From non-differentiability to discrete geometry

B-differential, hyperplanes and matroids

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Outline

Plan

Linear Complementarity Problems

General form [CPS92; FP03]

$$A, B \in \mathbb{R}^{n\times n}, a, b \in \mathbb{R}^n, \rightarrow \ \mathcal{A}(x) = Ax + a, \mathcal{B}(x) = Bx + b$$

$$0 \leq (Ax + a) \perp (Bx + b) \geq 0 \tag{1}$$

$$\forall\ i \in [1:n], \begin{cases} A_{i,:}x + a_i \geq 0 \\ B_{i,:}x + b_i \geq 0 \end{cases}, (A_{i,:}x + a_i)(B_{i,:}x + b_i) = 0$$

Remark: $u \geq 0, v \geq 0, uv = 0 \Leftrightarrow \min(u, v) = 0$

$(1) \Leftrightarrow \forall\ i \in [1:n], F_i(x) := \min(\mathcal{A}_i(x), \mathcal{B}_i(x)) = 0 \Leftrightarrow F(x) = 0$

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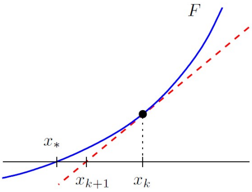
Nonlinear (nonsmooth) equations - Newton's method



1D Illustration

x^0 near x^*,
$F \in \mathcal{C}^{1,1}$,
$F'(x^*)$ non-singular
$\Rightarrow$ quadratic convergence

F' not defined everywhere

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F semismooth,
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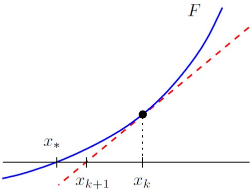

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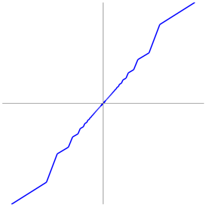

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Semismooth Newton's method

Adaptation of the usual method for this difficulty ([Qi93; QS93])
Replaces $F'(x_k)$ with a "generalized Jacobian" J_k

Algorithm's sketch

- take $x^0 \in \mathbb{R}^n$ (near x^*)
- for k = 1 2, . . . , solve $F(x^k) + J_k z^k = 0$ for z^k, with $J_k \in \partial_B F(x^k)$: $\partial_B F$ is the Bouligand differential
- then $x^{k+1} = x^k + (\alpha_k) z^k$

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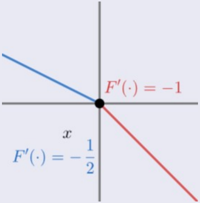
Generalized derivatives

Bouligand differential

$$\partial_{\mathrm{B}} F(x) = \{J \in \mathbb{R}^{n\times n} : \exists\ (x_k)_k \to x, F'(x_k) \to J\} \tag{2}$$

Example: $F(x) = \begin{cases} -x/2 & \text{if } x \leq 0 \\ -x & \text{if } x > 0 \end{cases}$,

$\partial_B F(0) = \{-1/2, -1\}$.



Summary

Minimum(LCPs) $\Rightarrow$ semismooth system, requires info on $\partial_B \min(\mathcal{A}, \mathcal{B})(\cdot) = \partial_B F(\cdot)$

One $J_B \in \partial_B F$: [Qi93]. But all of them?

The main question

Determine generalized Jacobians of $x \mapsto F(x) = \min(Ax + a, Bx + b)$

→ structure?
→ number?
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Plan

Computing the B-differential - 1

$$\min(\overbrace{f(x), g(x)}^{\in\mathbb{R}}) \text{ NOT diff} \Leftrightarrow f(x) \overset{C1}{=} g(x) \text{ and } f'(x) \overset{C2}{\neq} g'(x).$$

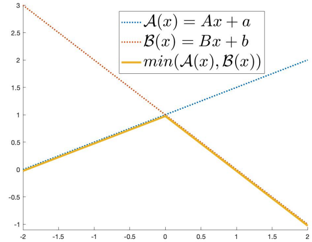

Illustration for 1D affine functions ($\rightarrow$ dimension n)

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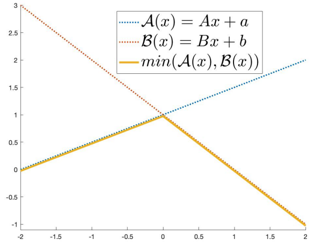

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Computing the B-differential - 2

$\min(\mathcal{A},\mathcal{B})(\overset{\simeq x}{x_k})$ non-diff $\Leftrightarrow \overset{\in I(x)}{\exists\ i}, (Ax_k + a)_i \overset{C1}{=} (Bx_k + b)_i \overset{x_k = x+d}{\Leftrightarrow}$
$(Ax + a)_i + A_{i,:}d = (Bx + b)_i + B_{i,:}d \Leftrightarrow A_{i,:}d = B_{i,:}d \Leftrightarrow d \in v_i^\perp$
$(v_i \neq 0$ by C2)

Hyperplanes $H_i := (B_{i,:} - A_{i,:})^\perp := v_i^\perp$; for ∂_B's def, $\mathbb{R}^n \setminus \cup H_i$

$$\mathbb{R}^n = H_i^- \cup H_i \cup H_i^+, \quad \begin{cases} H_i^- = \{x \in \mathbb{R}^n : v_i^\mathsf{T} x < 0\} \\ H_i^+ = \{x \in \mathbb{R}^n : v_i^\mathsf{T} x > 0\} \end{cases}$$

Convention: $\forall\ i \in [1:p]$,

$$\begin{aligned} H_i^+ &\Leftrightarrow B_{i,:}d - A_{i,:}d > 0 \Leftrightarrow \min(\dots) = \mathcal{A}_i(\dots) \Leftrightarrow J_{i,:} = A_{i,:} \\ H_i^- &\Leftrightarrow B_{i,:}d - A_{i,:}d < 0 \Leftrightarrow \min(\dots) = \mathcal{B}_i(\dots) \Leftrightarrow J_{i,:} = B_{i,:} \end{aligned}$$

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Computing the B-differential - 3

So far:

- vectorial problem in dimension n: derivatives $J \in \mathbb{R}^{n \times n}$
- function is piecewise affine, derivative is piecewise constant
- the matrices J are composed of lines of A and B
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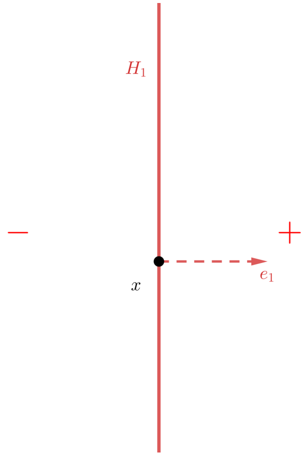

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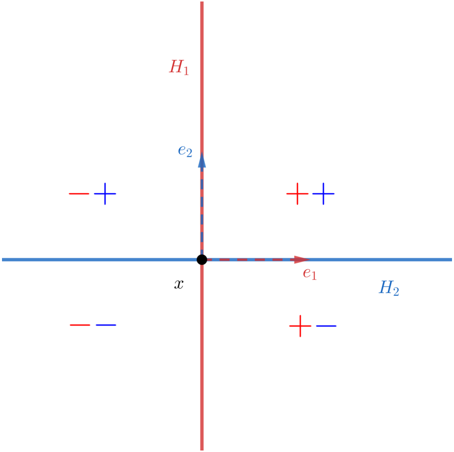

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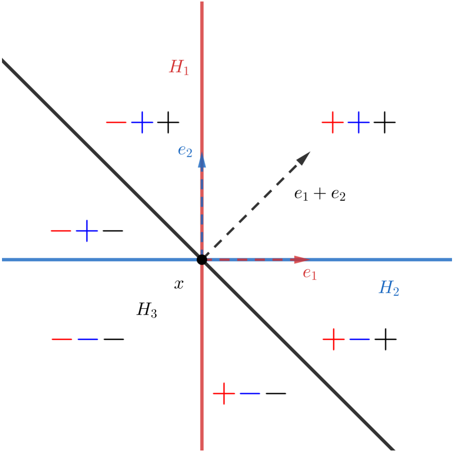
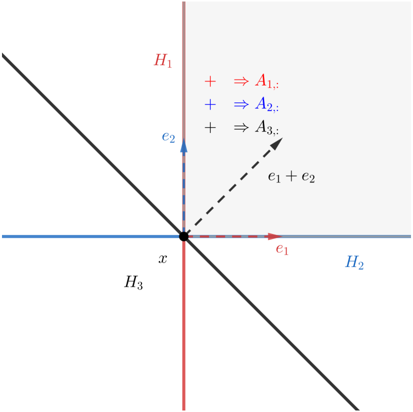


B-differential and hyperplanes



In the grey area, the points remain on the same sides of the hyperplanes: the Jacobian matrix remains constant.

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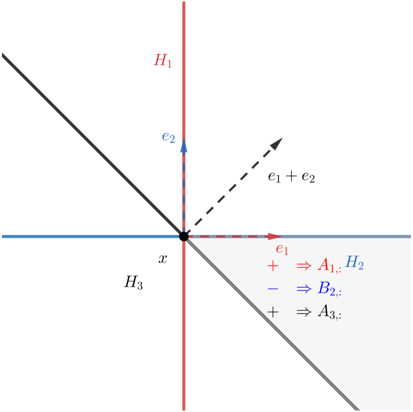

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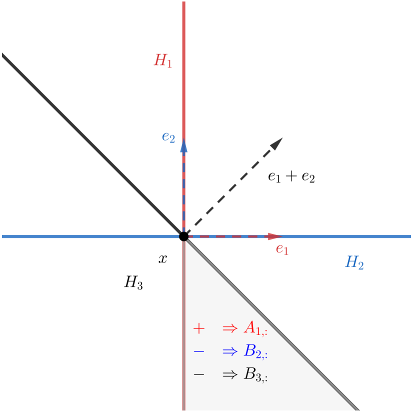

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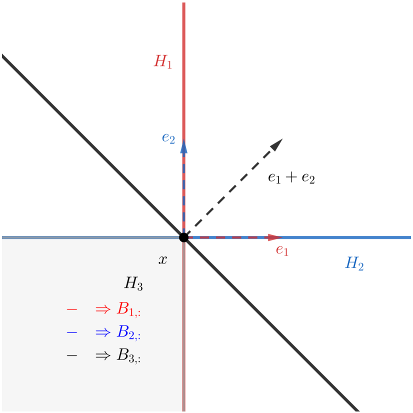

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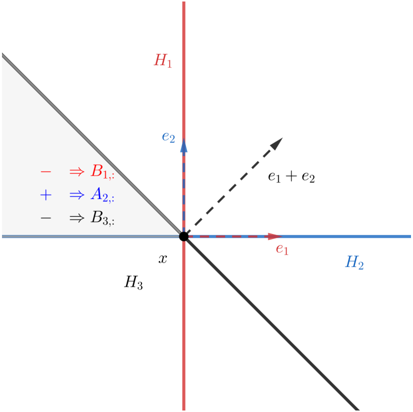

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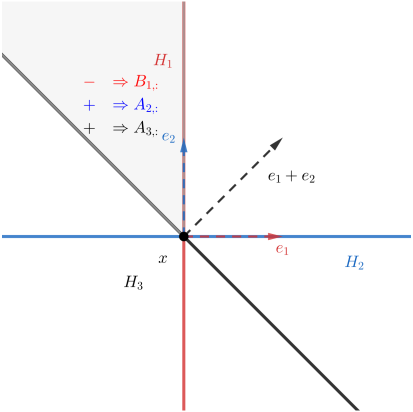

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Summary

$|I(x)| = p$ hyperplanes, $H_i = v_i^{\perp}, v_i = B_{i,:} - A_{i,:}$ [data]
$\mathbb{R}^n \setminus \bigcup H_i$ = differentiable points, on the $+$ or $-$ side of every H_i.
By convention: the $\pm$ becomes the sign s

Fundamental question

$$\text{given } V = [v_1 \ \dots \ v_p]$$
$$\text{find all } s = (s_1, \dots, s_p) \in \{\pm 1\}^p,$$
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2^p linear feasibility problems to solve... How to improve?

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Plan

1. From a nonsmooth question...
2. ... to combinatorics
3. Algorithmic details
   - Main principle
   - Improving on the structure
   - Dual approach: LO-free method
4. Some results

Main reasoning

Algorithm from [RČ18]:

- recursive tree that adds hyperplanes one at a time
- each node has one or two descendants,
- checked through Linear Optimization Problem (LOP)

at level k, with $s \in \{\pm 1\}^k$,

$$\forall\, i \in [1:k], \exists\, d_s, s_i v_i^\top d_s > 0 \Rightarrow \begin{cases} \forall\, i \in [1:k], s_i v_i^\top d > 0 \\ \qquad +v_{k+1}^\top d > 0 \end{cases} ? \quad \begin{cases} \forall\, i \in [1:k], s_i v_i^\top d > 0 \\ \qquad -v_{k+1}^\top d > 0 \end{cases} ?$$

The LOPs represent the main computational effort

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The LOPs represent the main computational effort

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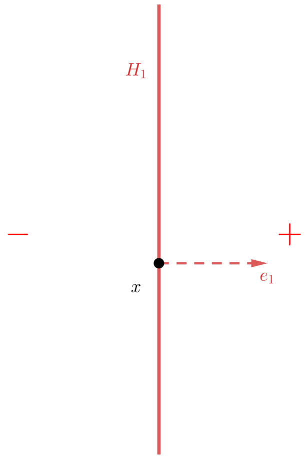

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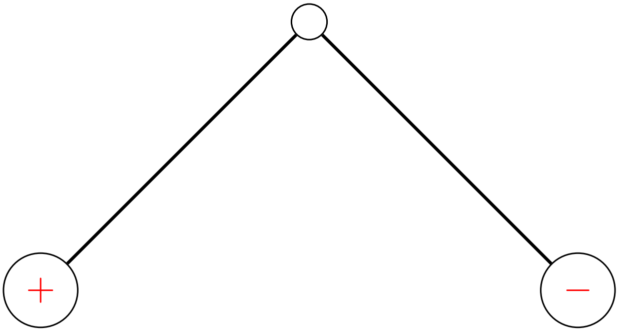

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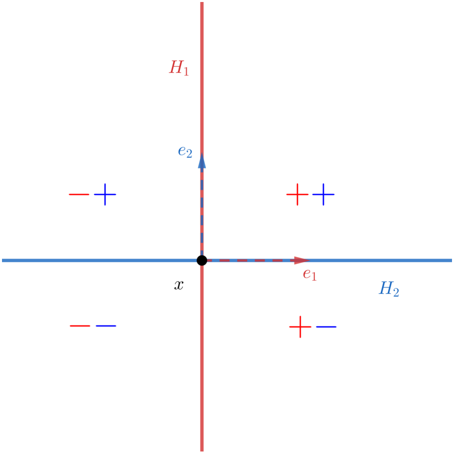

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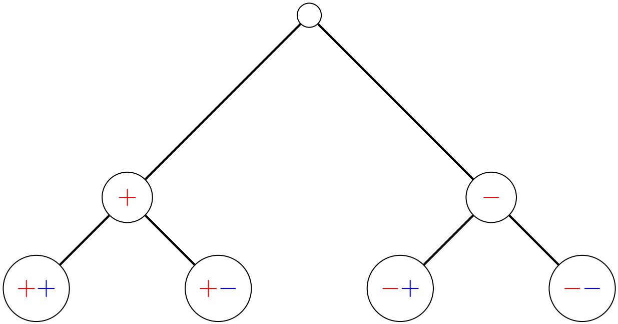

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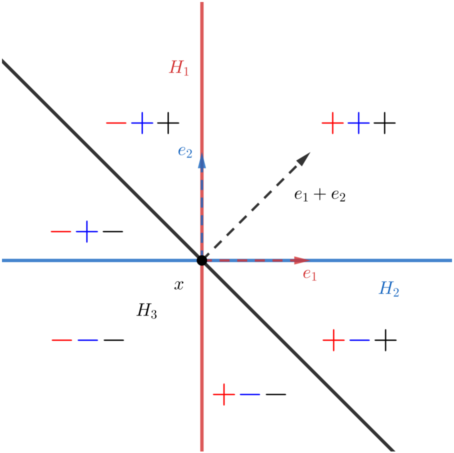

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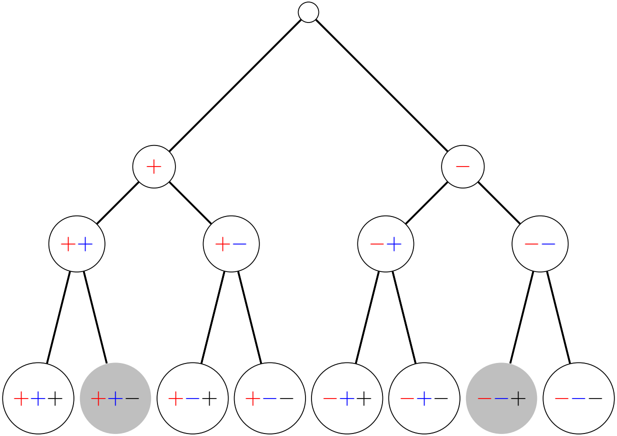

Reducing the LOP count - 1

- each tree node: a Linear Optimization Problem; small dimension, but the only 'real' task
- goal is to avoid solving LOPs

Each node is associated to a $s \in \{\pm 1\}^k$ and its $d_s \in \mathbb{R}^n$.
Between levels k and $k+1$, when hyperplane $k+1$ is added, d_s can belong to $H_{k+1} \Leftrightarrow v_{k+1}^\top d_s = 0$: $(i \in [1:k])$

$$\begin{cases} s_i v_i^\top d_s > 0 \\ v_{k+1}^\top d_s = 0 \end{cases} \Rightarrow \exists\, (d^+, d^-), \begin{cases} s_i v_i^\top d^\pm > 0 \\ \pm v_{k+1}^\top d^\pm > 0 \end{cases}$$

$v_{k+1}^\top d_s = 0$ is utopic, but formalized for $|v_{k+1}^\top d_s|$ small enough

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- each tree node: a Linear Optimization Problem; small dimension, but the only 'real' task
- goal is to avoid solving LOPs

Each node is associated to a $s \in \{\pm 1\}^k$ and its $d_s \in \mathbb{R}^n$.
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Using the "contrapositive"

$|v_{k+1}^T d_s|$ 'large' $\rightarrow$ less chance of both $(s, +1)$ and $(s, -1)$.

In s, hyperplanes $\overbrace{\{i_1, \dots, i_k\}}^{=I^s}$; $i_{k+1} = \arg\max_j \ |v_j^T d_s|, j \in [1:p] \setminus I^s$

Only a heuristic, but reasonably efficient.
Also, this order change is local - for each s it can change.

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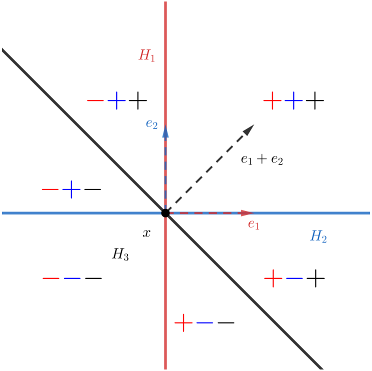
Infeasibility, matroids and circuits - 1



$++-$ (and $--+$) corresponds to an empty region: $+$ means right to H_1, $+$ over H_2, $-$ down left H_3: such a point does not exist. The system is $+ : d_1 > 0, + : d_2 > 0, - : -d_1 - d_2 > 0$

Infeasibility, matroids and circuits - 2

With $p > 3$, $++- \bullet \bullet \ldots \bullet \bullet$ always infeasible.

Gordan's alternative

$M \in \mathbb{R}^{p \times n}$, exactly one is true:

$$\begin{cases} \exists\, d \in \mathbb{R}^n : Md > 0_{\mathbb{R}^p} \\ \exists\, \gamma \in \mathbb{R}^p_+ \setminus \{0\} : M^\mathsf{T} \gamma = 0 \end{cases} \tag{3}$$

$s \in \{\pm 1\}^p$ arbitrary:
$M = \mathrm{diag}(s) V^\mathsf{T} \rightarrow Md = (s_1 v_1^\mathsf{T} d; \ldots; s_p v_p^\mathsf{T} d)$

"Feasibility of a system or element in the null space of the matrix"

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Instead: search for $\Gamma = \{\gamma\}$ and prune/stop the tree when an infeasibility is detected.
The γ's represent the "**circuits**" of the "**matroid**" defined by V

- the tree from [RČ18]
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Technical details

LO solver

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Plan

Summary

- LO only = ABC
- LO + a bit of duality = ABCD2
- LO + a lot of duality = ABCD3
- only duality = AD4

Not clear which is better: dual computations are sometimes not useful

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Results; blue = times, black = improvement factor

Name	RC	ABC		ABCD2		ABCD3		AD4	
R-4-8-2	1.70 10^{-2}	7.20 10^{-3}	2.36	6.53 10^{-3}	2.60	3.13 10^{-3}	**5.43**	8.03 10^{-3}	2.12
R-7-8-4	5.70 10^{-2}	3.38 10^{-2}	1.69	3.15 10^{-2}	1.81	2.24 10^{-2}	**2.54**	2.79 10^{-2}	2.04
R-7-9-4	9.97 10^{-2}	4.98 10^{-2}	2.00	4.96 10^{-2}	2.01	3.43 10^{-2}	**2.91**	5.16 10^{-2}	1.93
R-7-10-5	2.33 10^{-1}	1.16 10^{-1}	2.01	1.29 10^{-1}	1.81	1.05 10^{-1}	**2.22**	1.22 10^{-1}	1.91
R-7-11-4	2.36 10^{-1}	1.22 10^{-1}	1.93	1.20 10^{-1}	1.97	8.49 10^{-2}	**2.78**	1.32 10^{-1}	1.79
R-7-12-6	9.35 10^{-1}	5.05 10^{-1}	**1.85**	5.74 10^{-1}	1.63	5.13 10^{-1}	1.82	5.65 10^{-1}	1.65
R-7-13-5	9.11 10^{-1}	4.70 10^{-1}	**1.94**	5.41 10^{-1}	1.68	4.71 10^{-1}	1.93	5.33 10^{-1}	1.71
R-7-14-7	3.69	2.15	**1.72**	2.39	1.54	2.42	1.52	2.42	1.52
R-8-15-7	6.43	3.56	**1.81**	3.92	1.64	4.30	1.50	4.57	1.41
R-9-16-8	1.51 10^{+1}	8.88	**1.70**	1.03 10^{+1}	1.47	1.34 10^{+1}	1.13	1.41 10^{+1}	1.07
R-10-17-9	3.45 10^{+1}	2.08 10^{+1}	**1.66**	2.50 10^{+1}	1.38	4.04 10^{+1}	0.85	3.53 10^{+1}	0.98
2d-20-4	3.48 10^{-1}	1.76 10^{-1}	1.98	8.03 10^{-2}	4.33	6.96 10^{-2}	**5.00**	1.73 10^{-1}	2.01
2d-20-5	6.74 10^{-1}	3.54 10^{-1}	1.90	1.29 10^{-1}	**5.22**	1.32 10^{-1}	5.11	3.59 10^{-1}	1.88
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sR-2	1.71 10^{+1}	4.26	4.01	3.11	**5.50**	4.14	4.13	1.05 10^{+1}	1.63
sR-4	8.03 10^{+1}	3.68 10^{+1}	2.18	4.40 10^{+1}	**1.83**	1.41 10^{+2}	0.57	2.02 10^{+2}	0.40
sR-6	1.08 10^{+2}	1.54 10^{+2}	0.70	7.01 10^{+1}	**1.54**	2.58 10^{+2}	0.42	4.04 10^{+2}	0.27
perm-5	6.64 10^{-1}	1.89 10^{-1}	3.51	6.87 10^{-2}	**9.67**	8.53 10^{-2}	7.78	3.75 10^{-1}	1.77
perm-6	5.80	1.32	4.39	5.19 10^{-1}	**11.18**	1.03	5.63	3.81	1.52
perm-7	5.70 10^{+1}	1.10 10^{+1}	5.18	4.16	**13.70**	2.12 10^{+1}	2.69	6.37 10^{+1}	0.89
perm-8	5.98 10^{+2}	1.08 10^{+2}	5.54	4.41 10^{+1}	**13.56**	6.46 10^{+2}	0.93	1.59 10^{+3}	0.38
r-3-7	5.83 10^{-1}	3.16 10^{-1}	1.84	2.79 10^{-1}	2.09	2.27 10^{-1}	**2.57**	3.64 10^{-1}	1.60
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median/mean			1.93/2.23		2.05/3.70		1.93/2.48		1.52/1.32

Conclusion

- pretty far from the differentiability; but relevant in itself
- various elements: LO, LA, recursivity, implementation choices...
- also: affine hyperplanes ✓, version for rational data $\simeq$✓, dedicated package...

Thanks for your attention! Some questions?

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Theoretical detour

Very well-known in algebra / combinatorics...
... but very theoretically: Möbius function, lattices, matroids.

Very impressive results / algorithms for the cardinal (number of feasible systems, number of $J \in \partial_B$)
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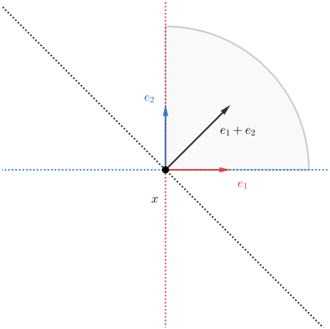
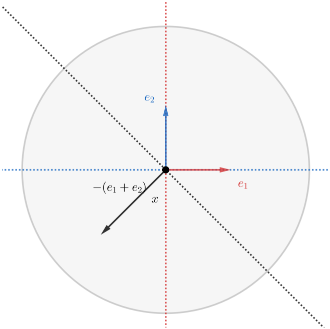
Various properties

-origin = center of symmetry ; $s_i v_i^\top d > 0 \Leftrightarrow (-s_i) v_i^\top (-d) > 0$



Feasible $\Leftrightarrow$ pointed cone



Infeasible $\Leftrightarrow$ non-pointed

-"connectedness" property (vertices = J's, edges = hyperplanes)

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With one more vector

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- $v_k^\top d_s^{k-1} = 0 \Rightarrow$ both systems ✓ by perturbation

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We look at subsets $I \subset [1:p]$, $\dim(\mathcal{N}(V_{:,I})) = \mathbf{1}$
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2^p LO feasibility $\leftrightarrow$ 2^p $\mathcal{N}$ searches; subsets of size $\leq 1 + \mathrm{rank}(V)$

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$\mathcal{N}(V_{:,I})$ gives 'unsigned' η's which define the sign $s_J = 1$ because

if ≥ 2, smaller subsets are of $\dim(\mathcal{N}) = 1$

2^p LO feasibility $\leftrightarrow$ 2^p $\mathcal{N}$ searches; subsets of size $\leq 1 + \mathrm{rank}(V)$

Issue (unresolved): "optimal" way to compute efficiently: if I s.t. $\dim(\mathcal{N}(V_{:,I})) = 1$, $I' \supsetneq I$ useless to check

Circuits of matroids

We look at subsets $I \subset [1:p]$, $\dim(\mathcal{N}(V_{:,I})) = \mathbf{1}$
and $\forall\ I' \subsetneq I$, $\dim(\mathcal{N}(V_{:,I'})) = 0$

$$\begin{aligned}\dim(\mathcal{N}(V_{:,I})) = 1 \Rightarrow & \mathcal{N}(V_{:,I}) = \mathrm{Vect}(\eta) \\ & \Rightarrow V_{:,I}\eta = 0 \Leftrightarrow \underbrace{V_{:,I}\mathrm{sign}(\eta)}_{V_{(:,I)}S_{(I)}} \underbrace{\mathrm{sign}(\eta)\eta}_{=\gamma_{(I)}\geq 0} = 0\end{aligned}$$

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