Submodular Functions, Optimization, and Applications to Machine Learning

— Fall Quarter, Lecture 20 —

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

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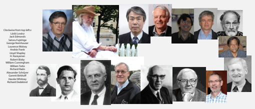
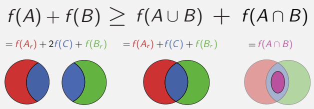
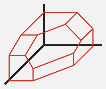
Dec 9th, 2020





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

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



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 → Polymatroids
- L11(11/4): Matroids → 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): Multilinear Extension, Submodular Max/polyhedral, Most Violated Ineq., Matroids Closure/Sat
- L19(12/7): Fund. Circuit/Dep, SFM, L.E. primal, Start SFM via Min-Norm Point
- L20(12/9): support for min-norm, proof that min-norm gives optimal, computing min-norm vector in B_f, SFM
- 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 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%).

Summary List of Concepts

- Most violated inequality $\max\{x(A) - f(A) : A \subseteq E\}$
- Matroid by circuits, and the fundamental circuit $C(I, e) \subseteq I + e$.
- Minimizers of submodular functions form a lattice.
- Minimal and maximal element of a lattice.
- x-tight sets, maximal and minimal tight set.
- sat function & Closure
- Saturation Capacity
- e-containing tight sets
- dep function & fundamental circuit of a matroid

Summary important definitions so far: tight, dep, & sat

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

$$\text{dep}(x, e) = \begin{cases} \bigcap\{A : e \in A \subseteq E, x(A) = f(A)\} & \text{if } e \in \text{sat}(x) \\ \emptyset & \text{else} \end{cases}$$

$$= \{e' : \exists \alpha > 0, \text{ s.t. } x + \alpha(\mathbf{1}_e - \mathbf{1}_{e'}) \in P_f\}$$

dep and sat in a lattice

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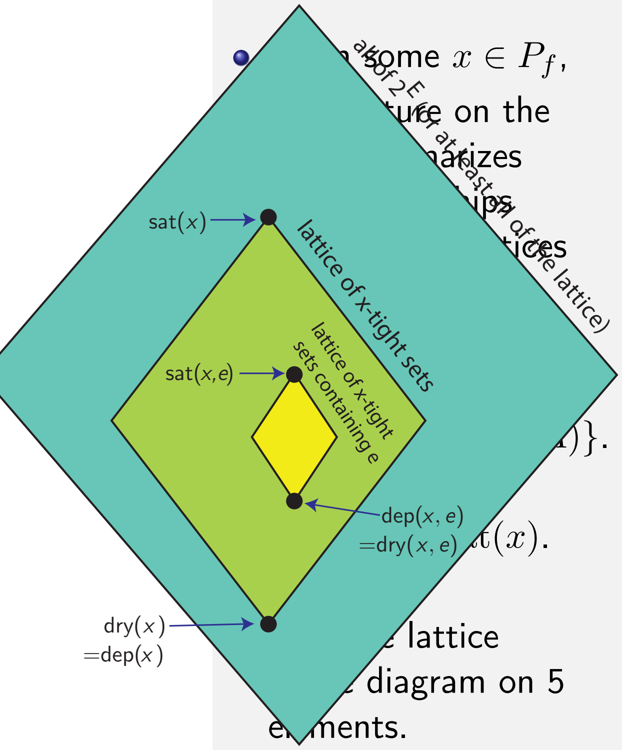
all of 2^E (or at least all of the lattice)
lattice of x-tight sets
lattice of x-tight sets containing e
sat(x)
sat(x,e)
dep(x, e)
=dry(x, e)
dry(x)
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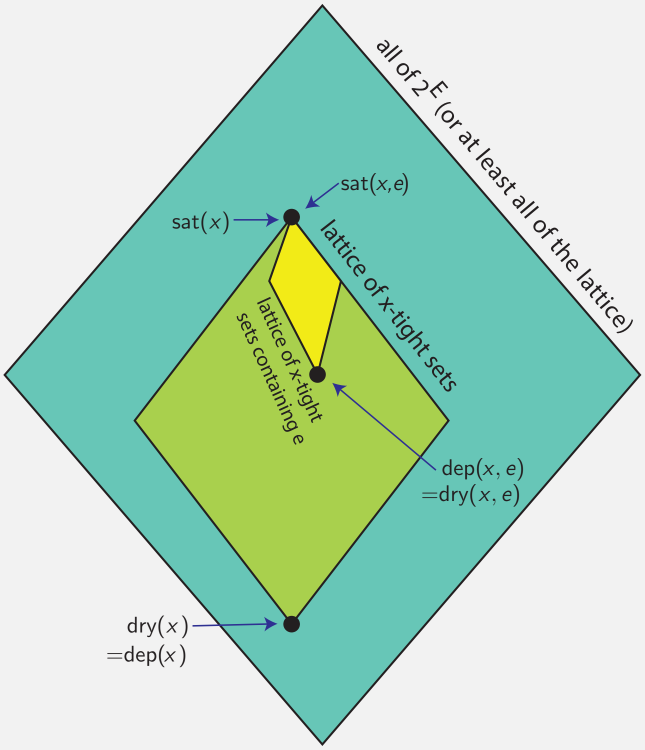
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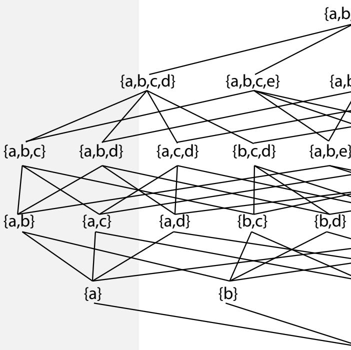

dep and sat in a lattice

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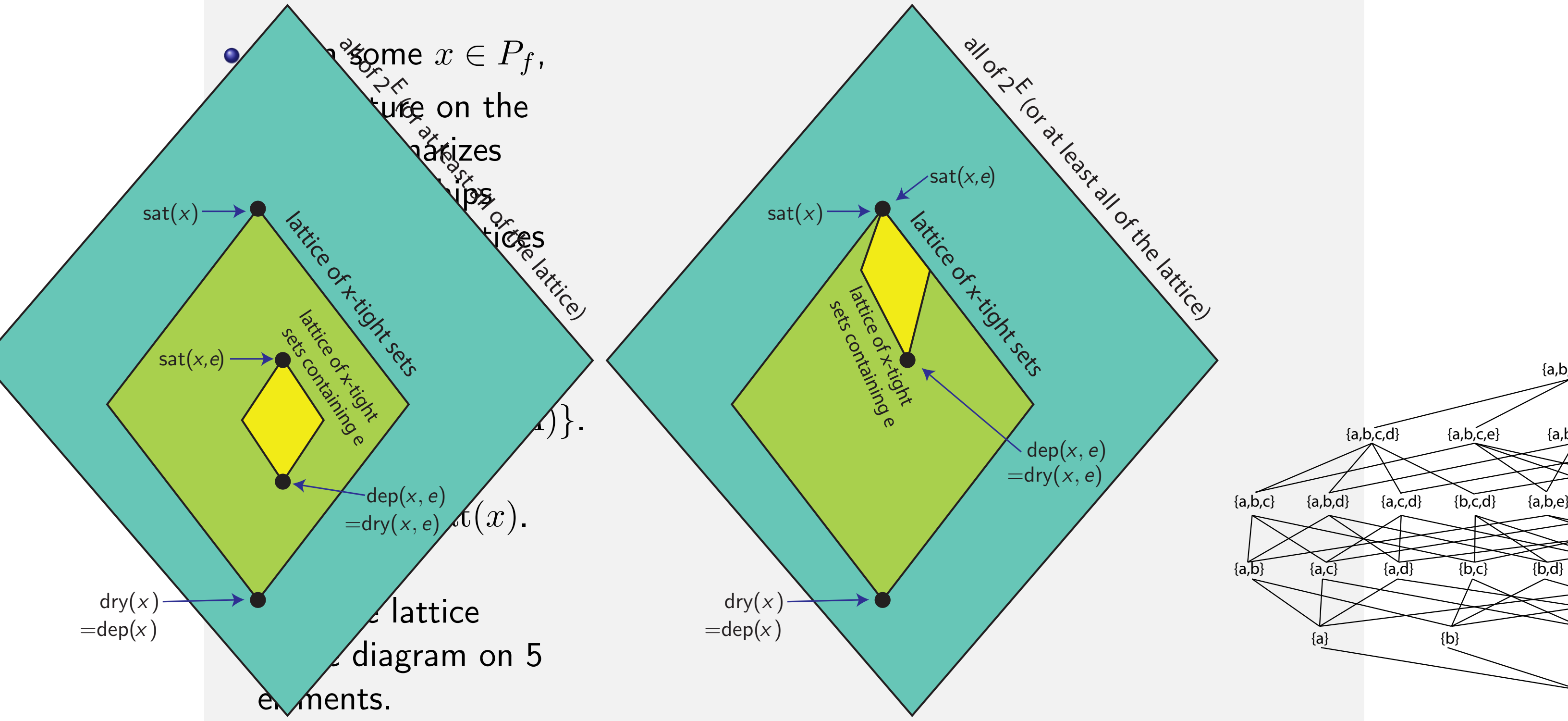

Minimizing $\breve{f}$ vs. minimizing f

In fact, we have:

Theorem 20.2.4

Let f be submodular and $\breve{f}$ be its Lovász extension. Then $\min\{f(A)|A \subseteq E\} = \min_{w\in\{0,1\}^E} \breve{f}(w) = \min_{w\in[0,1]^E} \breve{f}(w)$.

Proof.

- First, since $\breve{f}(\mathbf{1}_A) = f(A), \forall A \subseteq V$, we clearly have $\min\{f(A)|A \subseteq V\} = \min_{w\in\{0,1\}^E} \breve{f}(w) \geq \min_{w\in[0,1]^E} \breve{f}(w)$.
- Next, consider any $w \in [0,1]^E$, sort elements $E = \{e_1, \dots, e_m\}$ as $w(e_1) \geq w(e_2) \geq \dots \geq w(e_m)$, define $E_i = \{e_1, \dots, e_i\}$, and define $\lambda_m = w(e_m)$ and $\lambda_i = w(e_i) - w(e_{i+1})$ for $i \in \{1, \dots, m-1\}$.
- Then, as we have seen, $w = \sum_i \lambda_i \mathbf{1}_{E_i}$ and $\lambda_i \geq 0$.
- Also, $\sum_i \lambda_i = w(e_1) \leq 1$.

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Min-Norm Point: Definition

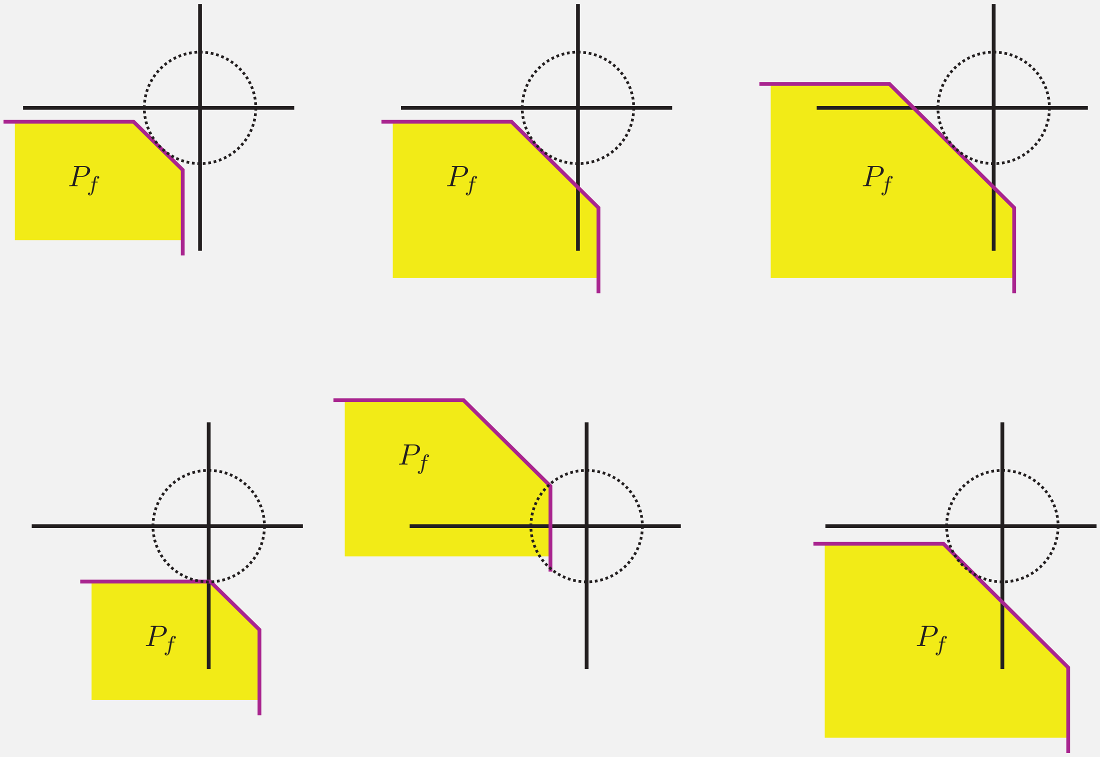
- Consider the optimization:

$$\text{minimize} \quad \|x\|_2^2 \qquad (20.25a)$$

$$\text{subject to} \quad x \in B_f \qquad (20.25b)$$

  where B_f is the base polytope of submodular f, and $\|x\|_2^2 = \sum_{e \in E} x(e)^2$ is the squared 2-norm. Let x^* be the optimal solution.
- Note, x^* is the unique optimal solution since we have a strictly convex objective over a set of convex constraints.
- x^* is called the minimum norm point of the base polytope.

Min-Norm Point: Examples



Min-Norm Point and Submodular Function Minimization

- Given optimal solution x^* to $[\min \|x\|_2^2 \text{ s.t. } x \in B_f]$, and consider:

$$y^* = x^* \wedge 0 = (\min(x^*(e), 0) | e \in E) \in P_f, \quad (20.25)$$

$$A_- = \{e : x^*(e) < 0\}, \qquad A_0 = \{e : x^*(e) \le 0\}. \quad (20.26)$$

- Thus, we immediately have that:

$$A_- \subseteq A_0 \quad (20.27)$$

and that

$$x^*(A_-) = x^*(A_0) = y^*(A_-) = y^*(A_0). \quad (20.28)$$

- These quantities will solve the SFM problem: we will see that $f(A_-) = f(A_0) = \min_{A \subseteq V} f(A)$ and that A_- is the unique minimal minimizer and A_0 is the unique maximal minimizer.
- The proof is nice since it uses recently developed tools (e.g., dep, sat).
- We'll also show both the Fujishige-Wolfe algorithm and the Frank-Wolfe algorithm (which are quite different from each other) can find the min-norm point relatively efficiently.

B_f dominates P_f

- In fact, every $x \in P_f$ is dominated by $x \le y \in B_f$.

Theorem 20.2.6

If $x \in P_f$ and T is tight for x (meaning $x(T) = f(T)$), then there exists $y \in B_f$ with $x \le y$ and $y(e) = x(e)$ for $e \in T$.

Proof.

- We construct the y algorithmically: initially set $y \leftarrow x$.
- $y \in P_f$, T is tight for y so $y(T) = f(T)$.
- Recall saturation capacity: for $y \in P_f$, $\hat{c}(y; e) = \min\{f(A) - y(A) | \forall A \ni e\} = \max\{\alpha : \alpha \in \mathbb{R}, y + \alpha \mathbf{1}_e \in P_f\}$
- Consider following algorithm:

```
$T' \leftarrow T$ ;
for $e \in E \setminus T$ do
    $y \leftarrow y + c(y;e)\mathbf{1}_e$ ; $T' \leftarrow T' \cup \{e\}$;
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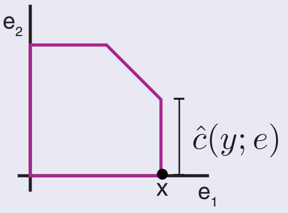

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Modified max-min theorem

- Min-max theorem (Thm 13.4.2) restated for $x = 0$.

$$\max\{y(E) | y \in P_f, y \le 0\} = \min\{f(X) | X \subseteq V\} \tag{20.27}$$

Theorem 20.2.6 (Edmonds-1970)

$$\min\{f(X) | X \subseteq E\} = \max\{x^-(E) | x \in B_f\} \tag{20.28}$$

where $x^-(e) = \min\{x(e), 0\}$ *for* $e \in E$.

Proof via the Lovász ext.

$$\min\{f(X)|X \subseteq E\} = \min_{w \in [0,1]^E} \breve{f}(w) = \min_{w \in [0,1]^E} \max_{x \in P_f} w^\intercal x \tag{20.29}$$

$$= \min_{w \in [0,1]^E} \max_{x \in B_f} w^\intercal x \tag{20.30}$$

$$= \max_{x \in B_f} \min_{w \in [0,1]^E} w^\intercal x \tag{20.31}$$

$$= \max_{x \in B_f} x^-(E) \tag{20.32}$$

□

Max-min theorem, all forms

We start directly from Theorem 13.4.2.

$$\max\left(y(E) : y \le 0, y \in P_f\right) = \min\left(f(A) : A \subseteq E\right) \tag{20.1}$$

Theorem 20.3.1 (Edmond's Max-Min Theorem (restated))

Given $y \in \mathbb{R}^E$, *define* $y^- \in \mathbb{R}^E$ *with* $y^-(e) = \min\{y(e), 0\}$ *for* $e \in E$.

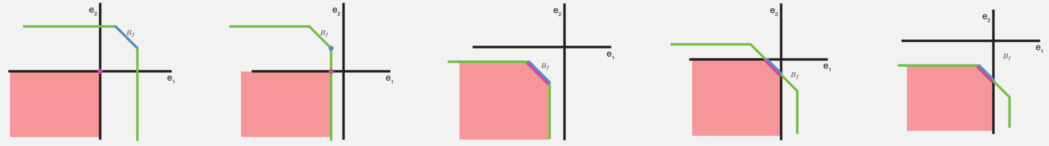
$$\max\left(y(E) : y \le 0, y \in P_f\right) = \max\left(y^-(E) : y \le 0, y \in P_f\right) \tag{20.2}$$

$$= \max\left(y^-(E) : y \in P_f\right) \tag{20.3}$$

$$= \max\left(y^-(E) : y \in B_f\right) \tag{20.4}$$

$$= \min\left(f(A) : A \subseteq E\right) \tag{20.5}$$

The first equality follows since $y \le 0$. The second equality (together with the first) shown on following slide. The third equality follows since for any $x \in P_f$ there exists a $y \in B_f$ with $x \le y$ (follows from Theorem 20.2.6).



Alt proof of $x^-(E)$ part of max-min theorem

Consider the following two problems for down-closed polyhedron P:

$$\max \sum_{e\in E} y(e) \quad (20.6a)$$
$$\text{s.t. } y \le x \quad (20.6b)$$
$$y \in P \quad (20.6c)$$

$$\max \sum_{e\in E} \min(y(e), x(e)) \quad (20.7a)$$
$$\text{s.t. } y \in P \quad (20.7b)$$

- Solutions identical cost. Let y_1^* be l.h.s. OPT and y_2^* be r.h.s. OPT.
- Consider l.h.s. OPT y_1^* in r.h.s. evaluation and suppose it is worse (lower) than r.h.s. OPT:

$$\sum_{e\in E} \min(y_1^*(e), x(e)) < \sum_{e\in E} \min(y_2^*(e), x(e)) \quad (20.8)$$

- But the vector $\bar{y}_1^*$ with entries $\bar{y}_1^*(e) = \min(y_2^*(e), x(e))$ has $\bar{y}_1^*(e) \le x(e)$ and $\bar{y}_1^* \in P$ since $y_2^* \in P$, $\bar{y}_1^* \le y_2^*$, and P is down-closed.
- Thus, $\bar{y}_1^*$ is l.h.s. feasible but a better l.h.s. evaluation, a contradiction of the optimality of y_1^* for l.h.s.
- Similarly, consider r.h.s. OPT y_2^* in l.h.s. evaluation and suppose it is worse (lower) than l.h.s. OPT

$$\sum_{e\in E} y_2^*(e) < \sum_{e\in E} y_1^*(e) \quad (20.9)$$

- But the vector $\bar{y}_2^*$ with entries $\bar{y}_2^*(e) = y_1^*(e)$ has $\bar{y}_2^* \in P$ and since $\bar{y}_2^*(e) \le x(e)$ for all e, we have

Greedy solves $\max\{w^\intercal x | x \in B_f\}$ for arbitrary $w \in \mathbb{R}^E$

Let $f(A)$ be an arbitrary submodular function, and $f(A) = f'(A) - m(A)$ where f' is polymatroidal, and $w \in \mathbb{R}^E$.

$$\begin{aligned}
\max\{w^\intercal x | x \in B_f\} &= \max\{w^\intercal x | x(A) \le f(A)\, \forall A, x(E) = f(E)\} \\
&= \max\left\{w^\intercal x | x(A) \le f'(A) - m(A)\, \forall A, x(E) = f'(E) - m(E)\right\} \\
&= \max\left\{w^\intercal x | x(A) + m(A) \le f'(A)\, \forall A, x(E) + m(E) = f'(E)\right\} \\
&= \max\{w^\intercal x + w^\intercal m | \\
&\qquad x(A) + m(A) \le f'(A)\, \forall A, x(E) + m(E) = f'(E)\} - w^\intercal m \\
&= \max\left\{w^\intercal y | y \in B_{f'}\right\} - w^\intercal m \\
&= w^\intercal y^* - w^\intercal m = w^\intercal (y^* - m)
\end{aligned}$$

where $y = x + m$, so that $x^* = y^* - m$.

So y^* uses greedy algorithm with positive orthant $B_{f'}$. To show, we use Theorem 12.4.1 in Lecture 11, but we don't require $y \ge 0$, and don't stop when w goes negative to ensure $y^* \in B_{f'}$. Then when we subtract off m from y^*, we get solution to the original problem.

$\min\{w^\intercal x : x \in B_f\}$

- Recall that the greedy algorithm solves, for $w \in \mathbb{R}_+^E$

$$\max\{w^\intercal x | x \in P_f\} = \max\{w^\intercal x | x \in B_f\} \tag{20.11}$$

  since for all $x \in P_f$, there exists $y \geq x$ with $y \in B_f$.
- For arbitrary $w \in \mathbb{R}^E$, we saw in Lecture 16 that the greedy algorithm will also solve:

$$\max\{w^\intercal x | x \in B_f\} \tag{20.12}$$

- Also, since $w \in \mathbb{R}^E$ is arbitrary, and since

$$\min\{w^\intercal x | x \in B_f\} = -\max\{-w^\intercal x | x \in B_f\} \tag{20.13}$$

  the greedy algorithm using ordering $(e_1, e_2, \dots, e_m)$ such that

$$w(e_1) \leq w(e_2) \leq \dots \leq w(e_m) \tag{20.14}$$

  will solve l.h.s. of Equation (20.13).

Greedy solves $\max\{w^\intercal x | x \in B_f\}$ for arbitrary $w \in \mathbb{R}^E$

Let $f(A)$ be arbitrary submodular function, and $f(A) = f'(A) - m(A)$ where f' is polymatroidal, and $w \in \mathbb{R}^E$.

$$\begin{aligned}
\max\{w^\intercal x | x \in B_f\} &= \max\{w^\intercal x | x(A) \leq f(A)\,\forall A, x(E) = f(E)\} \\
&= \max\left\{w^\intercal x | x(A) \leq f'(A) - m(A)\,\forall A, x(E) = f'(E) - m(E)\right\} \\
&= \max\left\{w^\intercal x | x(A) + m(A) \leq f'(A)\,\forall A, x(E) + m(E) = f'(E)\right\} \\
&= \max\big\{w^\intercal x + w^\intercal m | \\
&\qquad x(A) + m(A) \leq f'(A)\,\forall A, x(E) + m(E) = f'(E)\big\} - w^\intercal m \\
&= \max\left\{w^\intercal y | y \in B_{f'}\right\} - w^\intercal m \\
&= w^\intercal y^* - w^\intercal m = w^\intercal(y^* - m)
\end{aligned}$$

where $y = x + m$, so that $x^* = y^* - m$.
So y^* uses greedy algorithm with positive orthant $B_{f'}$. To show, we use Theorem 12.4.1 in Lecture 11, but we don't require $y \geq 0$, and don't stop when w goes negative to ensure $y^* \in B_{f'}$. Then when we subtract off m from y^*, we get solution to the original problem.

One last lemma

Lemma 20.3.2

Given function $\phi : \mathbb{R} \to \mathbb{R}$ and two points $a, b \in \mathbb{R}$ with $a < b$. Then ϕ is convex in the region $[a, b]$ if and only if

$$\phi(a) + \phi(b) \geq \phi(a + \alpha) + \phi(b - \alpha), \forall \alpha \in [0, b - a] \tag{20.15}$$

Proof.

This inequality is the same as

$$f(b) - f(b - \alpha) \geq f(a + \alpha) - f(a) \tag{20.16}$$

and the rest follows from Bilmes&Bai, "Deep Submodular Functions", Theorem 5.3 (which shows the corresponding theorem for concave functions). □

Min-Norm Point and Submodular Function Minimization

- Given optimal solution x^* to $[\min \|x\|_2^2$ s.t. $x \in B_f]$, and consider:

$$y^* = x^* \wedge 0 = (\min(x^*(e), 0) | e \in E) \in P_f, \tag{20.25}$$
$$A_- = \{e : x^*(e) < 0\}, \qquad A_0 = \{e : x^*(e) \leq 0\}. \tag{20.26}$$

- Thus, we immediately have that:

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  and that

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- These quantities will solve the SFM problem: we will see that $f(A_-) = f(A_0) = \min_{A \subseteq V} f(A)$ and that A_- is the unique minimal minimizer and A_0 is the unique maximal minimizer.
- The proof is nice since it uses recently developed tools (e.g., dep, sat).
- We'll also show both the Fujishige-Wolfe algorithm and the Frank-Wolfe algorithm (which are quite different from each other) can find the min-norm point relatively efficiently.

Min-Norm Point and SFM

Theorem 20.4.1

Let x^*, y^*, A_-, and A_0 be as given. Then y^* is a maximizer of $\max\{y(E) | y \in P_f, y \leq 0\} = \max(y^-(E) : y \in B_f)$, A_- is the unique minimal minimizer of f, and A_0 is the unique maximal minimizer of f.

Proof.

- First note, since $x^* \in B_f$, we have $x^*(E) = f(E)$, meaning $\text{sat}(x^*) = E$. Thus, we may consider any $e \in E$ within $\text{dep}(x^*, e)$.
- Consider any pair (e, e') with $e \in A_-$ and $e' \in \text{dep}(x^*, e)$. Then $x^*(e) < 0$, and $\exists \alpha > 0$ s.t. $x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'} \in P_f$.
- We have $x^*(E) = f(E)$ and x^* is minimum in l2 sense. We have $(x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'}) \in P_f$, and in fact

$$(x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'})(E) = x^*(E) + \alpha - \alpha = f(E) \tag{20.17}$$

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

...

Min-Norm Point and SFM

... proof of Thm. 20.4.1 cont.

- Then $(x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'})(E)$
  $= x^*(E \setminus \{e, e'\}) + \underbrace{(x^*(e) + \alpha)}_{x^*_{\text{new}}(e)} + \underbrace{(x^*(e') - \alpha)}_{x^*_{\text{new}}(e')} = f(E).$
- Minimality of $x^* \in B_f$ in l2 sense requires that, with such an $\alpha > 0$, $\Big(x^*(e)\Big)^2 + \Big(x^*(e')\Big)^2 < \Big(x^*_{\text{new}}(e)\Big)^2 + \Big(x^*_{\text{new}}(e')\Big)^2$
- Given that $e \in A_-$, $x^*(e) < 0$. Thus, if $x^*(e') > 0$, we would have $(x^*(e) + \alpha')^2 + (x^*(e') - \alpha')^2 < (x^*(e))^2 + (x^*(e'))^2$, for some $0 < \alpha' \leq \alpha$, contradicting the optimality of x^*.
- If $x^*(e') = 0$, we would have $(x^*(e) + \alpha')^2 + (\alpha')^2 < (x^*(e))^2$, for any $0 < \alpha' < |x^*(e)|$ by Lemma 20.3.2, again contradicting optimality of x^*.
- Thus, we must have $x^*(e') < 0$ (strict negativity).

...

Min-Norm Point and SFM

...proof of Thm. 20.4.1 cont.

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

...

Min-Norm Point and SFM

...proof of Thm. 20.4.1 cont.

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

$$x^*(A_-) = f(A_-) \tag{20.18}$$

$$x^*(A_0) = f(A_0) \tag{20.19}$$

$$x^*(A_-) = x^*(A_0) = y^*(E) = y^*(A_0) + \underbrace{y^*(E \setminus A_0)}_{=0} \tag{20.20}$$

and therefore, all together we have

$$f(A_-) = f(A_0) = x^*(A_-) = x^*(A_0) = y^*(E) \tag{20.21}$$

- Hence, $f(A_-) = f(A_0)$, meaning A_- and A_0 have the same valuation, but we have not yet shown they are the minimizers of the submodular function, nor that they are, resp. the maximal and minimal minimizers.

Min-Norm Point and SFM

. . . proof of Thm. 20.4.1 cont.

- Now, y^* is feasible for the l.h.s. of Eqn. (20.1) (recall, which is $\max\{y(E)|y \in P_f, y \leq 0\} = \min\{f(X)|X \subseteq V\}$). This follows since, we have $y^* = x^* \wedge 0 \leq 0$, and since $x^* \in B_f \subset P_f$, and $y^* \leq x^*$ and P_f is down-closed, we have that $y^* \in P_f$.
- Also, for any $y \in P_f$ with $y \leq 0$ and for any $X \subseteq E$, we have $y(E) \leq y(X) \leq f(X)$.
- Hence, we have found a feasible for l.h.s. of Eqn. (20.1), $y^* \leq 0$, $y^* \in P_f$, so $y^*(E) \leq f(X)$ for all X.
- So $y^*(E) \leq \min\{f(X)|X \subseteq V\}$.
- Considering Eqn. (20.22), we have found sets A_- and A_0 with tightness in Eqn. (20.1), meaning $y^*(E) = f(A_-) = f(A_0)$.
- Hence, y^* is a maximizer of l.h.s. of Eqn. (20.1), and A_- and A_0 are minimizers of f.

. . .

Min-Norm Point and SFM

. . . proof of Thm. 20.4.1 cont.

- We next show that, not only are they minimizers, but A_- is the unique minimal and A_0 is the unique maximal minimizer of f
- Now, for any $X \subset A_-$, we have

$$f(X) \geq x^*(X) > x^*(A_-) = f(A_-) \tag{20.22}$$

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

$$f(X) \geq x^*(X) > x^*(A_0) = f(A_0) \tag{20.23}$$

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

□

Min-Norm Point and SFM

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

Min-norm point and other minimizers of f

- Recall, that the set of minimizers of f forms a lattice.
- Q: If we take any A with $A_- \subset A \subset A_0$, is A also a minimizer? No. Consider graph cut function with graph with multiple connected components, so $A_- = \emptyset$, $A_0 = V$ but not all $A : A_- \subset A \subset A_0$ is a minimizer.
- In fact, with x^* the min-norm point, and A_- and A_0 as defined above, we have the following theorem:

Theorem 20.4.2

Let $A \subseteq E$ be any minimizer of submodular f, and let x^* be the minimum-norm point. Then A can be expressed in the form:

$$A = A_- \cup \bigcup_{a \in A_m} \text{dep}(x^*, a) \tag{20.24}$$

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

Min-norm point and other minimizers of f

proof of Thm. 20.4.2.

- If A is a minimizer, then $A_- \subseteq A \subseteq A_0$, and $f(A) = y^*(E)$ is the minimum valuation of f.
- But $x^* \in P_f$, so $x^*(A) \leq f(A)$ and $f(A) = x^*(A_-) \leq x^*(A)$.
- Also, since $A \subseteq A_0$ and $x^*(A_0 \setminus A) = 0$, $x^*(A_-) = x^*(A) = x^*(A_0)$
- Hence, $x^*(A) = x^*(A_-) = f(A)$ so that A is also a tight set for x^*.
- For any $a \in A$, A is a tight set containing a, and $\text{dep}(x^*, a)$ is the minimal tight containing a.
- Hence, for any $a \in A$, $\text{dep}(x^*, a) \subseteq A$.
- This means that $\bigcup_{a \in A} \text{dep}(x^*, a) = A$.
- Since $A_- \subseteq A \subseteq A_0$, then $\exists A_m \subseteq A \setminus A_-$ such that

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

...

Min-norm point and other minimizers of f

proof of Thm. 20.4.2.

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

$$A = A_- \cup \bigcup_{a \in A_m} \text{dep}(x^*, a) = \bigcup_{a \in A_-} \text{dep}(x^*, a) \cup \bigcup_{a \in A_m} \text{dep}(x^*, a) \tag{20.25}$$

- Then since A is a union of tight sets, A is also a tight set, and we have $f(A) = x^*(A)$.
- But since for any $a \in A_0$, $\text{dep}(x^*, a) \subseteq A_0$ then $A \subseteq A_0$ and we have that $x^*(A \setminus A_-) = 0$, so $f(A) = x^*(A) = x^*(A_-) = f(A_-)$ meaning A is also a minimizer of f.

□

Therefore, we can generate the entire lattice of minimizers of f starting from A_- and A_0 given access to $\text{dep}(x^*, e)$.

On a unique minimizer f

- Note that if $f(e|A) > 0, \forall A \subseteq E$ and $e \in E \setminus A$, then we have $A_- = A_0$ (there is one unique minimizer).
- On the other hand, if $A_- = A_0$, it does not imply $f(e|A) > 0$ for all $A \subseteq E \setminus \{e\}$.
- If $A_- = A_0$ then certainly $f(e|A_0) > 0$ for $e \in E \setminus A_0$ and $-f(e|A_0 \setminus \{e\}) > 0$ for all $e \in A_0$.

Duality: convex minimization of L.E. and min-norm alg.

- Let f be a submodular function with $\tilde{f}$ it's Lovász extension. Then the following two problems are duals (Bach-2013):

$$\underset{w \in \mathbb{R}^V}{\text{minimize}} \; \breve{f}(w) + \frac{1}{2}\|w\|_2^2 \qquad (20.26)$$

$$\text{maximize} \quad -\frac{1}{2}\|x\|_2^2 \qquad (20.27a)$$

$$\text{subject to} \quad x \in B_f \qquad (20.27b)$$

  where $B_f = P_f \cap \left\{x \in \mathbb{R}^V : x(V) = f(V)\right\}$ is the base polytope of submodular function f, and $\|x\|_2^2 = \sum_{e \in V} x(e)^2$ is squared 2-norm.
- Equation (20.26) is related to proximal methods to minimize the Lovász extension (see Parikh&Boyd, "Proximal Algorithms" 2013).
- Equation (20.27b) is solved by the minimum-norm point algorithm (Wolfe-1976, Fujishige-1984, Fujishige-2005, Fujishige-2011) is essentially an active-set procedure for quadratic programming, and uses Edmonds's greedy algorithm to make it efficient.
- These algorithms usually perform quite well in practice, they can be made to perform about the same, given a properly tuned implementation (also, the FrankWolfe based algorithm is much simpler).

Fujishige-Wolfe Min-Norm Algorithm

- Wolfe-1976 ("Finding the Nearest Point in a Polytope") developed an algorithm to compute the minimum norm point of a polytope, specified as a set of vertices (again, not same as Frank-Wolfe'1956).
- Given set of points $P = \{p_1, \cdots, p_m\}$ where $p_i \in \mathbb{R}^n$: find the minimum norm point in convex hull of P:

$$\min_{x \in \operatorname{conv} P} \|x\|_2 \tag{20.28}$$

- Wolfe's algorithm is guaranteed terminating, and explicitly uses a representation of x as a convex combination of points in P
- Fujishige-1984 "Submodular Systems and Related Topics" realized this algorithm can find the the min. norm point of B_f thanks to Edmond's greedy algorithm.
- Seems to still be (among) the fastest general purpose SFM algorithms in practice.

Convex and affine hulls, affinely independent

- Given points set $P = \{p_1, p_2, \dots, p_k\}$ with $p_i \in \mathbb{R}^V$, let $\operatorname{conv} P$ be the convex hull of P, i.e.,

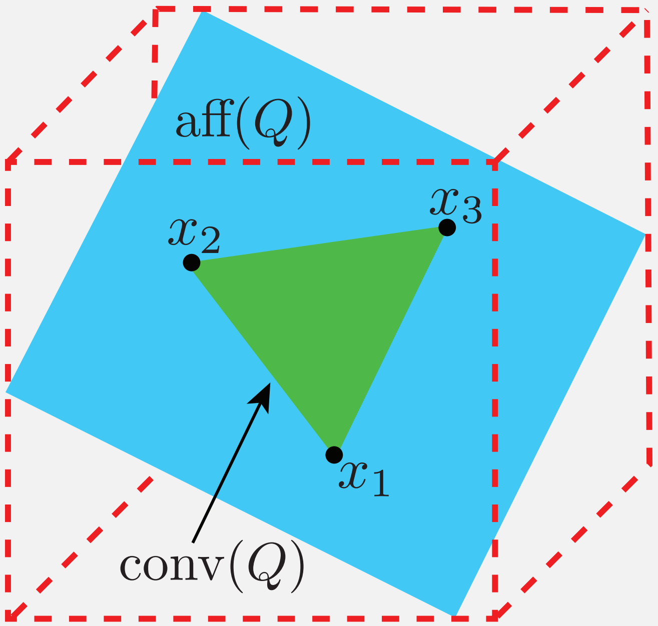
$$\operatorname{conv} P \triangleq \left\{ \sum_{i=1}^{k} \lambda_i p_i : \sum_{i} \lambda_i = 1,\ \lambda_i \geq 0, i \in [k] \right\}. \tag{20.29}$$

- For a set of points $Q = \{q_1, q_2, \dots, q_k\}$, with $q_i \in \mathbb{R}^V$, we define $\operatorname{aff} Q$ to be the affine hull of Q, i.e.:

$$\operatorname{aff} Q \triangleq \left\{ \sum_{i \in 1}^{k} \lambda_i q_i : \sum_{i=1}^{k} \lambda_i = 1 \right\} \supseteq \operatorname{conv} Q. \tag{20.30}$$

- A set of points Q is affinely independent if no point in Q belongs to the affine hull of the remaining points.

Convex vs. Affine hull, geometry



$\forall i, x_i \in \mathbb{R}^3$

$Q = \{x_1, x_2, x_3\}$

x_1, x_2, x_3 coplanar

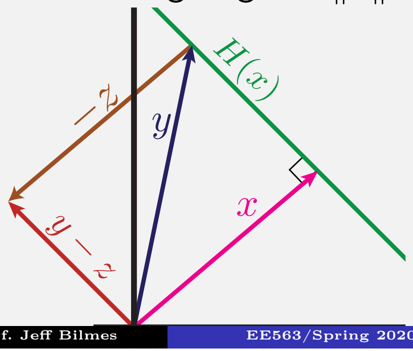
span(Q)

$H(x)$: Orthogonal x-containing hyperplane

- Define $H(x)$ as the hyperplane that is orthogonal to the line from 0 to x, while also containing x, i.e.

$$H(x) \triangleq \left\{ y \in \mathbb{R}^V \mid x^\intercal y = \|x\|_2^2 \right\} \tag{20.31}$$

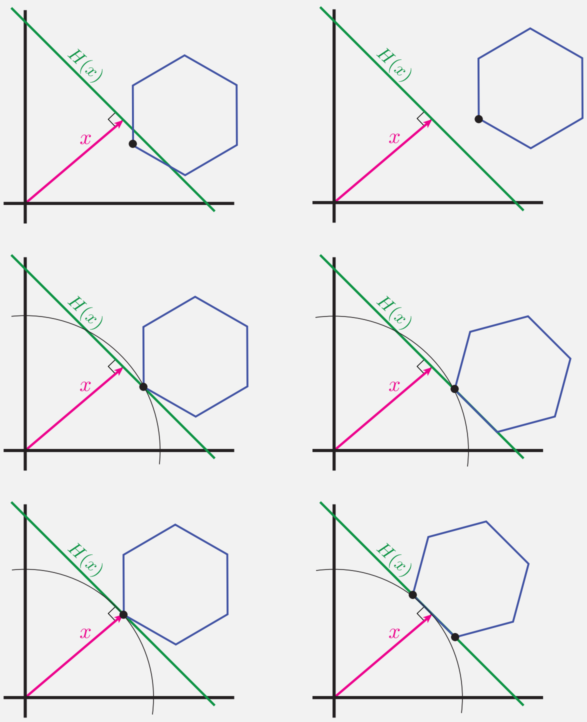
- Any set $\{y \in \mathbb{R}^V | x^\intercal y = c\}$ is orthogonal to the line from 0 to x. This follows since, for constant z, $\{y : (y-z)^\intercal x = 0\} = \{y : y^\intercal x = z^\intercal x\}$ is hyperplane orthogonal to x translated by z. Take $c = z^\intercal x$ for result, and $z = x$, giving $c = \|x\|^2$, to contain x.



- Note, $H(x)$ is translation of subspace of dimension $|V| - 1 = n - 1$ (i.e., $H(x) - \{x\}$ is a subspace, $H(x)$ is an affine set).

Ex: $H(x)$, polytopes, and supporting hyperplanes

- $H(x) = \left\{ y \in \mathbb{R}^V \,|\, x^\intercal y = \|x\|_2^2 \right\}$, any $z \in H(x)$ has $x^\intercal z = x^\intercal x$.
- Consider $\text{conv}\, P$ polytope for points $P = \{p_1, p_2, \dots\}$, and $\hat{p} \in \text{argmin}_{p \in P}\, x^\intercal p$. TL: $x^\intercal \hat{p} < x^\intercal x$; TR: $x^\intercal \hat{p} > x^\intercal x$; middle row: $x^\intercal p = x^\intercal x$.
- Bottom Row: In Algo, x is chosen so that if $x^\intercal \hat{p} = x^\intercal x$ then $H(x)$ separates P from the origin, and x is the min 2-norm point. Notice that $x^\intercal p \geq x^\intercal x$ for all $p \in P$.
- Middle/bottom row: $H(x)$ is a supporting hyperplane of $\text{conv}\, P$ (contained, touching).



Notation

- The line between x and y: given two points $x, y \in \mathbb{R}^V$, let $[x, y] \triangleq \{\lambda x + (1 - \lambda) y : \lambda \in [0, 1]\}$. Hence, $[x, y] = \text{conv}\, \{x, y\}$.
- Note, if we wish to minimize the 2-norm of a vector $\|x\|_2$, we can equivalently minimize its square $\|x\|_2^2 = \sum_i x_i^2$, and vice verse.

Fujishige-Wolfe Min-Norm Algorithm

- Algorithm maintains a set of points $Q \subseteq P$, which is always assuredly *affinely independent*, and also $|Q|$ doesn't grow large even if $|P|$ is large.
- When Q are affinely independent, minimum norm point in the affine hull of Q can easily be found, as a closed form solution for $\min_{x \in \text{aff } Q} \|x\|_2$ is available (see below).
- Algorithm repeatedly produces min. norm point x^* for selected set Q.
- If we find $w_i \geq 0, i = 1, \cdots, m$ for the minimum norm point, then x^* also belongs to $\text{conv}\, Q$ and also a minimum norm point over $\text{conv}\, Q$.
- If $Q \subseteq P$ is suitably chosen, x^* may even be the minimum norm point over $\text{conv}\, P$ solving the original problem.
- One of the most expensive parts of Wolfe's original 1976 algorithm is solving linear optimization problem over the polytope, doable by examining all the extreme points in the polytope.
- If number of extreme points is exponential, hard to do in general.
- Number of extreme points of submodular base polytope is exponentially large, but linear optimization over the base polytope B_f doable $O(n \log n)$ time via Edmonds's greedy algorithm.

Pseudocode of Fujishige-Wolfe Min-Norm (MN) algorithm

```
Input  : $P = \{p_1, \cdots, p_m\}, p_i \in \mathbb{R}^n, i = 1, \cdots, m.$
Output: $x^*$: the minimum-norm-point in $\text{conv}\, P$.
$x^* \longleftarrow p_{i^*}$ where $p_{i^*} \in \text{argmin}_{p \in P} \|p\|_2$      /* or choose it arbitrarily */ ;
$Q \longleftarrow \{x^*\}$;
while 1 do                                                  /* major loop */
    if $x^* = 0$ or $H(x^*)$ separates $P$ from origin then
        return : $x^*$
    else
        Choose $\hat{x} \in P$ on the near (closer to 0) side of $H(x^*)$;
        $Q = Q \cup \{\hat{x}\}$;
    while 1 do                                              /* minor loop */
        $x_0 \longleftarrow \text{argmin}_{x \in \text{aff } Q} \|x\|_2$;
        if $x_0 \in \text{conv}\, Q$ then
            $x^* \longleftarrow x_0$;
            break;
        else
            $y \longleftarrow \text{argmin}_{x \in \text{conv}\, Q \cap [x^*, x_0]} \|x - x_0\|_2$;
            Delete from $Q$ points not on the face of $\text{conv}\, Q$ where $y$ lies;
            $x^* \longleftarrow y$;
```

N: Pseudocode Fujishige-Wolfe Min-Norm (MN) algorithm

```
   Input  : $P = \{p_1, \cdots, p_m\}, p_i \in \mathbb{R}^n, i = 1, \cdots, m.$
   Output: $x^*$: the minimum-norm-point in $\text{conv}\, P$.
1  $p \longleftarrow p_{i^*}$ where $p_{i^*} \in \text{argmin}_{p \in P} \|p\|_2$, or choose $p \in P$ arbitrarily or
    heuristically ;
2  $Q \longleftarrow \{x^*\}$;
3  while 1 do                                                    /* major loop */
4      if $x^* = 0$ or $H(x^*)$ separates $P$ from origin then
           return : $x^*$
5      else
6          Choose $\hat{x} \in P$ on the near (closer to $0$) side of $H(x^*)$;
7          $Q = Q \cup \{\hat{x}\}$;
8      while 1 do                                                /* minor loop */
9          $x_0 \longleftarrow \text{argmin}_{x \in \text{aff}\, Q} \|x\|_2$;
10         if $x_0 \in \text{conv}\, Q$ then
11             $x^* \longleftarrow x_0$;
12             break;
13         else
14             $y \longleftarrow \text{argmin}_{x \in \text{conv}\, Q \cap [x^*, x_0]} \|x - x_0\|_2$;
15             Delete from $Q$ points not on the face of $\text{conv}\, Q$ where $y$ lies;
16             $x^* \longleftarrow y$;
```

Fujishige-Wolfe Min-Norm algorithm: Geometric Example

- It is advised that for the next set of slides, you have a print out of the previous MN algorithm available on display/paper somewhere.
- Algorithm maintains an invariant, namely that:

$$x^* \in \text{conv}\, Q \subseteq \text{conv}\, P, \tag{20.32}$$

  must hold at every possible assignment of x^* (Lines 1, 11, and 16):
  1. True after Line 1 since $Q = \{x^*\}$,
  2. True after Line 11 since $x_0 \in \text{conv}\, Q$,
  3. and true after Line 16 since $y \in \text{conv}\, Q$ even after deleting points.
- Note also for any $x^* \in \text{conv}\, Q \subseteq \text{conv}\, P$, we have

$$\min_{x \in \text{aff}\, Q} \|x\|_2 \leq \min_{x \in \text{conv}\, Q} \|x\|_2 \leq \|x^*\|_2 \tag{20.33}$$

- Note, the input, P, consists of m points. In the case of the base polytope, $P = B_f$ could be exponential in $n = |V|$.
- There are six places that might be seemingly tricky or expensive: Line 4, Line 6, Line 9, Line 10, Line 14, and Line 15.
- We will consider each in turn, but first we do a geometric example.

N: Pseudocode Fujishige-Wolfe Min-Norm (MN) algorithm

```
Input  : $P = \{p_1, \cdots, p_m\}, p_i \in \mathbb{R}^n, i = 1, \cdots, m$.
Output: $x^*$: the minimum-norm-point in conv $P$.
$p \longleftarrow p_{i^*}$ where $p_{i^*} \in \text{argmin}_{p \in P} \|p\|_2$, or choose $p \in P$ arbitrarily or
  heuristically ;
$Q \longleftarrow \{x^*\}$;
while 1 do                                                    /* major loop */
    if $x^* = 0$ or $H(x^*)$ separates $P$ from origin then
        return : $x^*$
    else
        Choose $\hat{x} \in P$ on the near (closer to 0) side of $H(x^*)$;
        $Q = Q \cup \{\hat{x}\}$;
    while 1 do                                                /* minor loop */
        $x_0 \longleftarrow \text{argmin}_{x \in \text{aff } Q} \|x\|_2$;
        if $x_0 \in \text{conv } Q$ then
            $x^* \longleftarrow x_0$;
            break;
        else
            $y \longleftarrow \text{argmin}_{x \in \text{conv } Q \cap [x^*, x_0]} \|x - x_0\|_2$;
            Delete from $Q$ points not on the face of conv $Q$ where $y$ lies;
            $x^* \longleftarrow y$;
```

Solved by Edmond's greedy procedure.

Solved via linear equation solver.

Linear equation solver represents x_0 as affine coefs, so this just checks >= 0.

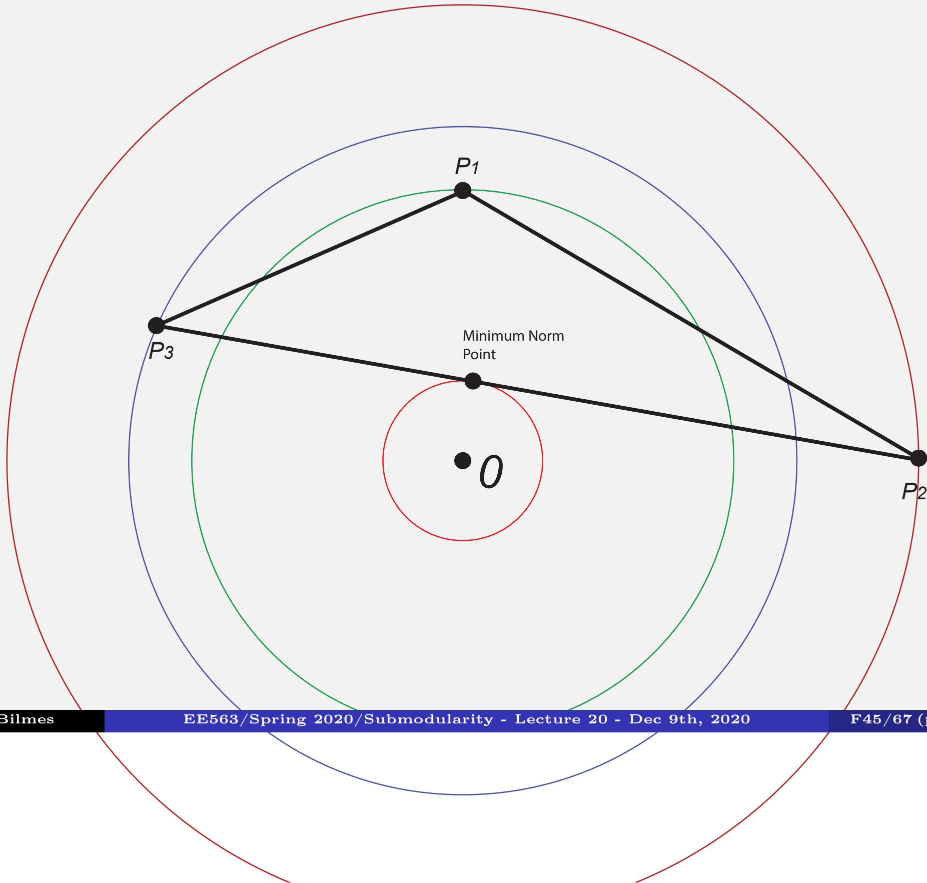
Doable since we're representing points as convex combinations of points within Q

Fujishige-Wolfe Min-Norm algorithm: Geometric Example

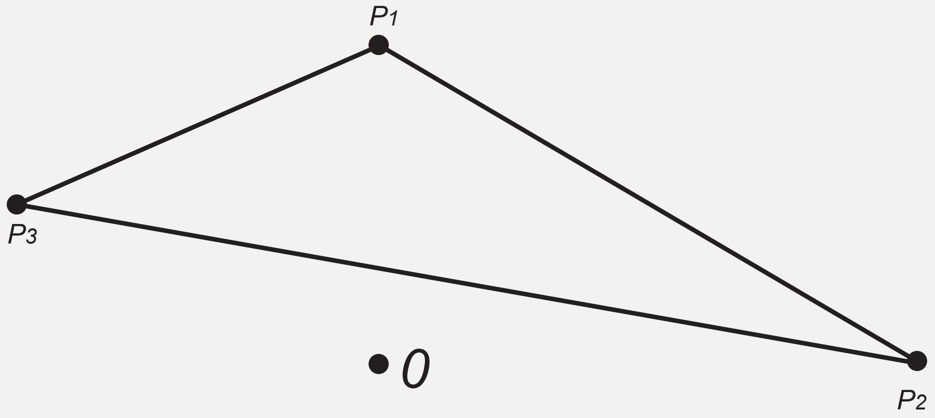
- In the following series of images, permanent (non-changing) named points on the polytope will be indicated by capital letters (i.e., P_1, P_2, P_3, R, S, T) while variables in the algorithm that are changing will use lower case letters (i.e., x^*, x_0, $\hat{x}$, y).
- Also, example is in 2D, so polytope given can't be a real base B_f for any f. Example meant to show only the geometry of the algorithm.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example

Polytope, and circles concentric at 0.

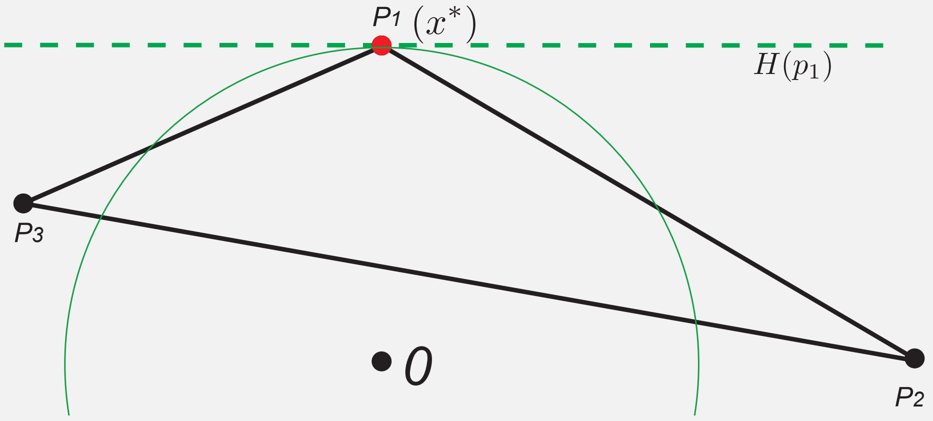


Fujishige-Wolfe Min-Norm algorithm: Geometric Example



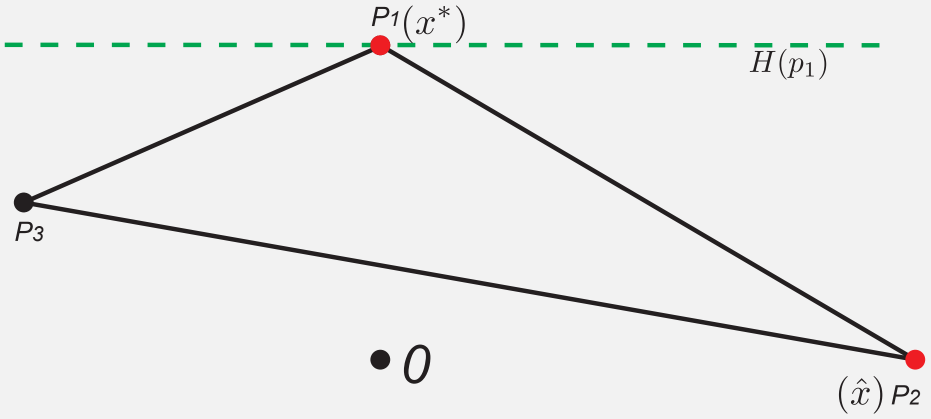
The initial polytope consisting of the convex hull of three points p_1, p_2, p_3, and the origin 0.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



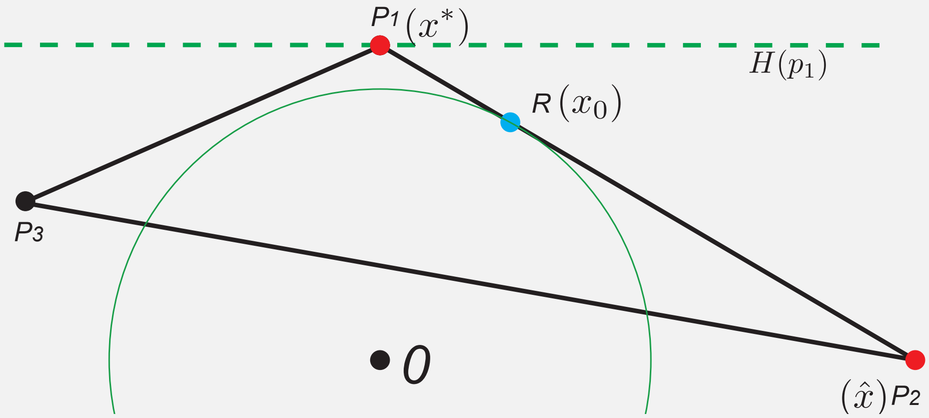
p_1 is the extreme point closest to 0 and so we choose it first, although we can choose any arbitrary extreme point as the initial point. We set $x^* \leftarrow p_1$ in Line 1, and $Q \leftarrow \{p_1\}$ in Line 2. $H(x^*) = H(p_1)$ (green dashed line) is not a supporting hyperplane of $\mathrm{conv}(P)$ in Line 4, so we move on to the else condition in Line 5.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



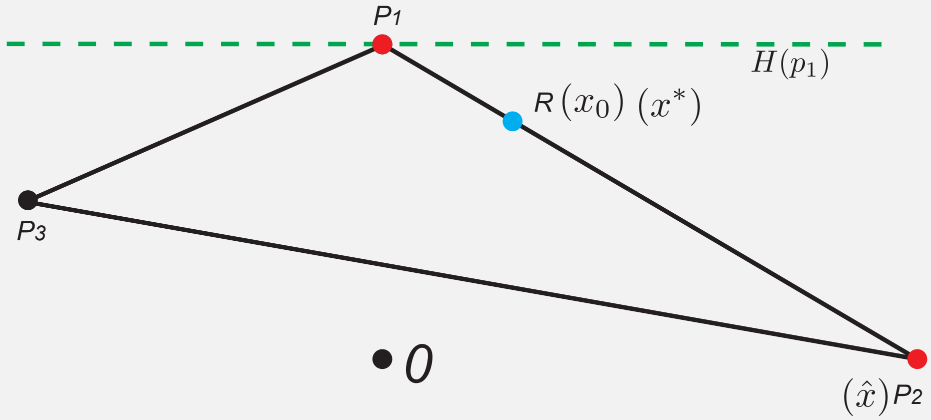
We need to add some extreme point $\hat{x}$ on the "near" side of $H(p_1)$ in Line 6, we choose $\hat{x} = p_2$. In Line 7, we set $Q \leftarrow Q \cup \{p_2\}$, so $Q = \{p_1, p_2\}$.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



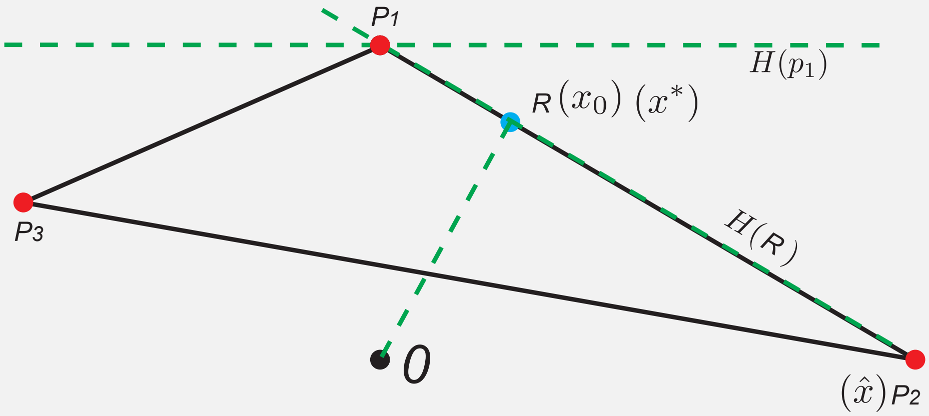
$x_0 = R$ is the min-norm point in $\text{aff}\,\{p_1, p_2\}$ computed in Line 9. Also, with $Q = \{p_1, p_2\}$, since $R \in \text{conv}\, Q$, we set $x^* \leftarrow x_0 = R$ in Line 11, not violating the invariant $x^* \in \text{conv}\, Q$. Note, after Line 11, we still have $x^* \in \text{conv}\, P$ and $\|x^*\|_2 = \|x^*_{\text{new}}\|_2 < \left\|x^*_{\text{old}}\right\|_2$ strictly.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



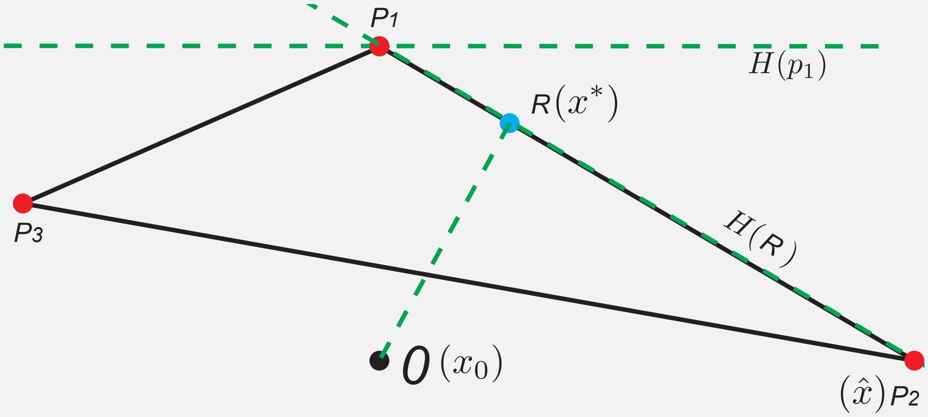
$x_0 = R$ is the min-norm point in $\text{aff}\,\{p_1, p_2\}$ computed in Line 9. Also, with $Q = \{p_1, p_2\}$, since $R \in \text{conv}\, Q$, we set $x^* \leftarrow x_0 = R$ in Line 11, not violating the invariant $x^* \in \text{conv}\, Q$. Note, after Line 11, we still have $x^* \in \text{conv}\, P$ and $\|x^*\|_2 = \|x^*_{\text{new}}\|_2 < \left\|x^*_{\text{old}}\right\|_2$ strictly.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



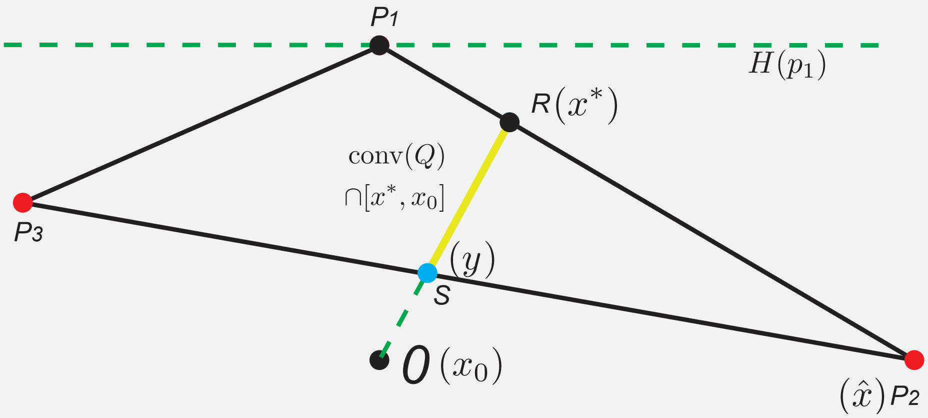
$R = x_0 = x^*$. We consider next $H(R) = H(x^*)$ in Line 4. $H(x^*)$ is not a supporting hyperplane of $\operatorname{conv} P$. So we choose p_3 on the "near" side of $H(x^*)$ in Line 6. Add $Q \leftarrow Q \cup \{p_3\}$ in Line 7. Now $Q = P = \{p_1, p_2, p_3\}$. The origin $x_0 = 0$ is the min-norm point in $\operatorname{aff} Q$ (Line 9), and it is not in the interior of $\operatorname{conv} Q$ (condition in Line 10 is false).

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



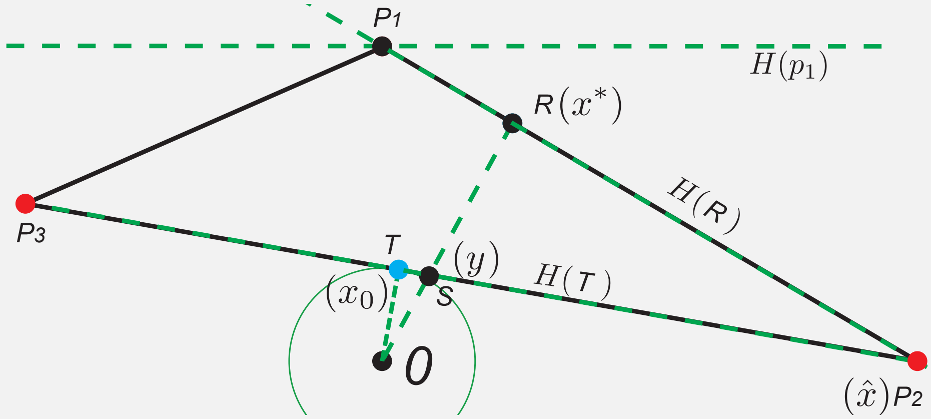
$R = x_0 = x^*$. We consider next $H(R) = H(x^*)$ in Line 4. $H(x^*)$ is not a supporting hyperplane of $\operatorname{conv} P$. So we choose p_3 on the "near" side of $H(x^*)$ in Line 6. Add $Q \leftarrow Q \cup \{p_3\}$ in Line 7. Now $Q = P = \{p_1, p_2, p_3\}$. The origin $x_0 = 0$ is the min-norm point in $\operatorname{aff} Q$ (Line 9), and it is not in the interior of $\operatorname{conv} Q$ (condition in Line 10 is false).

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



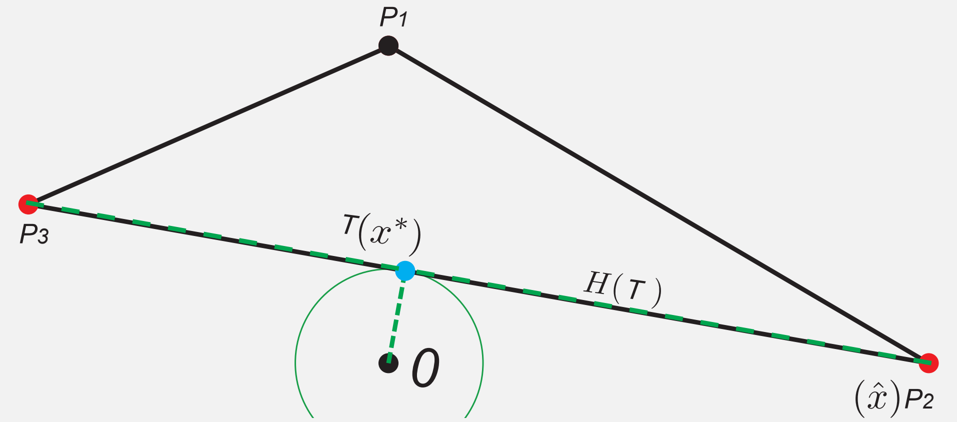
$Q = P = \{p_1, p_2, p_3\}$. Line 14: $S = y = \mathrm{argmin}_{x \in \mathrm{conv}\, Q \cap [x^*, x_0]} \|x - x_0\|_2$ where x_0 is 0 and x^* is R here. Thus, y lies on the boundary of $\mathrm{conv}\, Q$. Note, $\|y\|_2 < \|x^*\|_2$ since $x^* \in \mathrm{conv}\, Q$, $\|x_0\|_2 < \|x^*\|_2$.
Line 15: Delete p_1 from Q since not on face where $y = S$ lies. $Q = \{p_2, p_3\}$ after Line 15. We still have $y = S \in \mathrm{conv}\, Q$ for the updated Q. Line 16: $x^* \leftarrow y$, retain invariant $x^* \in \mathrm{conv}\, Q$, and again have $\|x^*\|_2 = \|x^*\|_2 < \|x^*\|$ strictly.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



$Q = \{p_2, p_3\}$, and so $x_0 = T$ computed in Line 9 is the min-norm point in $\mathrm{aff}\, Q$. We also have $x_0 \in \mathrm{conv}\, Q$ in Line 10 so we assign $x^* \leftarrow x_0$ in Line 11 and break.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



$H(T)$ separates P from the origin in Line 4, and therefore is a supporting hyperplane, and therefore x^* is the min-norm point in $\text{conv}\, P$, so we return with x^*.

Condition for Min-Norm Point

Theorem 20.5.1

$P = \{p_1, p_2, \dots, p_m\}$, $x^* \in \text{conv}\, P$ *is the min. norm point in* $\text{conv}\, P$ *iff*

$$p_i^\intercal x^* \geq \|x^*\|_2^2 \quad \forall i = 1, \cdots, m. \tag{20.34}$$

Proof.

- Assume x^* is the min-norm point, let $y \in \text{conv}\, P$, and $0 \leq \theta \leq 1$.
- Then $z \triangleq x^* + \theta(y - x^*) = (1-\theta)x^* + \theta y \in \text{conv}\, P$, and

$$\|z\|_2^2 = \|x^* + \theta(y - x^*)\|_2^2 \tag{20.35}$$

$$= \|x^*\|_2^2 + 2\theta(x^{*\intercal} y - x^{*\intercal} x^*) + \theta^2 \|y - x^*\|_2^2 \tag{20.36}$$

- It is possible for $\|z\|_2^2 < \|x^*\|_2^2$ for small θ, unless $x^{*\intercal} y \geq x^{*\intercal} x^*$ for all $y \in \text{conv}\, P \Rightarrow$ Equation (20.34).
- Conversely, given Eq (20.34), and given that $y = \sum_i \lambda_i p_i \in \text{conv}\, P$,

$$y^\intercal x^* = \sum_i \lambda_i p_i^\intercal x^* \geq \sum_i \lambda_i x^{*\intercal} x^* = x^{*\intercal} x^* \tag{20.37}$$

implying that $\|z\|_2^2 > \|x^*\|_2^2$ in Equation 20.36 for arbitrary $z \in \text{conv}\, P$. □

The set Q is always affinely independent

Lemma 20.5.2

The set Q in the MN Algorithm is always affinely independent.

Proof.

- Q is of course affinely independent when there is at most one point in it (e.g., after Line 2).
- After the initialization, it changes only by deletion of points, or adding a single point. Deletion does not change the independence.
- Before adding $\hat{x}$ at Line 7, we know x^* is the minimum norm point in $\text{aff}\, Q$ (since we break only at Line 12).
- Therefore, x^* is normal to $\text{aff}\, Q$, which implies $\text{aff}\, Q \subseteq H(x^*)$.
- Since $\hat{x} \notin H(x^*)$ chosen at Line 6, we have $\hat{x} \notin \text{aff}\, Q$.
- $\therefore$ update $Q \cup \{\hat{x}\}$ at Line 7 is affinely independent as long as Q is. □

Thus, by Lemma 20.5.2, we have for any $x \in \text{aff}\, Q$ such that $x = \sum_i w_i q_i$ with $\sum_i w_i = 1$, the weights w_i are uniquely determined.

The set Q is never too large

Lemma 20.5.3

The set Q in the MN Algorithm has size never more than $n + 1$.

Proof.

This is immediate, since Q is always affinely independent, and in $\mathbb{R}^V$, an affinely independent set can have at most $n + 1$ entries, with $|V| = n$. □

Minimum Norm in an affine set

- Line 9 of the algorithm requires $x_0 \leftarrow \min_{x \in \text{aff}\, Q} \|x\|_2$.
- When Q is affinely independent, this is relatively easy.
- Let Q represent $n \times k$ matrix with points as columns $q \in Q$. The following is solvable with matrix inversion/linear solver, where $x = Qw$:

$$\text{minimize} \qquad \|x\|_2^2 = w^\intercal Q^\intercal Q w \tag{20.38}$$

$$\text{subject to} \qquad \mathbf{1}^\intercal w = 1 \tag{20.39}$$

- Form Lagrangian $w^\intercal Q^\intercal Q w + 2\lambda(\mathbf{1}^\intercal w - 1)$, and differentiating w.r.t. λ and w, and setting to zero, we get:

$$\mathbf{1}^\intercal w = 1 \tag{20.40}$$

$$Q^\intercal Q w + \lambda \mathbf{1} = 0 \tag{20.41}$$

- $k+1$ variables and k unknowns, solvable with linear solver with matrices

$$\begin{bmatrix} 0 & \mathbf{1}^\intercal \\ \mathbf{1} & Q^\intercal Q \end{bmatrix} \begin{bmatrix} \lambda \\ w \end{bmatrix} = \begin{bmatrix} 1 \\ \mathbf{0} \end{bmatrix} \tag{20.42}$$

- Thanks to Q being affine, matrix on l.h.s. is invertable.

Minimum Norm in an affine set

- Note, this also solves Line 10, since feasibility requires $\sum_i w_i = 1$, we need only check $w \geq 0$ to ensure $x_0 = \sum_i w_i q_i \in \text{conv}\, Q$.
- In fact, a feature of the algorithm (in Wolfe's 1976 paper) is that we keep the convex coefficients $\{w_i\}_i$ where $x^* = \sum_i w_i p_i$ of x^* and from this vector. We also keep v such that $x_0 = \sum_i v_i q_i$ for points $q_i \in Q$, from Line 9.
- Given w and v, we can also easily solve Lines 14 and 15 (see "Step 3" on page 133 of Wolfe-1976, which also defines numerical tolerances).
- We have yet to see how to efficiently solve Lines 4 and 6, however.

MN Algorithm finds the MN point in finite time.

Theorem 20.5.4

The MN Algorithm finds the minimum norm point in $\operatorname{conv} P$ *after a finite number of iterations of the major loop.*

Proof.

- In minor loop, we always have $x^* \in \operatorname{conv} Q$, since whenever Q is modified, x^* is updated as well (Line 16) such that the updated x^* remains in new $\operatorname{conv} Q$.
- Hence, every time x^* is updated (in minor loop), its norm never increases, i.e., before Line 11, $\|x_0\|_2 \leq \|x^*\|_2$ since $x^* \in \operatorname{aff} Q$ and $x_0 = \min_{x \in \operatorname{aff} Q} \|x\|_2$. Similarly, before Line 16, $\|y\|_2 \leq \|x^*\|_2$, since invariant $x^* \in \operatorname{conv} Q$ but while $x_0 \in \operatorname{aff} Q$, we have $x_0 \notin \operatorname{conv} Q$, and $\|x_0\|_2 < \|x^*\|_2$.

...

MN Algorithm finds the MN point in finite time.

... proof of Theorem 20.5.4 continued.

- Moreover, there can be no more iterations within a minor loop than the dimension of $\operatorname{conv} Q$ for the initial Q given to the minor loop initially at Line 8 (dimension of $\operatorname{conv} Q$ is $|Q| - 1$ since Q is affinely independent).
- Each iteration of the minor loop removes at least one point from Q in Line 15.
- When Q reduces to a singleton, the minor loop always terminates.
- Thus, the minor loop terminates in finite number of iterations, at most dimension of Q.
- In fact, total number of iterations of minor loop in entire algorithm is at most number of points in P since we never add back in points to Q that have been removed.

...

MN Algorithm finds the MN point in finite time.

. . . proof of Theorem 20.5.4 continued.

- Each time Q is augmented with $\hat{x}$ at Line 7, followed by updating x^* with x_0 at Line 11, (i.e., when the minor loop returns with only one iteration), $\|x^*\|_2$ strictly decreases from what it was before.
- To see this, consider $x^* + \theta(\hat{x} - x^*)$ where $0 \le \theta \le 1$. Since both $\hat{x}, x^* \in \operatorname{conv} Q$, we have $x^* + \theta(\hat{x} - x^*) \in \operatorname{conv} Q$.
- Therefore, we have $\|x^* + \theta(\hat{x} - x^*)\|_2 \ge \|x_0\|_2$, which implies

$$\begin{aligned}\|x^* + \theta(\hat{x} - x^*)\|_2^2 &= \|x^*\|_2^2 + 2\theta\left((x^*)^\top \hat{x} - \|x^*\|_2^2\right) + \theta^2 \|\hat{x} - x^*\|_2^2 \\ &\ge \|x_0\|_2^2 \end{aligned} \tag{20.43}$$

and from Line 6, $\hat{x}$ is on the same side of $H(x^*)$ as the origin, i.e. $(x^*)^\top \hat{x} < \|x^*\|_2^2$, so middle term of r.h.s. of equality is negative.

. . .

MN Algorithm finds the MN point in finite time.

. . . proof of Theorem 20.5.4 continued.

- Therefore, for sufficiently small θ, specifically for

$$\theta < \frac{2\left(\|x^*\|_2^2 - (x^*)^\top \hat{x}\right)}{\|\hat{x} - x^*\|_2^2} \tag{20.44}$$

we have that $\|x^*\|_2^2 > \|x_0\|_2^2$.

- For a similar reason, we have $\|x^*\|_2$ strictly decreases each time Q is updated at Line 7 and followed by updating x^* with y at Line 16.
- Therefore, in each iteration of major loop, $\|x^*\|_2$ strictly decreases, and the MN Algorithm must terminate and it can only do so when the optimal is found.

□

Line: 6: Finding $\hat{x} \in P$ on the near side of $H(x^*)$

- The "near" side means the side that contains the origin.
- Ideally, find $\hat{x}$ such that the reduction of $\|x^*\|_2$ is maximized to reduce number of major iterations.
- From Eqn. 20.43, reduction on norm is lower-bounded:

$$\Delta = \|x^*\|_2^2 - \|x_0\|_2^2 \geq 2\theta\left(\|x^*\|_2^2 - (x^*)^\top \hat{x}\right) - \theta^2 \|\hat{x} - x^*\|_2^2 \triangleq \underline{\Delta} \tag{20.45}$$

- When $0 \leq \theta < \frac{2\left(\|x^*\|_2^2 - (x^*)^\top \hat{x}\right)}{\|\hat{x}-x^*\|_2^2}$, we can get the maximal value of the lower bound, over θ, as follows:

$$\max_{0 \leq \theta < \frac{2\left(\|x^*\|_2^2 - (x^*)^\top \hat{x}\right)}{\|\hat{x}-x^*\|_2^2}} \underline{\Delta} = \left(\frac{\|x^*\|_2^2 - (x^*)^\top \hat{x}}{\|\hat{x} - x^*\|_2}\right)^2 \tag{20.46}$$

Line: 6: Finding $\hat{x} \in P$ on the near side of $H(x^*)$

- To maximize lower bound of norm reduction at each major iteration, want to find an $\hat{x}$ such that the above lower bound (Equation 20.46) is maximized.
- That is, we want to find

$$\hat{x} \in \operatorname*{argmax}_{x \in P} \left(\frac{\|x^*\|_2^2 - (x^*)^\top x}{\|x - x^*\|_2}\right)^2 \tag{20.47}$$

to ensure that a large norm reduction is assured.
- This problem, however, is at least as hard as the MN problem itself as we have a quadratic term in the denominator.

Line: 6: Finding $\hat{x} \in P$ on the near side of $H(x^*)$

- As a surrogate, we maximize numerator in Eqn. 20.47, i.e., find

$$\hat{x} \in \underset{x \in P}{\operatorname{argmax}} \|x^*\|_2^2 - (x^*)^\top x = \underset{x \in P}{\operatorname{argmin}} (x^*)^\top x, \tag{20.48}$$

- Intuitively, by solving the above, we find $\hat{x}$ such that it has the largest "distance" to the hyperplane $H(x^*)$, and this is exactly the strategy used in the Wolfe-1976 algorithm.
- Also, solution $\hat{x}$ in Line 6 can be used to determine if hyperplane $H(x^*)$ separates $\operatorname{conv} P$ from the origin (Line 4): if the point in P having greatest distance to $H(x^*)$ is not on the side where origin lies, then $H(x^*)$ separates $\operatorname{conv} P$ from the origin.
- Mathematically and theoretically, we terminate the algorithm if

$$(x^*)^\top \hat{x} \geq \|x^*\|_2^2, \tag{20.49}$$

where $\hat{x}$ is the solution of Eq. 20.48.

Line: 6: Finding $\hat{x} \in P$ on the near side of $H(x^*)$

- In practice,the above optimality test might never hold numerically. Hence, as suggested by Wolfe, we introduce a tolerance parameter $\epsilon > 0$, and terminates the algorithm if

$$(x^*)^\top \hat{x} > \|x^*\|_2^2 - \epsilon \max_{x \in Q} \|x\|_2^2 \tag{20.50}$$

- When $\operatorname{conv} P$ is a submodular base polytope (i.e., $\operatorname{conv} P = B_f$ for a submodular function f), then the problem in Eqn 20.48 can be solved efficiently by Edmonds's greedy algorithm (even though there may be an exponential number of extreme points).
- Edmond's greedy algorithm, therefore, solves both Line 4 and Line 6 simultaneously.
- Hence, Edmonds's discovery is one of the main reasons that the MN algorithm is applicable to submodular function minimization.

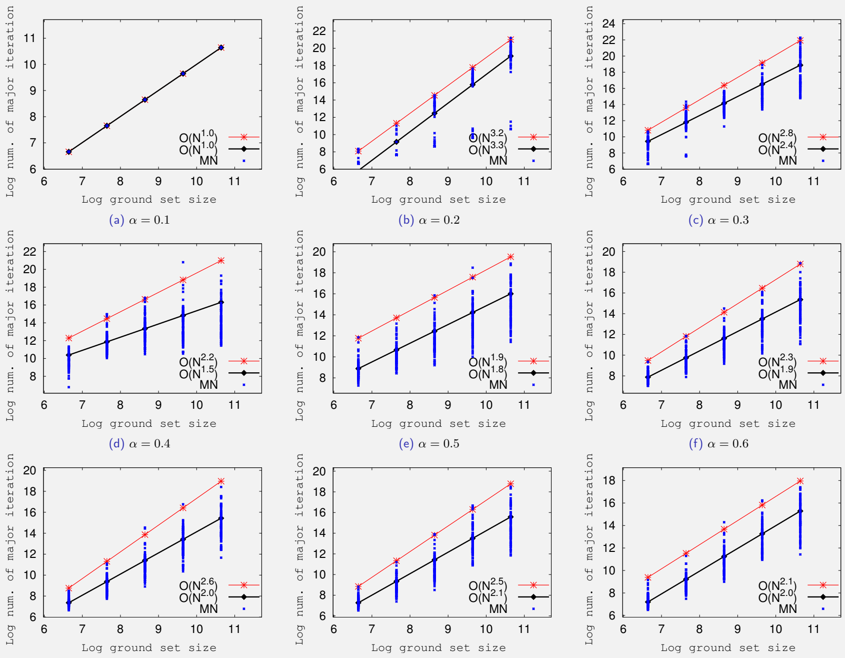
MN Algorithm Complexity

- The currently fastest strongly polynomial combinatorial algorithm for SFM achieves a running time of $O(n^5 T + n^6)$ (Orlin'09) where T is the time for function evaluation, far from practical for large problem instances.
- Fujishige & Isotani report that MN algorithm is fast in practice, but they use only a limited set of submodular functions.
- Complexity of MN Algorithm is still an unsolved problem.
- Obvious facts:
  - each major iteration requires $O(n)$ function oracle calls
  - complexity of each major iteration could be at least $O(n^3)$ due to the affine projection step (solving a linear system).
  - Therefore, the complexity of each major iteration is

$$O(n^3 + n^{1+p})$$

    where each function oracle call requires $O(n^p)$ time.
- Since the number of major iterations required is unknown, the complexity of MN is also unknown.

MN Algorithm Empirical Complexity



(a) $\alpha = 0.1$ (b) $\alpha = 0.2$ (c) $\alpha = 0.3$

(d) $\alpha = 0.4$ (e) $\alpha = 0.5$ (f) $\alpha = 0.6$

(g) $\alpha = 0.7$ (h) $\alpha = 0.8$ (i) $\alpha = 0.9$

Figure: The number of major iteration for $f(S) = -m_1(S) + 100 \cdot (w_1(\mathcal{N}(S)))^\alpha$. The red lines are the linear interpolations of the worst case points, and the black lines are the linear interpolations of the average case points. From Lin&Bilmes 2014 (unpublished)

MN Algorithm Complexity

- A lower bound complexity of the Fujishige-Wolfe min-norm procedure has not yet been established.
- In 2014, Chakrabarty, Jain, and Kothari in their NIPS 2014 paper "Provable Submodular Minimization using Wolfe's Algorithm" showed a pseudo-polynomial time bound of $O(n^7 g_f^2)$ where $n = |V|$ is the ground set, and g_f is the maximum gain of a particular function f.
- This is pseudo-polynomial since it depends on the function values.
- In 2020, in De Loera et. al. "The Minimum Euclidean-Norm Point in a Convex Polytope: Wolfe's Combinatorial Algorithm is Exponential", 2020, SIAM J. Computing, gave an example where the Wolfe procedure can run in exponential time, although this is not for the submodular polytope B_f that applies here, this is left as an open question. Hence, the lower bound complexity of the Fujishige-Wolfe procedure is still unknown.

Frank-Wolfe vs. Fujishige-Wolfe

Another algorithm we could use to find the min-norm is M. Frank & P. Wolfe "An algorithm for quadratic programming", 1956 (conditional gradient descent) for constrained convex minimization of convex function $f : \mathcal{D} \to \mathbb{R}$.

```
  Input  : Convex set $\mathcal{D} \subseteq \mathbb{R}^n$, convex $f : \mathcal{D} \to \mathbb{R}$, $x_0 \in \mathcal{D}$, $\tau > 0$
  Output: $x^* \in \mathcal{D}$, the minimizer of $f$ on $\mathcal{D}$.
1 $k \leftarrow 0$ and start with $x_0 \in \mathcal{D}$ ;
2 Let $s_k$ solve $\min\langle s, \nabla f(x_k)\rangle$ s.t. $s \in \mathcal{D}$ ;
3 Let $\lambda_k \in [0,1]$ minimize $f(\lambda s_k + (1-\lambda)x_k)$ ;
4 $x_{k+1} \leftarrow \lambda_k s_k + (1-\lambda_k)x_k$, $k \leftarrow k+1$ ;
5 Goto line 2 if $\|x_{k+1} - x_k\| > \tau$ ;
6 $x^* \leftarrow x_{k+1}$
```

- Above can also be used minimize Lovász extension, primal approach to SFM.
- The Frank-Wolfe and Fujishige-Wolfe are distinct procedures although Wolfe is the same person.

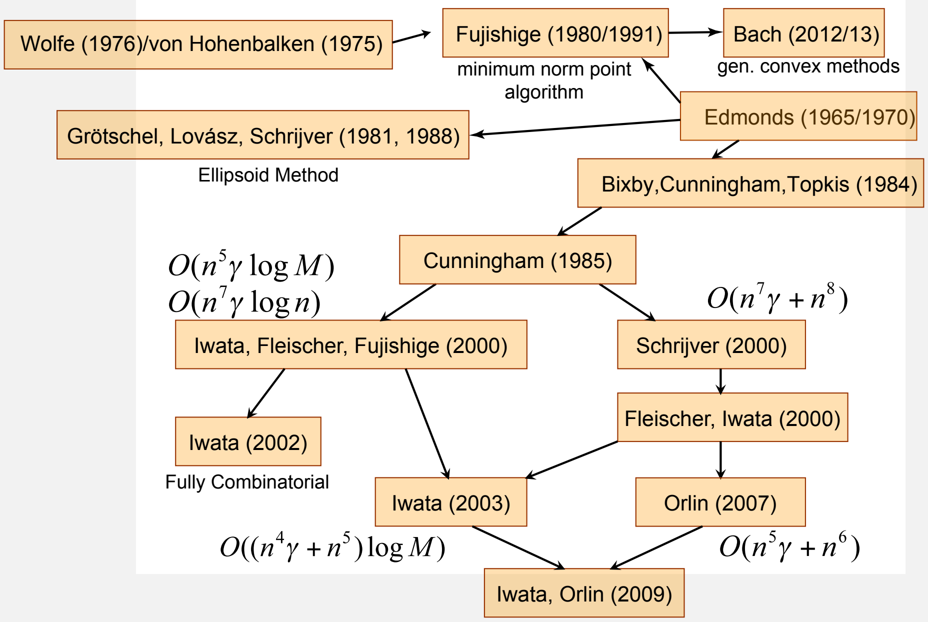
Other algorithms for approximate and/or pseudo-polynomial SFM

- In 2015, Lee, Sidford, and Wong, gave pseudo-poly algorithms for SFM that run in $O(n^2 \log nM\text{EO} + n^2 \log^{O(1)} nM)$ time nad $O(n^3 \log^2 n\text{EO} + n^4 \log^{O(1)} n)$ time respectively.
- In 2017, in Chakrabarty, Lee, Sidford, and Wong "Subquadratic Submodular Function Minimization", this was improved. I.e., for real-valued submodular functions, it runs in $\tilde{O}(n^{5/3}\text{EO}/\epsilon^3)$ giving an ϵ-additive approximate solution.
- In 2020, Axelrod, Liu, and Sidford "Near-optimal Approximate Discrete and Continuous Submodular Function Minimization" give a randomized algorithm that for a submodular function in the range $[-1, 1]$ runs in $\tilde{O}(n/\epsilon^2)$ for an ϵ-additive approximation to SFM. This can also be used to approximately minimize smooth DR-submodular (and not necessarily convex) functions.
- In 2020, Balkanski and Singer, "A Lower Bound for Parallel Submodular Minimization", give "adaptivity lower bounds" (see the paper for what this is) for the parallel complexity of SFM.
- Thus, quite a bit of recent work, and more soon to follow.

SFM Summary

modified from S. Iwata's slides

General Submodular Function Minimization



Wolfe (1976)/von Hohenbalken (1975)

Fujishige (1980/1991)

minimum norm point algorithm

Bach (2012/13)

gen. convex methods

Edmonds (1965/1970)

Grötschel, Lovász, Schrijver (1981, 1988)

Ellipsoid Method

Bixby,Cunningham,Topkis (1984)

Cunningham (1985)

$O(n^5\gamma \log M)$

$O(n^7\gamma \log n)$

$O(n^7\gamma + n^8)$

Iwata, Fleischer, Fujishige (2000)

Schrijver (2000)

Fleischer, Iwata (2000)

Iwata (2002)

Fully Combinatorial

Iwata (2003)

Orlin (2007)

$O((n^4\gamma + n^5)\log M)$

$O(n^5\gamma + n^6)$

Iwata, Orlin (2009)

Recent SFM Strongly Polynomial Summary

Table taken from Haotian Jiang's 2020 paper

Authors	Year	Oracle Complexity	Remarks
Grötschel, Lovász, Schrijver [GLS81, GLS88]	1981,88	$O(n^5)$ [McC05]	first strongly
Schrijver [Sch00]	2000	$O(n^8)$	first comb. strongly
Iwata, Fleischer, Fujishige [IFF01]	2000	$O(n^7 \log(n))$	first comb. strongly
Fleischer, Iwata [FI03]	2000	$O(n^7)$	
Iwata [Iwa03]	2002	$O(n^6 \log(n))$	
Vygen [Vyg03]	2003	$O(n^7)$	
Orlin [Orl09]	2007	$O(n^5)$	
Iwata, Orlin [IO09]	2009	$O(n^5 \log(n))$	
Lee, Sidford, Wong [LSW15]	2015	$O(n^3 \log^2(n))$	current best strongly
Lee, Sidford, Wong [LSW15]	2015	$O(n^3 \log(n))$	exponential time
Dadush, Végh, Zambelli [DVZ18]	2018	$O(n^3 \log^2(n))$	close to best
Haotain Jiang	2020	$O(n^3)$	currently best

Submodularity

This is only the beginning. Submodularity is still gaining in popularity in machine learning and data science, it has both a rich and long past and a promising future.