Submodular Functions, Optimization, and Applications to Machine Learning
— Spring Quarter, Lecture 15 —

http://www.ee.washington.edu/people/faculty/bilmes/classes/ee563_spring_2018/

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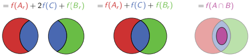
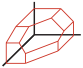
May 16th, 2018

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





Cumulative Outstanding Reading

- Read chapter 1 from Fujishige's book.
- Read chapter 2 from Fujishige's book.
- Read chapter 3 from Fujishige's book.
- Read chapter 4 from Fujishige's book.

Announcements, Assignments, and Reminders

- Next homework will be posted soon.
- As always, if you have any questions about anything, please ask then via our discussion board (https://canvas.uw.edu/courses/1216339/discussion_topics). Can meet at odd hours via zoom (send message on canvas to schedule time to chat).

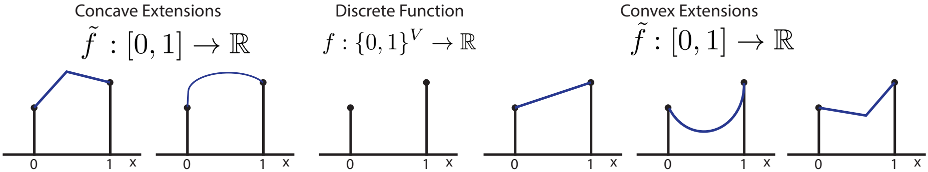
Class Road Map - EE563

- L1(3/26): Motivation, Applications, & Basic Definitions,
- L2(3/28): Machine Learning Apps (diversity, complexity, parameter, learning target, surrogate).
- L3(4/2): Info theory exs, more apps, definitions, graph/combinatorial examples
- L4(4/4): Graph and Combinatorial Examples, Matrix Rank, Examples and Properties, visualizations
- L5(4/9): More Examples/Properties/ Other Submodular Defs., Independence,
- L6(4/11): Matroids, Matroid Examples, Matroid Rank, Partition/Laminar Matroids
- L7(4/16): Laminar Matroids, System of Distinct Reps, Transversals, Transversal Matroid, Matroid Representation, Dual Matroids
- L8(4/18): Dual Matroids, Other Matroid Properties, Combinatorial Geometries, Matroids and Greedy.
- L9(4/23): Polyhedra, Matroid Polytopes, Matroids $\rightarrow$ Polymatroids
- L10(4/29): Matroids $\rightarrow$ Polymatroids, Polymatroids, Polymatroids and Greedy,
- L11(4/30): Polymatroids, Polymatroids and Greedy
- L12(5/2): Polymatroids and Greedy, Extreme Points, Cardinality Constrained Maximization
- L13(5/7): Constrained Submodular Maximization
- L14(5/9): Submodular Max w. Other Constraints, Cont. Extensions, Lovasz Extension
- L15(5/14): Cont. Extensions, Lovasz Extension, Choquet Integration, Properties
- L16(5/16):
- L17(5/21):
- L18(5/23):
- L–(5/28): Memorial Day (holiday)
- L19(5/30):
- L21(6/4): Final Presentations maximization.

Last day of instruction, June 1st. Finals Week: June 2-8, 2018.

Continuous Extensions of Discrete Set Functions

- Any function $f : 2^V \to \mathbb{R}$ (equivalently $f : \{0,1\}^V \to \mathbb{R}$) can be extended to a continuous function in the sense $\tilde{f} : [0,1]^V \to \mathbb{R}$.
- This may be tight (i.e., $\tilde{f}(\mathbf{1}_A) = f(A)$ for all A). I.e., the extension $\tilde{f}$ coincides with f at the hypercube vertices.
- In fact, any such discrete function defined on the vertices of the n-D hypercube $\{0,1\}^n$ has a variety of both convex and concave extensions tight at the vertices (Crama & Hammer'11). Example $n = 1$,



- Since there are an exponential number of vertices $\{0,1\}^n$, important questions regarding such extensions is:
  1. When are they computationally feasible to obtain or estimate?
  2. When do they have nice mathematical properties?
  3. When are they useful for something practical?

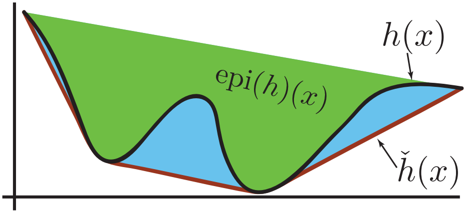
Def: Convex Envelope of a function

- Given any function $h : \mathbb{R}^n \to \mathbb{R}$, define new function $\check{h} : \mathbf{R}^n \to \mathbb{R}$ via:

$$\check{h}(x) = \sup \{g(x) : g \text{ is convex } \& \ g(y) \leq h(y), \forall y \in \mathbb{R}^n\} \qquad (15.6)$$

- I.e., (1) $\check{h}(x)$ is convex, (2) $\check{h}(x) \leq h(x), \forall x$, and (3) if $g(x)$ is any convex function having the property that $g(x) \leq h(x), \forall x$, then $g(x) \leq \check{h}(x)$.
- Alternatively,

$$\check{h}(x) = \inf \{t : (x,t) \in \text{convexhull}(\text{epigraph}(h))\} \qquad (15.7)$$



Convex Closure of Discrete Set Functions

- Given set function $f : 2^V \to \mathbb{R}$, an arbitrary (i.e., not necessarily submodular nor supermodular) set function, define a function $\check{f} : [0,1]^V \to \mathbb{R}$, as

$$\check{f}(x) = \min_{p \in \triangle^n(x)} \sum_{S \subseteq V} p_S f(S) \tag{15.1}$$

where $\triangle^n(x) =$ $\left\{ p \in \mathbb{R}^{2^n} : \sum_{S \subseteq V} p_S = 1,\ p_S \geq 0 \forall S \subseteq V,\ \&\ \sum_{S \subseteq V} p_S \mathbf{1}_S = x \right\}$

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- Hence, $\triangle^n(x)$ is the set of all probability distributions over the 2^n vertices of the hypercube, and where the expected value of the characteristic vectors of those points is equal to x, i.e., for any $p \in \triangle^n(x)$, $E_{S \sim p}(\mathbf{1}_S) = \sum_{S \subseteq V} p_S \mathbf{1}_S = x$.

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- Hence, $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$

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- Hence, $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$
- Note, this is not (necessarily) the Lovász extension, rather this is a convex extension.

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  3. That the convex closure $\check{f}$ is the convex envelope of the function defined only on the hypercube vertices, and that takes value $f(S)$ at $\mathbf{1}_S$.

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  3. That the convex closure $\check{f}$ is the convex envelope of the function defined only on the hypercube vertices, and that takes value $f(S)$ at $\mathbf{1}_S$.
  4. The definition of the Lovász extension of a set function, and that $\check{f}$ is the Lovász extension iff f is submodular.

Tightness of Convex Closure

Lemma 15.3.1

$\forall A \subseteq V$, *we have* $\check{f}(\mathbf{1}_A) = f(A)$.

Proof.

- Define p^x to be an achiving argmin in $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$.

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- Suppose $\exists S'$ with $S' \setminus A \neq 0$ having $p_{S'}^{\mathbf{1}_A} > 0$. This would mean, for any $v \in S' \setminus A$, that $\left(\sum_S p_S^{\mathbf{1}_A} \mathbf{1}_S\right)(v) > 0$, a contradiction.

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- Suppose $\exists S'$ s.t. $A \setminus S' \neq \emptyset$ with $p_{S'}^{\mathbf{1}_A} > 0$.
- Then, for any $v \in A \setminus S'$, consider below leading to a contradiction

$$\underbrace{p_{S'}\mathbf{1}_{S'}}_{>0} + \underbrace{\sum_{\substack{S \subseteq A \\ S \neq S'}} p_S \mathbf{1}_S}_{\text{can't sum to 1}} \Rightarrow \Big(\sum_{\substack{S \subseteq A \\ S \neq S'}} p_s \mathbf{1}_S\Big)(v) < 1 \tag{15.2}$$

I.e., $v \in A$ so it must get value 1, but since $v \notin S'$, v is deficient. □

Convexity of the Convex Closure

Lemma 15.3.2

$\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$ *is convex in* $[0,1]^V$.

Proof.

- Let $x, y \in [0,1]^V$, $0 \leq \lambda \leq 1$, and $z = \lambda x + (1-\lambda) y$, then

$$\lambda \check{f}(x) + (1-\lambda)\check{f}(y) = \lambda \sum_S p^x_S f(S) + (1-\lambda) \sum_S p^y_S f(S) \quad (15.3)$$

$$= \sum_S (\lambda p^x_S + (1-\lambda) p^y_S) f(S) \quad (15.4)$$

$$= \sum_S p^{z'}_S f(S) \geq \min_{p \in \triangle^n(z)} E_{S \sim p}[f(S)] \quad (15.5)$$

$$= \check{f}(z) = \check{f}(\lambda x + (1-\lambda) y) \quad (15.6)$$

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- Note that $p^{z'}_S = \lambda p^x_S + (1-\lambda) p^y_S$ and is feasible in the min since $\sum_S p^{z'}_S = 1$, $p^{z'}_S \geq 0$ and $\sum_S p^{z'}_S \mathbf{1}_S = z$.

Def: Convex Envelope of a function

- Given any function $h : \mathbb{R}^n \to \mathbb{R}$, define new function $\check{h} : \mathbf{R}^n \to \mathbb{R}$ via:

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Convex Closure is the Convex Envelope

Lemma 15.3.3

$\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$ *is the convex envelope.*

Proof.

- Suppose $\exists$ a convex $\bar{f}$ with $\bar{f}(\mathbf{1}_A) = f(A) = \check{f}(\mathbf{1}_A), \forall A \subseteq V$ and $\exists x \in [0,1]^V$ s.t. $\bar{f}(x) > \check{f}(x)$.
- Define p^x to be an achiving argmin in $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$. Hence, we have $x = \sum_S p^x_S \mathbf{1}_S$. Thus

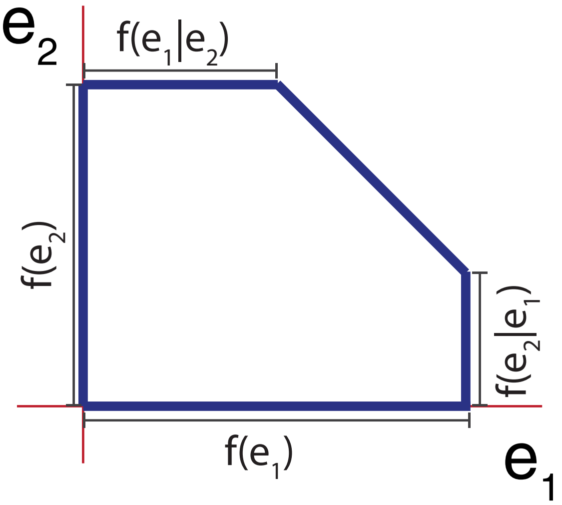
$$\check{f}(x) = \sum_S p^x_S f(S) = \sum_S p^x_S \bar{f}(\mathbf{1}_S) \tag{15.7}$$

$$< \bar{f}(x) = \bar{f}(\sum_S p^x_S \mathbf{1}_S) \tag{15.8}$$

but this contradicts the convexity of $\bar{f}$.

Polymatroid with labeled edge lengths

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



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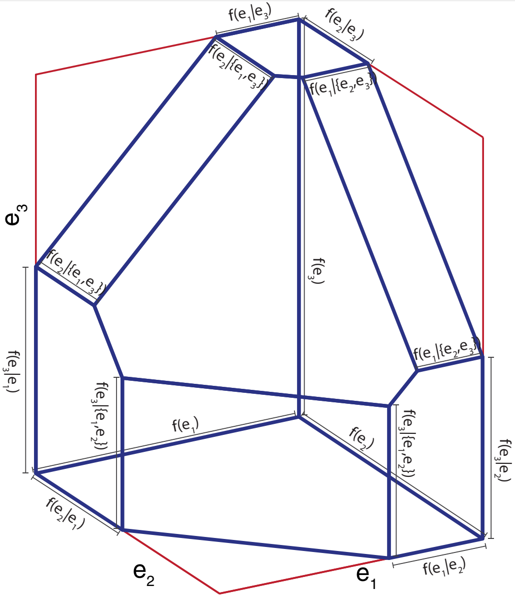

Optimization over P_f

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

$$\begin{aligned} \text{maximize} \quad & w^\intercal x & (15.9a) \\ \text{subject to} \quad & x \in P_f & (15.9b) \end{aligned}$$

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- Since P_f is down closed, if $\exists e \in E$ with $w(e) < 0$ then the solution above is unboundedly large. Hence, assume $w \in \mathbb{R}_+^E$.
- 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 $w^\intercal x \leq w^\intercal y$ when $w \in \mathbb{R}_+^E$.

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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

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

$$\begin{aligned} &\text{maximize} && w^\intercal x && (15.11a) \\ &\text{subject to} && x \in B_f && (15.11b) \end{aligned}$$

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

$$\breve{f}(w) = \max(wx : x \in B_f) \tag{15.12}$$

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- 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.

Edmond's Theorem: The Greedy Algorithm

- Edmonds proved that the solution to $\breve{f}(w) = \max(wx : x \in B_f)$ is solved by the greedy algorithm iff f is submodular.
- In particular, sort choose element order $(e_1, e_2, \ldots, e_m)$ based on decreasing w,so that $w(e_1) \geq w(e_2) \geq \cdots \geq w(e_m)$.
- Define the chain with i^{th} element $E_i = \{e_1, e_2, \ldots, e_i\}$.
- Define a vector $x^* \in \mathbb{R}^V$ where element e_i has value $x(e_i) = f(e_i | E_{i-1})$ for all $i \in V$.
- Then $\langle w, x^* \rangle = \max(wx : x \in B_f)$

Theorem 15.4.1 (Edmonds)

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

A continuous extension of submodular f

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

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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.

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

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- Convex analysis $\Rightarrow$ $\breve{f}(w) = \max(wx : x \in P)$ is always convex in w for any set $P \subseteq R^E$, since a maximum of a set of linear functions (true even when f is not submodular or P is not itself a convex set).

An extension of f

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

$$\begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \underbrace{(w_1 - w_2)}_{\lambda_1} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \underbrace{(w_2 - w_3)}_{\lambda_2} \begin{pmatrix} 1 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \cdots + \underbrace{(w_{n-1} - w_n)}_{\lambda_{m-1}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \end{pmatrix} + \underbrace{(w_m)}_{\lambda_m} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix} \tag{15.20}$$

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- If we take w in decreasing order, then each coefficient of the vectors is non-negative (except possibly the last one, $\lambda_m = w_m$).
- Often, we take $w \in \mathbb{R}_+^V$ or even $w \in [0,1]^V$, where $\lambda_m \geq 0$.

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

$$E_i \stackrel{\text{def}}{=} \{e_1, e_2, \ldots, e_i\} \tag{15.21}$$

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$$\mathbf{1}_{E_0} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \mathbf{1}_{E_1} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \ldots, \mathbf{1}_{E_\ell} = \begin{pmatrix} \left.\begin{matrix} 1 \\ 1 \\ \vdots \\ 1 \end{matrix}\right\} \ell\times \\ \left.\begin{matrix} 0 \\ 0 \\ \vdots \\ 0 \end{matrix}\right\} (n-\ell)\times \end{pmatrix}, \text{ etc.}$$

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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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- From the continuous $\breve{f}$, we can recover $f(A)$ for any $A \subseteq V$.

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

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

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- To summarize, with $\breve{f}(\mathbf{1}_A) = \sum_{i=1}^{m} \lambda_i f(E_i)$, we have

$$\breve{f}(\mathbf{1}_A) = f(A), \tag{15.25}$$

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

$$\breve{f}(\mathbf{1}_A) = \max\{\mathbf{1}_A{}^\intercal x : x \in B_f\} \tag{15.26}$$

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

$$\breve{f}(w) = \max \{w^\intercal x : x \in P_f\} \tag{15.28}$$

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 $\breve{f}(\mathbf{1}_A) = f(A)$, $\forall A$, in this way where

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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

$$\text{for } i \in \{1, \dots, m\}, \quad \lambda_i = \begin{cases} w(e_i) - w(e_{i+1}) & \text{if } i < m \\ w(e_m) & \text{if } i = m \end{cases} \tag{15.30}$$

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

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$$\text{for } i \in \{1, \dots, m\}, \quad \lambda_i = \begin{cases} w(e_i) - w(e_{i+1}) & \text{if } i < m \\ w(e_m) & \text{if } i = m \end{cases} \tag{15.30}$$

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.

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 $\breve{f}(\mathbf{1}_A) = f(A)$, $\forall A$, in this way where

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- $\breve{f}(w) = \sum_{i=1}^{m} \lambda_i f(E_i)$ is the associated interpolation of the values of f at sets corresponding to each hypercube vertex.
- This extension is called the Lovász extension!

Weighted gains vs. weighted functions

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

$$\breve{f}(w) = \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1}) \tag{15.31}$$

$$= \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1})) \tag{15.32}$$

$$= w(e_m) f(E_m) + \sum_{i=1}^{m-1} (w(e_i) - w(e_{i+1})) f(E_i) \tag{15.33}$$

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- So $\breve{f}(w)$ seen either as sum of weighted gain evaluations (Eqn. (15.31)), or as sum of weighted function evaluations (Eqn. (15.34)).

Summary: comparison of the two extension forms

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

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- In both Eq. (15.35) and Eq. (15.36), we have $\breve{f}(\mathbf{1}_A) = f(A)$, $\forall A$, but Eq. (15.36), might not be convex.
- Submodularity is sufficient for convexity, but is it necessary?

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

- Lovász showed that if a function $\breve{f}(w)$ defined as in Eqn. (15.29) is convex, then f must be submodular.

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- This continuous extension $\breve{f}$ of f, in any case (f being submodular or not), is typically called the Lovász extension of f (but also sometimes called the Choquet integral, or the Lovász-Edmonds extension).

Lovász Extension, Submodularity and Convexity

Theorem 15.4.2

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

Proof.

- We've already seen that if f is submodular, its extension can be written via Eqn.(15.29) due to the greedy algorithm, and therefore is also equivalent to $\breve{f}(w) = \max\{wx : x \in P_f\}$, and thus is convex.

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- Conversely, suppose the Lovász extension $\breve{f}(w) = \sum_i \lambda_i f(E_i)$ of some function $f : 2^E \to \mathbb{R}$ is a convex function.

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- We note that, based on the extension definition, in particular the definition of the $\{\lambda_i\}_i$, we have that $\breve{f}(\alpha w) = \alpha \breve{f}(w)$ for any $\alpha \in \mathbb{R}_+$. I.e., f is a positively homogeneous convex function.

...

Lovász Extension, Submodularity and Convexity

. . . proof of Thm. 15.4.2 cont.

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... proof of Thm. 15.4.2 cont.

- Earlier, we saw that $\breve{f}(\mathbf{1}_A) = f(A)$ for all $A \subseteq E$.
- Now, given $A, B \subseteq E$, we will show that

$$\breve{f}(\mathbf{1}_A + \mathbf{1}_B) = \breve{f}(\mathbf{1}_{A \cup B} + \mathbf{1}_{A \cap B}) \tag{15.37}$$

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

$$w = (w(e_1), w(e_2), \dots, w(e_m)) \tag{15.39}$$

$$= (\underbrace{2, 2, \dots, 2}_{i \in C}, \underbrace{1, 1, \dots, 1}_{i \in A \triangle B}, \underbrace{0, 0, \dots, 0}_{i \in E \setminus (A \cup B)}) \tag{15.40}$$

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

. . .

Lovász Extension, Submodularity and Convexity

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

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$$\leq 0.5\breve{f}(\mathbf{1}_A) + 0.5\breve{f}(\mathbf{1}_B) \tag{15.43}$$

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$$\leq 0.5\breve{f}(\mathbf{1}_A) + 0.5\breve{f}(\mathbf{1}_B) \tag{15.43}$$

$$= 0.5(f(A) + f(B)) \tag{15.44}$$

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$$= 0.5(f(A) + f(B)) \tag{15.44}$$

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

$$f(A \cup B) + f(A \cap B) \leq f(A) + f(B) \tag{15.45}$$

so f must be submodular.

□

Lovász ext. vs. the concave closure of submodular function

- The above theorem showed that the Lovász extension is convex iff f is submodular.

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- I.e., not only is the Lovász extension convex for f submodular, it is the convex closure when f is convex.
- Hence, convex closure is easy to evaluate when f is submodular and is this particular form iff f is submodular.

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Theorem 15.4.3

Let $\breve{f}(w) = \max(wx : x \in B_f) = \sum_{i=1}^{m} \lambda_i f(E_i)$ *be the Lovász extension and* $\breve{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$ *be the convex closure. Then* $\breve{f}$ *and* $\breve{f}$ *coincide iff* f *is submodular.*

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- Assume f is submodular.

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- Given x, let p^x be an achieving argmin in $\breve{f}(x)$ that also maximizes $\sum_S p^x_S |S|^2$.

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- Assume f is submodular.
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- Suppose $\exists A, B \subseteq V$ that are crossing (i.e., $A \not\subseteq B$, $B \not\subseteq A$) and positive and w.l.o.g., $p_A^x \geq p_B^x > 0$.

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- Then we may update p^x as follows:

$$\bar{p}^x_A \leftarrow p^x_A - p^x_B \qquad \bar{p}^x_B \leftarrow p^x_B - p^x_B \tag{15.46}$$

$$\bar{p}^x_{A \cup B} \leftarrow p^x_{A \cup B} + p^x_B \qquad \bar{p}^x_{A \cap B} \leftarrow p^x_{A \cap B} + p^x_B \tag{15.47}$$

and by submodularity, this does not increase $\sum_S p^x_S f(S)$.

...

Lovász ext. vs. the concave closure of submodular function

. . . proof cont.

- This does increase $\sum_S p^x_S |S|^2$ however since

$$|A \cup B|^2 + |A \cap B|^2 = (|A| + |B \setminus A|)^2 + (|B| - |B \setminus A|)^2 \quad (15.48)$$

$$= |A|^2 + |B|^2 + 2|B \setminus A|(|A| - |B| + |B \setminus A|) \quad (15.49)$$

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- Contradiction! Hence, there can be no crossing sets A, B and we must have, for any A, B with $p^x_A > 0$ and $p^x_B > 0$ either $A \subset B$ or $B \subset A$.

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- Contradiction! Hence, there can be no crossing sets A, B and we must have, for any A, B with $p^x_A > 0$ and $p^x_B > 0$ either $A \subset B$ or $B \subset A$.
- Hence, the sets $\{A \subseteq V : p^x_A > 0\}$ form a chain and can be as large only as size $n = |V|$.

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... proof cont.

- This does increase $\sum_S p_S^x |S|^2$ however since

$$|A \cup B|^2 + |A \cap B|^2 = (|A| + |B \setminus A|)^2 + (|B| - |B \setminus A|)^2 \quad (15.48)$$
$$= |A|^2 + |B|^2 + 2|B \setminus A|(|A| - |B| + |B \setminus A|) \quad (15.49)$$
$$\geq |A|^2 + |B|^2 \quad (15.50)$$

- Contradiction! Hence, there can be no crossing sets A, B and we must have, for any A, B with $p_A^x > 0$ and $p_B^x > 0$ either $A \subset B$ or $B \subset A$.
- Hence, the sets $\{A \subseteq V : p_A^x > 0\}$ form a chain and can be as large only as size $n = |V|$.
- This is the same chain that defines the Lovász extension $\breve{f}(x)$, namely $\emptyset = E_0 \subseteq E_1 \subseteq E_2 \subset \ldots$ where $E_i = \{e_1, e_2, \ldots, e_i\}$ and e_i is orderd so that $x(e_1) \geq x(e_2) \geq \cdots \geq x(e_n)$.

Lovász ext. vs. the concave closure of submodular function

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- Consider $x = \mathbf{1}_S + \frac{1}{2}\mathbf{1}_{\{i,j\}}$.

Lovász ext. vs. the concave closure of submodular function

...proof cont.

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- Consider $x = \mathbf{1}_S + \frac{1}{2}\mathbf{1}_{\{i,j\}}$.
- Then $\breve{f}(x) = \frac{1}{2}f(S) + \frac{1}{2}f(S+i+j)$ and p^x is feasible for $\check{f}$ with $p^x_S = 1/2$ and $p^x_{S+i+j} = 1/2$.

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- An alternate feasible distribution for x in the convex closure is $\bar{p}^x_{S+i} = \bar{p}^x_{S+j} = 1/2$.

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- This gives

$$\breve{f}(x) \leq \frac{1}{2}[f(S+i) + f(S+j)] < \breve{f}(x) \tag{15.51}$$

meaning $\breve{f}(x) \neq \breve{f}(x)$.

Integration and Aggregation

- Integration is just summation (e.g., the $\int$ symbol has as its origins a sum).

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- Lebesgue integration allows integration w.r.t. an underlying measure μ of sets. E.g., given measurable function f, we can define

$$\int_X f du = \sup I_X(s) \tag{15.52}$$

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 $c_i > 0$.

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Integration, Aggregation, and Weighted Averages

$$\text{WAVG}(x) = \sum_{e \in E} x(e)w(e) \tag{15.56}$$

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

$$\text{WAVG}_{w_1+w_2}(x) = \text{WAVG}_{w_1}(x) + \text{WAVG}_{w_2}(x), \tag{15.57}$$

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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 $\alpha \geq 0$).

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

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- 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 15.5.1

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

$$C_f(w) = \sum_{i=1}^{m} (w_{e_i} - w_{e_{i+1}}) f(E_i) \tag{15.63}$$

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:

$$C_f(w) = \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1})) \tag{15.64}$$

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

$$\sum_{k=m}^{n} a_k b_k = \sum_{k=m}^{n} A_k (b_k - b_{k+1}) + A_n b_{n+1} - A_{m-1} b_m \tag{15.65}$$

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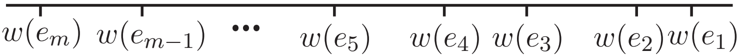
- Consider segmenting the real-axis at boundary points w_{e_i}, right most is w_{e_1}.



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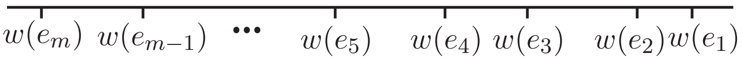

- A function can be defined on a segment of $\mathbb{R}$, namely $w_{e_i} > \alpha \geq w_{e_{i+1}}$. This function $F_i : [w_{e_{i+1}}, w_{e_i}) \to \mathbb{R}$ is defined as

$$F_i(\alpha) = f(\{e \in E : w_e > \alpha\}) = f(E_i) \tag{15.66}$$

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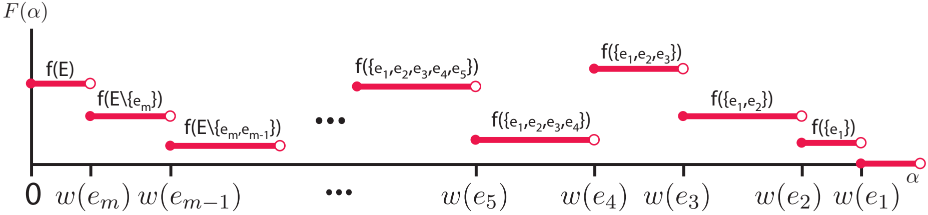
- Visualizing a piecewise constant function, where the constant values are given by f evaluated on E_i for each i



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

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

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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 $w_{m+1} \stackrel{\text{def}}{=} 0$.

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- 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.

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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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where the function F is defined as before.

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- 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:

$$\mathsf{AG}(x) = \sum_{A \subseteq E} x(A) w_A = \sum_{A \subseteq E} x(A) \mathsf{AG}(\mathbf{1}_A) \tag{15.73}$$

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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 $x \in \operatorname{conv}(\mathcal{V}(x))$.

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:

$$\alpha_0^x(A) + \sum_{j=1}^{m} \alpha_j^x(A) x_j \in \mathbb{R} \tag{15.74}$$

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  Note that many of these coefficient are often zero.

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

$$\text{AG}(x) \stackrel{\text{def}}{=} \sum_{A:\mathbf{1}_A \in \mathcal{V}(x)} \Big(\alpha_0^x(A) + \sum_{j=1}^{m} \alpha_j^x(A) x_j \Big) \text{AG}(\mathbf{1}_A) \tag{15.75}$$

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

$$\text{conv}(\mathcal{V}_\sigma) = \left\{x \in [0,1]^n | x_{\sigma(1)} \geq x_{\sigma(2)} \geq \cdots \geq x_{\sigma(m)}\right\} \tag{15.76}$$

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

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Proposition 15.5.3

The above linear interpolation in Eqn. (15.75) 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 $A = E_i = \{e_{\sigma_1}, \ldots, e_{\sigma_i}\}$ for appropriate order σ.

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- Hence, Lovász extension is a generalized aggregation function.

Lovász extension as max over orders

- We can also write the Lovász extension as follows:

$$\tilde{f}(w) = \max_{\sigma \in \Pi_{[m]}} w^\intercal c^\sigma \tag{15.77}$$

where $\Pi_{[m]}$ is the set of $m!$ permutations of $[m] = E$, $\sigma \in \Pi_{[m]}$ is a particular permutation, and c^σ is a vector associated with permutation σ defined as:

$$c_i^\sigma = f(E_{\sigma_i}) - f(E_{\sigma_{i-1}}) \tag{15.78}$$

where $E_{\sigma_i} = \{e_{\sigma_1}, e_{\sigma_2}, \dots, e_{\sigma_i}\}$.

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- Note this immediately follows from the definition of the Lovász extension in the form:

$$\tilde{f}(w) = \max_{x \in P_f} w^\intercal x = \max_{x \in B_f} w^\intercal x \tag{15.79}$$

since we know that the maximum is achieved by an extreme point of the base B_f and all extreme points are obtained by a permutation-of-E-parameterized greedy instance.

Lovász extension, defined in multiple ways

- As shorthand notation, lets use $\{w \geq \alpha\} \equiv \{e \in E : w(e) \geq \alpha\}$, called the weak α-sup-level set of w.

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- Given any $w \in \mathbb{R}^E$, sort E as $w(e_1) \geq w(e_2) \geq \cdots \geq w(e_m)$. Also, w.l.o.g., number elements of w so that $w_1 \geq w_2 \geq \cdots \geq w_m$.

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- We have already seen how we can define the Lovász extension for any (not necessarily submodular) function f in the following equivalent ways:

$$\tilde{f}(w) = \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1}) \tag{15.80}$$

$$= \sum_{i=1}^{m-1} f(E_i)(w(e_i) - w(e_{i+1})) + f(E) w(e_m) a \tag{15.81}$$

$$= \sum_{i=1}^{m-1} \lambda_i f(E_i) \tag{15.82}$$

Lovász extension, as integral

- Additional ways we can define the Lovász extension for any (not necessarily submodular) but normalized function f include:

$$\tilde{f}(w) = \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1}) = \sum_{i=1}^{m} \lambda_i f(E_i) \tag{15.83}$$

$$= \sum_{i=1}^{m-1} f(E_i)(w(e_i) - w(e_{i+1})) + f(E) w(e_m) \tag{15.84}$$

$$= \int_{\min\{w_1,\ldots,w_m\}}^{+\infty} f(\{w \geq \alpha\}) d\alpha + f(E) \min\{w_1, \ldots, w_m\} \tag{15.85}$$

$$= \int_{0}^{+\infty} f(\{w \geq \alpha\}) d\alpha + \int_{-\infty}^{0} [f(\{w \geq \alpha\}) - f(E)] d\alpha \tag{15.86}$$

general Lovász extension, as simple integral

- In fact, we have that, given function f, and any $w \in \mathbb{R}^E$:

$$\tilde{f}(w) = \int_{-\infty}^{+\infty} \hat{f}(\alpha) d\alpha \tag{15.87}$$

where

$$\hat{f}(\alpha) = \begin{cases} f(\{w \geq \alpha\}) & \text{if } \alpha >= 0 \\ f(\{w \geq \alpha\}) - f(E) & \text{if } \alpha < 0 \end{cases} \tag{15.88}$$

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- So we can write it as a simple integral over the right function.
- These make it easier to see certain properties of the Lovász extension. But first, we show the above.

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- To show Eqn. (15.85), first note that the r.h.s. terms are the same since $w(e_m) = \min\{w_1, \ldots, w_m\}$.

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$$f(\{w \geq \alpha\}) = \begin{cases} 0 & \text{if } \alpha > w(e_1) \\ f(E_k) & \text{if } \alpha \in (w(e_{k+1}), w(e_k)), k \in \{1, \ldots, m-1\} \\ f(E) & \text{if } \alpha < w(e_m) \end{cases} \tag{15.89}$$

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  we may use open intervals since sets of zero measure don't change integration.
- Inside the integral, then, this recovers Eqn. (15.84).

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- To show Eqn. (15.86), start with Eqn. (15.85), note $w_m = \min\{w_1, \dots, w_m\}$, take any $\beta \leq \min\{0, w_1, \dots, w_m\}$, and form:

$$\tilde{f}(w)$$

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&= \int_0^{+\infty} f(\{w \geq \alpha\})d\alpha + \int_{\beta}^{0} f(\{w \geq \alpha\})d\alpha - \int_{\beta}^{0} f(E)d\alpha
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and then let $\beta \to \infty$ and we get Eqn. (15.86), i.e.:

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\end{aligned}$$

and then let $\beta \to \infty$ and we get Eqn. (15.86), i.e.:

$$= \int_{0}^{+\infty} f(\{w \geq \alpha\})d\alpha + \int_{-\infty}^{0} [f(\{w \geq \alpha\}) - f(E)]d\alpha$$

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Equality (a) follows since $\int_{-\infty}^{\infty} f(\alpha)d\alpha = \int_{-\infty}^{\infty} f(a\alpha + b)d\alpha$ for any b and $a \in \pm 1$, and equality (b) follows since $f(A) = f(E \setminus A)$, so $f(\{w \leq \alpha\}) = f(\{w > \alpha\})$.

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- Hence, for $w \in [0,1]^m$, we can also define the Lovász extension as

$$\tilde{f}(w) = \mathbb{E}_{p(\alpha)}[\underbrace{f(\{w \geq \alpha\})}_{h(\alpha)}] = \mathbb{E}_{p(\alpha)}[\underbrace{f(e \in E : w(e_i) \geq \alpha)}_{h(\alpha)}] \quad (15.93)$$

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  where α is uniform random variable in $[0,1]$.
- Useful for showing results for randomized rounding schemes in solving submodular opt. problems subject to constraints via relaxations to convex optimization problems subject to linear constraints.

Simple expressions for Lovász E. with $m = 2$, $E = \{1, 2\}$

- If $w_1 \geq w_2$, then

$$\tilde{f}(w) = w_1 f(\{1\}) + w_2 f(\{2\}|\{1\}) \quad (15.94)$$

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$$= \frac{1}{2} f(1)(w_1 - w_2) + \frac{1}{2} f(1)(w_1 - w_2) \quad (15.100)$$

$$+ \frac{1}{2} f(\{1, 2\})(w_1 + w_2) - \frac{1}{2} f(\{1, 2\})(w_1 - w_2) \quad (15.101)$$

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- A similar (symmetric) expression holds when $w_1 \leq w_2$.

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- This gives, for general w_1, w_2, that

$$\tilde{f}(w) = \frac{1}{2}\left(f(\{1\}) + f(\{2\}) - f(\{1,2\})\right)|w_1 - w_2| \tag{15.103}$$

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- Thus, if $f(A) = H(X_A)$ is the entropy function, we have $\tilde{f}(w) = H(e_1)w_1 + H(e_2)w_2 - I(e_1; e_2)\min\{w_1, w_2\}$ which must be convex in w, where $I(e_1; e_2)$ is the mutual information.

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- This "simple" but general form of the Lovász extension with $m = 2$ can be useful.

Example: $m = 2$, $E = \{1, 2\}$, contours

- If $w_1 \geq w_2$, then

$$\tilde{f}(w) = w_1 f(\{1\}) + w_2 f(\{2\}|\{1\}) \tag{15.108}$$

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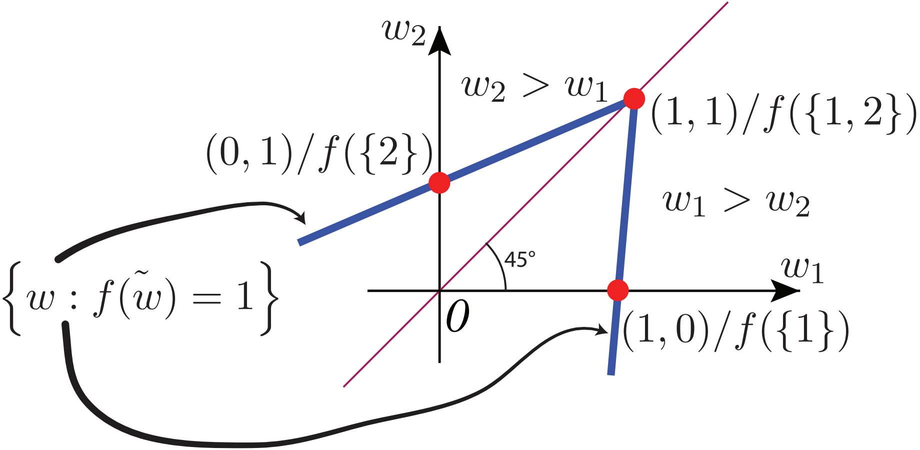
- Contour plot of $m = 2$ Lovász extension (from Bach-2011).



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- Thus, we can look "down" on the contour plot of the Lovász extension, $\left\{ w : \tilde{f}(w) = 1 \right\}$, from a vantage point right on the line $\{x : x = \alpha \mathbf{1}_E, \alpha > 0\}$ since moving in direction $\mathbf{1}_E$ changes nothing.

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- Example 1 (from Bach-2011): $f(A) = \mathbf{1}_{|A| \in \{1,2\}}$ $= \min\{|A|, 1\} + \min\{|E \setminus A|, 1\} - 1$ is submodular, and $\tilde{f}(w) = \max_{k \in \{1,2,3\}} w_k - \min_{k \in \{1,2,3\}} w_k$.

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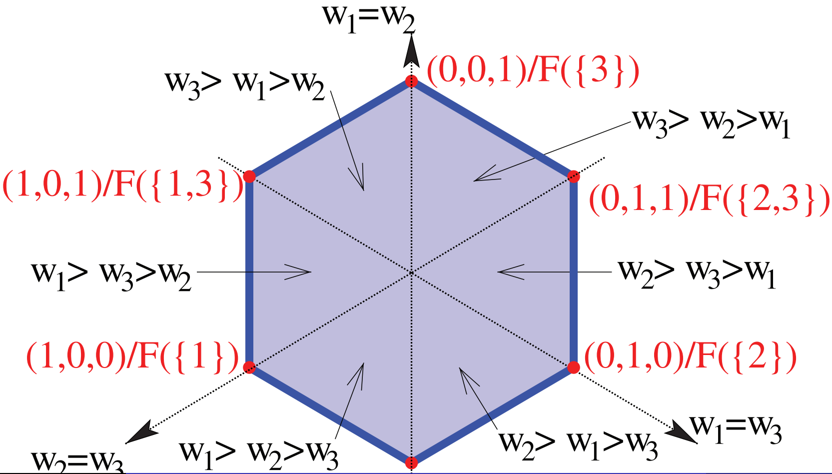

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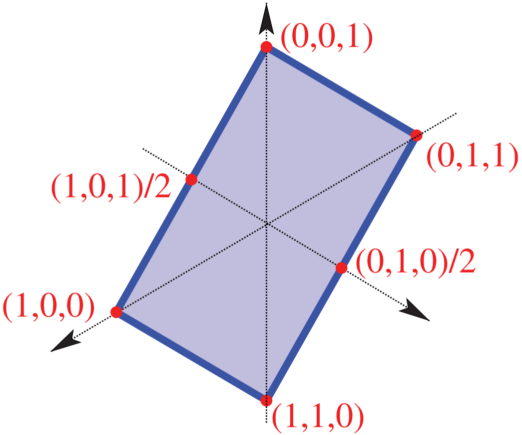
- Example 2 (from Bach-2011): $f(A) = |\mathbf{1}_{1 \in A} - \mathbf{1}_{2 \in A}| + |\mathbf{1}_{2 \in A} - \mathbf{1}_{3 \in A}|$



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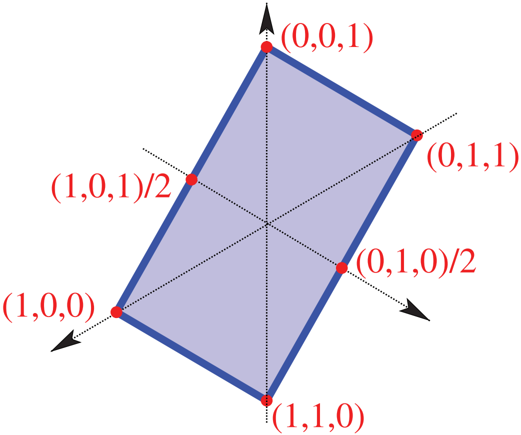
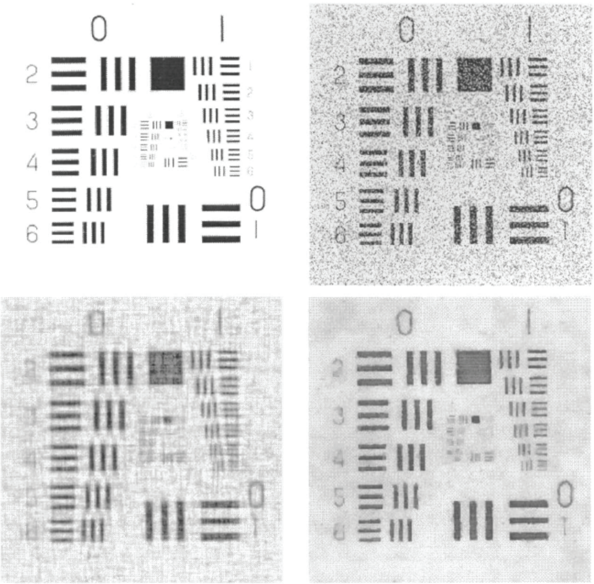
- This gives a "total variation" function for the Lovász extension, with $\tilde{f}(w) = |w_1 - w_2| + |w_2 - w_3|$, a prior to prefer piecewise-constant signals.



Total Variation Example

From "Nonlinear total variation based noise removal algorithms" Rudin, Osher, and Fatemi, 1992. Top left original, bottom right total variation.



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- And if $m(A) = |A|$, we get

$$\tilde{f}(w) = \sum_{i=1}^{m} w(e_i)\big(g(i) - g(i-1)\big) \tag{15.111}$$

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- Cut Function: Given a non-negative weighted graph $G = (V, E, m)$ where $m : E \to \mathbb{R}_+$ is a modular function over the edges, we know from Lecture 2 that $f : 2^V \to \mathbb{R}_+$ with $f(X) = m(\Gamma(X))$ where $\Gamma(X) = \{(u, v) | (u, v) \in E, u \in X, v \in V \setminus X\}$ is non-monotone submodular.

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- This is also a form of "total variation"

A few more Lovász extension examples

Some additional submodular functions and their Lovász extensions, where $w(e_1) \geq w(e_2) \geq \cdots \geq w(e_m) \geq 0$. Let $W_k \triangleq \sum_{i=1}^{k} w(e_i)$.

$f(A)$	$\tilde{f}(w)$
$\|A\|$	$\\|w\\|_1$
$\min(\|A\|, 1)$	$\\|w\\|_\infty$
$\min(\|A\|, 1) - \max(\|A\| - m + 1, 0)$	$\\|w\\|_\infty - \min_i w_i$
$\min(\|A\|, k)$	W_k
$\min(\|A\|, k) - \max(\|A\| - (n-k) + 1, 1)$	$2W_k - W_m$
$\min(\|A\|, \|E \setminus A\|)$	$2W_{\lfloor m/2 \rfloor} - W_m$

(thanks to K. Narayanan).

Supervised And Unsupervised Machine Learning

- Given training data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^m$ with $(x_i, y_i) \in \mathbb{R}^n \times \mathbb{R}$, perform the following risk minimization problem:

$$\min_{w \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^m \ell(y_i, w^\intercal x_i) + \lambda \Omega(w), \tag{15.114}$$

  where $\ell(\cdot)$ is a loss function (e.g., squared error) and $\Omega(w)$ is a norm.
- When data has multiple responses $(x_i, y_i) \in \mathbb{R}^n \times \mathbb{R}^k$, learning becomes:

$$\min_{w^1, \dots, w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^k, (w^k)^\intercal x_i) + \lambda \Omega(w^k), \tag{15.115}$$

- When data has multiple responses only that are observed, $(y_i) \in R^k$ we get dictionary learning (Krause & Guestrin, Das & Kempe):

$$\min_{x_1, \dots, x_m} \min_{w^1, \dots, w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^k, (w^k)^\intercal x_i) + \lambda \Omega(w^k), \tag{15.116}$$

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- Points of difference should be "sparse" (frequently zero).

(Rodriguez, 2009)

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- Ex: total variation is Lovász-ext. of graph cut, but $\exists$ many more!

Lovász extension and norms

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- Hence, not all norms come from the Lovász extension of some submodular function.
- Similarly, not all convex functions are the Lovász extension of some submodular function.

Lovász extension and norms

- Using Lovász extension to define various norms of the form $\|w\|_{\tilde{f}} = \tilde{f}(|w|)$, renders the function symmetric about all orthants (i.e., $\|w\|_{\tilde{f}} = \|b \odot w\|_{\tilde{f}}$ where $b \in \{-1, 1\}^m$ and $\odot$ is element-wise multiplication).
- Simple example. The Lovász extension of the modular function $f(A) = |A|$ is the ℓ_1 norm, and the Lovász extension of the modular function $f(A) = m(A)$ is the weighted ℓ_1 norm.
- With more general submodular functions, one can generate a large and interesting variety of norms, all of which have polyhedral contours (unlike, say, something like the ℓ_2 norm).
- Hence, not all norms come from the Lovász extension of some submodular function.
- Similarly, not all convex functions are the Lovász extension of some submodular function.
- Bach-2011 has a complete discussion of this.