Submodular Functions, Optimization, and Applications to Machine Learning

— Spring Quarter, Lecture 18 —

http://j.ee.washington.edu/~bilmes/classes/ee596b_spring_2014/

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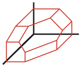
$$f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$$

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



Cumulative Outstanding Reading

- Good references for today: Schrijver-2003, Oxley-1992/2011, Welsh-1973, Goemans-2010, Cunningham-1984, Edmonds-1969, Choquet-1955, Grabisch/Marichal/Mesiar/Pap "Aggregation Functions", Lovász-1983, Bach-2011.
- Read Tom McCormick's overview paper on SFM `http://people.commerce.ubc.ca/faculty/mccormick/sfmchap8a.pdf`
- Read chapters 1 - 4 from Fujishige book.
- Matroid properties `http://www-math.mit.edu/~goemans/18433S09/matroid-notes.pdf`
- Read lecture 14 slides on lattice theory at our web page (`http://j.ee.washington.edu/~bilmes/classes/ee596b_spring_2014/`)
- Wolfe "Finding the Nearest Point in a Polytope", 1976.
- Fujishige & Isotani, "A Submodular Function Minimization Algorithm Based on the Minimum-Norm Base", 2009.

Announcements, Assignments, and Reminders

- Weekly Office Hours: Wednesdays, 5:00-5:50, or by skype or google hangout (email me).

Class Road Map - IT-I

- L1 (3/31): Motivation, Applications, & Basic Definitions
- L2: (4/2): Applications, Basic Definitions, Properties
- L3: More examples and properties (e.g., closure properties), and examples, spanning trees
- L4: proofs of equivalent definitions, independence, start matroids
- L5: matroids, basic definitions and examples
- L6: More on matroids, System of Distinct Reps, Transversals, Transversal Matroid, Matroid and representation
- L7: Dual Matroids, other matroid properties, Combinatorial Geometries
- L8: Combinatorial Geometries, matroids and greedy, Polyhedra, Matroid Polytopes,
- L9: From Matroid Polytopes to Polymatroids.
- L10: Polymatroids and Submodularity
- L11: More properties of polymatroids, SFM special cases
- L12: polymatroid properties, extreme points polymatroids,
- L13: sat, dep, supp, exchange capacity, examples
- L14: Lattice theory: partially ordered sets; lattices; distributive, modular, submodular, and boolean lattices; ideals and join irreducibles.
- L15: Supp, Base polytope, polymatroids and entropic Venn diagrams, exchange capacity,
- L16: proof that minimum norm point yields min of submodular function, and the lattice of minimizers of a submodular function, Lovasz extension
- L17: Lovasz extension, Choquet Integration, more properties/examples of Lovasz extension, convex minimization and SFM.
- L18: Lovasz extension examples and structured convex norms, The Min-Norm Point Algorithm detailed.
- L19: symmetric submodular function minimization, maximizing monotone submodular function w. card constraints.
- L20: maximizing monotone submodular function w. other constraints, non-monotone maximization.

Finals Week: June 9th-13th, 2014.

Choquet integral

Definition 18.2.1

Let f be any capacity on E and $w \in \mathbb{R}_+^E$. The Choquet integral (1954) of w w.r.t. f is defined by

$$C_f(w) = \sum_{i=1}^{m} (w_{e_i} - w_{e_{i+1}}) f(E_i) \tag{18.12}$$

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

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

$$C_f(w) = \sum_{i=1}^{m} w(e_i)(f(E_i) - f(E_{i-1})) \tag{18.13}$$

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

Lovász extension, as integral

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

$$\tilde{f}(w) = \sum_{i=1}^{m} w(e_i) f(e_i | E_{i-1}) = \sum_{i=1}^{m} \lambda_i f(E_i) \tag{18.22}$$

$$= \sum_{i=1}^{m-1} f(E_i)(w(e_i) - w(e_{i+1})) + f(E) w(e_m) \tag{18.23}$$

$$= \int_{\min\{w_1,\ldots,w_m\}}^{+\infty} f(\{w \geq \alpha\}) d\alpha + f(E) \min\{w_1, \ldots, w_m\} \tag{18.24}$$

$$= \int_{0}^{+\infty} f(\{w \geq \alpha\}) d\alpha + \int_{-\infty}^{0} [f(\{w \geq \alpha\}) - f(E)] d\alpha \tag{18.25}$$

Lovász extension properties

- Using the above, have the following (some of which we've seen):

Theorem 18.2.2

Let $f, g : 2^E \to \mathbb{R}$ be normalized ($f(\emptyset) = g(\emptyset) = 0$). Then

1. *Superposition of LE operator: Given f and g with Lovász extensions $\tilde{f}$ and $\tilde{g}$ then $\tilde{f} + \tilde{g}$ is the Lovász extension of $f + g$ and $\lambda \tilde{f}$ is the Lovász extension of λf for $\lambda \in \mathbb{R}$.*
2. *If $w \in \mathbb{R}_+^E$ then $\tilde{f}(w) = \int_0^{+\infty} f(\{w \geq \alpha\}) d\alpha$.*
3. *For $w \in \mathbb{R}^E$, and $\alpha \in \mathbb{R}$, we have $\tilde{f}(w + \alpha \mathbf{1}_E) = \tilde{f}(w) + \alpha f(E)$.*
4. *Positive homogeneity: I.e., $\tilde{f}(\alpha w) = \alpha \tilde{f}(w)$ for $\alpha \geq 0$.*
5. *For all $A \subseteq E$, $\tilde{f}(\mathbf{1}_A) = f(A)$.*
6. *f symmetric as in $f(A) = f(E \setminus A), \forall A$, then $\tilde{f}(w) = \tilde{f}(-w)$ ($\tilde{f}$ is even).*
7. *Given partition $E^1 \cup E^2 \cup \dots \cup E^k$ of E and $w = \sum_{i=1}^k \gamma_i \mathbf{1}_{E_k}$ with $\gamma_1 \geq \gamma_2 \geq \dots \geq \gamma_k$, and with $E^{1:i} = E^1 \cup E^2 \cup \dots \cup E^i$, then $\tilde{f}(w) = \sum_{i=1}^k \gamma_i f(E^i | E^{1:i-1}) = \sum_{i=1}^{k-1} f(E^{1:i})(\gamma_i - \gamma_{i+1}) + f(E)\gamma_k$.*

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

In fact, we have:

Theorem 18.2.5

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

Proof.

- First, since $\tilde{f}(\mathbf{1}_A) = f(A), \forall A \subseteq V$, we clearly have $\min\{f(A)|A \subseteq V\} = \min_{w\in\{0,1\}^E} \tilde{f}(w) \geq \min_{w\in[0,1]^E} \tilde{f}(w)$.
- 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, $\sum_i \lambda_i = w(e_1) \leq 1$.

...

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

- If $w_1 \geq w_2$, then

$$\begin{aligned} \tilde{f}(w) &= w_1 f(\{1\}) + w_2 f(\{2\}|\{1\}) && (18.1) \\ &= (w_1 - w_2) f(\{1\}) + w_2 f(\{1, 2\}) && (18.2) \end{aligned}$$

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- If $w_1 \leq w_2$, then

$$\tilde{f}(w) = w_2 f(\{2\}) + w_1 f(\{1\}|\{2\}) \tag{18.3}$$

$$= (w_2 - w_1) f(\{2\}) + w_1 f(\{1, 2\}) \tag{18.4}$$

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- If $w_1 \geq w_2$, then

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&= (w_1 - w_2) f(\{1\}) + w_2 f(\{1,2\}) && (18.6)\\
&= \frac{1}{2} f(1)(w_1 - w_2) + \frac{1}{2} f(1)(w_1 - w_2) && (18.7)\\
&\quad + \frac{1}{2} f(\{1,2\})(w_1 + w_2) - \frac{1}{2} f(\{1,2\})(w_1 - w_2) && (18.8)\\
&\quad + \frac{1}{2} f(2)(w_1 - w_2) + \frac{1}{2} f(2)(w_2 - w_1) && (18.9)
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\end{aligned}$$

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

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

- This gives, for general w_1, w_2, that

$$\tilde{f}(w) = \frac{1}{2}\left(f(\{1\}) + f(\{2\}) - f(\{1,2\})\right)|w_1 - w_2| \tag{18.10}$$

$$+ \frac{1}{2}\left(f(\{1\}) - f(\{2\}) + f(\{1,2\})\right)w_1 \tag{18.11}$$

$$+ \frac{1}{2}\left(-f(\{1\}) + f(\{2\}) + f(\{1,2\})\right)w_2 \tag{18.12}$$

$$= -\left(f(\{1\}) + f(\{2\}) - f(\{1,2\})\right)\min\{w_1, w_2\} \tag{18.13}$$

$$+ f(\{1\})w_1 + f(\{2\})w_2 \tag{18.14}$$

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

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- Thus, if $f(A) = H(X_A)$ is the entropy function, we have $\tilde{f}(w) = H(e_1)w_1 + H(e_2)w_2 - I(e_1; e_2)\min\{w_1, w_2\}$ which must be convex in w, where $I(e_1; e_2)$ is the mutual information.
- This "simple" but general form of the Lovász extension with $m = 2$ can be useful.

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

- If $w_1 \geq w_2$, then

$$\tilde{f}(w) = w_1 f(\{1\}) + w_2 f(\{2\}|\{1\}) \tag{18.15}$$

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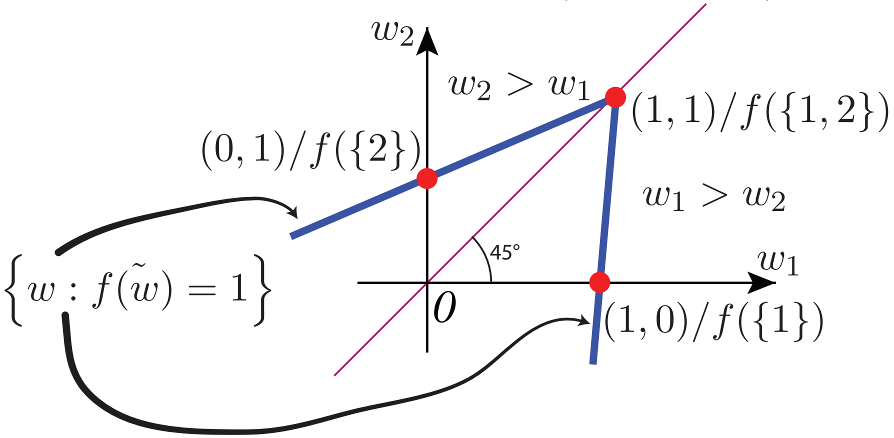
  - If $w = (1, 1)/f(\{1, 2\})$ then $\tilde{f}(w) = 1$.

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

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

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



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- Consider any submodular f' and $x \in B_{f'}$. Then $f(A) = f'(A) - x(A)$ is submodular, and moreover $f(E) = f'(E) - x(E) = 0$.
- Hence, from $\tilde{f}(w + \alpha \mathbf{1}_E) = \tilde{f}(w) + \alpha f(E)$, we have that $\tilde{f}(w + \alpha \mathbf{1}_E) = \tilde{f}(w)$.

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

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

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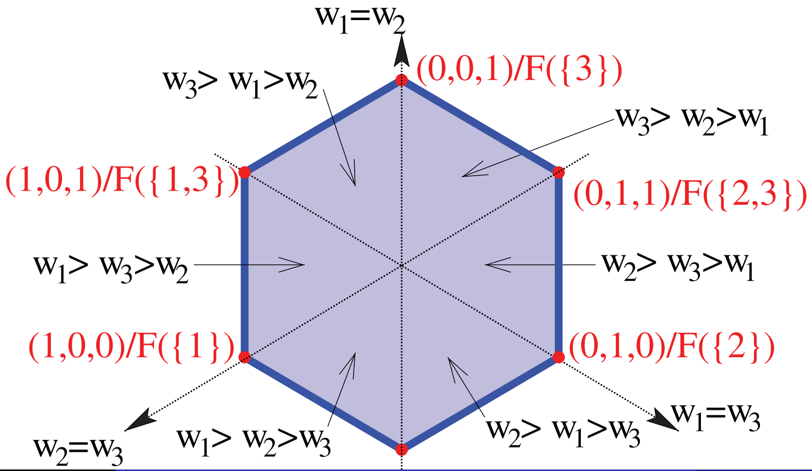
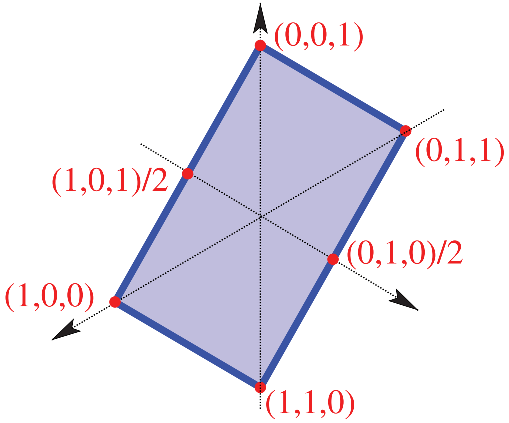


Example: $m = 3$, $E = \{1, 2, 3\}$

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



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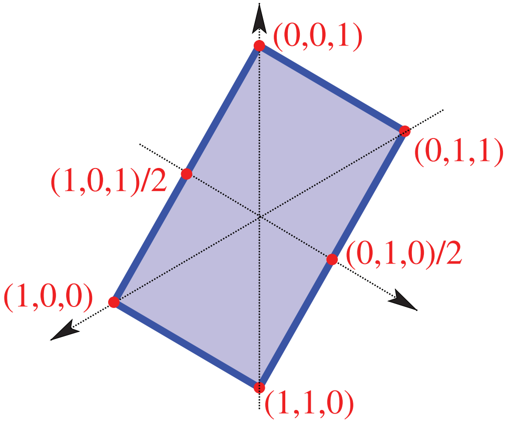
- Example 2 (from Bach-2011): $f(A) = |\mathbf{1}_{1 \in A} - \mathbf{1}_{2 \in A}| + |\mathbf{1}_{2 \in A} - \mathbf{1}_{3 \in A}|$
- This gives a "total variation" function for the Lovász extension, with $\tilde{f}(w) = |w_1 - w_2| + |w_2 - w_3|$, a prior to prefer piecewise-constant signals.



Total Variation Example

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

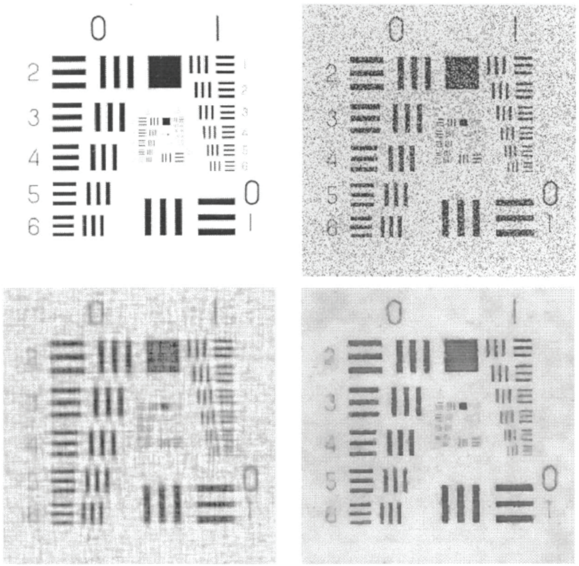


Fig. 3. (a) "Resolution Chart". (b) Noisy "Resolution Chart", SNR = 1.0. (c) Wiener filter reconstruction from (b). (d) TV reconstruction from (b).

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$$\tilde{f}(w) = \sum_{i=1}^{m} w(e_i)\big(g(M_i) - g(M_{i-1})\big) \tag{18.17}$$

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

$$\tilde{f}(w) = \sum_{i=1}^{m} w(e_i)\big(g(i) - g(i-1)\big) \tag{18.18}$$

Example: Lovász extension and cut functions

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

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$$\tilde{f}(w) = \sum_{i,j \in V} m_{ij} \max\{(w_i - w_j), 0\} \tag{18.20}$$

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- This is also a form of "total variation"

A few more Lovász extension examples

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

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

(thanks to K. Narayanan).

Supervised And Unsupervised Machine Learning

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

$$\min_{w \in \mathbb{R}^n} \frac{1}{m} \sum_{i=1}^m \ell(y_i, w^\intercal x_i) + \lambda \Omega(w), \tag{18.21}$$

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

$$\min_{w^1, \dots, w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^k, (w^k)^\intercal x_i) + \lambda \Omega(w^k), \tag{18.22}$$

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

$$\min_{x_1, \dots, x_m} \min_{w^1, \dots, w^k \in \mathbb{R}^n} \sum_{j=1}^k \frac{1}{m} \sum_{i=1}^m \ell(y_i^k, (w^k)^\intercal x_i) + \lambda \Omega(w^k), \tag{18.23}$$

Norms, sparse norms, and computer vision

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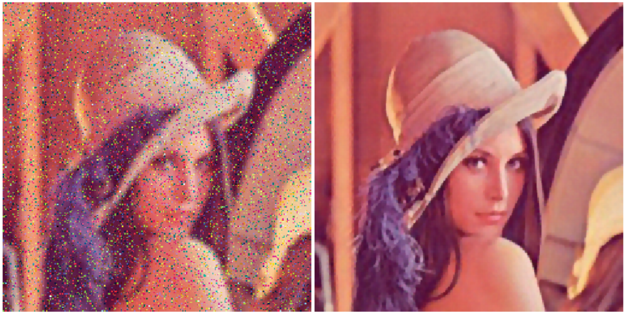
- Points of difference should be "sparse" (frequently zero).



(Rodriguez, 2009)

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- Submodular functions thus parameterize structured convex sparse norms via the Lovász-extension!
- Ex: total variation is Lovász-ext. of graph cut, but $\exists$ many more!

Lovász extension and norms

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

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- Hence, not all norms come from the Lovász extension of some submodular function.
- Similarly, not all convex functions are the Lovász extension of some submodular function.
- Bach-2011 has a complete discussion of this.

Review

The following four slides are review, and are from Lectures 12, 15, and 16.

A polymatroid function's polyhedron is a polymatroid.

Theorem 18.4.1

Let f be a submodular function defined on subsets of E. For any $x \in \mathbb{R}^E$, we have:

$$\textit{rank}(x) = \max\left(y(E) : y \leq x, y \in P_f\right) = \min\left(x(A) + f(E \setminus A) : A \subseteq E\right) \tag{18.5}$$

Essentially the same theorem as Theorem **??**. Taking $x = 0$ we get:

Corollary 18.4.2

Let f be a submodular function defined on subsets of E. $x \in \mathbb{R}^E$, we have:

$$\textit{rank}(0) = \max\left(y(E) : y \leq 0, y \in P_f\right) = \min\left(f(A) : A \subseteq E\right) \tag{18.6}$$

Min-Norm Point: Definition

- Restating what we saw before, we have:

$$\max\{y(E) | y \in P_f, y \leq 0\} = \min\{f(X) | X \subseteq V\} \tag{18.12}$$

- Consider the optimization:

$$\begin{aligned} &\text{minimize} && \|x\|_2^2 && (18.13a)\\ &\text{subject to} && x \in B_f && (18.13b)\end{aligned}$$

  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 and Submodular Function Minimization

- Given optimal solution x^* to the above, consider the quantities

$$\begin{aligned} y^* &= x^* \wedge 0 = (\min(x^*(e), 0) | e \in E) && (18.1)\\ A_- &= \{e : x^*(e) < 0\} && (18.2)\\ A_0 &= \{e : x^*(e) \leq 0\} && (18.3) \end{aligned}$$

- Thus, we immediately have that:

$$A_- \subseteq A_0 \qquad (18.4)$$

and that

$$x^*(A_-) = x^*(A_0) = y^*(A_-) = y^*(A_0) \qquad (18.5)$$

- It turns out, these quantities will solve the submodular function minimization problem, as we now show.
- The proof is nice since it uses the tools we've been recently developing.

Min-Norm Point and SFM

Theorem 18.4.1

*Let y^*, A_-, and A_0 be as given. Then y^* is a maximizer of the l.h.s. of Eqn. (**??**). Moreover, 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 can consider any $e \in E$ within $\text{dep}(x^*, e)$.
- Consider any pair (e, e') with $e' \in \text{dep}(x^*, e)$ and $e \in A_-$. 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

$$(x^* + \alpha \mathbf{1}_e - \alpha \mathbf{1}_{e'})(E) = x^*(E) + \alpha - \alpha = f(E) \qquad (18.1)$$

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

...

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):

$$\underset{w \in \mathbb{R}^V}{\text{minimize}} \; \tilde{f}(w) + \frac{1}{2}\|w\|_2^2 \tag{18.25}$$

$$\begin{aligned} &\text{maximize} && -\|x\|_2^2 && (18.26a) \\ &\text{subject to} && x \in B_f && (18.26b) \end{aligned}$$

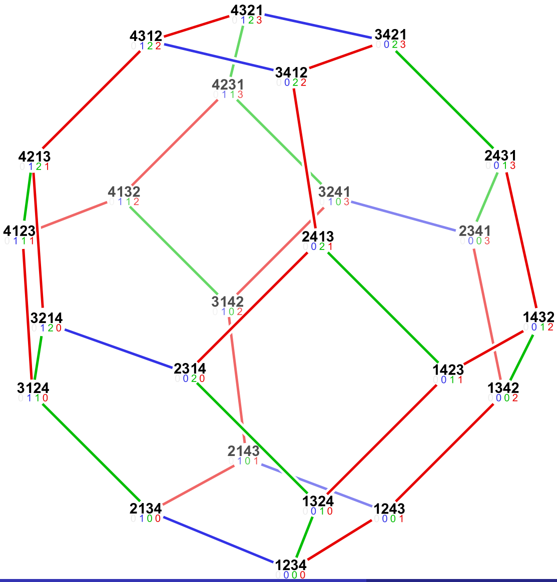
  where $B_f = P_f \cap \left\{x \in \mathbb{R}^V : x(V) = f(V)\right\}$ is the base polytope of submodular function f, and $\|x\|_2^2 = \sum_{e \in V} x(e)^2$ is squared 2-norm.
- Equation (18.25) is related to proximal methods to minimize the Lovász extension (see Parikh&Boyd, "Proximal Algorithms" 2013).
- Equation (18.26b) is solved by the minimum-norm point algorithm (Wolfe-1976, Fujishige-1984, Fujishige-2005, Fujishige-2011) is (as we will see) essentially an active-set procedure for quadratic programming, and uses Edmonds's greedy algorithm to make it efficient.
- Unknown worst-case running time, although in practice it usually performs quite well (see below).

Ex: 3D base B_f: permutahedron

- Consider submodular function $f : 2^V \to \mathbb{R}$ with $|V| = 4$, and for $X \subseteq V$, concave g,

$$f(X) = g(|X|)$$
$$= \sum_{i=1}^{|X|}(4 - i + 1)$$

- Then B_f is a 3D polytope, and in this particular case gives us a permutahedron with 24 distinct extreme points, on the right (from wikipedia).



Modified max-min theorem

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Theorem 18.4.1 (Edmonds-1970)

$$\min\{f(X) | X \subseteq E\} = \max\left\{x^-(E) | x \in B_f\right\} \tag{18.27}$$

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

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Proof.

$$\begin{aligned}
\min \{f(X) | X \subseteq E\} &= \min_{w \in [0,1]^E} \tilde{f}(w) = \min_{w \in [0,1]^E} \max_{x \in P_f} w^\intercal x && (18.28)\\
&= \min_{w \in [0,1]^E} \max_{x \in B_f} w^\intercal x && (18.29)\\
&= \max_{x \in B_f} \min_{w \in [0,1]^E} w^\intercal x && (18.30)\\
&= \max_{x \in B_f} x^-(E) && (18.31)
\end{aligned}$$

Convexity, Strong duality, and min/max swap

The min/max switch follows from strong duality. I.e., consider $g(w, x) = w^\intercal x$ and we have domains $w \in [0,1]^E$ and $x \in B_f$. then for any $(w, x) \in [0,1]^E \times B_f$, we have

$$\min_{w' \in [0,1]^E} g(w', x) \leq g(w, x) \leq \max_{x' \in B_f} g(w, x') \tag{18.32}$$

which means that we have weak duality

$$\max_{x \in B_f} \min_{w' \in [0,1]^E} g(w', x) \leq \min_{w \in [0,1]^E} \max_{x' \in B_f} g(w, x') \tag{18.33}$$

but since $g(w, x)$ is linear, we have strong duality, meaning

$$\max_{x \in B_f} \min_{w' \in [0,1]^E} g(w', x) = \min_{w \in [0,1]^E} \max_{x' \in B_f} g(w, x') \tag{18.34}$$

Alternate proof of modified max-min theorem

We start directly from Theorem 12.5.2.

$$\max\left(y(E) : y \le 0, y \in P_f\right) = \min\left(f(A) : A \subseteq E\right) \tag{18.35}$$

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

$$\begin{aligned}\max\left(y(E) : y \le 0, y \in P_f\right) &= \max\left(y^-(E) : y \le 0, y \in P_f\right) && (18.36)\\ &= \max\left(y^-(E) : y \in P_f\right) && (18.37)\\ &= \max\left(y^-(E) : y \in B_f\right) && (18.38)\end{aligned}$$

The first equality follows since $y \le 0$. For the second equality, clearly l.h.s. $\le$ r.h.s. Also, l.h.s. $\ge$ r.h.s. since the positive parts don't matter.

$$\begin{aligned}\max\left(y^-(E) : y \in P_f\right) &= \max\left(y^-(E) : y(A) \le f(A) \forall A\right) && (18.39)\\ &= \max\left(y^-(E) : y^-(A) + y^+(A) \le f(A) \forall A\right)\end{aligned}$$

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 **??**).

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

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

$$\max\{w^\intercal x | x \in P_f\} = \max\{w^\intercal x | x \in B_f\} \tag{18.40}$$

  since for all $x \in P_f$, there exists $y \geq x$ with $y \in B_f$.

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- For arbitrary $w \in \mathbb{R}^E$, greedy algorithm will also solve:

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- For arbitrary $w \in \mathbb{R}^E$, greedy algorithm will also solve:

$$\max \{w^\intercal x | x \in B_f\} \tag{18.41}$$

- Also, since

$$\min \{w^\intercal x | x \in B_f\} = -\max \{-w^\intercal x | x \in B_f\} \tag{18.42}$$

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

$$w(e_1) \leq w(e_2) \leq \dots \leq w(e_m) \tag{18.43}$$

will solve Equation (18.42).

$\max\{w^\intercal x | x \in B_f\}$ 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 12, 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.

Orthogonal x-containing hyperplane & convex/affine hulls

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

$$H(x) \triangleq \left\{ y \in \mathbb{R}^V \mid x^\intercal y = \|x\|_2^2 \right\} \tag{18.44}$$

Any set $\{y \in \mathbb{R}^V | x^\intercal y = c\}$ is orthogonal to the line from 0 to x. To also contain x, we need $\|x\|_2 \|x\|_2 \cos 0 = c$ giving $c = \|x\|_2^2$.

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

$$\operatorname{conv} P \triangleq \left\{ \sum_{i=1}^k \lambda_i p_i : \sum_i \lambda_i = 1, \ \lambda_i \geq 0, i \in [k] \right\}. \tag{18.45}$$

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  and for $Q = \{q_1, q_2, \dots, q_k\}$, with $q_i \in \mathbb{R}^V$, let $\text{aff}\, Q$ be the affine hull of Q, i.e.,

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  and for $Q = \{q_1, q_2, \dots, q_k\}$, with $q_i \in \mathbb{R}^V$, let $\text{aff}\, Q$ be the affine hull of Q, i.e.,

$$\text{aff}\, Q \triangleq \left\{ \sum_{i \in 1}^k \lambda_i q_i : \sum_{i=1}^k \lambda_i = 1 \right\} \supseteq \text{conv}\, Q. \tag{18.46}$$

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, $[x, y] = \text{conv}\,\{x, y\}$.

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- 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

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- 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:

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- Wolfe's algorithm is guaranteed terminating, and explicitly uses a representation of x as a convex combination of points in P
- Algorithm maintains a set of points $Q \subseteq P$, which is always assuredly *affinely independent*.

Fujishige-Wolfe Min-Norm Algorithm

- 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).

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- 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 $\operatorname{conv} P$.
1  $x^* \longleftarrow p_{i^*}$ where $p_{i^*} \in \operatorname{argmin}_{p \in P} \|p\|_2$      /* or choose it arbitrarily */ ;
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          $x_0 \longleftarrow \min_{x \in \operatorname{aff} Q} \|x\|_2$;
10         if $x_0 \in \operatorname{conv} Q$ then
11             $x^* \longleftarrow x_0$;
12             break;
13         else
14             $y \longleftarrow \min_{x \in \operatorname{conv} Q \cap [x^*, x_0]} \|x - x_0\|_2$;
15             Delete from $Q$ points not on the face of $\operatorname{conv} Q$ 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.

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- Algorithm maintains an invariant, namely that:

$$x^* \in \operatorname{conv} Q \subseteq \operatorname{conv} P, \tag{18.48}$$

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 $x_0 \in \operatorname{conv} Q$,
3. and true after Line 16 since $y \in \operatorname{conv} Q$ even after deleting points.

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- Note also for any $x^* \in \operatorname{conv} Q \subseteq \operatorname{conv} P$, we have

$$\min_{x \in \operatorname{aff} Q} \|x\|_2 \leq \min_{x \in \operatorname{conv} Q} \|x\|_2 \leq \|x^*\|_2 \tag{18.49}$$

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- There are six places that might be seemingly tricky or expensive: Line 4, Line 6, Line 9, Line 10, Line 14, and Line 15.

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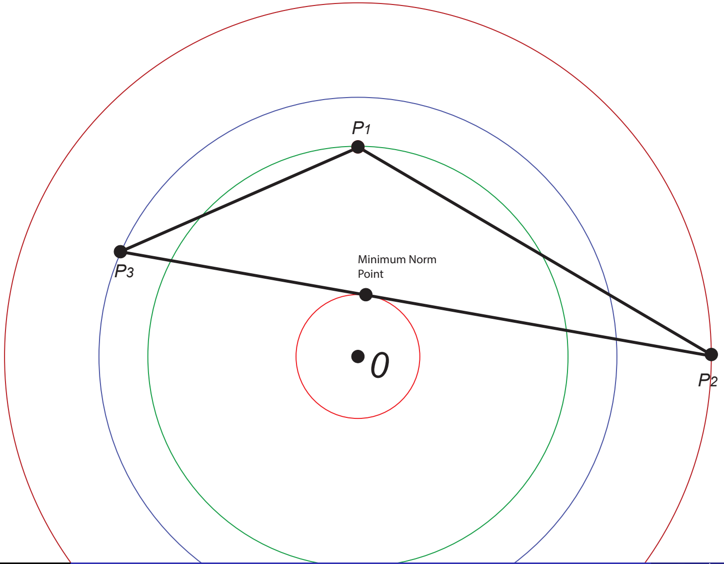
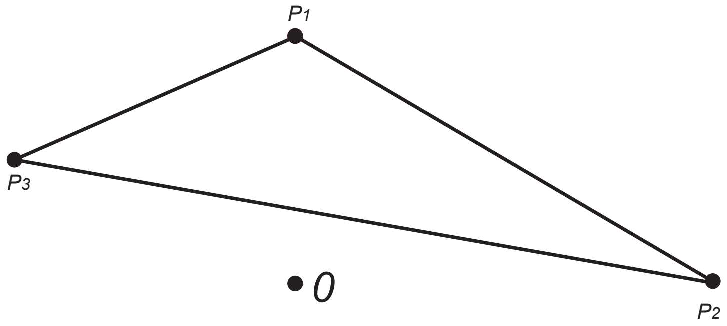
- There are six places that might be seemingly tricky or expensive: Line 4, Line 6, Line 9, Line 10, Line 14, and Line 15.
- We will consider each in turn, but first we do a geometric example.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example

Polytope, and circles concentric at 0.

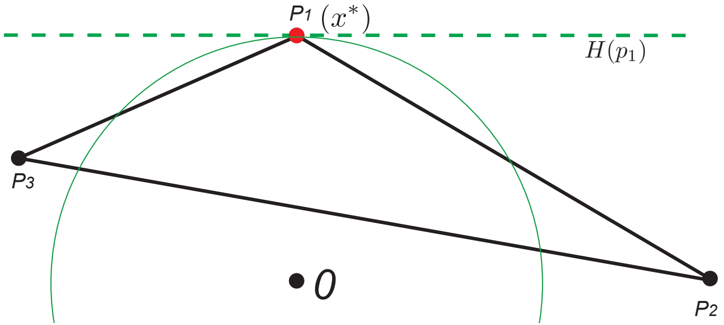


Fujishige-Wolfe Min-Norm algorithm: Geometric Example



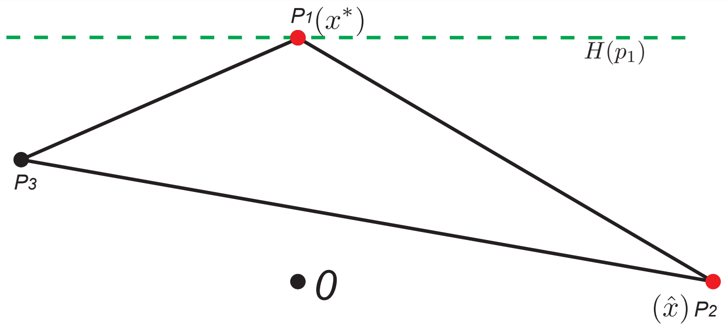
The initial polytope consisting of the convex hull of three points p_1, p_2, p_3, and the origin 0.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



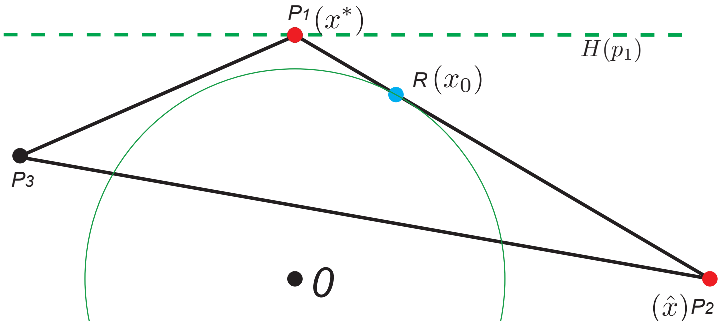
p_1 is the extreme point closest to 0 and so we choose it first, although we can choose any arbitrary extreme point as the initial point. We set $x^* \leftarrow p_1$ in Line 1, and $Q \leftarrow \{p_1\}$ in Line 2. $H(x^*) = H(p_1)$ (green dashed line) is not a supporting hyperplane of $\text{conv}(P)$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

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



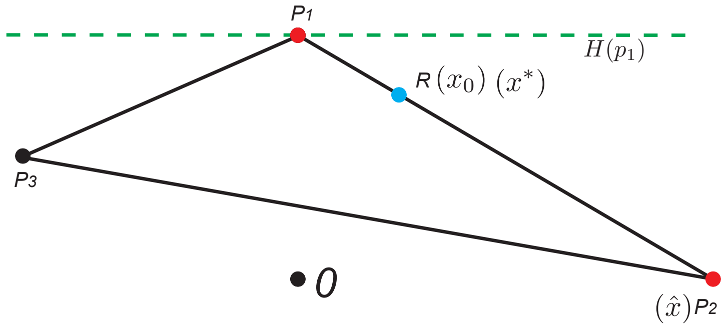
We need to add some extreme point $\hat{x}$ on the "near" side of $H(p_1)$ in Line 6, we choose $\hat{x} = p_2$. In Line 7, we set $Q \leftarrow Q \cup \{p_2\}$, so $Q = \{p_1, p_2\}$.

Fujishige-Wolfe Min-Norm algorithm: Geometric Example



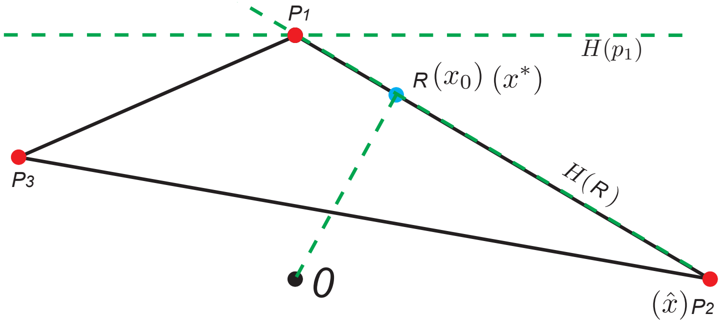
$x_0 = R$ is the min-norm point in $\text{aff}\,\{p_1, p_2\}$ computed in Line 9.

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. Note, after Line 11, we still have $x^* \in P$ and $\|x^*\|_2 = \|x^*_{\text{new}}\|_2 < \|x^*_{\text{old}}\|_2$ 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 $Q = P = \{p_1, p_2, p_3\}$.

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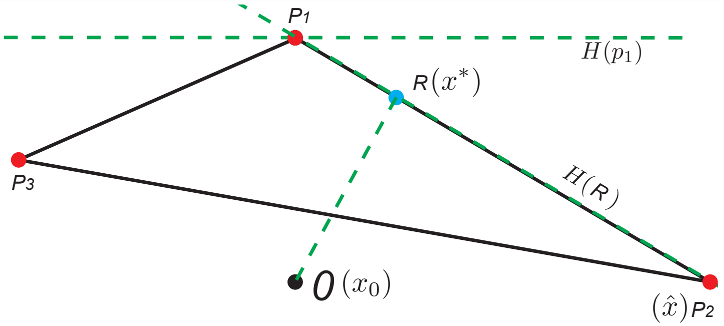
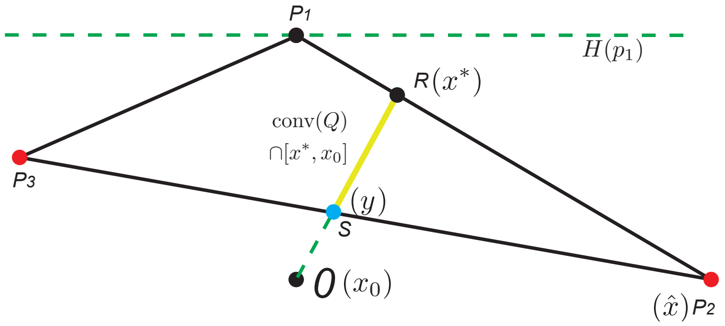


$R = x_0 = x^*$. We consider next $H(R) = H(x^*)$ in Line 4. $H(x^*)$ is not a supporting hyperplane of $\operatorname{conv} P$. So we choose p_3 on the "near" side of $H(x^*)$ in Line 6. Add $Q \leftarrow Q \cup \{p_3\}$ in Line 7. Now $Q = P = \{p_1, p_2, p_3\}$. The origin $x_0 = 0$ is the min-norm 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: $S = y = \min_{x \in \text{conv}\, Q \cap [x^*, x_0]} \|x - x_0\|_2$ where x_0 is 0 and x^* is R here. Thus, y lies on the boundary of $\text{conv}\, Q$. Note, $\|y\|_2 < \|x^*\|_2$ since $x^* \in \text{conv}\, Q$, $\|x_0\|_2 < \|x^*\|_2$.

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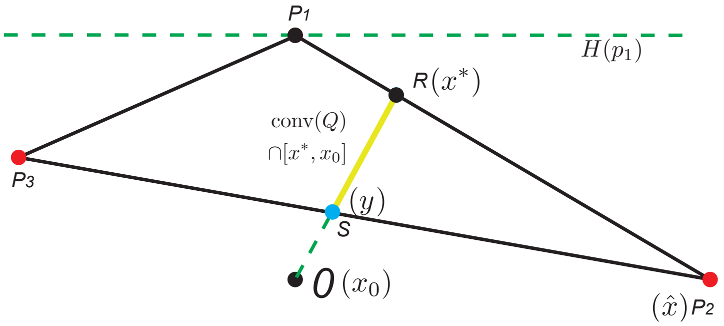

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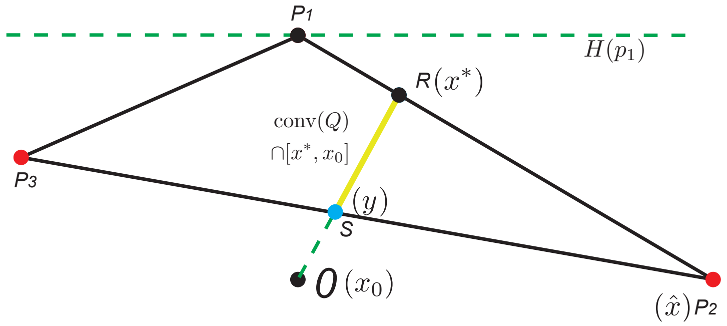

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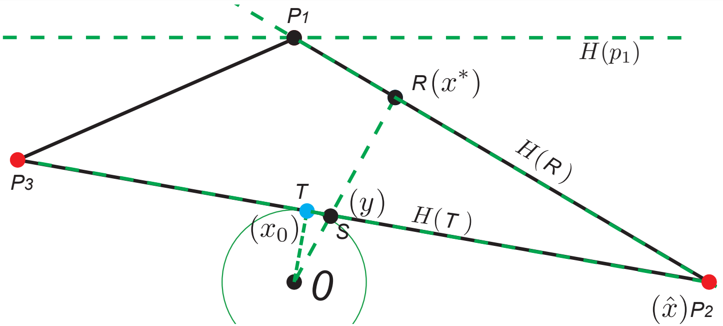

$Q = \{p_2, p_3\}$, and so $x_0 = T$ computed in Line 9 is the min-norm point in $\operatorname{aff} Q$. We also have $x_0 \in \operatorname{conv} Q$ in Line 10 so we assign $x^* \leftarrow x_0$ in Line 11 and break.

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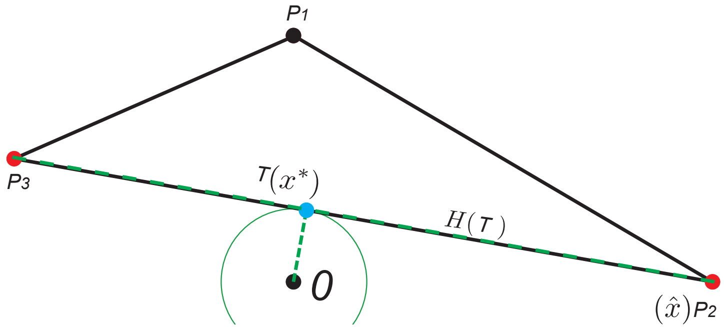

$H(T)$ separates P from the origin in Line 4, and therefore is a supporting hyperplane, and therefore x^* is the min-norm point in $\operatorname{conv} P$, so we return with x^*.

Condition for Min-Norm Point

Theorem 18.4.2

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

$$p_i^\intercal x^* \geq \|x^*\|_2^2 \quad \forall i = 1, \cdots, m. \tag{18.50}$$

Proof.

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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

$$\|z\|_2^2 = \|x^* + \theta(y - x^*)\|_2^2 \tag{18.51}$$

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- Conversely, given Eq (18.50), and given that $y = \sum_i \lambda_i p_i \in \operatorname{conv} P$,
$$y^\intercal x^* = \sum_i \lambda_i p_i^\intercal x^* \geq \sum_i \lambda_i x^{*\intercal} x^* = x^{*\intercal} x^* \tag{18.53}$$
implying that $\|z\|_2^2 > \|x^*\|_2^2$ in Equation 18.52 for arbitrary $z \in \operatorname{conv} P$. □

The set Q is always affinely independent

Lemma 18.4.3

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Thus, by Lemma 18.4.3, we have for any $x \in \operatorname{aff} Q$ such that $x = \sum_i w_i q_i$ with $\sum_i w_i = 1$, the weights w_i are uniquely determined.

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- Let Q also represent the $n \times k$ matrix with points as columns $q \in Q$. We get the following, solvable with matrix inversion/linear solver:

$$\begin{aligned} &\text{minimize} && \|x\|_2^2 = w^\intercal Q^\intercal Q w && (18.54) \\ &\text{subject to} && \mathbf{1}^\intercal w = 1 && (18.55) \end{aligned}$$

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  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).

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  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 18.4.4

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 $\operatorname{conv} Q$.

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- 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).

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- 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.

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- 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.

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- Therefore, we have $\|x^* + \theta(\hat{x} - x^*)\|_2 \geq \|x_0\|_2$, which implies

$$\begin{aligned}\|x^* + \theta(\hat{x} - x^*)\|_2^2 &= \|x^*\|_2^2 + 2\theta\left((x^*)^\top \hat{x} - \|x^*\|_2^2\right) + \theta^2 \|\hat{x} - x^*\|_2^2 \\ &\geq \|x_0\|_2^2 \end{aligned} \tag{18.56}$$

$\hat{x}$ is on the same side of $H(x^*)$ as the origin, i.e. $(x^*)^\top \hat{x} < \|x^*\|_2^2$.

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- Therefore, for sufficiently small θ, specifically for

$$\theta < \frac{2\left(\|x^*\|_2^2 - (x^*)^\top \hat{x}\right)}{\|\hat{x} - x^*\|_2^2} \tag{18.57}$$

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- 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.

$\square$

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$$\Delta = \|x^*\|_2^2 - \|x_0\|_2^2 \geq 2\theta \left(\|x^*\|_2^2 - (x^*)^\top \hat{x} \right) - \theta^2 \|\hat{x} - x^*\|_2^2 \triangleq \underline{\Delta} \tag{18.58}$$

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- 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:

$$\max_{0 \leq \theta < \frac{2\left(\|x^*\|_2^2 - (x^*)^\top \hat{x}\right)}{\|\hat{x} - x^*\|_2^2}} \underline{\Delta} = \left(\frac{\|x^*\|_2^2 - (x^*)^\top \hat{x}}{\|\hat{x} - x^*\|_2} \right)^2 \tag{18.59}$$

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- This problem, however, is at least as hard as the MN problem itself as we have a quadratic term in the denominator.

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- As a surrogate, we maximize numerator in Eqn. 18.60, i.e., find

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- Also, solution $\hat{x}$ 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.

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- Mathematically, we terminate the algorithm if

$$(x^*)^\top \hat{x} \geq \|x^*\|_2^2\,, \tag{18.62}$$

where $\hat{x}$ is the solution of Eq. 18.61.

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- 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

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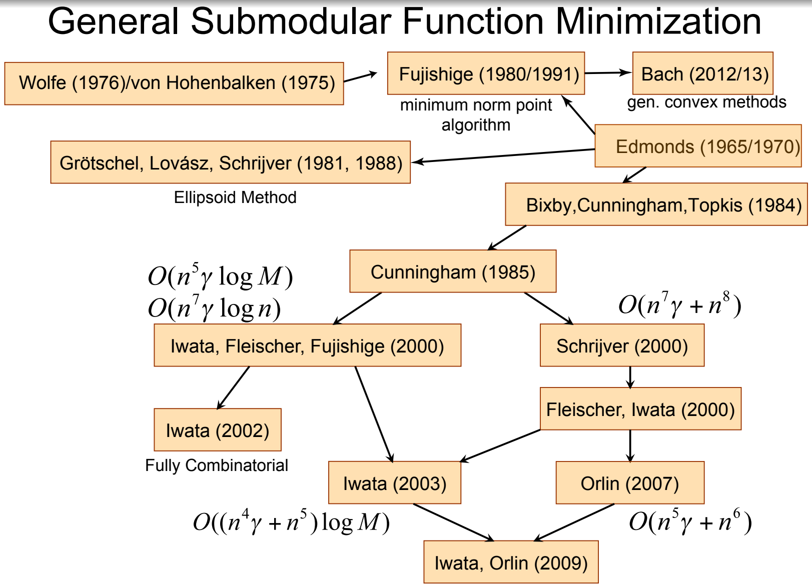
- Hence, Edmonds's discovery is one of the main reasons that the MN algorithm is applicable to submodular function minimization.

SFM Summary (modified from S. Iwata's slides)



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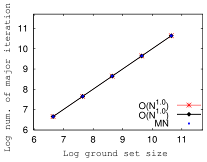
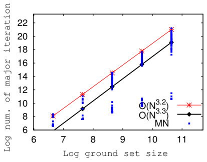
- Since the number of major iterations required is unknown, the complexity of MN is also unknown.

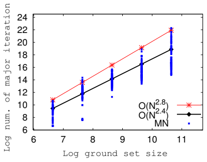
MN Algorithm Empirical Complexity



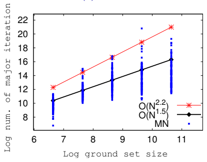
(a) $\alpha = 0.1$



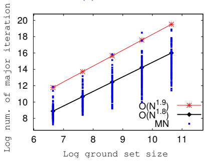
(b) $\alpha = 0.2$



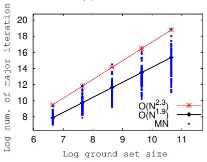
(c) $\alpha = 0.3$



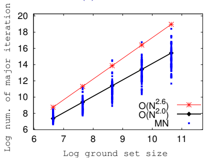
(d) $\alpha = 0.4$



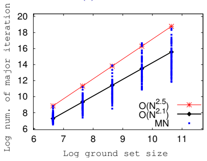
(e) $\alpha = 0.5$



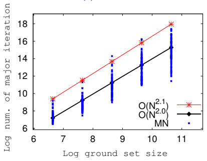
(f) $\alpha = 0.6$



(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)