Submodular Functions, Optimization, and Applications to Machine Learning

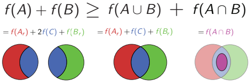
— Spring Quarter, Lecture 14 —

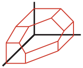
http://www.ee.washington.edu/people/faculty/bilmes/classes/ee563_spring_2018/

Prof. Jeff Bilmes

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

May 14th, 2018





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 is posted on canvas. Due Thursday 5/10, 11:59pm.
- 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 $\to$ Polymatroids
- L10(4/29): Matroids $\to$ 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):
- 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.

Priority Queue

- Use a priority queue Q as a data structure: operations include:
  - Insert an item (v, α) into queue, with $v \in V$ and $\alpha \in \mathbb{R}$.

$$\text{insert}(Q, (v, \alpha)) \tag{14.14}$$

  - Pop the item (v, α) with maximum value α off the queue.

$$(v, \alpha) \leftarrow \text{pop}(Q) \tag{14.15}$$

  - Query the value of the max item in the queue

$$\max(Q) \in \mathbb{R} \tag{14.16}$$

- On next slide, we call a popped item "fresh" if the value (v, α) popped has the correct value $\alpha = f(v|S_i)$. Use extra "bit" to store this info
- If a popped item is fresh, it must be the maximum — this can happen if, at given iteration, v was first popped and neither fresh nor maximum so placed back in the queue, and it then percolates back to the top at which point it is fresh — thereby avoid extra queue check.

Minoux's Accelerated Greedy Algorithm Submodular Max

Algorithm 1: Minoux's Accelerated Greedy Algorithm

1 Set $S_0 \leftarrow \emptyset$; $i \leftarrow 0$; Initialize priority queue Q ;
2 **for** $v \in E$ **do**
3   INSERT$(Q, f(v))$
4 **repeat**
5     $(v, \alpha) \leftarrow$ pop(Q) ;
6   **if** α *not "fresh"* **then**
7   recompute $\alpha \leftarrow f(v|S_i)$
8   **if** *(popped* α *in line 5 was "fresh") OR (*$\alpha \geq$ max(Q)*)* **then**
9   Set $S_{i+1} \leftarrow S_i \cup \{v\}$;
10         $i \leftarrow i + 1$;
11   **else**
12   insert$(Q, (v, \alpha))$
13 **until** $i = |E|$;

(Minimum) Submodular Set Cover

- Given polymatroid f, goal is to find a covering set of minimum cost:

$$S^* \in \underset{S \subseteq V}{\operatorname{argmin}} |S| \text{ such that } f(S) \geq \alpha \tag{14.14}$$

  where α is a "cover" requirement.
- Normally take $\alpha = f(V)$ but defining $f'(A) = \min \{f(A), \alpha\}$ we can take any α. Hence, we have equivalent formulation:

$$S^* \in \underset{S \subseteq V}{\operatorname{argmin}} |S| \text{ such that } f'(S) \geq f'(V) \tag{14.15}$$

- Note that this immediately generalizes standard set cover, in which case $f(A)$ is the cardinality of the union of sets indexed by A.
- Greedy Algorithm: Pick the first chain item S_i chosen by aforementioned greedy algorithm such that $f(S_i) \geq \alpha$ and output that as solution.

(Minimum) Submodular Set Cover: Approximation Analysis

- For integer valued f, this greedy algorithm an $O(\log(\max_{s \in V} f(\{s\})))$ approximation. Let S^* be optimal, and S^{G} be greedy solution, then

$$|S^{\mathsf{G}}| \leq |S^*| H(\max_{s \in V} f(\{s\})) = |S^*| O(\log_e(\max_{s \in V} f(\{s\}))) \tag{14.14}$$

  where H is the harmonic function, i.e., $H(d) = \sum_{i=1}^{d}(1/i)$.
- If f is not integral value, then bounds we get are of the form:

$$|S^{\mathsf{G}}| \leq |S^*| \left(1 + \log_e \frac{f(V)}{f(V) - f(S_{T-1})}\right) \tag{14.15}$$

  wehre S_T is the final greedy solution that occurs at step T.
- Set cover is hard to approximate with a factor better than $(1-\epsilon)\log \alpha$, where α is the desired cover constraint.

Curvature of a Submodular function

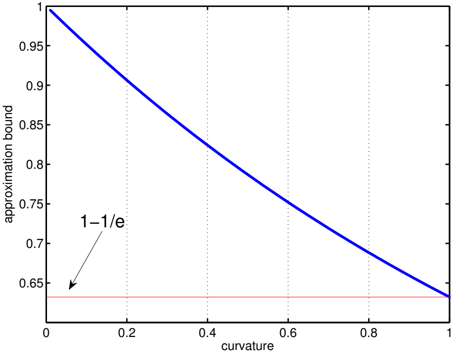
- By submodularity, total curvature can be computed in either form:

$$c \triangleq 1 - \min_{S, j \notin S : f(j|\emptyset) \neq 0} \frac{f(j|S)}{f(j|\emptyset)} = 1 - \min_{j : f(j|\emptyset) \neq 0} \frac{f(j|V \setminus \{j\})}{f(j|\emptyset)} \quad (14.17)$$

- Note: Matroid rank is either modular $c = 0$ or maximally curved $c = 1$ — hence, matroid rank can have only the extreme points of curvature, namely 0 or 1.
- Polymatroid functions are, in this sense, more nuanced, in that they allow non-extreme curvature, with $c \in [0, 1]$.
- It will be remembered the notion of "partial dependence" within polymatroid functions.

Curvature and approximation

- Curvature limitation can help the greedy algorithm in terms of approximation bounds.
- Conforti & Cornuéjols showed that greedy gives a $1/(1+c)$ approximation to $\max\{f(S) : S \in \mathcal{I}\}$ when f has total curvature c.
- Hence, greedy subject to matroid constraint is a $\max(1/(1+c), 1/2)$ approximation algorithm, and if $c < 1$ then it is better than 1/2 (e.g., with $c = 1/4$ then we have a 0.8 algorithm).
- For k-uniform matroid (i.e., k-cardinality constraints), then approximation factor becomes $\frac{1}{c}(1 - e^{-c})$



Generalizations

- Consider a k-uniform matroid $\mathcal{M} = (V, \mathcal{I})$ where $\mathcal{I} = \{S \subseteq V : |S| \leq k\}$, and consider problem $\max\{f(A) : A \in \mathcal{I}\}$

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- Combinations of the above (e.g., knapsack & multiple matroid constraints).

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- For one matroid, we have a 1/2 approximation.
- Very easy algorithm, Minoux trick still possible, while addresses multiple matroid constraints — but the bound is not that good when there are many matroids.

Matroid Intersection and Bipartite Matching

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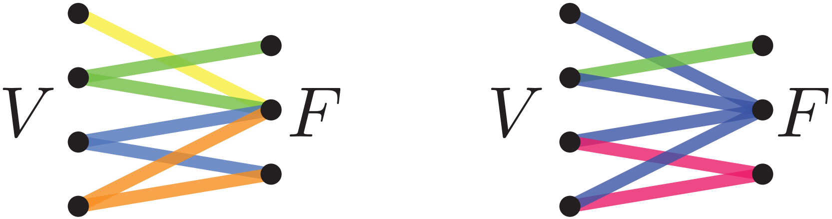

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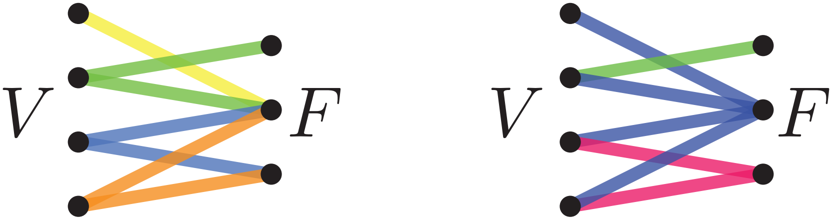

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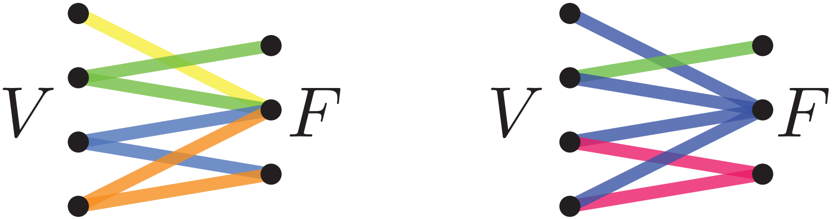

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- In bipartite graph case, therefore, can be solved in polynomial time.

Matroid Intersection and Network Communication

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- We may wish to find the maximum size edge-induced subgraph that is still forest in both graphs (i.e., adding any edges will create a circuit in either M_1, M_2, or both).
- This is again a matroid intersection problem.

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- From G with n nodes, create G' with $n+1$ nodes by duplicating (w.l.o.g.) a particular node $v_1 \in V(G)$ to v_1^+, v_1^-, and have all outgoing edges from v_1 come instead from v_1^- and all edges incoming to v_1 go instead to v_1^+.

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- Let M_1 be the cycle matroid on G'.
- Let M_2 be the partition matroid having as independent sets those that have no more than one edge leaving any node — i.e., $I \in \mathcal{I}(M_2)$ if $|I \cap \delta^-(v)| \leq 1$ for all $v \in V(G')$.

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- Definition: a Hamiltonian cycle is a cycle that passes through each node exactly once.
- Given directed graph G, goal is to find such a Hamiltonian cycle.
- From G with n nodes, create G' with $n+1$ nodes by duplicating (w.l.o.g.) a particular node $v_1 \in V(G)$ to v_1^+, v_1^-, and have all outgoing edges from v_1 come instead from v_1^- and all edges incoming to v_1 go instead to v_1^+.
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- Then a Hamiltonian cycle exists iff there is an n-element intersection of M_1, M_2, and M_3.

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- Since TSP is NP-complete, we obviously can't solve matroid intersections of 3 more matroids, unless P=NP.
- But bipartite graph example gives us hope for 2 matroids, as in that case we can easily solve $\max |X|$ s.t. $x \in \mathcal{I}_1 \cap \mathcal{I}_2$.

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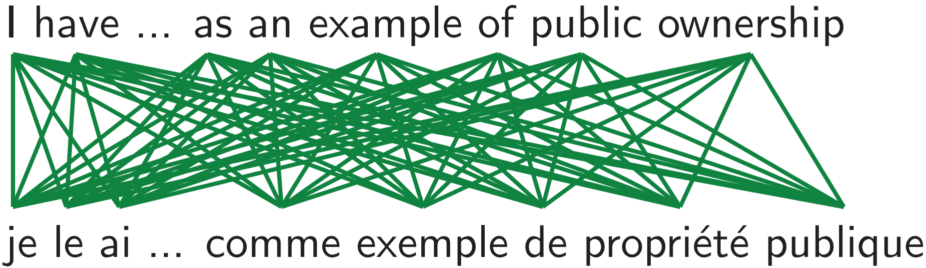
- Consider bipartite graph $G = (E, F, V)$ where E and F are the left/right set of nodes, respectively, and V is the set of edges.
- E corresponds to, say, an English language sentence and F corresponds to a French language sentence — goal is to form a matching (an alignment) between the two.

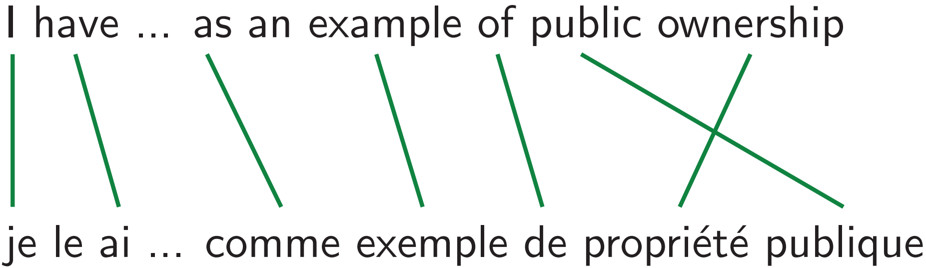
Greedy over > 1 matroids: Multiple Language Alignment

- Consider English string and French string, set up as a bipartite graph.



Greedy over > 1 matroids: Multiple Language Alignment

- One possible alignment, a matching, with score as sum of edge weights.



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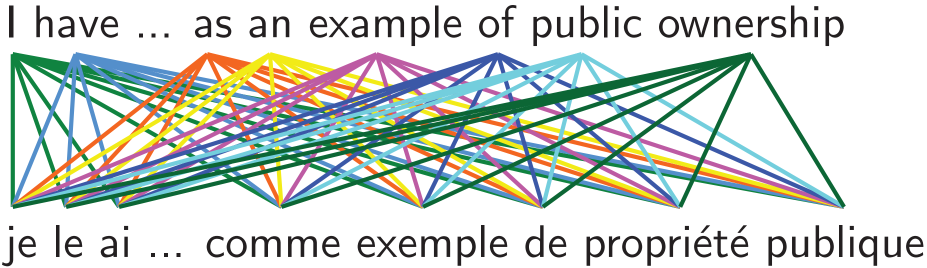

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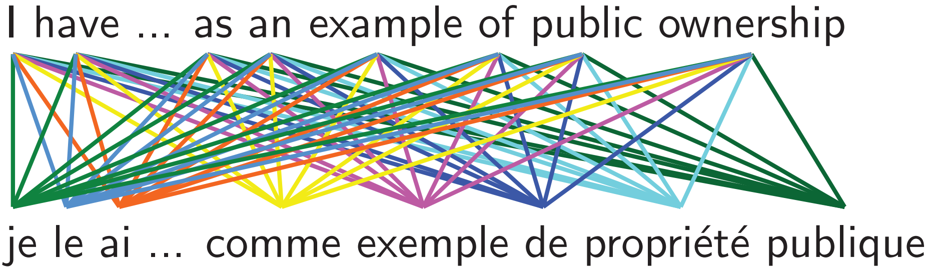

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- Generalizing further, each block of edges in each partition matroid can have its own "fertility" limit:
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- Maximizing submodular function subject to multiple matroid constraints addresses this problem.

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- We can solve this via submodular maximization subject to multiple matroid independence constraints as we next describe ...

Submodular Welfare: Submodular Max over matroid partition

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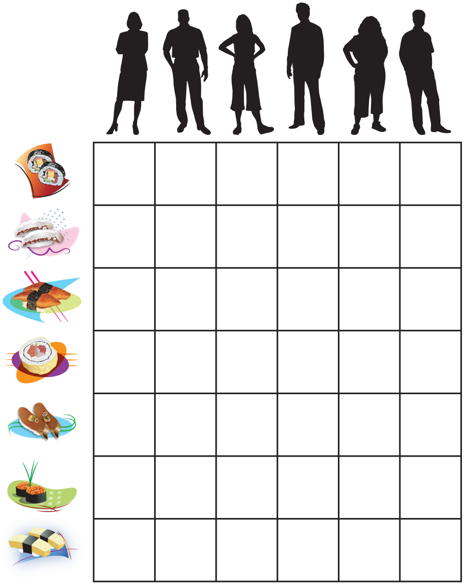

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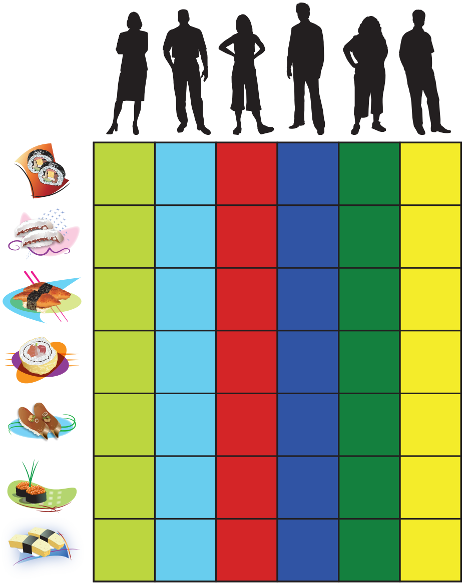

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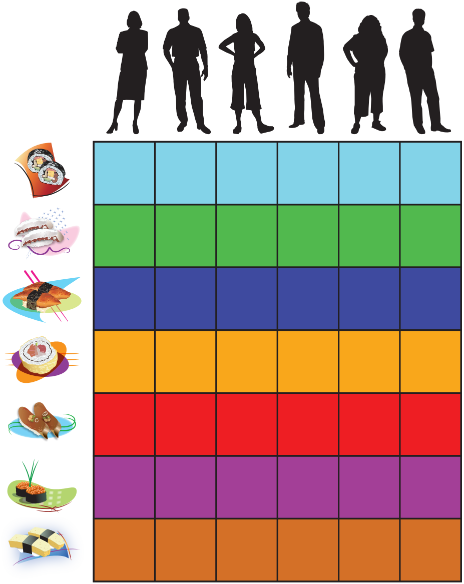

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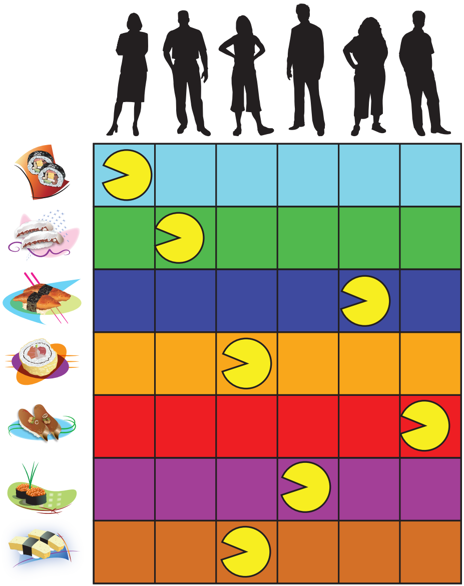

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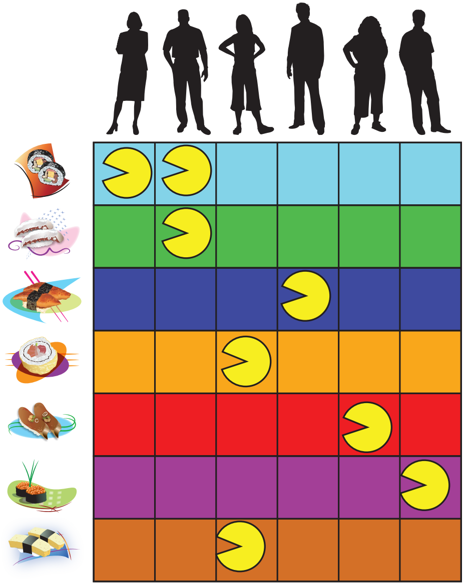

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- Important: A knapsack constraint yields an independence system (down closed) but it is not a matroid!
- $c(e)$ may be seen as the cost of item e and if $c(e) = 1$ for all e, then we recover the cardinality constraint we saw earlier.

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- Greedy can be seen as choosing the best gain: Starting with $S_0 = \emptyset$, we repeat the following greedy step

$$S_{i+1} = S_i \cup \left\{ \operatorname*{argmax}_{v \in V \setminus S_i} \Big(f(S_i \cup \{v\}) - f(S_i) \Big) \right\} \tag{14.5}$$

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- Core idea in knapsack case: Greedy can be extended to choose next whatever looks cost-normalized best, i.e., Starting some initial set S_0, we repeat the following cost-normalized greedy step

$$S_{i+1} = S_i \cup \left\{ \operatorname*{argmax}_{v \in V \setminus S_i} \frac{f(S_i \cup \{v\}) - f(S_i)}{c(v)} \right\} \tag{14.6}$$

  which we repeat until $c(S_{i+1}) > b$ and then take S_i as the solution.

A Knapsack Constraint

- There are a number of ways of getting approximation bounds using this strategy.
- If we run the normalized greedy procedure starting with $S_0 = \emptyset$, and compare the solution found with the max of the singletons $\max_{v \in V} f(\{v\})$, choosing the max, then we get a $(1 - e^{-1/2}) \approx 0.39$ approximation, in $O(n^2)$ time (Minoux trick also possible for further speed)
- Partial enumeration: On the other hand, we can get a $(1 - e^{-1}) \approx 0.63$ approximation in $O(n^5)$ time if we run the above procedure starting from all sets of cardinality three (so restart for all S_0 such that $|S_0| = 3$), and compare that with the best singleton and pairwise solution.
- Extending something similar to this to d simultaneous knapsack constraints is possible as well.

Local Search Algorithms

From J. Vondrak

- Local search involves switching up to t elements, as long as it provides a (non-trivial) improvement; can iterate in several phases. Some examples follow:
- 1/3 approximation to unconstrained non-monotone maximization [Feige, Mirrokni, Vondrak, 2007]
- $1/(k + 2 + \frac{1}{k} + \delta_t)$ approximation for non-monotone maximization subject to k matroids [Lee, Mirrokni, Nagarajan, Sviridenko, 2009]
- $1/(k + \delta_t)$ approximation for monotone submodular maximization subject to $k \geq 2$ matroids [Lee, Sviridenko, Vondrak, 2010].

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- Thus, any approximation algorithm must be for unipolar submodular functions. E.g., non-negative but otherwise arbitrary submodular functions.
- We may get a $(\frac{1}{3} - \frac{\epsilon}{n})$ approximation for maximizing non-monotone non-negative submodular functions, with most $O(\frac{1}{\epsilon} n^3 \log n)$ function calls using approximate local maxima.

Submodularity and local optima

- Given any submodular function f, a set $S \subseteq V$ is a local maximum of f if $f(S - v) \leq f(S)$ for all $v \in S$ and $f(S + v) \leq f(S)$ for all $v \in V \setminus S$ (i.e., local in a Hamming ball of radius 1).

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- This is the approach that yields the $(\frac{1}{3} - \frac{\epsilon}{n})$ approximation algorithm.

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Algorithm 5: Randomized Linear-time non-monotone submodular max

Set $L \leftarrow \emptyset$; $U \leftarrow V$ /* Lower L, upper U. Invariant: $L \subseteq U$ */ ;
Order elements of $V = (v_1, v_2, \ldots, v_n)$ arbitrarily ;
for $i \leftarrow 0 \ldots |V|$ **do**
  $a \leftarrow [f(v_i|L)]_+$; $b \leftarrow [-f(U|U \setminus \{v_i\})]_+$;
  if $a = b = 0$ **then** $p \leftarrow 1/2$;
  ;
  else $p \leftarrow a/(a+b)$;
  ;
  if *Flip of coin with* $\Pr($*heads*$) = p$ *draws heads* **then**
    $L \leftarrow L \cup \{v_i\}$;
  Otherwise /* if the coin drew tails, an event with prob. $1 - p$ */
    $U \leftarrow U \setminus \{v\}$
return L *(which is the same as* U *at this point)*

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- It may be possible to choose the random order smartly to get better results in practice.

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- Often the computational costs of the algorithms are prohibitive (e.g., exponential in k) with large constants, so these algorithms might not scale.
- On the other hand, these algorithms offer deep and interesting intuition into submodular functions, beyond what we have covered here.

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- We can recover $1 - 1/e$ approximation using the continuous greedy algorithm on the multilinear extension and then using pipage rounding to re-integerize the solution (see J. Vondrak's publications).
- More general constraints are possible too, as we see on the next table (for references, see Jan Vondrak's publications http://theory.stanford.edu/~jvondrak/).

Submodular Max Summary - From J. Vondrak

Monotone Maximization

Constraint	Approximation	Hardness	Technique
$\lvert S\rvert \leq k$	$1-1/e$	$1-1/e$	greedy
matroid	$1-1/e$	$1-1/e$	multilinear ext.
$O(1)$ knapsacks	$1-1/e$	$1-1/e$	multilinear ext.
k matroids	$k+\epsilon$	$k/\log k$	local search
k matroids and $O(1)$ knapsacks	$O(k)$	$k/\log k$	multilinear ext.

Nonmonotone Maximization

Constraint	Approximation	Hardness	Technique
Unconstrained	$1/2$	$1/2$	combinatorial
matroid	$1/e$	0.48	multilinear ext.
$O(1)$ knapsacks	$1/e$	0.49	multilinear ext.
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Continuous Extensions of Discrete Set Functions

- Any function $f : 2^V \rightarrow \mathbb{R}$ (equivalently $f : \{0,1\}^V \rightarrow \mathbb{R}$) can be extended to a continuous function in the sense $\tilde{f} : [0,1]^V \rightarrow \mathbb{R}$.

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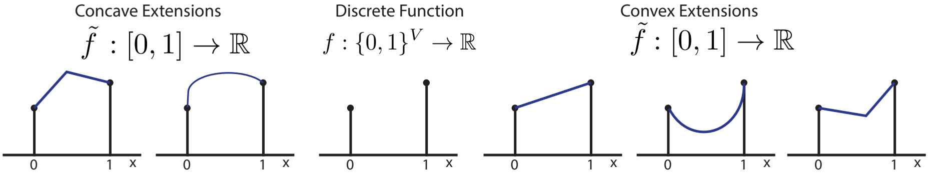

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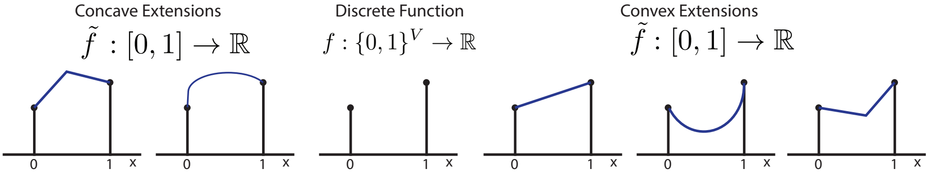

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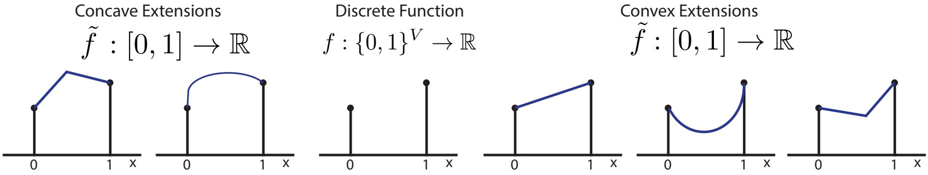

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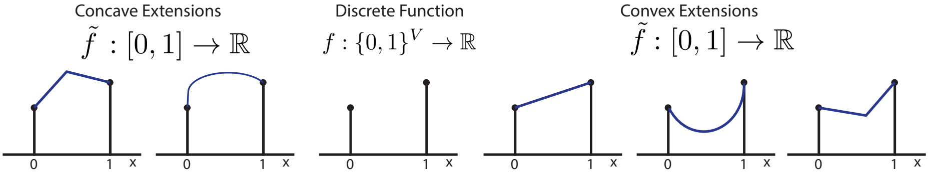

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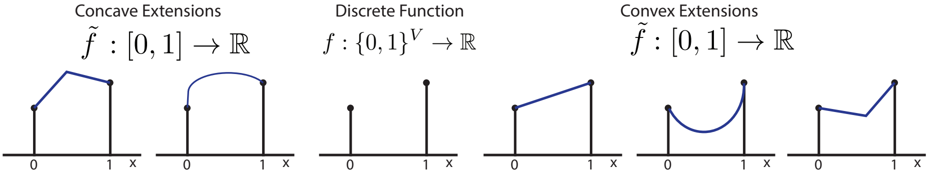

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Def: Convex Envelope of a function

- 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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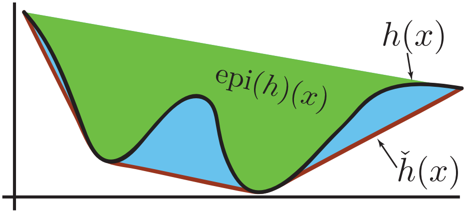
- Alternatively,

$$\check{h}(x) = \inf \{t : (x,t) \in \text{convexhull}(\text{epigraph}(h))\} \quad (14.8)$$



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where $\triangle^n(x) =$
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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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  2. That $\breve{f}$ is convex (and consequently, that any arbitrary set function has a tight convex extension).
  3. That the convex closure $\breve{f}$ is the convex envelope of the function defined only on the hypercube vertices, and that takes value $f(S)$ at $\mathbf{1}_S$.

Convex Closure of Discrete Set Functions

- Given, $\check{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$, there are several things we'd like to 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.

Tightness of Convex Closure

Lemma 14.4.1

$\forall A \subseteq V$, *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 $p_{S'}^{\mathbf{1}_A} > 0$.

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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

$$\underbrace{p_{S'} \mathbf{1}_{S'}}_{>0} + \underbrace{\sum_{\substack{S \subseteq A \\ S \neq S'}} p_S \mathbf{1}_S}_{\text{can't sum to 1}} \Rightarrow \Bigg(\sum_{\substack{S \subseteq A \\ S \neq S'}} p_s \mathbf{1}_S \Bigg)(v) < 1 \tag{14.10}$$

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 14.4.2

$\breve{f}(x) = \min_{p \in \triangle^n(x)} E_{S \sim p}[f(S)]$ *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

$$\lambda \breve{f}(x) + (1-\lambda)\breve{f}(y) = \lambda \sum_S p^x_S f(S) + (1-\lambda) \sum_S p^y_S f(S) \tag{14.11}$$

$$= \sum_S (\lambda p^x_S + (1-\lambda) p^y_S) f(S) \tag{14.12}$$

$$= \sum_S p^{z'}_S f(S) \geq \min_{p \in \triangle^n(z)} E_{S \sim p}[f(S)] \tag{14.13}$$

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

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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:

$$\check{h}(x) = \sup \{g(x) : g \text{ is convex } \& \; g(y) \leq h(y), \forall y \in \mathbb{R}^n\} \tag{14.7}$$

Convex Closure is the Convex Envelope

Lemma 14.4.3

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

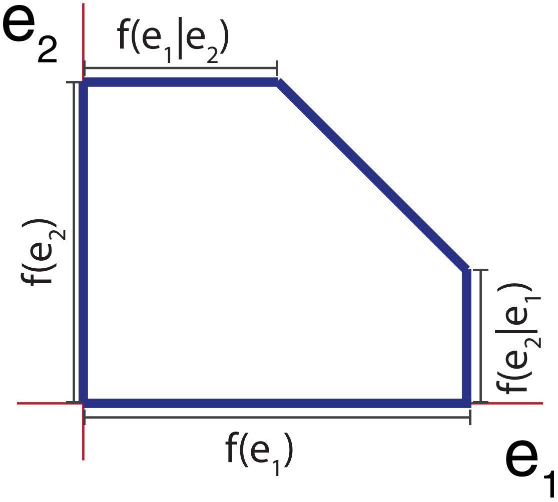
$$\check{f}(x) = \sum_S p^x_S f(S) = \sum_S p^x_S \bar{f}(\mathbf{1}_S) \tag{14.15}$$

$$< \bar{f}(x) = \bar{f}\Big(\sum_S p^x_S \mathbf{1}_S\Big) \tag{14.16}$$

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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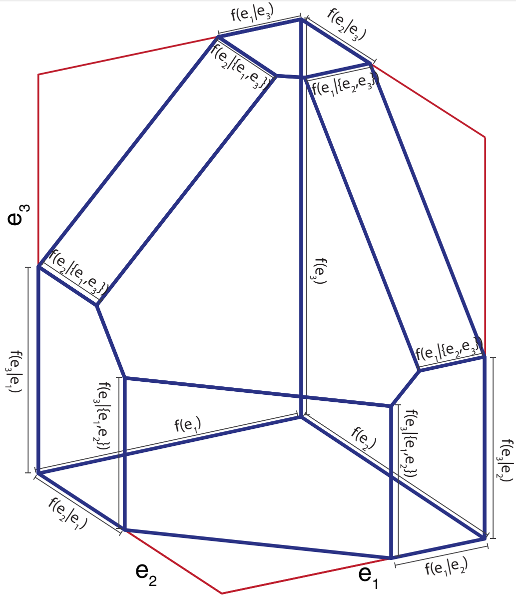

Optimization over P_f

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

$$\begin{aligned} &\text{maximize} && w^\intercal x && (14.17a) \\ &\text{subject to} && x \in P_f && (14.17b) \end{aligned}$$

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- 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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- Hence, the problem is equivalent to: given $w \in \mathbb{R}_+^E$,

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

A continuous extension of f

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

$$\breve{f}(w) = \max(wx : x \in B_f) \quad (14.20)$$

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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 14.5.1 (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).

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- 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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- 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

$$\begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \underbrace{(w_1 - w_2)}_{\lambda_1} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \underbrace{(w_2 - w_3)}_{\lambda_2} \begin{pmatrix} 1 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \cdots + \underbrace{(w_{n-1} - w_n)}_{\lambda_{m-1}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \end{pmatrix} + \underbrace{(w_m)}_{\lambda_m} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix} \tag{14.28}$$

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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 $\lambda_m \geq 0$.

An extension of f

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

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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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- 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

$$\breve{f}(w) = \max \{ w^\intercal x : x \in P_f \} \tag{14.36}$$

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:

$$\breve{f}(w) = \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1}) \tag{14.39}$$

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- So $\breve{f}(w)$ seen either as sum of weighted gain evaluations (Eqn. (14.39)), or as sum of weighted function evaluations (Eqn. (14.42)).

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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- 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. (14.37) 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 14.5.2

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.(14.37) 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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- 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. 14.5.2 cont.

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

. . .

Lovász Extension, Submodularity and Convexity

. . . proof of Thm. 14.5.2 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

$$\breve{f}(\mathbf{1}_A + \mathbf{1}_B) = \breve{f}(\mathbf{1}_{A \cup B} + \mathbf{1}_{A \cap B}) \tag{14.45}$$

$$= f(A \cup B) + f(A \cap B). \tag{14.46}$$

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Lovász Extension, Submodularity and Convexity

. . . proof of Thm. 14.5.2 cont.

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$$= f(A \cup B) + f(A \cap B). \quad (14.46)$$

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

$$w = (w(e_1), w(e_2), \dots, w(e_m)) \quad (14.47)$$

$$= (\underbrace{2, 2, \dots, 2}_{i\in C}, \underbrace{1, 1, \dots, 1}_{i\in A\triangle B}, \underbrace{0, 0, \dots, 0}_{i\in E\setminus(A\cup B)}) \quad (14.48)$$

. . .

Lovász Extension, Submodularity and Convexity

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- Then, considering $\breve{f}(w) = \sum_i \lambda_i f(E_i)$, we have $\lambda_{|C|} = 1$, $\lambda_{|A\cup B|} = 1$, and $\lambda_i = 0$ for $i \notin \{|C|, |A \cup B|\}$.

. . .

Lovász Extension, Submodularity and Convexity

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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

. . . proof of Thm. 14.5.2 cont.

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

$$0.5[f(A \cap B) + f(A \cup B)] \tag{14.52}$$

□

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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(14.52)

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Lovász Extension, Submodularity and Convexity

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$$= \breve{f}(0.5\mathbf{1}_A + 0.5\mathbf{1}_B) \tag{14.50}$$

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Lovász Extension, Submodularity and Convexity

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$$\leq 0.5\breve{f}(\mathbf{1}_A) + 0.5\breve{f}(\mathbf{1}_B) \quad (14.51)$$

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Lovász Extension, Submodularity and Convexity

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Lovász Extension, Submodularity and Convexity

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

$$f(A \cup B) + f(A \cap B) \leq f(A) + f(B) \tag{14.53}$$

so f must be submodular.

□

Lovász ext. vs. <u>the</u> concave closure of submodular function

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Lovász ext. vs. the concave closure of submodular function

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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.

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- The above theorem showed that the Lovász extension is convex iff f is submodular.
- Our next theorem shows that the Lovász extension coincides precisely with the convex closure iff f is submodular.
- 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.

Lovász ext. vs. the concave closure of submodular function

Theorem 14.5.3

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

Proof.

- Assume f is submodular.

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Lovász ext. vs. the concave closure of submodular function

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Proof.

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

...

Lovász ext. vs. the concave closure of submodular function

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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., $p_A^x \geq p_B^x > 0$.

. . .

Lovász ext. vs. the concave closure of submodular function

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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.

Proof.

- Assume f is submodular.
- Given x, let p^x be an achieving argmin in $\breve{f}(x)$ that also maximizes $\sum_S p^x_S |S|^2$.
- 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., $p^x_A \geq p^x_B > 0$.
- Then we may update p^x as follows:

$$\bar{p}^x_A \leftarrow p^x_A - p^x_B \qquad \bar{p}^x_B \leftarrow p^x_B - p^x_B \tag{14.54}$$

$$\bar{p}^x_{A \cup B} \leftarrow p^x_{A \cup B} + p^x_B \qquad \bar{p}^x_{A \cap B} \leftarrow p^x_{A \cap B} + p^x_B \tag{14.55}$$

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

$$|A \cup B|^2 + |A \cap B|^2 = (|A| + |B \setminus A|)^2 + (|B| - |B \setminus A|)^2 \quad (14.56)$$

$$= |A|^2 + |B|^2 + 2|B \setminus A|(|A| - |B| + |B \setminus A|) \quad (14.57)$$

$$\geq |A|^2 + |B|^2 \quad (14.58)$$

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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 $B \subset A$.

Lovász ext. vs. the concave closure of submodular function

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- Hence, the sets $\{A \subseteq V : p^x_A > 0\}$ form a chain and can be as large only as size $n = |V|$.

Lovász ext. vs. the concave closure of submodular function

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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 $n = |V|$.
- 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

. . . proof cont.

- Next, assume f is not submodular. We must show that the Lovász extension $\breve{f}(x)$ and the concave closure $\breve{f}(x)$ need not coincide.

Lovász ext. vs. the concave closure of submodular function

. . . proof cont.

- Next, assume f is not submodular. We must show that the Lovász extension $\breve{f}(x)$ and the concave closure $\check{f}(x)$ need not coincide.
- Since f is not submodular, $\exists S$ and $i, j \notin S$ such that $f(S) + f(S + i + j) > f(S + i) + f(S + j)$, a strict violation of submodularity.

Lovász ext. vs. the concave closure of submodular function

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- Next, assume f is not submodular. We must show that the Lovász extension $\breve{f}(x)$ and the concave closure $\check{f}(x)$ need not coincide.
- Since f is not submodular, $\exists S$ and $i, j \notin S$ such that $f(S) + f(S+i+j) > f(S+i) + f(S+j)$, a strict violation of submodularity.
- Consider $x = \mathbf{1}_S + \frac{1}{2}\mathbf{1}_{\{i,j\}}$.

Lovász ext. vs. the concave closure of submodular function

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

Lovász ext. vs. the concave closure of submodular function

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

Lovász ext. vs. the concave closure of submodular function

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- Since f is not submodular, $\exists S$ and $i, j \notin S$ such that $f(S) + f(S+i+j) > f(S+i) + f(S+j)$, a strict violation of submodularity.
- 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 $\breve{f}$ with $p^x_S = 1/2$ and $p^x_{S+i+j} = 1/2$.
- An alternate feasible distribution for x in the convex closure is $\bar{p}^x_{S+i} = \bar{p}^x_{S+j} = 1/2$.
- This gives

$$\breve{f}(x) \leq \frac{1}{2}[f(S+i) + f(S+j)] < \breve{f}(x) \tag{14.59}$$

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