

Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 18 —

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Prof. Jeff Bilmes

University of Washington, Seattle
Department of Electrical Engineering
<http://melodi.ee.washington.edu/~bilmes>

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$$\begin{aligned} f(A) + f(B) &\geq f(A \cup B) + f(A \cap B) \\ &= f(A_1) + 2f(C) + f(B_2) = f(A_1) + f(C) + f(B_2) = f(A \cap B) \end{aligned}$$



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

[//canvas.uw.edu/courses/1039754/discussion_topics](https://canvas.uw.edu/courses/1039754/discussion_topics))).

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 \leq , 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:

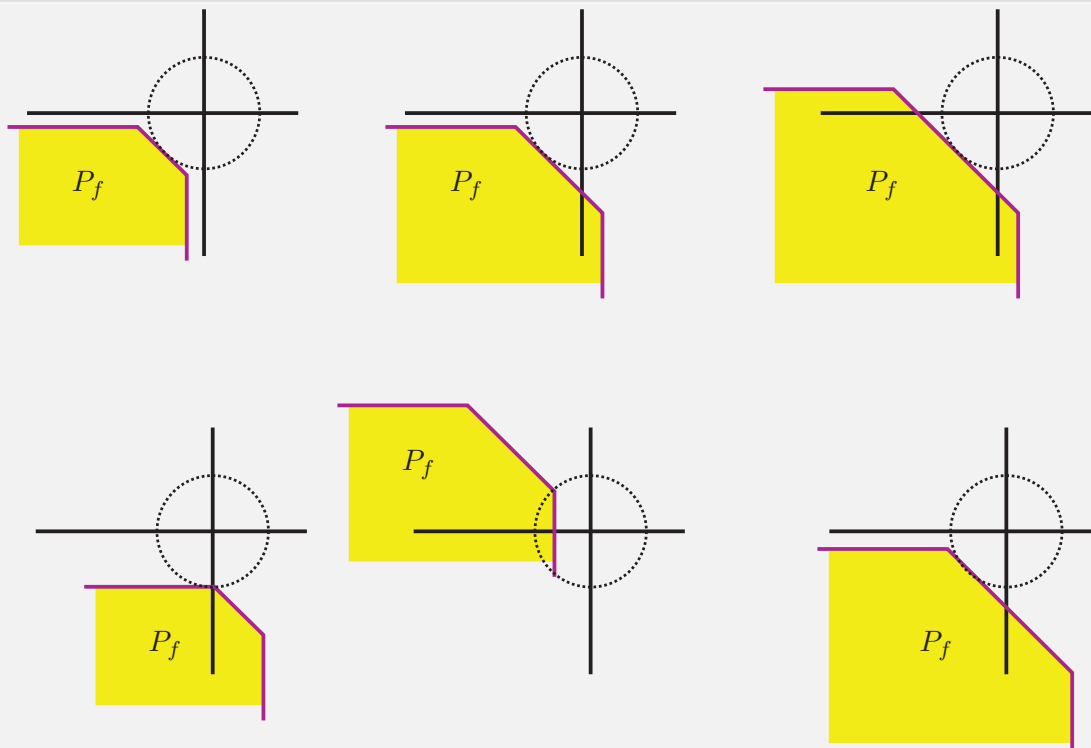
$$\text{minimize} \quad \|x\|_2^2 \quad (18.1a)$$

$$\text{subject to} \quad x \in B_f \quad (18.1b)$$

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

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

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

$$A_0 = \{e : x^*(e) \leq 0\} \quad (18.3)$$

- Thus, we immediately have that:

$$A_- \subseteq A_0 \quad (18.4)$$

and that

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

- 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:

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

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:

$$\text{rank}(0) = \max (y(E) : y \leq 0, y \in P_f) = \min (f(A) : A \subseteq E) \quad (18.2)$$

Summary of sat, and dep

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

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

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

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

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

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

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 $0 \leq \alpha' < \alpha$.

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 $x \in P_f$, $\text{sat}(x) \triangleq \bigcup \{A : A \in \mathcal{D}(x)\} = \{e : e \in E, \forall \alpha > 0, x + \alpha \mathbf{1}_e \notin P_f\}$.
- Saturation capacity: for $x \in P_f$, $0 \leq \hat{c}(x; e) \triangleq \min \{f(A) - x(A) \mid \forall A \ni e\} = \max \{\alpha : \alpha \in \mathbb{R}, x + \alpha \mathbf{1}_e \in P_f\}$
- Recall: $\text{sat}(x) = \{e : \hat{c}(x; e) = 0\}$ and $E \setminus \text{sat}(x) = \{e : \hat{c}(x; e) > 0\}$.
- e -containing x -tight sets: For $x \in P_f$, $\mathcal{D}(x, e) = \{A : e \in A \subseteq E, x(A) = f(A)\} \subseteq \mathcal{D}(x)$.
- Minimal e -containing x -tight set/polymatroidal fundamental circuit/:
For $x \in P_f$,

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

Min-Norm Point and SFM

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 $\text{sat}(x^*) = E$. Thus, we can consider any $e \in E$ within $\text{dep}(x^*, e)$.
- Consider any pair (e, e') with $e' \in \text{dep}(x^*, e)$ 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 l2 sense. We have $(x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'}) \in P_f$, and in fact

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

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

...

Min-Norm Point and SFM

... proof of Thm. 18.3.1 cont.

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

$$= x^*(E \setminus \{e, e'\}) + \underbrace{(x^*(e) + \alpha)}_{x_{\text{new}}^*(e)} + \underbrace{(x^*(e') - \alpha)}_{x_{\text{new}}^*(e')} = f(E).$$
- Minimality of $x^* \in B_f$ in l2 sense requires that, with such an $\alpha > 0$,

$$(x^*(e))^2 + (x^*(e'))^2 < (x_{\text{new}}^*(e))^2 + (x_{\text{new}}^*(e'))^2$$
- 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).

...

Min-Norm Point and SFM

... proof of Thm. 18.3.1 cont.

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

...

Min-Norm Point and SFM

... proof of Thm. 18.3.1 cont.

- Therefore, we have $\cup_{e \in A_-} \text{dep}(x^*, e) = A_-$ and $\cup_{e \in A_0} \text{dep}(x^*, e) = A_0$
- i.e., $\{\text{dep}(x^*, e)\}_{e \in A_-}$ is cover for A_- , as is $\{\text{dep}(x^*, e)\}_{e \in A_0}$ for A_0 .
- $\text{dep}(x^*, e)$ is minimal tight set containing e , meaning $x^*(\text{dep}(x^*, e)) = f(\text{dep}(x^*, e))$, and since tight sets are closed under union, we have that A_- and A_0 are also tight, meaning:

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

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

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

and therefore, all together we have

$$f(A_-) = f(A_0) = x^*(A_-) = x^*(A_0) = y^*(E) \tag{18.5}$$

...

Min-Norm Point and SFM

... 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 $y^* \in P_f$.
- Also, for any $y \in P_f$ with $y \leq 0$ and for any $X \subseteq E$, we have $y(E) \leq y(X) \leq f(X)$.
- Hence, we have found a feasible for l.h.s. of Eqn. (17.7), $y^* \leq 0$, $y^* \in P_f$, so $y^*(E) \leq f(X)$ for all X .
- So $y^*(E) \leq \min \{f(X) | X \subseteq V\}$.
- Considering Eqn. (18.6), 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 .

Min-Norm Point and SFM

... proof of Thm. 18.3.1 cont.

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

$$f(X) \geq x^*(X) > x^*(A_-) = f(A_-) \quad (18.6)$$

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

$$f(X) \geq x^*(X) > x^*(A_0) = f(A_0) \quad (18.7)$$

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



Min-Norm Point and SFM

- So, if we have a procedure to compute the min-norm point computation, we can solve SFM.
- Nice thing about previous proof is that it uses both expressions for dep for different purposes.
- This was discovered by Fujishige (in fact the proof above is an expanded version of the one found in the book).
- As we saw last time, the algorithm (by F. Wolfe) can find this min-norm point, essentially an active-set procedure for quadratic programming. It uses Edmonds's greedy algorithm to make it efficient.
- This is currently the best practical algorithm for **general purpose** submodular function minimization.
- But recall, its underlying lower-bound complexity is unknown.

Min-norm point and other minimizers of f

- Recall, that the set of minimizers of f forms a lattice.
- 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:

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

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

Min-norm point and other minimizers of f

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 .
- But $x^* \in P_f$, so $x^*(A) \leq f(A)$ and $f(A) = x^*(A_-) \leq x^*(A)$ (or alternatively, just note that $x^*(A_0 \setminus A) = 0$).
- Hence, $x^*(A) = x^*(A_-) = f(A)$ so that A is also a tight set for x^* .
- For any $a \in A$, A is a tight set containing a , and $\text{dep}(x^*, a)$ is the minimal tight containing a .
- Hence, for any $a \in A$, $\text{dep}(x^*, a) \subseteq A$.
- This means that $\bigcup_{a \in A} \text{dep}(x^*, a) = A$.
- Since $A_- \subseteq A \subseteq A_0$, then $\exists A_m \subseteq A \setminus A_-$ such that

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

...

Min-norm point and other minimizers of f

proof of Thm. 18.3.2.

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

$$A = A_- \cup \bigcup_{a \in A_m} \text{dep}(x^*, a) = \bigcup_{a \in A_-} \text{dep}(x^*, a) \cup \bigcup_{a \in A_m} \text{dep}(x^*, a) \quad (18.9)$$

- 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 $\text{dep}(x^*, e)$.

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).
- 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):

$$\underset{w \in \mathbb{R}^V}{\text{minimize}} \quad \tilde{f}(w) + \frac{1}{2} \|w\|_2^2 \quad (18.10)$$

$$\underset{x \in B_f}{\text{maximize}} \quad -\|x\|_2^2 \quad (18.11a)$$

$$\text{subject to} \quad x \in B_f \quad (18.11b)$$

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

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

Optimization over P_f

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

$$\text{maximize} \quad w^\top x \quad (18.12a)$$

$$\text{subject to} \quad x \in P_f \quad (18.12b)$$

- Since P_f is down closed, if $\exists e \in E$ with $w(e) < 0$ then the solution above is unboundedly large. Hence, assume $w \in \mathbb{R}_+^E$.
- 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 $x \leq y \in B_f$ which can only increase $w^\top x \leq w^\top y$.
- Hence, the problem is equivalent to: given $w \in \mathbb{R}_+^E$,

$$\text{maximize} \quad w^\top x \quad (18.13a)$$

$$\text{subject to} \quad x \in B_f \quad (18.13b)$$

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

A continuous extension of f

- Consider again optimization problem. Given $w \in \mathbb{R}^E$,

$$\text{maximize} \quad w^\top x \quad (18.14a)$$

$$\text{subject to} \quad x \in B_f \quad (18.14b)$$

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

$$\check{f}(w) = \max(w^\top x : x \in B_f) \quad (18.15)$$

- 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.

A continuous extension of submodular f

- 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 $w(e_1) \geq w(e_2) \geq \dots \geq w(e_m)$.
- Define the chain with i^{th} element $E_i = \{e_1, e_2, \dots, e_i\}$, we have

$$\check{f}(w) = \max\{wx : x \in P_f\} \quad (18.16)$$

$$= \sum_{i=1}^m w(e_i) f(e_i | E_{i-1}) \quad (18.17)$$

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

$$= w(e_m) f(E_m) + \sum_{i=1}^{m-1} (w(e_i) - w(e_{i+1})) f(E_i) \quad (18.19)$$

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

A continuous extension of submodular f

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

$$\check{f}(w) = \max\{wx : x \in B_f\} \quad (18.20)$$

- Therefore, if f is a submodular function, we can write

$$\check{f}(w) = w(e_m) f(E_m) + \sum_{i=1}^{m-1} (w(e_i) - w(e_{i+1})) f(E_i) \quad (18.21)$$

$$= \sum_{i=1}^m \lambda_i f(E_i) \quad (18.22)$$

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 $P \subseteq \mathbb{R}^E$, 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).

An extension of f

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

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

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

An extension of f

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

$$E_i \stackrel{\text{def}}{=} \{e_1, e_2, \dots, e_i\} \quad (18.24)$$

- Note that

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

$\left. \begin{matrix} 1 \\ 1 \\ \vdots \\ 1 \end{matrix} \right\} \ell \times$
 $\left. \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} \right\} (n - \ell) \times$

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

From \check{f} back to f , even when f is not submodular

- From the continuous \check{f} , we can recover $f(A)$ for any $A \subseteq V$.
- Take $w = \mathbf{1}_A$ for some $A \subseteq E$, so w is vertex of the hypercube.
- Order the elements of E in decreasing order of w so that $w(e_1) \geq w(e_2) \geq w(e_3) \geq \dots \geq w(e_m)$.
- This means

$$w = (w(e_1), w(e_2), \dots, w(e_m)) = (\underbrace{1, 1, 1, \dots, 1}_{|A| \text{ times}}, \underbrace{0, 0, \dots, 0}_{m-|A| \text{ times}}) \quad (18.25)$$

so that $\mathbf{1}_A(i) = 1$ if $i \leq |A|$, and $\mathbf{1}_A(i) = 0$ otherwise.

- For any $f : 2^E \rightarrow \mathbb{R}$, $w = \mathbf{1}_A$, since $E_{|A|} = \{e_1, e_2, \dots, e_{|A|}\} = A$:

$$\begin{aligned} \check{f}(w) &= \sum_{i=1}^m \lambda_i f(E_i) = w(e_m) f(E_m) + \sum_{i=1}^{m-1} (w(e_i) - w(e_{i+1})) f(E_i) \\ &= \mathbf{1}_A(m) f(E_m) + \sum_{i=1}^{m-1} (\mathbf{1}_A(i) - \mathbf{1}_A(i+1)) f(E_i) \end{aligned} \quad (18.26)$$

$$= (\mathbf{1}_A(|A|) - \mathbf{1}_A(|A| + 1)) f(E_{|A|}) = f(E_{|A|}) = f(A) \quad (18.27)$$

From \check{f} back to f

- We can view $\check{f} : [0, 1]^E \rightarrow \mathbb{R}$ defined on the hypercube, with f defined as \check{f} evaluated on the hypercube extreme points (vertices).
- To summarize, with $\check{f}(A) = \sum_{i=1}^m \lambda_i f(E_i)$, we have

$$\check{f}(\mathbf{1}_A) = f(A), \quad (18.28)$$

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

$$\check{f}(\mathbf{1}_A) = \max \{ \mathbf{1}_A^\top x : x \in B_f \} \quad (18.29)$$

$$= \max \{ \mathbf{1}_A^\top x : x(B) \leq f(B), \forall B \subseteq E \} \quad (18.30)$$

$$(18.31)$$

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

$$\check{f}(w) = \max \{ w^\top x : x \in P_f \} \quad (18.32)$$

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

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

$$\check{f}(w) = \sum_{i=1}^m \lambda_i f(E_i) \quad (18.33)$$

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

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

so that $w = \sum_{i=1}^m \lambda_i \mathbf{1}_{E_i}$.

- $w = \sum_{i=1}^m \lambda_i \mathbf{1}_{E_i}$ 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:

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

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

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

$$= \sum_{i=1}^m \lambda_i f(E_i) \quad (18.38)$$

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

Summary: comparison of the two extension forms

- 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:

$$\check{f}(w) = \max(wx : x \in P_f) = \sum_{i=1}^m \lambda_i f(E_i) \quad (18.39)$$

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 $w(e_1) \geq w(e_2) \geq \dots \geq w(e_m)$.

- On the other hand, **for any f (even non-submodular)**, we can produce an extension \check{f} having the form

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

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 $w(e_1) \geq w(e_2) \geq \dots \geq w(e_m)$.

- In both Eq. (18.39) and Eq. (18.40), we have $\check{f}(\mathbf{1}_A) = f(A)$, $\forall A$, but Eq. (18.40), might not be convex.
- Submodularity is sufficient for convexity, but is it necessary?

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

- Lovász showed that if a function $\check{f}(w)$ defined as in Eqn. (18.33) is convex, then f must be submodular.
- 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).

Lovász Extension, Submodularity and Convexity

Theorem 18.4.1

A function $f : 2^E \rightarrow \mathbb{R}$ 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.
- Conversely, suppose the Lovász extension $\check{f}(w) = \sum_i \lambda_i f(E_i)$ of some function $f : 2^E \rightarrow \mathbb{R}$ 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.

...

Lovász Extension, Submodularity and Convexity

... proof of Thm. 18.4.1 cont.

- Earlier, we saw that $\check{f}(\mathbf{1}_A) = f(A)$ for all $A \subseteq E$.

- Now, given $A, B \subseteq E$, we will show that

$$\check{f}(\mathbf{1}_A + \mathbf{1}_B) = \check{f}(\mathbf{1}_{A \cup B} + \mathbf{1}_{A \cap B}) \quad (18.41)$$

$$= f(A \cup B) + f(A \cap B). \quad (18.42)$$

- Let $C = A \cap B$, order E based on decreasing $w = \mathbf{1}_A + \mathbf{1}_B$ so that

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

$$= (\underbrace{2, 2, \dots, 2}_{i \in C}, \underbrace{1, 1, \dots, 1}_{i \in A \Delta B}, \underbrace{0, 0, \dots, 0}_{i \in E \setminus (A \cup B)}) \quad (18.44)$$

- Then, considering $\check{f}(w) = \sum_i \lambda_i f(E_i)$, we have $\lambda_{|C|} = 1$, $\lambda_{|A \cup B|} = 1$, and $\lambda_i = 0$ for $i \notin \{|C|, |A \cup B|\}$.
- But then $E_{|C|} = A \cap B$ and $E_{|A \cup B|} = A \cup B$. Therefore,
 $\check{f}(w) = \check{f}(\mathbf{1}_A + \mathbf{1}_B) = f(A \cap B) + f(A \cup B)$.

...

Lovász Extension, Submodularity and Convexity

... proof of Thm. 18.4.1 cont.

- Also, since \check{f} is convex (by assumption) and positively homogeneous, we have for any $A, B \subseteq E$,

$$0.5[f(A \cap B) + f(A \cup B)] = 0.5[\check{f}(\mathbf{1}_A + \mathbf{1}_B)] \quad (18.45)$$

$$= \check{f}(0.5\mathbf{1}_A + 0.5\mathbf{1}_B) \quad (18.46)$$

$$\leq 0.5\check{f}(\mathbf{1}_A) + 0.5\check{f}(\mathbf{1}_B) \quad (18.47)$$

$$= 0.5(f(A) + f(B)) \quad (18.48)$$

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

$$f(A \cup B) + f(A \cap B) \leq f(A) + f(B) \quad (18.49)$$

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 sciences. Convexity is a very natural property of various functions and domains occurring in such models; quite often the only non-trivial property which can be stated in general.

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 μ of sets. E.g., given measurable function f , we can define

$$\int_X f d\mu = \sup I_X(s) \quad (18.50)$$

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 $0 \leq s \leq f$ 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 $c_i > 0$.

Integration, Aggregation, and Weighted Averages

- In finite discrete spaces, Lebesgue integration is just a weighted average, and can be seen as an **aggregation** function.
- 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:

$$\text{WAVG}(x) = \sum_{e \in E} x(e)w(e) \quad (18.51)$$

- Consider $\mathbf{1}_e$ for $e \in E$, we have

$$\text{WAVG}(\mathbf{1}_e) = w(e) \quad (18.52)$$

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

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

Integration, Aggregation, and Weighted Averages

$$\text{WAVG}(x) = \sum_{e \in E} x(e)w(e) \quad (18.54)$$

- 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 $\alpha \in \mathbb{R}$,

$$\text{WAVG}_{w_1+w_2}(x) = \text{WAVG}_{w_1}(x) + \text{WAVG}_{w_2}(x), \quad (18.55)$$

$$\text{WAVG}_w(x_1 + x_2) = \text{WAVG}_w(x_1) + \text{WAVG}_w(x_2), \quad (18.56)$$

and,

$$\text{WAVG}(\alpha x) = \alpha \text{WAVG}(x). \quad (18.57)$$

- 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 $\alpha \geq 0$).

Integration, Aggregation, and Weighted Averages

- 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 $A \subseteq E$):

$$\text{AG}(\mathbf{1}_A) = w_A \quad (18.58)$$

- What then might $\text{AG}(x)$ be for some $x \in \mathbb{R}^E$? Our weighted average functions might look **something** more like the r.h.s. in:

$$\text{AG}(x) = \sum_{A \subseteq E} x(A) w_A = \sum_{A \subseteq E} x(A) \text{AG}(\mathbf{1}_A) \quad (18.59)$$

- Note, we can define $w(e) = w'(e)$ and $w(A) = 0, \forall A : |A| > 1$ and get back previous (normal) weighted average, in that

$$\text{WAVG}_{w'}(x) = \text{AG}_w(x) \quad (18.60)$$

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

Integration, Aggregation, and Weighted Averages

- Set function $f : 2^E \rightarrow \mathbb{R}$ is called a **capacity** if it is monotone non-decreasing, i.e., $f(A) \leq f(B)$ whenever $A \subseteq B$.
- A **Boolean function** f is any function $f : \{0, 1\}^m \rightarrow \{0, 1\}$ and is a **pseudo-Boolean function** if $f : \{0, 1\}^m \rightarrow \mathbb{R}$.
- Any set function corresponds to a pseudo-Boolean function. I.e., given $f : 2^E \rightarrow \mathbb{R}$, form $f_b : \{0, 1\}^m \rightarrow \mathbb{R}$ as $f_b(x) = f(A_x)$ where the A, x bijection is $A = \{e \in E : x_e = 1\}$ and $x = \mathbf{1}_A$.
- Also, if we have an expression for f_b we can construct a set function f as $f(A) = f_b(\mathbf{1}_A)$. We can also often relax f_b to any $x \in [0, 1]^m$.
- 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.

Choquet integral

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

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

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

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

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

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

Choquet integral

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

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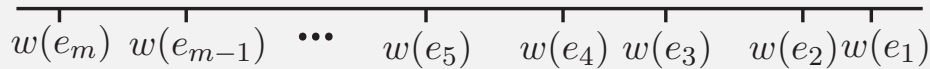
where in the sum, we have sorted and renamed the elements of E so that $w_{e_1} \geq w_{e_2} \geq \dots \geq w_{e_m} \geq w_{e_{m+1}} \triangleq 0$, and where $E_i = \{e_1, e_2, \dots, e_i\}$.

- 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

$$\sum_{k=m}^n a_k b_k = \sum_{k=m}^n A_k (b_k - b_{k+1}) + A_n b_{n+1} - A_{m-1} b_m \quad (18.63)$$

The “integral” in the Choquet integral

- Thought of as an integral over \mathbb{R} of a piece-wise constant function.
- First note, assuming E is ordered according to descending w , so that $w(e_1) \geq w(e_2) \geq \dots \geq w(e_{m-1}) \geq w(e_m)$, then $E_i = \{e_1, e_2, \dots, e_i\} = \{e \in E : w_e \geq w_{e_i}\}$.
- For any $w_{e_i} > \alpha \geq w_{e_{i+1}}$ we also have $E_i = \{e_1, e_2, \dots, e_i\} = \{e \in E : w_e > \alpha\}$.
- Consider segmenting the real-axis at boundary points w_{e_i} , right most is 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 $F_i : [w_{e_{i+1}}, w_{e_i}) \rightarrow \mathbb{R}$ is defined as

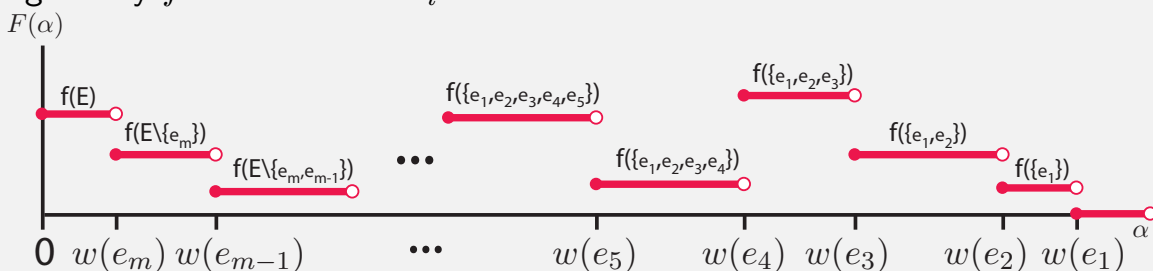
$$F_i(\alpha) = f(\{e \in E : w_e > \alpha\}) = f(E_i) \quad (18.64)$$

The “integral” in the Choquet integral

- 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:

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

- 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?

The “integral” in the Choquet integral

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

$$\tilde{f}(w) \stackrel{\text{def}}{=} \int_0^\infty F(\alpha) d\alpha \quad (18.65)$$

$$= \int_0^\infty f(\{e \in E : w_e > \alpha\}) d\alpha \quad (18.66)$$

$$= \int_{w_{m+1}}^\infty f(\{e \in E : w_e > \alpha\}) d\alpha \quad (18.67)$$

$$= \sum_{i=1}^m \int_{w_{i+1}}^{w_i} f(\{e \in E : w_e > \alpha\}) d\alpha \quad (18.68)$$

$$= \sum_{i=1}^m \int_{w_{i+1}}^{w_i} f(E_i) d\alpha = \sum_{i=1}^m f(E_i)(w_i - w_{i+1}) \quad (18.69)$$

The “integral” in the Choquet integral

- But we saw before that $\sum_{i=1}^m f(E_i)(w_i - w_{i+1})$ is just the Lovász extension of a function f .
- Thus, we have the following definition:

Definition 18.5.2

Given $w \in \mathbb{R}_+^E$, the Lovász extension (equivalently Choquet integral) may be defined as follows:

$$\tilde{f}(w) \stackrel{\text{def}}{=} \int_0^\infty F(\alpha) d\alpha \quad (18.70)$$

where the function F is defined as before.

- Note that it is not necessary in general to require $w \in \mathbb{R}_+^E$ (i.e., we can take $w \in \mathbb{R}^E$) nor that f be non-negative, but it is a bit more involved. Above is the simple case.
- The above integral will be further generalized a bit later.

Choquet integral and aggregation

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

$$\text{AG}(x) = \sum_{A \subseteq E} x(A)w_A = \sum_{A \subseteq E} x(A)\text{AG}(\mathbf{1}_A) \quad (18.71)$$

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 $\mathcal{V}_1, \mathcal{V}_2, \dots, \mathcal{V}_q$.
- 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 \mathcal{V}_i defines the i^{th} polytope.
- 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 $x \in \text{conv}(\mathcal{V}(x))$.

Choquet integral and aggregation

- 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 $\mathbf{1}_A \in \text{conv}(\mathcal{V}(x))$. The affine transformation is as follows:

$$\alpha_0^x(A) + \sum_{j=1}^m \alpha_j^x(A)x_j \in \mathbb{R} \quad (18.72)$$

Note that many of these coefficient are often zero.

- From this, we can define an aggregation function of the form

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

Choquet integral and aggregation

- We can define a canonical triangulation of the hypercube in terms of permutations of the coordinates. I.e., given some permutation σ , define

$$\text{conv}(\mathcal{V}_\sigma) = \{x \in [0, 1]^n | x_{\sigma(1)} \geq x_{\sigma(2)} \geq \dots \geq x_{\sigma(m)}\} \quad (18.74)$$

Then these $m!$ blocks of the partition are called the **canonical partitions** of the hypercube.

- With this, we can define $\{\mathcal{V}_i\}_i$ as the vertices of $\text{conv}(\mathcal{V}_\sigma)$ for each permutation σ . In this case, we have:

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 σ .

- Hence, Lovász extension is a generalized aggregation function.