Submodular Functions, Optimization, and Applications to Machine Learning
— Fall Quarter, Lecture 17 —

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

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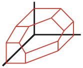
Nov 30th, 2020

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

$= f(A_r) + 2f(C) + f(B_r)$ $\quad = f(A_r) + f(C) + f(B_r)$ $\quad = f(A \cap B)$



Class Road Map - EE563

- L1(9/30): Motivation, Applications, Definitions, Properties
- L2(10/5): Sums concave(modular), uses (diversity/costs, feature selection), information theory
- L3(10/7): Monge, More Definitions, Graph and Combinatorial Examples,
- L4(10/12): Graph & Combinatorial Examples, Matrix Rank, Properties, Other Defs, Independence
- L5(10/14): Properties, Defs of Submodularity, Independence
- L6(10/19): Matroids, Matroid Examples, Matroid Rank,
- L7(10/21): Matroid Rank, More on Partition Matroid, Laminar Matroids, System of Distinct Reps, Transversals
- L8(10/26): Transversal Matroid, Matroid and representation, Dual Matroid
- L9(10/28): Other Matroid Properties, Combinatorial Geometries, Matroid and Greedy, Polyhedra, Matroid Polytopes
- L10(11/2): Matroid Polytopes, Matroids $\rightarrow$ Polymatroids
- L11(11/4): Matroids $\rightarrow$ Polymatroids, Polymatroids
- L12(11/9): Polymatroids, Polymatroids and Greedy
- L–(11/11): Veterans Day, Holiday
- L13(11/16): Polymatroids and Greedy, Possible Polytopes, Extreme Points, Cardinality Constrained Maximization
- L14(11/18): Cardinality Constrained Maximization, Curvature
- L15(11/23): Curvature, Submodular Max w. Other Constraints, Start Cont. Extensions
- L16(11/25): Submodular Max w. Other Constraints, Cont. Extensions, Lovász extension
- L17(11/30): Choquet Integration, Non-linear Measure/Aggregation, Definitions/Properties, Examples.
- L18(12/2):
- L19(12/7):
- L20(12/9):
- L21(12/14): final meeting (presentations) maximization.

Last day of instruction, Fri. Dec 11th. Finals Week: Dec 12-18, 2020

Rest of class

- Homework 4 posted, due Thursday Dec 17th, 2020, 11:55pm.
- Final project paper proposal, due Sunday Dec 6th, 11:59pm.
- Final project 4-page paper and presentation slides, due Sunday Dec 13th, 11:59pm.
- Final project presentation, Monday Dec 14th, starting at 10:30am.
- Final project: Read and present a recent (past 5 years) paper on submodular/supermodular optimization. Paper should have both a theoretical and practical component. What is due: (1) 4-page paper summary, and (2) 10 minute presentation about the paper, will be giving presentations on Monday 12/14/2020. You must choose your paper before the 14th (this will be HW5), and you must turn in your slides and 4-page paper (this will be HW6).
- Recall, grades will be based on a combination of a final project (40%) and the four homeworks (60%).

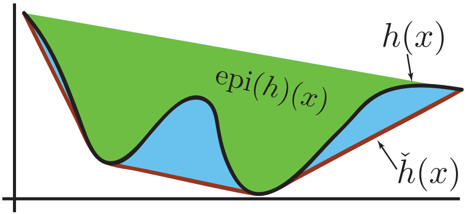
Def: Convex Envelope of a function

- Given any function $h : \mathcal{D}_h \to \mathbb{R}$, where $\mathcal{D}_h \subseteq \mathbb{R}^n$, define the new function $\check{h} : \mathbf{R}^n \to \mathbb{R}$ via:

$$\check{h}(x) = \sup \{g(x) : g \text{ is convex } \& \ g(y) \le h(y), \forall y \in \mathcal{D}_h\} \tag{17.1}$$

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

$$\check{h}(x) = \inf \{t : (x,t) \in \text{convexhull}(\text{epigraph}(h))\} \tag{17.2}$$



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

$$\check{f}(x) = \min_{p \in \triangle^n(x)} \sum_{S \subseteq V} p_S f(S) \tag{17.1}$$

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

- 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 $x \in [0,1]^V$, i.e., for any $p \in \triangle^n(x)$, $E_{S \sim p}(\mathbf{1}_S) = \sum_{S \subseteq V} p_S \mathbf{1}_S = x$.
- Hence, $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$
- We will show that this is **a** convex extension. Does it have any special properties?

Convex Closure of Discrete Set Functions

- Given, $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$, we ~~can~~ did show:
  1. that $\check{f}$ is tight (i.e., $\forall S \subseteq V$, we have $\check{f}(\mathbf{1}_S) = f(S)$).
  2. that $\check{f}$ is convex (and consequently, that any arbitrary set function has a tight convex extension).
  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.
- Note that the **concave** closure can also be defined, as $\hat{f}(x) = \max_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$, but it is in general impossible to obtain exactly even for submodular functions.

Greedy-based continuous extension of submodular f

- Given a submodular function f, a $w \in \cancel{\mathbb{R}^E_+}$ $[0,1]^E$, choose element order $(e_1, e_2, \dots, e_m)$ based on decreasing w,so that $1 \geq w(e_1) \geq w(e_2) \geq \dots \geq w(e_m) \geq 0$.
- Define chain $\emptyset \triangleq E_0 \subset E_1 \subset E_2 \subset \dots \subset E_m = E$ based on w, so the i^{th} element of this change has $E_i = \{e_1, e_2, \dots, e_i\}$.

We have, for $w \in \cancel{\mathbb{R}^E_+}$ $[0,1]^E$ that

$$\breve{f}(w) = \max(wx : x \in P_f) = \max(wx : x \in B_f) \tag{17.12}$$

$$= \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1}) = \sum_{i=1}^{m} w(e_i) x(e_i) \tag{17.13}$$

$$= \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1})) \tag{17.14}$$

$$= (1 - w(e_1))f(E_0) + w(e_m)f(E_m) + \sum_{i=1}^{m-1} (w(e_i) - w(e_{i+1}))f(E_i) \tag{17.15}$$

Greedy-based continuous extension of submodular f

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

$$\breve{f}(w) = \max(wx : x \in B_f) \tag{17.12}$$

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

$$\breve{f}(w) = w(e_m)f(E_m) + \sum_{i=1}^{m-1}(w(e_i) - w(e_{i+1}))f(E_i) \tag{17.13}$$

$$= \sum_{i=1}^{m} \lambda_i f(E_i) \tag{17.14}$$

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.

The Lovász 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

$$\breve{f}(w) = \sum_{i=1}^{m} \lambda_i f(E_i) \tag{17.20}$$

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

$$\text{for } i \in \{1, \ldots, m\}, \quad \lambda_i = \begin{cases} w(e_i) - w(e_{i+1}) & \text{if } i < m \\ w(e_m) & \text{if } i = m \end{cases} \tag{17.21}$$

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

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:

$$\breve{f}(w) = \max(wx : x \in B_f) = \sum_{i=1}^{m} \lambda_i f(E_i) \qquad (17.24)$$

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

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

$$\breve{f}(w) = \sum_{i=1}^{m} \lambda_i f(E_i) \qquad (17.25)$$

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

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

Lovász Extension, Submodularity and Convexity

Theorem 17.2.6

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.(??) due to the greedy algorithm, and therefore is also equivalent to $\breve{f}(w) = \max\{wx : x \in P_f\}$, and thus is convex.
- 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.
- 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 ext. vs. the concave closure of submodular function

Theorem 17.2.6

Let $\breve{f}(w) = \max(wy : y \in B_f) = \sum_{i=1}^{m} \lambda_i f(E_i)$ *be the Lovász extension and* $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$ *be the convex closure. Then* $\breve{f}$ *and* $\check{f}$ *coincide iff* f *is submodular, i.e.,* $\breve{f}(w) = \check{f}(w), \forall w \in [0,1]$.

Proof.

- Assume f is submodular.
- Given x, let p^x be an achieving argmin in $\check{f}(x)$ that also maximizes $\sum_S p_S^x |S|^2$.
- Suppose $\exists A, B \subseteq V$ that are crossing (i.e., $A \not\subseteq B$, $B \not\subseteq A$) with positive p_A^x, p_B^x. W.l.o.g., $p_A^x \geq p_B^x > 0$.
- Then we may update p^x, keeping it a distribution, as follows:

$$\bar{p}_A^x \leftarrow p_A^x - p_B^x \qquad \bar{p}_B^x \leftarrow p_B^x - p_B^x \tag{17.33}$$

$$\bar{p}_{A\cup B}^x \leftarrow p_{A\cup B}^x + p_B^x \qquad \bar{p}_{A\cap B}^x \leftarrow p_{A\cap B}^x + p_B^x \tag{17.34}$$

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

...

Integration

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- Lebesgue integration (See Rudin 1987, Definition 1.23, for details) allows integration w.r.t. an underlying measure μ of sets. Formal definition (from Rudin): given measurable function f, we can define

$$\int_X f du = \sup I_X(s) \tag{17.1}$$

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 $c_i > 0$.

Review

- Recall, a Boolean function f is any function $f : \{0,1\}^m \rightarrow \{0,1\}$ and is a pseudo-Boolean function if $f : \{0,1\}^m \rightarrow \mathbb{R}$.

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- 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 $x = \mathbf{1}_A$.

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- 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.

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- 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 17.3.1

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

$$C_f(w) = \sum_{i=1}^{m} (w_{e_i} - w_{e_{i+1}}) f(E_i) \tag{17.2}$$

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

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

$$C_f(w) = \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1})) \tag{17.3}$$

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

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- 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

$$\sum_{k=m}^{n} a_k b_k = \sum_{k=m}^{n} A_k(b_k - b_{k+1}) + A_n b_{n+1} - A_{m-1} b_m \tag{17.4}$$

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

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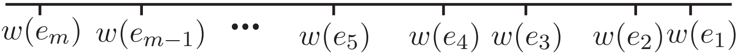
- Can segment real-axis at boundary points w_{e_i}, right most is w_{e_1}.



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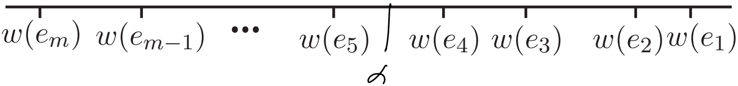

- A function can be defined on a segment $w_{e_i} > \alpha \geq w_{e_{i+1}}$ of $\mathbb{R}$. This function $F_i : [w_{e_{i+1}}, w_{e_i}) \to \mathbb{R}$ is defined as

$$F_i(\alpha) = f(\{e \in E : w_e > \alpha\}) = f(E_i) \tag{17.5}$$

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:

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

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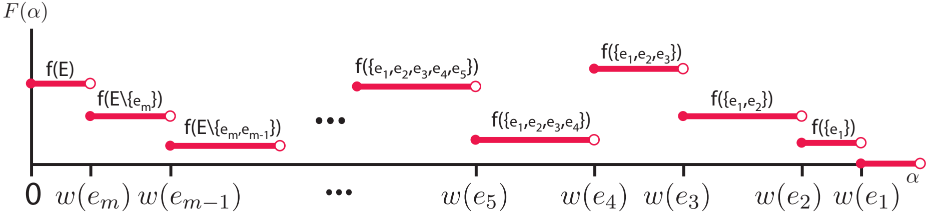
- Visualizing a piecewise constant function, where the constant values are given by f evaluated on E_i for each i



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

$$\tilde{f}(w) \stackrel{\text{def}}{=} \int_0^\infty F(\alpha) d\alpha \tag{17.6}$$

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$$= \sum_{i=1}^m \int_{w_{i+1}}^{w_i} f(\{e \in E : w_e > \alpha\}) d\alpha \tag{17.9}$$

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$$= \sum_{i=1}^m \int_{w_{i+1}}^{w_i} f(\{e \in E : w_e > \alpha\}) d\alpha \tag{17.9}$$

$$= \sum_{i=1}^m \int_{w_{i+1}}^{w_i} f(E_i) d\alpha = \sum_{i=1}^m f(E_i)(w_i - w_{i+1}) \tag{17.10}$$

The "integral" in the Choquet integral

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

$$\tilde{f}(w) \stackrel{\text{def}}{=} \int_0^\infty F(\alpha) d\alpha \tag{17.11}$$

where the function F is defined as before.

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

Integration, Aggregation, and Weighted Averages

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

mean, max, min,
harmonic mean, geometric mean,
...

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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:

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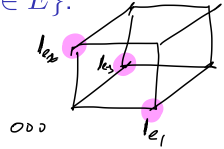

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so seen as a function on the hypercube vertices, the entire WAVG function is given based on values on a size $m = |E|$ subset of the vertices of this hypercube, i.e., $\{\mathbf{1}_e : e \in E\}$. Moreover, we are interpolating as in

$$\text{WAVG}(x) = \sum_{e \in E} x(e)w(e) = \sum_{e \in E} x(e)\text{WAVG}(\mathbf{1}_e) \tag{17.14}$$

Integration, Aggregation, and Weighted Averages

$$\mathsf{WAVG}(x) = \sum_{e \in E} x(e) w(e) \tag{17.15}$$

- WAVG function is linear in weights w **and** 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 $\alpha \in \mathbb{R}$,

$$\mathsf{WAVG}_{w_1+w_2}(x) = \mathsf{WAVG}_{w_1}(x) + \mathsf{WAVG}_{w_2}(x), \tag{17.16}$$

$$\mathsf{WAVG}_{w}(x_1 + x_2) = \mathsf{WAVG}_{w}(x_1) + \mathsf{WAVG}_{w}(x_2), \tag{17.17}$$

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Integration, Aggregation, and Weighted Averages

$LE_f(x)$

$LE_{f_1+f_2}(x) = LE_{f_1}(x) + LE_{f_2}(x)$

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and is homogeneous, $\forall \alpha \in \mathbb{R}$,

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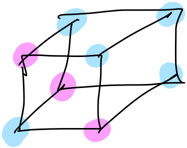
- How related? The Lovász extension $\breve{f}(x)$ is still linear in "weights" (i.e., the submodular function f), but will not be linear in x and will only be positively homogeneous (for $\alpha \geq 0$).

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 $A \subseteq E$):

$$\text{AG}(\mathbf{1}_A) = w_A \tag{17.19}$$



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

$$\mathsf{AG}(x) = \sum_{A \subseteq E} x(A) w_A = \sum_{A \subseteq E} x(A) \mathsf{AG}(\mathbf{1}_A) \tag{17.20}$$

$$= \sum_{e \in E} x(e) \sum_{A : A \ni e} w_A = \sum_{e \in E} x(e) w'_e$$

Choquet integral and aggregation

- We wish to produce some notion of generalized aggregation function having the flavor of:

$$\mathsf{AG}(x) = \sum_{A \subseteq E} x(A) w_A = \sum_{A \subseteq E} x(A) \mathsf{AG}(\mathbf{1}_A) \tag{17.21}$$

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

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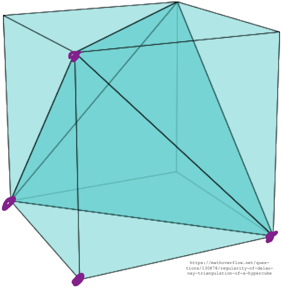
- E.g., for each i, $\mathcal{V}_i = \{\mathbf{1}_{A_1}, \mathbf{1}_{A_2}, \dots, \mathbf{1}_{A_k}\}$ (k vertices) and the convex hull of $\mathcal{V}_i$ defines the i^{th} polytope. This forms a "triangulation" of the hypercube.



https://mathoverflow.net/questions/130878/regularity-of-delaunay-triangulation-of-a-hypercube

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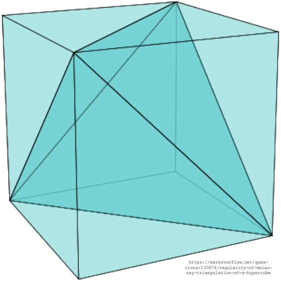

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- For any $x \in [0,1]^m$ there is a (not necessarily unique) $\mathcal{V}(x) = \mathcal{V}_j$ for some j such that $x \in \text{conv}(\mathcal{V}(x))$.

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:

$$\alpha_0^x(A) + \sum_{j=1}^{m} \alpha_j^x(A) x_j \in \mathbb{R} \tag{17.22}$$

Note that many of these coefficient are often zero.

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$$\mathsf{AG}(x) \stackrel{\text{def}}{=} \sum_{A:\mathbf{1}_A \in \mathcal{V}(x)} \Big(\alpha_0^x(A) + \sum_{j=1}^m \alpha_j^x(A) x_j\Big) \mathsf{AG}(\mathbf{1}_A) \tag{17.23}$$

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- Note, no longer necessarily linear in x.

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

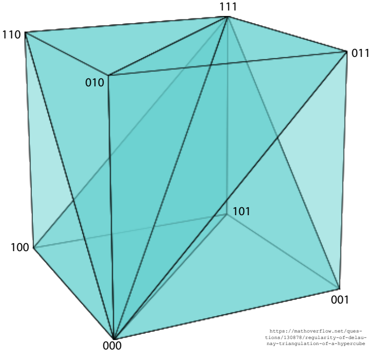
$$\text{conv}(\mathcal{V}_\sigma) = \{x \in [0,1]^n | x_{\sigma(1)} \geq x_{\sigma(2)} \geq \cdots \geq x_{\sigma(m)}\} \qquad (17.24)$$

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

$m = 3$

$m! = 6$

$\therefore$ 6 blocks in the partition



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The above linear interpolation in Eqn. (17.23) 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 can be seen as a form of generalized aggregation function. non-linear measure theory.

Lovász extension as max over orders

- We can also write the Lovász extension as follows:

$$\tilde{f}(w) = \max_{\sigma \in \Pi_{[m]}} w^{\intercal} c^{\sigma} \tag{17.25}$$

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:

$$c_i^{\sigma} = f(E_{\sigma_i}) - f(E_{\sigma_{i-1}}) \tag{17.26}$$

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

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

$$\tilde{f}(w) = \max_{x \in P_f} w^\intercal x = \max_{x \in B_f} w^\intercal x \tag{17.27}$$

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

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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:

$$\tilde{f}(w) = \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1}) \tag{17.28}$$

$$= \sum_{i=1}^{m-1} f(E_i)(w(e_i) - w(e_{i+1})) + f(E)w(e_m) \tag{17.29}$$

$$= \sum_{i=1}^{m-1} \lambda_i f(E_i) \tag{17.30}$$

Lovász extension, as integral

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

$$\tilde{f}(w) = \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1}) = \sum_{i=1}^{m} \lambda_i f(E_i) \tag{17.31}$$

$$= \sum_{i=1}^{m-1} f(E_i)(w(e_i) - w(e_{i+1})) + f(E) w(e_m) \tag{17.32}$$

$$= \int_{\min\{w_1,\dots,w_m\}}^{+\infty} f(\{w \geq \alpha\}) d\alpha + f(E) \min\{w_1, \dots, w_m\} \tag{17.33}$$

$$\stackrel{\text{(a)}}{=} \int_0^{+\infty} f(\{w \geq \alpha\}) d\alpha + \int_{-\infty}^{0} [f(\{w \geq \alpha\}) - f(E)] d\alpha \tag{17.34}$$

We will show (a) in a few slides.

general Lovász extension, as simple integral

- Assuming (a), we have that, given function f, and any $w \in \mathbb{R}^E$:

$$\tilde{f}(w) = \int_{-\infty}^{+\infty} \hat{f}(\alpha) d\alpha \tag{17.35}$$

where

$$\hat{f}(\alpha) = \begin{cases} f(\{w \geq \alpha\}) & \text{if } \alpha \geq 0 \\ f(\{w \geq \alpha\}) - f(E) & \text{if } \alpha < 0 \end{cases} \tag{17.36}$$

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

Lovász extension, as integral

- To show Eqn. (17.33), first note that the r.h.s. terms are the same since $w(e_m) = \min\{w_1, \dots, w_m\}$.

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We will show (a) in a few slides.

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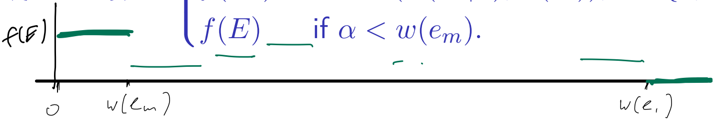

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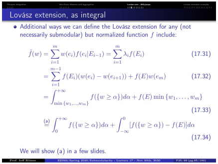

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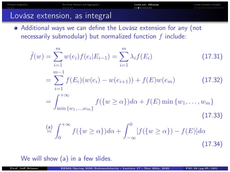
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Prof. Jeff Bilmes EE563/Spring 2020/Submodularity - Lecture 17 - Nov 30th, 2020 F25/49 (pg.65/160)

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$\tilde{f}(w)$ $\therefore \beta \leq \min(0, w_m)$

Choquet Integration | Non-linear Measure and Aggregation | Lovász extn., defs/props | Lovász extension examples

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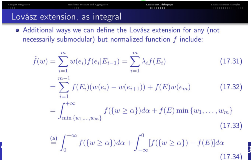

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$$\cancel{LE(\lambda x) = \lambda LE(x)}$$

$$LE_{\lambda f}(x) = \lambda \cdot LE_f(x)$$

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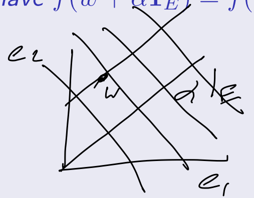

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6. *f symmetric as in $f(A) = f(E \setminus A), \forall A$, then $\tilde{f}(w) = \tilde{f}(-w)$ ($\tilde{f}$ is even).*

$f(A) = f'(A) + f'(V \setminus A)$

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7. *Given partition* $E^1 \cup E^2 \cup \cdots \cup E^k$ *of* E *and* $w = \sum_{i=1}^k \gamma_i \mathbf{1}_{E_k}$ *with* $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_k$*, and with* $E^{1:i} = E^1 \cup E^2 \cup \cdots \cup E^i$*, then* $\tilde{f}(w) = \sum_{i=1}^k \gamma_i f(E^i | E^{1:i-1}) = \sum_{i=1}^{k-1} f(E^{1:i})(\gamma_i - \gamma_{i+1}) + f(E)\gamma_k$*.*

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- And if $f(E) = 0$, then the Lovász extension is constant along the direction $\mathbf{1}_E$.

Lovász extension properties

- Given Eqns. (17.31) through (17.34), most of the above properties are relatively easy to derive.
- For example, if f is symmetric, and since $f(E) = f(\emptyset) = 0$, we have

$$\tilde{f}(-w) = \int_{-\infty}^{\infty} f(\{-w \geq \alpha\})d\alpha \tag{17.40}$$

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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$$\{w > \alpha\} = E \setminus \{w \leq \alpha\} \tag{17.40}$$

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

$$\tilde{f}(w) = \mathbb{E}_{p(\alpha)}[\underbrace{f(\{w \geq \alpha\})}_{h(\alpha)}] = \mathbb{E}_{p(\alpha)}[\underbrace{f(e \in E : w(e_i) \geq \alpha)}_{h(\alpha)}] \quad (17.41)$$

where α is uniform random variable in $[0,1]$.

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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.

One slide review of ~~co~~ncave relaxation

[illegible]

- convex closure $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$, where where $\triangle^n(x) = \left\{ p \in \mathbb{R}^{2^n} : \sum_{S \subseteq V} p_S = 1,\ p_S \geq 0 \forall S \subseteq V, \ \&\ \sum_{S \subseteq V} p_S \mathbf{1}_S = x \right\}$
- "Edmonds" extension $\breve{f}(w) = \max(wx : x \in B_f)$
- Lovász extension $f_{\mathsf{LE}}(w) = \sum_{i=1}^m \lambda_i f(E_i)$, with λ_i such that $w = \sum_{i=1}^m \lambda_i \mathbf{1}_{E_i}$
- $\tilde{f}(w) = \max_{\sigma \in \Pi_{[m]}} w^\intercal c^\sigma$, $\Pi_{[m]}$ set of $m!$ permutations of $[m]$, $\sigma \in \Pi_{[m]}$ a permutation, c^σ vector with $c_i^\sigma = f(E_{\sigma_i}) - f(E_{\sigma_{i-1}})$, $E_{\sigma_i} = \{e_{\sigma_1}, e_{\sigma_2}, \ldots, e_{\sigma_i}\}$.
- Choquet integral $C_f(w) = \sum_{i=1}^m (w_{e_i} - w_{e_{i+1}}) f(E_i)$
- $\tilde{f}(w) = \int_{-\infty}^{+\infty} \hat{f}(\alpha) d\alpha$, $\hat{f}(\alpha) = \begin{cases} f(\{w \geq \alpha\}) & \text{if } \alpha \geq 0 \\ f(\{w \geq \alpha\}) - f(E) & \text{if } \alpha < 0 \end{cases}$
- All the same when f is submodular.

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

- If $w_1 \geq w_2$, then

$$\tilde{f}(w) = w_1 f(\{1\}) + w_2 f(\{2\}|\{1\}) \tag{17.42}$$

$$= (w_1 - w_2) f(\{1\}) + w_2 f(\{1, 2\}) \tag{17.43}$$

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- If $w_1 \geq w_2$, then

$$\tilde{f}(w) = w_1 f(\{1\}) + w_2 f(\{2\}|\{1\}) \tag{17.46}$$

$$= (w_1 - w_2) f(\{1\}) + w_2 f(\{1,2\}) \tag{17.47}$$

$$= \frac{1}{2} f(1)(w_1 - w_2) + \frac{1}{2} f(1)(w_1 - w_2) \tag{17.48}$$

$$+ \frac{1}{2} f(\{1,2\})(w_1 + w_2) - \frac{1}{2} f(\{1,2\})(w_1 - w_2) \tag{17.49}$$

$$+ \frac{1}{2} f(2)(w_1 - w_2) + \frac{1}{2} f(2)(w_2 - w_1) \tag{17.50}$$

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

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

- This gives, for general w_1, w_2, that

$$\tilde{f}(w) = \frac{1}{2}\left(f(\{1\}) + f(\{2\}) - f(\{1,2\})\right)|w_1 - w_2| \tag{17.51}$$

$$+ \frac{1}{2}\left(f(\{1\}) - f(\{2\}) + f(\{1,2\})\right) w_1 \tag{17.52}$$

$$+ \frac{1}{2}\left(-f(\{1\}) + f(\{2\}) + f(\{1,2\})\right) w_2 \tag{17.53}$$

$$= -\left(f(\{1\}) + f(\{2\}) - f(\{1,2\})\right) \min\{w_1, w_2\} \tag{17.54}$$

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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.

Combinatorial MI.

$I_f(e_1; e_2) = f(e_1) + f(e_2) - f(e_1, e_2)$

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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

$$\tilde{f}(w) = w_1 f(\{1\}) + w_2 f(\{2\}|\{1\}) \tag{17.56}$$

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$$= \left(\frac{1}{f(1,2)}, \frac{1}{f(1,2)} \right)$$

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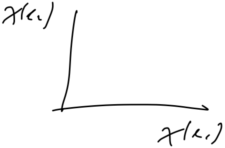

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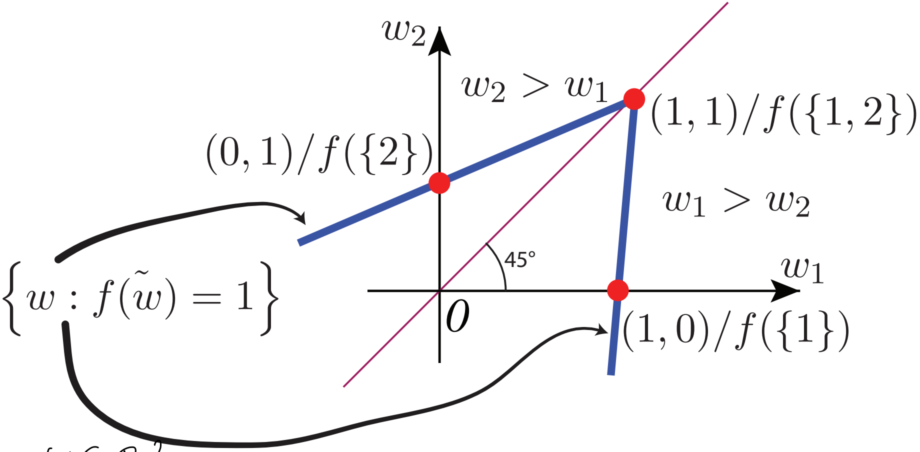
  - If $w = (1, 1)/f(\{1, 2\})$ then $\tilde{f}(w) = 1$.
- Can plot contours of the form $\left\{w \in \mathbb{R}^2 : \tilde{f}(w) = 1\right\}$, particular marked points of form $w = \mathbf{1}_A \times \frac{1}{f(A)}$ for certain A, where $\tilde{f}(w) = 1$.

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

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



$w \in \mathbb{R}^2$

Example: $m = 3$, $E = \{1, 2, 3\}$

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- Consider any submodular f' and $x \in B_{f'}$. Then $f(A) = f'(A) - x(A)$ is submodular, and moreover $f(E) = f'(E) - x(E) = 0$.

$x \in B_{f'}$, a vertex of $B_{f'}$ generated from greedy according to the order σ,

$$E_i = \{e_{\sigma_1}, e_{\sigma_2}, \dots, e_{\sigma_i}\}$$

$$\therefore \quad f(E_i) = 0 \quad \forall i.$$

$$E_m = E$$

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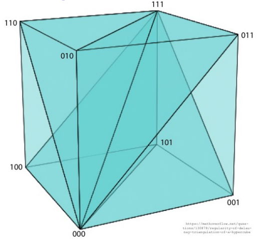
- Thus, we can look "down" on the contour plot of the Lovász extension, $\left\{ w : \tilde{f}(w) = 1 \right\}$, from a vantage point of being right on the ray $\{x : x = \alpha \mathbf{1}_E, \alpha > 0\}$ since moving in direction $\mathbf{1}_E$ changes nothing.



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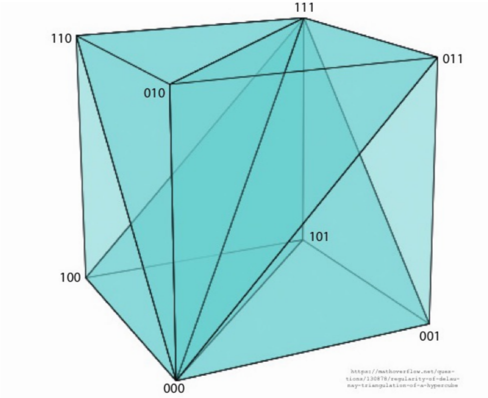
- I.e., consider 2D plane perpendicular to the ray $\{x : x = \alpha \mathbf{1}_E, \alpha > 0\}$ at any point along that ray, then Lovász extension is surface plot with coordinates on that 2D plane, or alternatively we can view contours (which we will do).

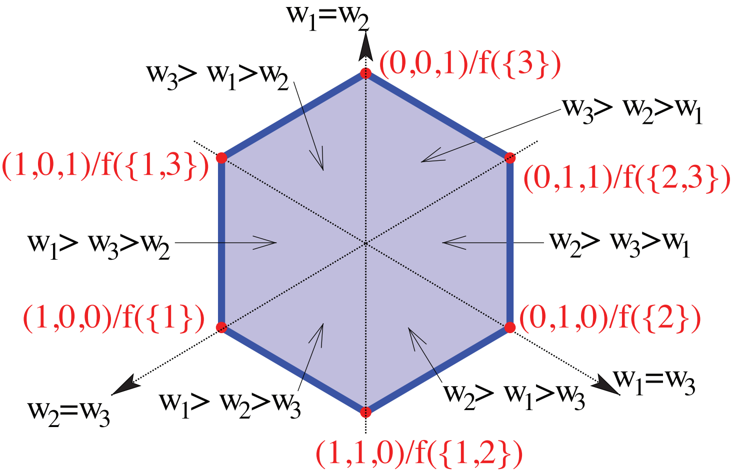
Example: $m = 3$, $E = \{1, 2, 3\}$

- 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 $\tilde{f}(w) = \max_{k \in \{1,2,3\}} w_k - \min_{k \in \{1,2,3\}} w_k$.



Example: $m = 3$, $E = \{1, 2, 3\}$

- 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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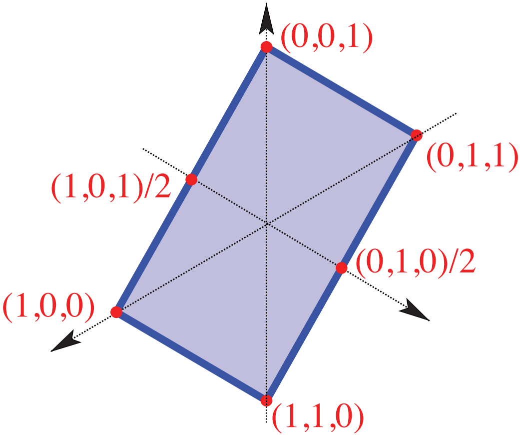

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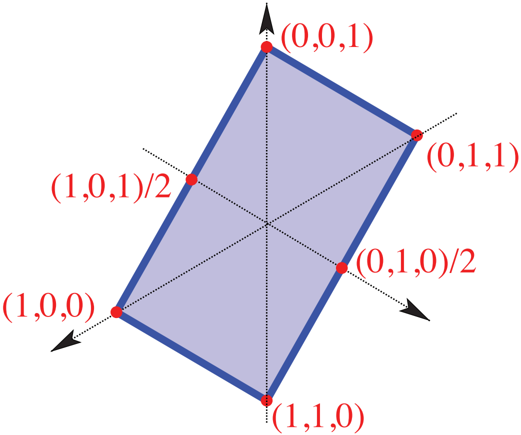

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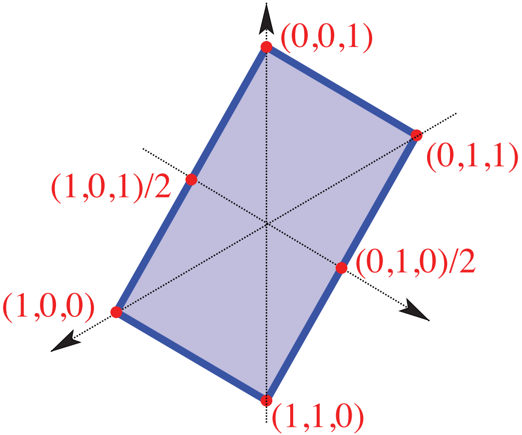
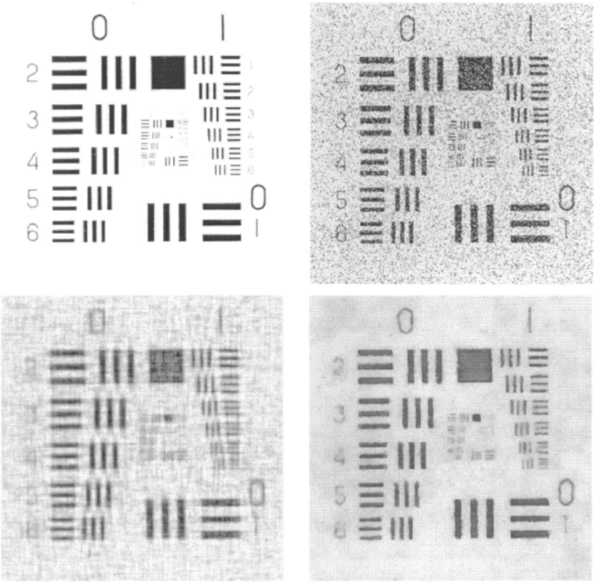


Total Variation Example

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

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Example: Lovász extension and cut functions

- 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 $W_k \triangleq \sum_{i=1}^{k} w(e_i)$.

$f(A)$	$\tilde{f}(w)$
$\lvert A\rvert$	$\lVert w\rVert_1$
$\min(\lvert A\rvert, 1)$	$\lVert w\rVert_\infty$
$\min(\lvert A\rvert, 1) - \max(\lvert A\rvert - m + 1, 0)$	$\lVert w\rVert_\infty - \min_i w_i$
$\min(\lvert A\rvert, k)$	W_k
$\min(\lvert A\rvert, k) - \max(\lvert A\rvert - (n-k) + 1, 1)$	$2W_k - W_m$
$\min(\lvert A\rvert, \lvert E \setminus A\rvert)$	$2W_{\lfloor m/2 \rfloor} - W_m$

(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:

ERM

$$\min_{w \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^m \ell(y_i, w^\intercal x_i) + \lambda \Omega(w), \tag{17.62}$$

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:

$$\min_{w^1,\dots,w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^k, (w^k)^\intercal x_i) + \lambda \Omega(w^k), \tag{17.63}$$

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

$$\min_{x_1,\dots,x_m} \min_{w^1,\dots,w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^k, (w^k)^\intercal x_i) + \lambda \Omega(w^k), \tag{17.64}$$

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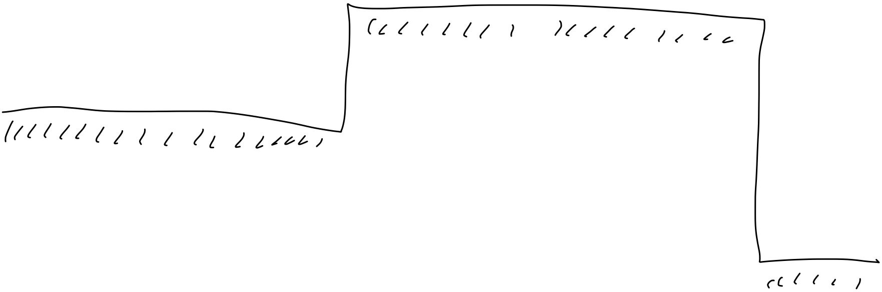

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- Points of difference should be "sparse" (frequently zero).

(Rodriguez, 2009)

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$\sqrt{\mathrm{supp}(w)}$

$\sqrt{\mathrm{supp}(w)(V_1)} + \sqrt{\mathrm{supp}(w)(V_2)}$

$f(A) = \sqrt{|A \cap V_1|} + \sqrt{|A \cap V_2|}$

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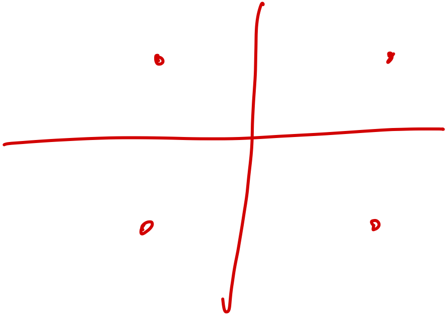
- Ex: total variation is Lovász-ext. of graph cut, but $\exists$ many more!

Lovász extension and norms

- Using Lovász extension to define various norms of the form $\|w\|_{\tilde{f}} = \tilde{f}(|w|)$. This renders the function symmetric about all orthants (meaning, $\|w\|_{\tilde{f}} = \|b \odot w\|_{\tilde{f}}$ for any $b \in \{-1, 1\}^m$ and $\odot$ is element-wise multiplication).

• Note, $\|w\|_{\tilde{f}}$ is an actual norm ?



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- Bach-2011 has a complete discussion of this. (now book).