(x) = \{e : \hat{c}(x; e) > 0\}$ .
- e-containing x-tight sets: For  $x \in P_f$ ,  $\mathcal{D}(x,e) = \{A : e \in A \subseteq E, x(A) = f(A)\} \subseteq \mathcal{D}(x).$

• Saturation capacity: for  $x \in P_f$ ,  $0 \le \hat{c}(x; e) \triangleq$ 

 Minimal e-containing x-tight set/polymatroidal fundamental circuit/: For  $x \in P_f$ ,

$$\begin{split} \operatorname{r} x &\in P_f, \\ \operatorname{dep}(x,e) &= \begin{cases} \bigcap \left\{A: e \in A \subseteq E, x(A) = f(A)\right\} & \text{if } e \in \operatorname{sat}(x) \\ \emptyset & \text{else} \end{cases} \\ &= \left\{e': \exists \alpha > 0, \text{ s.t. } x + \alpha(\mathbf{1}_e - \mathbf{1}_{e'}) \in P_f\right\}$$

#### Theorem 18.3.1

Let  $y^*$ ,  $A_-$ , and  $A_0$  be as given. Then  $y^*$  is a maximizer of the l.h.s. of Eqn. (17.7). Moreover,  $A_-$  is the unique minimal minimizer of f and  $A_0$  is the unique maximal minimizer of f.

#### Proof.

• First note, since  $x^* \in B_f$ , we have  $x^*(E) = f(E)$ , meaning  $\operatorname{sat}(x^*) = E$ . Thus, we can consider any  $e \in E$  within  $\operatorname{dep}(x^*, e)$ .

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- Consider any pair (e,e') with  $e' \in \operatorname{dep}(x^*,e)$  and  $e \in A_-$ . Then  $x^*(e) < 0$ , and  $\exists \alpha > 0$  s.t.  $x^* + \alpha \mathbf{1}_e \alpha \mathbf{1}_{e'} \in P_f$ .

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- Consider any pair (e,e') with  $e'\in \operatorname{dep}(x^*,e)$  and  $e\in A_-$ . Then  $x^*(e)<0$ , and  $\exists \alpha>0$  s.t.  $x^*+\alpha \mathbf{1}_e-\alpha \mathbf{1}_{e'}\in P_f$ .
- We have  $x^*(E)=f(E)$  and  $x^*$  is minimum in I2 sense. We have  $(x^*+\alpha \mathbf{1}_e-\alpha \mathbf{1}_{e'})\in P_f$ , and in fact

$$(x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'})(E) = x^*(E) + \alpha - \alpha = f(E)$$
 (18.1)

so  $x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'} \in B_f$  also.

$$\begin{array}{l} \bullet \ \, \text{Then} \, \left( x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'} \right) (E) \\ = x^* (E \setminus \{e,e'\}) + \underbrace{\left( x^*(e) + \alpha \right)}_{x^*_{\text{new}}(e)} + \underbrace{\left( x^*(e') - \alpha \right)}_{x^*_{\text{new}}(e')} = f(E). \end{array}$$

- Then  $(x^* + \alpha \mathbf{1}_e \alpha \mathbf{1}_{e'})(E)$ =  $x^*(E \setminus \{e, e'\}) + \underbrace{(x^*(e) + \alpha)}_{x^*_{\text{new}}(e)} + \underbrace{(x^*(e') - \alpha)}_{x^*_{\text{new}}(e')} = f(E).$
- $\bullet \ \ \mbox{Minimality of} \ x^* \in B_f \ \mbox{in I2 sense requires that, with such an} \ \alpha > 0,$

$$\left( x^*(e) \right)^2 + \left( x^*(e') \right)^2 < \left( x^*_{\mathsf{new}}(e) \right)^2 + \left( x^*_{\mathsf{new}}(e') \right)^2$$

- Then  $(x^* + \alpha \mathbf{1}_e \alpha \mathbf{1}_{e'})(E)$ =  $x^*(E \setminus \{e, e'\}) + \underbrace{(x^*(e) + \alpha)}_{x^*_{\text{new}}(e)} + \underbrace{(x^*(e') - \alpha)}_{x^*_{\text{new}}(e')} = f(E).$
- Minimality of  $x^* \in B_f$  in I2 sense requires that, with such an  $\alpha > 0$ ,  $\left(x^*(e)\right)^2 + \left(x^*(e')\right)^2 < \left(x^*_{\mathsf{new}}(e)\right)^2 + \left(x^*_{\mathsf{new}}(e')\right)^2$
- Given that  $e \in A_-$ ,  $x^*(e) < 0$ . Thus, if  $x^*(e') > 0$ , we could have  $(x^*(e) + \alpha)^2 + (x^*(e') \alpha)^2 < (x^*(e))^2 + (x^*(e'))^2$ , contradicting the optimality of  $x^*$ .

## . . . proof of Thm. 18.3.1 cont.

- Then  $(x^* + \alpha \mathbf{1}_e \alpha \mathbf{1}_{e'})(E)$ =  $x^*(E \setminus \{e, e'\}) + \underbrace{(x^*(e) + \alpha)}_{x^*_{\mathsf{new}}(e)} + \underbrace{(x^*(e') - \alpha)}_{x^*_{\mathsf{new}}(e')} = f(E).$
- Minimality of  $x^* \in B_f$  in I2 sense requires that, with such an  $\alpha > 0$ ,  $\left(x^*(e)\right)^2 + \left(x^*(e')\right)^2 < \left(x^*_{\mathsf{new}}(e)\right)^2 + \left(x^*_{\mathsf{new}}(e')\right)^2$
- Given that  $e \in A_-$ ,  $x^*(e) < 0$ . Thus, if  $x^*(e') > 0$ , we could have  $(x^*(e) + \alpha)^2 + (x^*(e') \alpha)^2 < (x^*(e))^2 + (x^*(e'))^2$ , contradicting the optimality of  $x^*$ .
- If  $x^*(e') = 0$ , we would have  $(x^*(e) + \alpha)^2 + (\alpha)^2 < (x^*(e))^2$ , for any  $0 < \alpha < |x^*(e)|$  (Exercise:), again contradicting the optimality of  $x^*$ .

•••

## $\dots$ proof of Thm. $18.\overline{3}.1$ cont.

- Then  $(x^* + \alpha \mathbf{1}_e \alpha \mathbf{1}_{e'})(E)$ =  $x^*(E \setminus \{e, e'\}) + \underbrace{(x^*(e) + \alpha)}_{x^*_{\text{new}}(e)} + \underbrace{(x^*(e') - \alpha)}_{x^*_{\text{new}}(e')} = f(E).$
- Minimality of  $x^* \in B_f$  in I2 sense requires that, with such an  $\alpha > 0$ ,  $\left(x^*(e)\right)^2 + \left(x^*(e')\right)^2 < \left(x^*_{\mathsf{new}}(e)\right)^2 + \left(x^*_{\mathsf{new}}(e')\right)^2$
- Given that  $e \in A_-$ ,  $x^*(e) < 0$ . Thus, if  $x^*(e') > 0$ , we could have  $(x^*(e) + \alpha)^2 + (x^*(e') \alpha)^2 < (x^*(e))^2 + (x^*(e'))^2$ , contradicting the optimality of  $x^*$ .
- If  $x^*(e') = 0$ , we would have  $(x^*(e) + \alpha)^2 + (\alpha)^2 < (x^*(e))^2$ , for any  $0 < \alpha < |x^*(e)|$  (Exercise:), again contradicting the optimality of  $x^*$ .
- Thus, we must have  $x^*(e') < 0$  (strict negativity).

#### ... proof of Thm. 18.3.1 cont.

• Thus, for a pair (e,e') with  $e'\in \operatorname{dep}(x^*,e)$  and  $e\in A_-$ , we have x(e')<0 and hence  $e'\in A_-$ .

. . .

- Thus, for a pair (e,e') with  $e' \in dep(x^*,e)$  and  $e \in A_-$ , we have x(e') < 0 and hence  $e' \in A_-$ .
- Hence,  $\forall e \in A_-$ , we have  $dep(x^*, e) \subseteq A_-$ .

#### ... proof of Thm. 18.3.1 cont.

- Thus, for a pair (e,e') with  $e' \in dep(x^*,e)$  and  $e \in A_-$ , we have x(e') < 0 and hence  $e' \in A_-$ .
- Hence,  $\forall e \in A_-$ , we have  $dep(x^*, e) \subseteq A_-$ .
- A very similar argument can show that,  $\forall e \in A_0$ , we have  $dep(x^*, e) \subseteq A_0$ .

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- Thus, for a pair (e,e') with  $e' \in dep(x^*,e)$  and  $e \in A_-$ , we have x(e') < 0 and hence  $e' \in A_-$ .
- Hence,  $\forall e \in A_-$ , we have  $dep(x^*, e) \subseteq A_-$ .
- A very similar argument can show that,  $\forall e \in A_0$ , we have  $dep(x^*, e) \subseteq A_0$ .
- Also, recall that  $e \in dep(x^*, e)$ .

- ... proof of Thm. 18.3.1 cont.
  - ullet Therefore, we have  $\cup_{e\in A_-} \operatorname{dep}(x^*,e) = A_-$  and  $\cup_{e\in A_0} \operatorname{dep}(x^*,e) = A_0$

- Therefore, we have  $\bigcup_{e \in A_-} \operatorname{dep}(x^*, e) = A_-$  and  $\bigcup_{e \in A_0} \operatorname{dep}(x^*, e) = A_0$
- ullet le.,  $\{\operatorname{dep}(x^*,e)\}_{e\in A_-}$  is cover for  $A_-$ , as is  $\{\operatorname{dep}(x^*,e)\}_{e\in A_0}$  for  $A_0$ .

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- $dep(x^*, e)$  is minimal tight set containing e, meaning  $x^*(dep(x^*, e)) = f(dep(x^*, e))$ , and since tight sets are closed under union, we have that  $A_-$  and  $A_0$  are also tight, meaning:

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$$x^*(A_-) = f(A_-) (18.2)$$

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$$x^*(A_-) = f(A_-) \tag{18.2}$$

$$x^*(A_0) = f(A_0) \tag{18.3}$$

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$$x^*(A_-) = f(A_-) (18.2)$$

$$x^*(A_0) = f(A_0) (18.3)$$

$$x^*(A_-) = x^*(A_0) = y^*(E) = y^*(A_0) + \underbrace{y^*(E \setminus A_0)}_{0}$$
 (18.4)

#### ... proof of Thm. 18.3.1 cont.

- Therefore, we have  $\bigcup_{e \in A_-} \operatorname{dep}(x^*, e) = A_-$  and  $\bigcup_{e \in A_0} \operatorname{dep}(x^*, e) = A_0$
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and therefore, all together we have

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$$x^*(A_-) = x^*(A_0) = y^*(E) = y^*(A_0) + \underbrace{y^*(E \setminus A_0)}_{=0}$$
 (18.4)

and therefore, all together we have

$$f(A_{-}) = f(A_{0}) = x^{*}(A_{-}) = x^{*}(A_{0}) = y^{*}(E)$$
 (18.5)

## ... proof of Thm. 18.3.1 cont.

• Now,  $y^*$  is feasible for the l.h.s. of Eqn. (17.7) (recall, which is  $\max\{y(E)|y\in P_f,y\leq 0\}=\min\{f(X)|X\subseteq V\}$ ).

#### ... proof of Thm. 18.3.1 cont.

• Now,  $y^*$  is feasible for the l.h.s. of Eqn. (17.7) (recall, which is  $\max{\{y(E)|y\in P_f,y\leq 0\}}=\min{\{f(X)|X\subseteq V\}}$ ). This follows since, we have  $y^*=x^*\wedge 0\leq 0$ , and since  $x^*\in B_f\subset P_f$ , and  $y^*\leq x^*$  and  $P_f$  is down-closed, we have that  $y^*\in P_f$ .

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- Also, for any  $y \in P_f$  with  $y \le 0$  and for any  $X \subseteq E$ , we have  $y(E) \le y(X) \le f(X)$ .

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- Considering Eqn. (18.2), we have found sets  $A_-$  and  $A_0$  with tightness in Eqn. (17.7), meaning  $y^*(E)=f(A_-)=f(A_0)$ .
- Hence,  $y^*$  is a maximizer of l.h.s. of Eqn. (17.7), and  $A_-$  and  $A_0$  are minimizers of f.

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• Now, for any  $X \subset A_-$ , we have

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• And for any  $X \supset A_0$ , we have

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ullet Hence,  $A_-$  must be the unique minimal minimizer of f, and  $A_0$  is the unique maximal minimizer of f.



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- In fact, with  $x^*$  the min-norm point, and  $A_-$  and  $A_0$  as defined above, we have the following theorem:

#### Theorem 18.3.2

Let  $A \subseteq E$  be any minimizer of submodular f, and let  $x^*$  be the minimum-norm point. Then A can be expressed in the form:

$$A = A_{-} \cup \bigcup_{a \in A_m} \operatorname{dep}(x^*, a) \tag{18.8}$$

for some set  $A_m \subseteq A_0 \setminus A_-$ . Conversely, for any set  $A_m \subseteq A_0 \setminus A_-$ , then  $A \triangleq A_- \cup \bigcup_{a \in A_m} \operatorname{dep}(x^*, a)$  is a minimizer.

#### proof of Thm. 18.3.2.

• If A is a minimizer, then  $A_- \subseteq A \subseteq A_0$ , and  $f(A) = y^*(E)$  is the minimum valuation of f.

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- For any  $a \in A$ , A is a tight set containing a, and  $dep(x^*, a)$  is the minimal tight containing a.
- Hence, for any  $a \in A$ ,  $dep(x^*, a) \subseteq A$ .
- This means that  $\bigcup_{a \in A} \operatorname{dep}(x^*, a) = A$ .
- Since  $A_- \subseteq A \subseteq A_0$ , then  $\exists A_m \subseteq A \setminus A_-$  such that

$$A = \bigcup_{a \in A_{-}} \operatorname{dep}(x^{*}, a) \cup \bigcup_{a \in A_{m}} \operatorname{dep}(x^{*}, a) = A_{-} \cup \bigcup_{a \in A_{m}} \operatorname{dep}(x^{*}, a)$$

#### proof of Thm. 18.3.2.

ullet Conversely, consider any set  $A_m \subseteq A_0 \setminus A_-$ , and define A as

$$A = A_{-} \cup \bigcup_{a \in A_{m}} \operatorname{dep}(x^{*}, a) = \bigcup_{a \in A_{-}} \operatorname{dep}(x^{*}, a) \cup \bigcup_{a \in A_{m}} \operatorname{dep}(x^{*}, a)$$
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Therefore, we can generate the entire lattice of minimizers of f starting from  $A_-$  and  $A_0$  given access to  $dep(x^*, e)$ .

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• Then since A is a union of tight sets, A is also a tight set, and we have  $f(A) = x^*(A)$ .



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- Then since A is a union of tight sets, A is also a tight set, and we have  $f(A) = x^*(A)$ .
- But  $x^*(A \setminus A_-) = 0$ , so  $f(A) = x^*(A) = x^*(A_-) = f(A_-)$  meaning A is also a minimizer of f.

Therefore, we can generate the entire lattice of minimizers of f starting from  $A_-$  and  $A_0$  given access to  $dep(x^*, e)$ .

# On a unique minimizer f

• Note that if f(e|A) > 0,  $\forall A \subseteq E$  and  $e \in E \setminus A$ , then we have  $A_- = A_0$  (there is one unique minimizer).

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- On the other hand, if  $A_-=A_0$ , it does not imply f(e|A)>0 for all  $A\subseteq E\setminus\{e\}$ .
- If  $A_- = A_0$  then certainly  $f(e|A_0) > 0$  for  $e \in E \setminus A_0$  and  $-f(e|A_0 \setminus \{e\}) > 0$  for all  $e \in A_0$ .

# Duality: convex minimization of L.E. and min-norm alg.

• Let f be a submodular function with  $\tilde{f}$  it's Lovász extension. Then the following two problems are duals (Bach-2013):

where  $B_f = P_f \cap \{x \in \mathbb{R}^V : x(V) = f(V)\}$  is the base polytope of submodular function f, and  $||x||_2^2 = \sum_{e \in V} x(e)^2$  is squared 2-norm.

- Equation (18.10) is related to proximal methods to minimize the Lovász extension (see Parikh&Boyd, "Proximal Algorithms" 2013).
- Equation (18.11b) is solved by the minimum-norm point algorithm (Wolfe-1976, Fujishige-1984, Fujishige-2005, Fujishige-2011) is (as we will see) essentially an active-set procedure for quadratic programming, and uses Edmonds's greedy algorithm to make it efficient.
- Unknown worst-case running time, although in practice it usually performs quite well (see below).

### Review

The next slide comes from lecture 13.

### 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 18.4.1

Proof that min-norm gives optimal

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).

ullet Consider the following optimization. Given  $w \in \mathbb{R}^E$ ,

maximize 
$$w^{\mathsf{T}}x$$
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- The greedy algorithm will solve this, and the proof almost identical.
- Due to Theorem ??, any  $x \in P_f$  with  $x \notin B_f$  is dominated by  $x \le y \in B_f$  which can only increase  $w^\intercal x \le w^\intercal y$ .

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• Moreover, we can have  $w \in \mathbb{R}^E$  if we insist on  $x \in B_f$ .

## A continuous extension of f

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• We may consider this optimization problem a function  $\check{f}:\mathbb{R}^E\to\mathbb{R}$  of  $w\in\mathbb{R}^E$ , defined as:

$$\check{f}(w) = \max(wx : x \in B_f) \tag{18.15}$$

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ullet Hence, for any w, from the solution to the above theorem (as we have seen), we can compute the value of this function using Edmond's greedy algorithm.

• That is, given a submodular function f, a  $w \in \mathbb{R}^E$ , choose element order  $(e_1, e_2, \dots, e_m)$  based on decreasing w,so that  $w(e_1) \geq w(e_2) \geq \dots \geq w(e_m)$ .

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$$= \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1}))$$
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$$= \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1}))$$
(18.18)

$$= w(e_m)f(E_m) + \sum_{i=1}^{m-1} (w(e_i) - w(e_{i+1}))f(E_i)$$
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- That is, given a submodular function f, a  $w \in \mathbb{R}^E$ , choose element order  $(e_1, e_2, \dots, e_m)$  based on decreasing w, so that  $w(e_1) \geq w(e_2) \geq \dots \geq w(e_m)$ .
- ullet Define the chain with  $i^{\mathsf{th}}$  element  $E_i = \{e_1, e_2, \dots, e_i\}$  , we have

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• We say that  $\emptyset \triangleq E_0 \subset E_1 \subset E_2 \subset \cdots \subset E_m = E$  forms a chain based on w.

• Definition of the continuous extension, once again, for reference:

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where  $\lambda_m = w(e_m)$  and otherwise  $\lambda_i = w(e_i) - w(e_{i+1})$ , where the elements are sorted descending according to w as before.

• From convex analysis, we know  $\check{f}(w) = \max(wx : x \in P)$  is always convex in w for any set  $P \subseteq R^E$ , since it is the maximum of a set of linear functions (true even when f is not submodular or P is not a convex set).

 $\bullet$  Recall, for any such  $w \in \mathbb{R}^E$ , we have

$$\begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \underbrace{\begin{pmatrix} w_1 - w_2 \end{pmatrix}}_{\lambda_1} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \underbrace{\begin{pmatrix} w_2 - w_3 \end{pmatrix}}_{\lambda_2} \begin{pmatrix} 1 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \underbrace{\begin{pmatrix} w_1 - w_2 \end{pmatrix}}_{\lambda_m} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \underbrace{\begin{pmatrix} w_1 - w_2 \end{pmatrix}}_{\lambda_m} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \underbrace{\begin{pmatrix} w_1 - w_2 \end{pmatrix}}_{\lambda_m} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 0 \end{pmatrix} + \underbrace{\begin{pmatrix} w_1 - w_2 \end{pmatrix}}_{\lambda_m} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix}$$
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$$\cdots + \underbrace{(w_{n-1} - w_n)}_{\lambda_{m-1}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \end{pmatrix} + \underbrace{(w_m)}_{\lambda_m} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix} \tag{18.23}$$

• If we take w in decreasing order, then each coefficient of the vectors is non-negative (except possibly the last one,  $\lambda_m = w_m$ ).

• Define sets  $E_i$  based on this decreasing order of w as follows, for  $i=0,\ldots,n$ 

$$E_i \stackrel{\text{def}}{=} \{e_1, e_2, \dots, e_i\}$$
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Note that

$$\mathbf{1}_{E_0} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \mathbf{1}_{E_1} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \dots, \mathbf{1}_{E_\ell} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \text{ etc. }$$

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• Hence, from the previous and current slide, we have  $w = \sum_{i=1}^m \lambda_i \mathbf{1}_{E_i}$ 

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$$w = (w(e_1), w(e_2), \dots, w(e_m)) = (\underbrace{1, 1, 1, \dots, 1}_{|A| \text{ times}}, \underbrace{0, 0, \dots, 0}_{m-|A| \text{ times}})$$
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Proof that min-norm gives optima

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$$= \mathbf{1}_A(m) f(E_m) + \sum_{i=1}^{m-1} (\mathbf{1}_A(i) - \mathbf{1}_A(i+1)) f(E_i) \qquad (18.26)$$

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## From $\check{f}$ back to f

• We can view  $\check{f}:[0,1]^E\to\mathbb{R}$  defined on the hypercube, with f defined as  $\check{f}$  evaluated on the hypercube extreme points (vertices).

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ullet ...and when f is submodular, we also have have

$$\check{f}(\mathbf{1}_A) = \max\{\mathbf{1}_A^{\mathsf{T}} x : x \in B_f\}$$
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$$= \max \left\{ \mathbf{1}_A^{\mathsf{T}} x : x(B) \le f(B), \forall B \subseteq E \right\} \tag{18.30}$$

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• Note when considering only  $\check{f}:[0,1]^E\to\mathbb{R}$ , then any  $w\in[0,1]^E$  is in positive orthant, adn we have

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## An extension of an arbitrary $f: 2^V \to \mathbb{R}$

• Thus, for any  $f: 2^E \to \mathbb{R}$ , even non-submodular f, we can define an extension, having  $\check{f}(\mathbf{1}_A) = f(A), \ \forall A$ , in this way where

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with the  $E_i=\{e_1,\ldots,e_i\}$ 's defined based on sorted descending order of w as in  $w(e_1)\geq w(e_2)\geq \cdots \geq w(e_m)$ , and where

for 
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,  $\lambda_i = \begin{cases} w(e_i) - w(e_{i+1}) & \text{if } i < m \\ w(e_m) & \text{if } i = m \end{cases}$  (18.34)

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•  $w = \sum_{i=1}^{m} \lambda_i \mathbf{1}_{E_i}$  is an interpolation of certain hypercube vertices.

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- $w = \sum_{i=1}^{m} \lambda_i \mathbf{1}_{E_i}$  is an interpolation of certain hypercube vertices.
- $\check{f}(w) = \sum_{i=1}^{m} \lambda_i f(E_i)$  is the associated interpolation of the values of f at sets corresponding to each hypercube vertex.

### Weighted gains vs. weighted functions

• Again sorting E descending in w, the extension summarized:

$$\check{f}(w) = \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1})$$
(18.35)

$$= \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1}))$$
(18.36)

$$= w(e_m)f(E_m) + \sum_{i=1}^{m-1} (w(e_i) - w(e_{i+1}))f(E_i)$$
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 (18.37)

$$=\sum_{i=1}^{m}\lambda_{i}f(E_{i})\tag{18.38}$$

• So  $\check{f}(w)$  seen either as sum of weighted gain evaluatiosn (Eqn. (18.35), or as sum of weighted function evaluations (Eqn. (18.38)).

• So if f is submodular, then we can write  $\check{f}(w) = \max(wx : x \in P_f)$  (which is clearly convex) in the form:

$$\check{f}(w) = \max(wx : x \in P_f) = \sum_{i=1}^{m} \lambda_i f(E_i)$$
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ullet On the other hand, for any f (even non-submodular), we can produce an extension  $\check{f}$  having the form

$$\check{f}(w) = \sum_{i=1}^{m} \lambda_i f(E_i)$$
(18.40)

where  $w = \sum_{i=1}^m \lambda_i \mathbf{1}_{E_i}$  and  $E_i = \{e_1, \dots, e_i\}$  defined based on sorted descending order  $w(e_1) \geq w(e_2) \geq \dots \geq w(e_m)$ .

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- Submodularity is sufficient for convexity, but is it necessary?

# The Lovász extension of $f: 2^E \to \mathbb{R}$

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- This continuous extension  $\check{f}$  of f, in any case (f being submodular or not), is called the Lovász extension of f.
- Note, also possible to define this when  $f(\emptyset) \neq 0$  (but doesn't really add any generality).

### Theorem 18.4.1

A function  $f: 2^E \to \mathbb{R}$  is submodular iff its Lovász extension  $\check{f}$  of f is convex.

### Proof.

• We've already seen that if f is submodular, its extension can be written via Eqn.(18.33) due to the greedy algorithm, and therefore is also equivalent to  $\check{f}(w) = \max\{wx : x \in P_f\}$ , and thus is convex.

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- Conversely, suppose the Lovász extension  $\check{f}(w) = \sum_i \lambda_i f(E_i)$  of some function  $f: 2^E \to \mathbb{R}$  is a convex function.
- We note that, based on the extension definition, in particular the definition of the  $\{\lambda_i\}_i$ , we have that  $\check{f}(\alpha w) = \alpha \check{f}(w)$  for any  $\alpha \in \mathbb{R}_+$ . I.e., f is a positively homogeneous convex function.

### ... proof of Thm. 18.4.1 cont.

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$$\check{f}(\mathbf{1}_A + \mathbf{1}_B) = \check{f}(\mathbf{1}_{A \cup B} + \mathbf{1}_{A \cap B})$$
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$$= f(A \cup B) + f(A \cap B).$$
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• Let 
$$C = A \cap B$$
, order  $E$  based on decreasing  $w = \mathbf{1}_A + \mathbf{1}_B$  so that

$$w = (w(e_1), w(e_2), \dots, w(e_m))$$
(18.43)

$$= (\underbrace{2, 2, \dots, 2}_{i \in C}, \underbrace{1, 1, \dots, 1}_{i \in A \triangle B}, \underbrace{0, 0, \dots, 0}_{i \in E \setminus (A \cup B)})$$

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- But then  $E_{|C|}=A\cap B$  and  $E_{|A\cup B|}=A\cup B.$  Therefore,  $\check{f}(w)=\check{f}(\mathbf{1}_A+\mathbf{1}_B)=f(A\cap B)+f(A\cup B).$

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ullet Thus, we have shown that for any  $A,B\subseteq E$ ,

$$f(A \cup B) + f(A \cap B) \le f(A) + f(B)$$
 (18.49)

so f must be submodular.



### Edmonds - Submodularity - 1969

SUBMODULAR FUNCTIONS, MATROIDS, AND CERTAIN POLYHEDRA\*

Jack Edmonds

National Bureau of Standards, Washington, D.C., U.S.A.

I.

The viewpoint of the subject of matroids, and related areas of lattice theory, has always been, in one way or another, abstraction of algebraic dependence or, equivalently, abstraction of the incidence relations in geometric representations of algebra. Often one of the

### Lovász - Submodularity - 1983

### Submodular functions and convexity

#### L. Lovász

Eötvös Loránd University, Department of Analysis I, Múzeum krt. 6-8, H-1088 Budapest, Hungary

#### 0. Introduction

In "continuous" optimization convex functions play a central role. Besides elementary tools like differentiation, various methods for finding the minimum of a convex function constitute the main body of nonlinear optimization. But even linear programming may be viewed as the optimization of very special (linear) objective functions over very special convex domains (polyhedra). There are several reasons for this popularity of convex functions:

- Convex functions occur in many mathematical models in economy, engineering, and other sciencies. Convexity is a very natural property of various functions and domains occuring in such models; quite often the only non-trivial property which can be stated in general.

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### Integration and Aggregation

- Integration is just summation (e.g., the  $\int$  symbol has as its origins a sum).
- Lebesgue integration allows integration w.r.t. an underlying measure  $\mu$  of sets. E.g., given measurable function f, we can define

$$\int_{X} f du = \sup I_X(s) \tag{18.50}$$

where  $I_X(s) = \sum_{i=1}^n c_i \mu(X \cap X_i)$ , and where we take the sup over all measurable functions s such that  $0 \le s \le f$  and  $s(x) = \sum_{i=1}^n c_i I_{X_i}(x)$  and where  $I_{X_i}(x)$  is indicator of membership of set  $X_i$ , with  $c_i > 0$ .

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- I.e., given a weight vector  $w \in [0,1]^E$  for some finite ground set E, then for any  $x \in \mathbb{R}^E$  we have the weighted average of x as:

$$WAVG(x) = \sum_{e \in E} x(e)w(e)$$
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so seen as a function on the hypercube vertices, the entire WAVG function is given based on values on a size m=|E| subset of the vertices of this hypercube, i.e.,  $\{\mathbf{1}_e:e\in E\}$ . Moreover, we are interpolating as in

$$WAVG(x) = \sum_{e \in E} x(e)w(e) = \sum_{e \in E} x(e)WAVG(\mathbf{1}_e)$$
 (18.53)

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• Clearly, WAVG function is linear in weights w, in the argument x, and is homogeneous. That is, for all  $w, w_1, w_2, x, x_1, x_2 \in \mathbb{R}^E$  and  $\alpha \in \mathbb{R}$ ,

$$WAVG_{w_1+w_2}(x) = WAVG_{w_1}(x) + WAVG_{w_2}(x),$$
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• We will see: The Lovász extension is still be linear in "weights" (i.e., the submodular function f), but will not be linear in x and will only be positively homogeneous (for  $\alpha \geq 0$ ).

• More complex "nonlinear" aggregation functions can be constructed by defining the aggregation function on all vertices of the hypercube. I.e., for each  $\mathbf{1}_A:A\subseteq E$  we might have (for all  $A\subseteq E$ ):

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ullet Set function  $f:2^E \to \mathbb{R}$  is a game if f is normalized  $f(\emptyset)=0$ .

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- We saw this for Lovász extension.
- It turns out that a concept essentially identical to the Lovász extension was derived much earlier, in 1954, and using this derivation (via integration) leads to deeper intuition.

#### Definition 18.5.1

Let f be any capacity on E and  $w \in \mathbb{R}_+^E$ . The Choquet integral (1954) of w w.r.t. f is defined by

$$C_f(w) = \sum_{i=1}^{m} (w_{e_i} - w_{e_{i+1}}) f(E_i)$$
(18.61)

where in the sum, we have sorted and renamed the elements of E so that  $w_{e_1} \ge w_{e_2} \ge \cdots \ge w_{e_m} \ge w_{e_{m+1}} \triangleq 0$ , and where  $E_i = \{e_1, e_2, \dots, e_i\}$ .

• We immediately see that an equivalent formula is as follows:

$$C_f(w) = \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1}))$$
 (18.62)

where  $E_0 \stackrel{\text{def}}{=} \emptyset$ .

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• BTW: this again essentially Abel's partial summation formula: Given two arbitrary sequences  $\{a_n\}$  and  $\{b_n\}$  with  $A_n = \sum_{k=1}^n a_k$ , we have

$$\sum_{k=m}^{n} a_k b_k = \sum_{k=m}^{n} A_k (b_k - b_{k+1}) + A_n b_{n+1} - A_{m-1} b_m$$
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- First note, assuming E is ordered according to descending w, so that  $w(e_1) \geq w(e_2) \geq \cdots \geq w(e_{m-1}) \geq w(e_m)$ , then  $E_i = \{e_1, e_2, \ldots, e_i\} = \{e \in E : w_e \geq w_{e_i}\}.$

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- For any  $w_{e_i} > \alpha \ge w_{e_{i+1}}$  we also have  $E_i = \{e_1, e_2, \dots, e_i\} = \{e \in E : w_e > \alpha\}.$

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- Consider segmenting the real-axis at boundary points  $w_{e_i}$ , right most is  $w_{e_1}$ .

$$w(e_m) \ w(e_{m-1}) \ \cdots \ w(e_5) \ w(e_4) \ w(e_3) \ w(e_2)w(e_1)$$

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$$\overline{w(e_m)} \ w(e_{m-1}) \ \cdots \ w(e_5) \ w(e_4) \ w(e_3) \ w(e_2) w(e_1)$$

• A function can be defined on a segment of  $\mathbb{R}$ , namely  $w_{e_i} > \alpha \geq w_{e_{i+1}}$ . This function  $F_i : [w_{e_{i+1}}, w_{e_i}) \to \mathbb{R}$  is defined as

$$F_i(\alpha) = f(\{e \in E : w_e > \alpha\}) = f(E_i)$$
 (18.64)

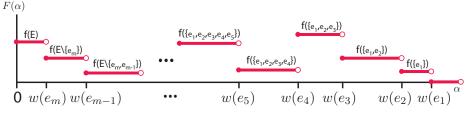
• We can generalize this to multiple segments of  $\mathbb{R}$  (for now, take  $w \in \mathbb{R}_+^E$ ). The piecewise-constant function is defined as:

$$F(\alpha) = \begin{cases} f(E) & \text{if } 0 \leq \alpha < w_m \\ f(\{e \in E : w_e > \alpha\}) & \text{if } w_{e_{i+1}} \leq \alpha < w_{e_i}, \ i \in \{1, \dots, m-1\} \\ 0 \ (= f(\emptyset)) & \text{if } w_1 < \alpha \end{cases}$$

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 $\bullet$  Visualizing a piecewise constant function, where the constant values are given by f evaluated on  $E_i$  for each i



Note, what is depicted may be a game but not a capacity. Why?

• Now consider the integral, with  $w \in \mathbb{R}_+^E$ , and normalized f so that  $f(\emptyset) = 0$ . Recall  $w_{m+1} \stackrel{\mathrm{def}}{=} 0$ .

$$\tilde{f}(w) \stackrel{\text{def}}{=} \int_{0}^{\infty} F(\alpha) d\alpha$$
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$$= \sum_{i=1}^{m} \int_{w_{i+1}}^{w_i} f(E_i) d\alpha = \sum_{i=1}^{m} f(E_i) (w_i - w_{i+1})$$
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Given  $w \in \mathbb{R}_+^E$ , the Lovász extension (equivalently Choquet integral) may be defined as follows:

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- The above integral will be further generalized a bit later.

 Recall, we want to produce some notion of generalized aggregation function having the flavor of:

$$AG(x) = \sum_{A \subseteq E} x(A)w_A = \sum_{A \subseteq E} x(A)AG(\mathbf{1}_A)$$
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how does this correspond to Lovász extension?

• Let us partition the hypercube  $[0,1]^m$  into q polytopes, each defined by a set of vertices  $\mathcal{V}_1, \mathcal{V}_2, \dots, \mathcal{V}_q$ .

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- E.g., for each i,  $\mathcal{V}_i = \{\mathbf{1}_{A_1}, \mathbf{1}_{A_2}, \dots, \mathbf{1}_{A_k}\}$  (k vertices) and the convex hull of  $V_i$  defines the  $i^{\text{th}}$  polytope.

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- This forms a "triangulation" of the hypercube.
- For any  $x \in [0,1]^m$  there is a (not necessarily unique)  $\mathcal{V}(x) = \mathcal{V}_j$  for some j such that  $x \in \text{conv}(\mathcal{V}(x))$ .

• Most generally, for  $x \in [0,1]^m$ , let us define the (unique) coefficients  $\alpha_0^x(A)$  and  $\alpha_i^x(A)$  that define the affine transformation of the coefficients of x to be used with the particular hypercube vertex  $\mathbf{1}_A \in \operatorname{conv}(\mathcal{V}(x))$ . The affine transformation is as follows:

$$\alpha_0^x(A) + \sum_{j=1}^m \alpha_j^x(A) x_j \in \mathbb{R}$$
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• From this, we can define an aggregation function of the form

$$\mathsf{AG}(x) \stackrel{\text{def}}{=} \sum_{A: \mathbf{1}_A \in \mathcal{V}(x)} \left( \alpha_0^x(A) + \sum_{j=1}^m \alpha_j^x(A) x_j \right) \mathsf{AG}(\mathbf{1}_A) \tag{18.73}$$

• We can define a canonical triangulation of the hypercube in terms of permutations of the coordinates. I.e., given some permutation  $\sigma$ , define

$$\operatorname{conv}(\mathcal{V}_{\sigma}) = \left\{ x \in [0, 1]^n | x_{\sigma(1)} \ge x_{\sigma(2)} \ge \dots \ge x_{\sigma(m)} \right\}$$
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#### Proposition 18.5.3

The above linear interpolation in Eqn. (18.73) using the canonical partition yields the Lovász extension with  $\alpha_0^x(A) + \sum_{j=1}^m \alpha_j^x(A) x_j = x_{\sigma_i} - x_{\sigma_{i-1}}$  for  $A = E_i = \{e_{\sigma_1}, \dots, e_{\sigma_i}\}$  for appropriate order  $\sigma$ .

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• Hence, Lovász extension is a generalized aggregation function.