Introduction to Submodular Functions

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Teaching plan

- First hour: Tom McCormick on submodular functions

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- Next half hour: Satoru Iwata on Lovàsz extension

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- Next half hour: Satoru Iwata on Lovàsz extension
- Later: Tom, Satoru, Francis, Seffi on more advanced topics

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- Motivating example
- What is a submodular function?
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  - For example, if you are already producing iPhones, then the setup cost for also producing iPads is small, but if you are not producing iPhones, the setup cost for producing iPads is large.
- Suppose that we choose to produce the subset of products $S \subseteq E$. Then we write the setup cost of subset S as $c(S)$.

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  - We typically think that $\mathrm{EO} = \Omega(n)$, i.e., that it takes at least linear time to evaluate f on S.

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- Suppose that $S \subset T$ and that $e \notin T$. Since T includes everything in S and more, it is reasonable to guess that the marginal setup cost of adding e to T is not larger than the marginal setup cost of adding e to S. That is,

$$\forall S \subset T \subset T + e,\ c(T + e) - c(T) \leq c(S + e) - c(S). \quad (1)$$

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- When a set function satisfies (1) we say that it is submodular.

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Submodularity definitions

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Homework. □

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  - Many set functions arising in applications are monotone, but not all of them.
- A set function that is both submodular and monotone is called a polymatroid.
  - Polymatroids generalize matroids, and are a special case of the submodular polyhedra we'll see later.

Even more definitions

- We say that set function f is supermodular if it satisfies these definitions with the inequalities reversed, i.e., if

$$\forall S \subset T \subset T + e, \; f(T + e) - f(T) \geq f(S + e) - f(S). \quad (4)$$

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- The lemma suggest a natural way to extend a vector $a \in \mathbb{R}^E$ to a modular set function: Define $a(S) = \sum_{e \in S} a_e$. Note that $a(\emptyset) = 0$. (Queyranne: "$a \cdot S$" is better notation?)

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- In this example we naturally want to find a subset to produce that maximizes our net revenue, i.e, to solve $\max_{S \subseteq E}(p(S) - c(S))$, or equivalently

$$\min_{S \subseteq E}(c(S) - p(S)).$$

More examples of submodularity

- Let $G = (N, A)$ be a directed graph. For $S \subseteq N$ define $\delta^+(S) = \{i \to j \in A \mid i \in S,\ j \notin S\}$, $\delta^-(S) = \{i \to j \in A \mid i \notin S,\ j \in S\}$. Then $|\delta^+(S)|$ and $|\delta^-(S)|$ are submodular.

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- More generally, suppose that $w \in \mathbb{R}^A$ are weights on the arcs. If $w \geq 0$, then $w(\delta^+(S))$ and $w(\delta^-(S))$ are submodular, and if $w \ngeq 0$ then they are not necessarily submodular (homework).

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- Now specialize the previous example slightly to Max Flow / Min Cut: Let $N = \{s\} \cup \{t\} \cup E$ be the node set with source s and sink t. We have arc capacities $u \in \mathbb{R}^A_+$, i.e., arc $i \to j$ has capacity $u_{ij} \geq 0$. An s–t cut is some $S \subseteq E$, and the capacity of cut S is $\mathrm{cap}(S) = u(\delta^+(S + s))$, which is submodular.

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  - Here $\mathrm{cap}(\emptyset) = \sum_{e \in E} u_{se}$ is usually positive.

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Theorem (Ford & Fulkerson)

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- Now we want to sketch part of the proof of this, since some later proofs will use the same technique.

Algorithmic proof of Max Flow / Min Cut

- First, weak duality. For any feasible flow x and cut S:

$$\begin{aligned}
\mathrm{val}(x) &= x(\delta^+(\{s\})) - x(\delta^-(\{s\})) \\
&\quad + \textstyle\sum_{i \in S} [x(\delta^+(\{i\})) - x(\delta^-(\{i\}))] \\
&= x(\delta^+(S+s)) - x(\delta^-(S+s)) \\
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- An augmenting path w.r.t. feasible flow x is a directed path P such that $i \to j \in P$ implies either (i) $i \to j \in A$ and $x_{ij} < u_{ij}$, or (ii) $j \to i \in A$ and $x_{ji} > 0$.

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  - Many SFMin algorithms are based on Push-Relabel.
- Min Cut is a canonical example of minimizing a submodular function, and many of the algorithms are based on analogies with Max Flow / Min Cut.

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- Entropy: The *Shannon entropy* of a random vector.
- Sensor location: If we have a joint probability distribution over two random vectors $P(X, Y)$ indexed by E and the X variables are *conditionally independent* given Y, then the expected reduction in the uncertainty of about Y given the values of X on subset S is submodular. Think of placing sensors at a subset S of locations in the ground set E in order to measure Y; a sort of stochastic coverage.

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  - Thus for the SFMax problems, we will be interested in approximation algorithms.
  - An algorithm for an maximization problem is a α-approximation if it always produces a feasible solution with objective value at least $\alpha \cdot \text{OPT}$.

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  - Unfortunately, exactly computing M is NP Hard (SFMax), but we can compute a good enough bound on M in $O(n\mathrm{EO})$ time.

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  - There is no apparent reason why an SFMin/Max algorithm needs multiplication or division, so we call an algorithm fully combinatorial if it is strongly polynomial, and uses only addition/subtraction and comparisons.

Is submodularity concavity or convexity?

- Submodular functions are sort of *concave*: Suppose that set function f has $f(S) = g(|S|)$ for some $g : \mathbb{R} \to \mathbb{R}$. Then f is submodular iff g is concave (homework). This is the "decreasing returns to scale" point of view.

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- Continuous convex functions are easy to minimize, hard to maximize; SFMin looks easy, SFMax is hard. Thus the convex view looks better.
- There is a whole theory of discrete convexity starting from the Lovász extension that parallels continuous convex analysis, see Murota's book.

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  - It further implies that the optimal value for SFMin is non-positive, and the optimal value for SFMax is non-negative, since we can always get 0 by choosing $S = \emptyset$.

Submodular polyhedra

- Let's associate submodular functions with polyhedra.
- It turns out that the right thing to do is to think about vectors $x \in \mathbb{R}^E$, and so polyhedra in $\mathbb{R}^E$.
- The key constraint for us is for some subset $S \subseteq E$

$$x(S) \leq f(S).$$

- We can think of this as a sort of generalized upper bound on sums over subsets of components of x.
- What about when $S = \emptyset$? We get $x(\emptyset) \equiv 0 \leq f(\emptyset)$???
  - To get this to make sense we will *normalize* all our submodular functions via $f(S) \leftarrow f(S) - f(\emptyset)$ in order to be able to assume that $f(\emptyset) = 0$.
  - Notice that this normalization does not change the optimal subset for SFMin and SFMax.
  - It further implies that the optimal value for SFMin is non-positive, and the optimal value for SFMax is non-negative, since we can always get 0 by choosing $S = \emptyset$.
  - This normalization is non-trivial for Min Cut.

The submodular polyhedron

- Now that we've normalized s.t. $f(\emptyset) = 0$, define the submodular polyhedron associated with set function f by

$$P(f) \equiv \{x \in \mathbb{R}^E \mid x(S) \leq f(S) \ \forall S \subseteq E\}.$$

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- It turns out to be convenient to also consider the face of $P(f)$ induced by the constraint $x(E) \leq f(E)$, called the base polyhedron of f:

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- We will soon show that $B(f)$ is always non-empty when f is submodular.

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- Intuitively, with $w \geq 0$ a maximum solution will be forced up against the $x(E) \leq f(E)$ constraint, and so it will become tight, and so an optimal solution will be in $B(f)$. So we consider $\max_{x \in \mathbb{R}^E} w^T x$ s.t. $x \in B(f)$.

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- The naive thing to do is to try to solve this *greedily*: Order the elements such that $w_1 \geq w_2 \geq \cdots \geq w_n$.

Outline

Introduction
- Motivating example
- What is a submodular function?
- Review of Max Flow / Min Cut

Optimizing submodular functions
- SFMin versus SFMax
- Tools for submodular optimization
- The Greedy Algorithm

The Greedy Algorithm (Edmonds)

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    and $2^{\prec_1} = \{1, 3, 4, 5\}$, $2^{\prec_2} = \{1\}$.
- In this notation we can re-express the main step of Greedy on the ith element in $\prec$ as
  "Make $x_{e_i} \leftarrow f(e_i^{\prec} + e_i) - f(e_i^{\prec})$."

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  - Thus $x(S) \leq f(S - e_k) + (f(e_k^{\prec} + e_k) - f(e_k^{\prec})) = f(e_{k+1}^{\prec}) + f(S - e_k) - f(e_k^{\prec}) \leq f(S)$.

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- In order to show optimality of the x coming from Greedy, we construct a dual optimal solution.

Dual feasibility

- Here are the dual LPs:

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  - We chose $\prec$ s.t. $w_{e_{i-1}} - w_{e_i} \geq 0$, and so $\pi_S \geq 0$.
  - Now $\sum_{S \ni e_k} \pi_S = \sum_{i=k+1}^{n+1} (w_{e_{i-1}} - w_{e_i})$ $= w_{e_k} - w_{e_{n+1}} = w_{e_k}$, as desired.

Optimality from duality

- For any $x \in B(f)$ and π feasible for the dual, note that

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  - Thus we get equality, and so x is (primal) optimal (and π is dual optimal).

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  - Although $B(f)$ has 2^n constraints, the linear order $\prec$ is a succinct certificate that $v^{\prec} \in B(f)$.
  - This proves that $B(f) \neq \emptyset$.
  - Greedy works on $B(f)$ for *any* w; it works on $P(f)$ if $w \geq 0$.

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  - As we saw in the proof, the constraint for $S = e_k^{\prec}$ is tight for each $e_k \in E$.
- Therefore M is the lower triangular matrix:

$$M = \begin{array}{c} \\ e_2^{\prec} \\ e_3^{\prec} \\ \vdots \\ e_{n+1}^{\prec} \end{array} \begin{array}{c} \begin{array}{cccc} e_1 & e_2 & \dots & e_n \end{array} \\ \begin{pmatrix} 1 & 0 & \dots & 0 \\ 1 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \dots & 1 \end{pmatrix} \end{array}$$

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- Again this triangular system easily solves to $\pi_{e_i^\prec} = w_{i-1} - w_i$.
- This also shows that $v^\prec$ is a vertex, as it follows from M being nonsingular.