Short Course on Submodular Functions

S. Thomas McCormick Maurice Queyranne

Sauder School of Business, UBC JPOC Summer School, June 2013

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

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- Because of this, we talk about set functions using an value oracle model: we assume that we have an algorithm *E* whose input is some S ⊆ E, and whose output is f(S). We denote the running time of *E* by EO.

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- Because of this, we talk about set functions using an value oracle model: we assume that we have an algorithm *E* whose input is some *S* ⊆ *E*, and whose output is *f*(*S*). We denote the running time of *E* by EO.
 - We typically think that EO = Ω(n), i.e., that it takes at least linear time to evaluate f on S.

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

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

Back to the motivating example

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

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► In general, if f is a set function on E, we say that f is submodular if

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The classic definition of submodularity looks quite different. We also say that set function f is submodular if

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

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

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

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

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

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- More generally, suppose that w ∈ ℝ^A are weights on the arcs. If w ≥ 0, then w(δ⁺(S)) and w(δ⁻(S)) are submodular, and if w ≥ 0 then they are not necessarily submodular (homework).

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

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

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

Algorithmic proof of Max Flow / Min Cut

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

$$\begin{aligned} \operatorname{val}(x) &= x(\delta^+(\{s\})) - x(\delta^-(\{s\})) \\ &+ \sum_{i \in S} [x(\delta^+(\{i\})) - x(\delta^-(\{i\}))] \\ &= x(\delta^+(S+s)) - x(\delta^-(S+s)) \\ &\leq u(\delta^+(S+s)) - 0 = \operatorname{cap}(S). \end{aligned}$$

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An augmenting path w.r.t. feasible flow x is a directed path P such that i → j ∈ P implies either (i) i → j ∈ A and x_{ij} < u_{ij}, or (ii) j → i ∈ A and x_{ji} > 0.

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► For
$$i \in S + s$$
 and $j \notin S + s$ we must have $x_{ij} = u_{ij}$ and $x_{ji} = 0$, and so $val(x) = x(\delta^+(S+s)) - x(\delta^-(S+s)) = u(\delta^+(S+s)) - 0 = cap(S).$

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

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- Coverage: There is a set F a facilities we can open, and a set C of clients we want to service. There is a bipartite graph $B = (F \cup C, A)$ from F to C such that if we open $S \subseteq F$, we serve the set of clients $\Gamma(S) \equiv \{j \in C \mid i \to j \in A, \text{ some } i \in S\}$. If $w \ge 0$ then $w(\Gamma(S))$ is submodular.

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

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- ▶ By contrast, in other contexts we want to *maximize*. For example, in an undirected graph with weights $w \ge 0$ on the edges, the Max Cut problem is to $\max_{S \subseteq E} w(\delta(S))$.
- Generically, Submodular Function Maximization (SFMax) is:

 $\label{eq:given submodular f, solve} \mbox{ Given submodular } f, \mbox{ solve } \max_{S \subseteq E} f(S).$

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 - Or we could have multiple budgets, or . . .

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 - When f is integer-valued, define $M = \max_{S \subseteq E} |f(S)|$.
 - ▶ Unfortunately, exactly computing *M* is NP Hard (SFMax), but we can compute a good enough bound on *M* in *O*(*n*EO) time.

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- ▶ If non-integral data is allowed, then the running time cannot depend on *M* at all.
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 - There is no apparent reason why an SFMin/Max algorithm needs multiplication or division, so we call an algorithm fully combinatorial if it is strongly polynomial, and uses only addition/subtraction and comparisons.

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

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- Submodular functions are sort of *convex*: Set function f induces values on {0,1}^E via f̂(χ(S)) = f(S), where χ(S)_e = 1 if e ∈ S, 0 otherwise. There is a canonical piecewise linear way to extend f̂ to [0,1]^E called the Lovász extension. Then f is submodular iff f̂ is convex.

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

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- ▶ What about when $S = \emptyset$? We get $x(\emptyset) \equiv 0 \leq f(\emptyset)$???
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 - This normalization is non-trivial for Min Cut.

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

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

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

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- ▶ Intuitively, with $w \ge 0$ a maximum solution will be forced up against the $x(E) \le f(E)$ constraint, and so it will become tight, and so an optimal solution will be in B(f). So we consider $\max_{x \in \mathbb{R}^E} w^T x$ s.t. $x \in B(f)$.
- ► The naive thing to do is to try to solve this greedily: Order the elements such that w₁ ≥ w₂ ≥ ··· ≥ w_n.

Outline

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Optimizing submodular functions

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An algorithmic framework

Schrijver's Algorithm for SFMin

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Other SFMin topics

Extensions and the future of SFMin

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- In this notation we can re-express the main step of Greedy on the *i*th element in ≺ as

"Make $x_{e_i} \leftarrow f(e_i^{\prec} + e_i) - f(e_i^{\prec})$."

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

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

▶ Define π_S like this: Put $\pi_S = w_{e_{i-1}} - w_{e_i}$ if $S = e_i^{\prec}$, $\pi_E = w_{e_n} - 0$ (using " $w_{e_{n+1}} = 0$ "), and $\pi_S = 0$ otherwise.

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 $= w_{e_k} - w_{e_{n+1}} = w_{e_k}$, as desired.

$$w^{T}x = \sum_{e \in E} (\sum_{S \ni e} \pi_{S})x_{e}$$

= $\sum_{S \subseteq E} \pi_{S} \sum_{e \in S} x_{e}$
= $\sum_{S \subseteq E} \pi_{S}x(S)$
 $\leq \sum_{S \subseteq E} \pi_{S}f(S).$

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

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

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 - Greedy works on B(f) for any w; it works on P(f) if $w \ge 0$.

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 - As we saw in the proof, the constraint for S = e[≺]_k is tight for each e_k ∈ E.
- Therefore *M* is the lower triangular matrix:

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

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- ▶ Triangular systems like this are easy to solve, and indeed gives that $x_{e_i} = f(e_i^{\prec} + e_i) f(e_i^{\prec})$.

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- ► This also shows that v[≺] is a vertex, as it follows from M being nonsingular.

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- We are going to show that v^{≺'} − v[≺] = α(χ_k − χ_l) for a step length α.

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 - ► Thus for $e \neq k, l$ we have that $v_e^{\prec} = f(e^{\prec} + e) - f(e^{\prec}) = f(e^{\prec'} + e) - f(e^{\prec'}) = v_e^{\prec'}.$

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Thus for e ≠ k, l we have that v[≺]_e = f(e[≺] + e) - f(e[≺]) = f(e^{≺'} + e) - f(e^{≺'}) = v^{≺'}_e.
For e = k we have v[≺]_k = f(k[≺] + k) - f(k[≺]) = f(l[≺] + k + l) - f(l[≺] + l) and v[≺]_k = f(k^{≺'} + k) - f(k^{≺'}) = f(l[≺] + k) - f(l[≺]).

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move k later in \prec , v_k^\prec gets smaller.

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- ► It turns out that all the edges of B(f) come from consecutive exchanges like this.

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- Since x(E) = f(E) is a constraint of B(f), all $x \in B(f)$ have the constant sum f(E). Thus it is not a surprise that $|v_k^{\prec} v_k^{\prec'}| = |v_l^{\prec} v_l^{\prec'}| = c(k, l; v^{\prec}).$
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 - Unfortunately it turns out that computing c(k, l; x) is provably as difficult as SFMin.

Outline

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

Optimizing submodular functions

SFMin versus SFMax Tools for submodular optimization The Greedy Algorithm

SFMin algorithms An algorithmic framework

Schrijver's Algorithm for SFMin

Motivating the algorithm Analyzing the algorithm

Other SFMin topics

Extensions and the future of SFMin

An algorithmic framework for SFMin

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 - GLS then extend this to show a strongly polynomial running time.

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- Even better, we guess (see below) that there exists an optimal solution to the dual where only one π_S is positive, say π_{S*} = 1.

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 - ► Thus x(E) = x(S*) + x(E S*) = f(S*) + u(E S*), proving that S* induces a dual optimal solution.

• Our LP strong duality says that $\max_{x \in P(f): x \leq u} x(E) = \min_{S \subseteq E} (f(S) + u(E - S)).$

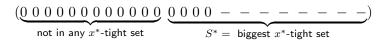
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- ▶ Thus we can use the modified primal LP $\max_{y \in B(f)} y^{-}(E)$.
 - This is the form of the LP that we will use.
 - ▶ This LP is quite close to the Greedy LP, except that the objective is the piecewise linear $y^-(E)$ instead of x(E), and this makes solving the problem *much* harder.

• Here is weak duality for these LPs:

$$\begin{array}{rcl} y^-(E) & \leq & y^-(S) & \text{tight if } y_e < 0 \implies e \in S \\ & \leq & y(S) & \text{tight if } e \in S \implies y_e \leq 0 \\ & \leq & f(S) & \text{tight if } S \text{ is } y\text{-tight.} \end{array}$$

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- Or does it? What is missing?

How do we know that $y \in B(f)$?

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 - We keep multipliers $\lambda_i \geq 0$ for $i \in \mathcal{I}$ satisfying $\sum_{i \in \mathcal{I}} \lambda_i = 1$.
 - Then $y = \sum_{i \in \mathcal{I}} \lambda_i v^i$ is a succinct certificate proving that $y \in B(f)$.

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- ► The task of subroutine REDUCEV is to eliminate redundant columns of V while maintaining $V\lambda = \begin{pmatrix} 1 & y \end{pmatrix}$ and $\lambda \ge 0$.
- This can be done with standard linear algebra techniques in ${\cal O}(n^3)$ time.

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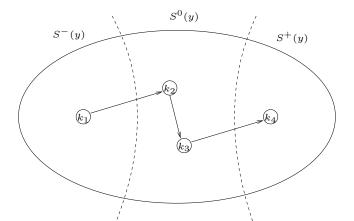
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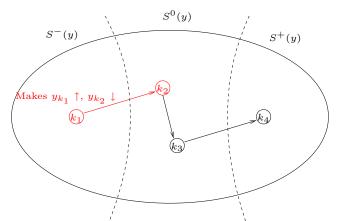
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 - But unfortunately computing c(k, l; y) is as hard as SFMin.
 - And if we don't have any \prec_i with (l,k) consecutive in \prec_i , then how can we change the representation $y = \sum_{i \in \mathcal{I}} \lambda_i v^i$ to track this $\chi_k \chi_l$ direction?

Assume that we have the situation as in the picture below, where (k_2, k_1) is consecutive in \prec_1 , (k_3, k_2) is consecutive in \prec_2 , and (k_4, k_3) is consecutive in \prec_3 .



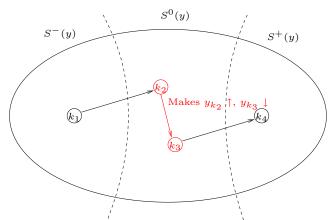
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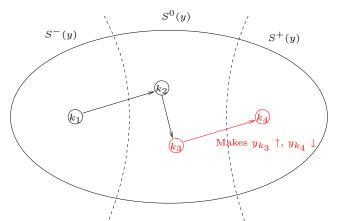
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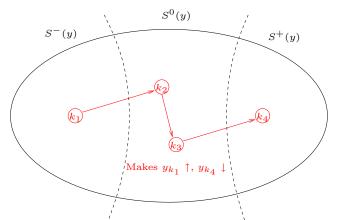
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But if we do all three swaps at the same time this would $\uparrow y_{k_1}$ and $\downarrow y_{k_4}$, and this would increase $y^-(E)$.



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- ▶ The same proof works with a more general definition of arcs: Put $e \rightarrow g \in A$ whenever $g \prec_i e$ for some $i \in \mathcal{I}$.
- The "only" remaining thing to do is to find some way to arrange augmentations so there is only a polynomial number of them.

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- These are some of the reasons why it took many, many years to figure out how to get a combinatorial SFMin algorithm, and why Cunningham's SFMin algorithm was only pseudo-polynomial.

Outline

Introduction

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

Optimizing submodular functions

SFMin versus SFMax Tools for submodular optimization The Greedy Algorithm

SFMin algorithms

An algorithmic framework

Schrijver's Algorithm for SFMin Motivating the algorithm Analyzing the algorithm

Other SFMin topics

Extensions and the future of SFMin

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 - When (l, k) is consecutive in ≺, then |(l, k]≺| = 1; as |[l, k]≺| becomes larger than 1, computing c(k, l; y) becomes more difficult.

Suppose that we have identified *l* ∈ S⁺(y) and *k* ∈ S⁻(y), so we want to ↓ y_l and ↑ y_k by moving *l* to the right and *k* to the left in some ≺_h, call it just ≺.

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Doing this block swap that moves in the direction v^{l,j} − v[≺] would indeed ↓ y_l, but it wouldn't affect y_k.

- Suppose that we have identified *l* ∈ S⁺(y) and *k* ∈ S⁻(y), so we want to ↓ y_l and ↑ y_k by moving *l* to the right and *k* to the left in some ≺_h, call it just ≺.
- Suppose that \prec looks like this for some $j \in (l, k]_{\prec}$:

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- Doing this block swap that moves in the direction v^{l,j} − v[≺] would indeed ↓ y_l, but it wouldn't affect y_k.
- But ≺^{l,j} does have the nice property that (l, k]_{≺l,j} ⊂ (l, k]_≺, so it gets closer to being a c(k, j; y) that we can compute.

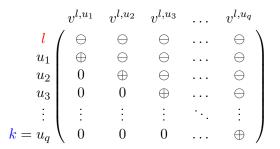
The block swap matrix

Index the elements of (l, k] ≺ as l ≺ u₁ ≺ u₂ · · · ≺ u_q = k and consider the submatrix of the matrix of columns v^{l,u_b} − v[≺]:

$$v^{l,u_1}$$
 v^{l,u_2} v^{l,u_3} \dots v^{l,u_q}
 $l \ (\ominus \ \ominus \ \ominus \ \dots \ \ominus \) \ (\ominus \ \ominus \ \ominus \ \dots \ \ominus \) \ (\ominus \ \ominus \ \ominus \ \dots \ \ominus \) \ (\ominus \ \ominus \) \ (\ominus \ \ominus \) \ (\ominus \) \ ($

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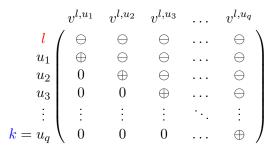
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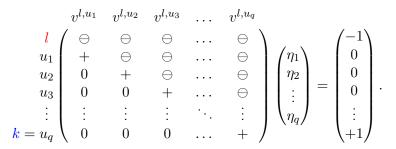
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Now we are free to assume that all v_j^{l,j} > v_j[≺], i.e., the diagonal entries of the matrix are strictly positive.

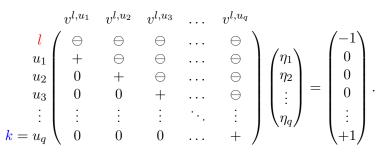
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- Since this system is triangular with positive diagonal, it has a solution η ≥ 0.
- ▶ Put $\alpha = 1/\sum_{j} \eta_{j}$ and $\mu = \alpha \eta$. Then $(v^{l,j} v^{\prec})\eta = \chi_{k} \chi_{l}$ becomes $(v^{l,j} - v^{\prec})\mu = \alpha(\chi_{k} - \chi_{l})$, or $v^{\prec} + \alpha(\chi_{k} - \chi_{l}) = \sum_{j \in (l,k]_{\prec}} \mu_{j} v^{l,j}$ which is (6) as desired.

The ExcHBD subroutine

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- ► Return to using v^h for v^{\prec} . If we replace the term $\lambda_h v^h$ in $y = \sum_i \lambda_i v^i$ by $\lambda_h (\sum_{j \in (l,k]_{\prec}} \mu_j v^{l,j})$, then y will change by $\lambda_h \alpha(\chi_k \chi_l)$, and so we'll move in the direction we want.

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- ▶ We call this operation EXCHBD, since it gives us the bound α on $c(k, l; v^{\prec})$.

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 - ► Non-saturating PUSHes exit, so worry only about saturating PUSHes.
 - ► Each saturating PUSH(l, k) either reduces max_i |(l, k]_{≺i}| or the number of i achieving this max. Since |(l, k]_{≺i}| ≤ n, there are O(n²) iterations.

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- 4. Compute $S = \{e \mid e \text{ is reachable from } S_1(y)\}$ and return S as an optimal SFMin solution.

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- We already noted that other operations preserve validity.

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- Thus the Push-Relabel version of Schrijver's Algorithm is a strongly polynomial SFMin algorithm.

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 - ► It comes from a general algorithm for minimizing l₂ distance to a polytope.
 - ▶ It has no known polynomial bound, but its empirical performance beat all other algorithms that Fujishige et al tested: *O*(*n*^{3.3}).

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 - ... and more, see Goemans and Ramakrishnan.

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 - \mathcal{F} is closed under \cap and \cup (a ring family).
 - *F* is closed under ∩ and ∪ only when S ∩ T ≠ ∅ (an intersecting family).
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- ▶ But don't get carried away: Solving min_{S⊆E:|S|=k} f(S) is NP Hard.

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 - Minimization of bisubmodular functions, a "signed" analogue of submodular functions.