Polling Set Construction and Worst-Case Complexity for Direct Search under Polyhedral Convex Constraints

Joint work with Clément Royer (U. Paris Dauphine-PSL)

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Key references

This talk is based on:

- LR & C. W. Royer, Poll Set Construction and Worst-Case Complexity for Direct Search under Polyhedral Convex Constraints, arXiv:2605.27814 (2026).

Software available on Github: `https://github.com/lindonroberts/directsearch`

Direct Search Methods

Considering direct search methods with sufficient decrease: [Kolda, Lewis & Torczon, 2003]

Direct Search Iteration

- Given $\boldsymbol{x}_k \in \mathbb{R}^n$ and $\alpha_k > 0$, choose a set $\mathcal{D}_k \subset \mathbb{R}^n$ of p vectors
- If there exists $\boldsymbol{d}_k \in \mathcal{D}_k$ with $f(\boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k) < f(\boldsymbol{x}_k) - \frac{1}{2}\alpha_k^2$
  - Set $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$ and increase α_k
  - Otherwise, set $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k$ and decrease α_k

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For convergence, need poll set $\mathcal{D}_k$ to satisfy:

$$\max_{\boldsymbol{d} \in \mathcal{D}_k} \frac{\boldsymbol{d}^T(-\nabla f(\boldsymbol{x}_k))}{\|\boldsymbol{d}\|_2 \, \|\nabla f(\boldsymbol{x}_k)\|_2} \geq \kappa \in (0, 1]$$

i.e. there is a vector $\boldsymbol{d}$ making a (sufficiently small) acute angle with $-\nabla f(\boldsymbol{x}_k)$.

To quantify the quality of the poll set, look at the cosine measure of $\mathcal{D}_k$:

$$\mathrm{cm}(\mathcal{D}_k) = \min_{\boldsymbol{v}\neq\boldsymbol{0}} \max_{\boldsymbol{d}\in\mathcal{D}_k} \frac{\boldsymbol{d}^T\boldsymbol{v}}{\|\boldsymbol{d}\|_2 \, \|\boldsymbol{v}\|_2}$$

i.e. (cosine of the) largest angle between $\boldsymbol{v}$ and the closest (in angle) $\boldsymbol{d} \in \mathcal{D}_k$ to $\boldsymbol{v}$.

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For $\pm$ coordinate directions, $\kappa = 1/\sqrt{n} \to \mathcal{O}(n\epsilon^{-2})$ iterations, or $\mathcal{O}(n^2\epsilon^{-2})$ objective evaluations (up to $|\mathcal{D}_k| = 2n$ evaluations per iteration).

An alternative perspective

Link 1: A classical result is:

Theorem (Davis, 1954)

A set $\mathcal{D}$ has $\text{cm}(\mathcal{D}) > 0$ if and only if $\mathcal{D}$ is a positive spanning set (PSS) (i.e. can write every $\boldsymbol{v} \in \mathbb{R}^n$ as a positive combination of vectors in $\mathcal{D}$, or $\text{cone}(\mathcal{D}) = \mathbb{R}^n$).

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Link 2: In model-based DFO, suppose we build a linear interpolant $m(\cdot)$ using perturbations $\boldsymbol{d}_1, \ldots, \boldsymbol{d}_n$ around $\boldsymbol{x}$. Then

$$|m(\boldsymbol{x}+\boldsymbol{d}) - f(\boldsymbol{x}) - \nabla f(\boldsymbol{x})^T \boldsymbol{d}| \leq \frac{L_{\nabla f}}{2} d_{\max}^2 \sum_{i=1}^n |c_i(\boldsymbol{d})|,$$

where the $c_i(\boldsymbol{d})$ satisfy $\boldsymbol{d} = \sum_{i=1}^n c_i(\boldsymbol{y})\boldsymbol{d}_i$ (exist whenever $\boldsymbol{d}_i$ linearly span $\mathbb{R}^n$).

This corresponds to Λ-poisedness or Lebesgue measure.

[Trefethen, 2020], [LR, 2025]

Positive Spanning Sets

These two ideas motivate an alternative measure of poll set quality, generalizing the Lebesgue measure to positive spanning sets.

Definition

A set $\mathcal{D} = \{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_p\}$ is a Λ-positive spanning set (Λ-PSS) for $B(\boldsymbol{x}, \alpha)$ if, for any $\|\boldsymbol{v}\|_2 \leq \alpha$, we can write $\boldsymbol{v} = \sum_{i=1}^{p} c_i(\boldsymbol{v})\boldsymbol{d}_i$ with $c_i(\boldsymbol{v}) \geq 0$ and $\sum_{i=1}^{p} c_i(\boldsymbol{v}) \leq \Lambda$.

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This is essentially equivalent to a lower bound $\mathrm{cm}(\mathcal{D}) \geq \kappa$ with $\kappa = 1/\Lambda$.

Theorem (LR & Royer, 2026)

(a) *If $\mathcal{D}$ is a Λ-PSS and and $\|\boldsymbol{d}_i\|_2 \leq d_{\max}\alpha$, then $\mathrm{cm}(\mathcal{D}) \geq 1/(d_{\max}\Lambda)$*

(b) *If $\mathrm{cm}(\mathcal{D}) \geq \kappa$ and $\|\boldsymbol{d}_i\|_2 \geq d_{\min}\alpha$, then $\mathcal{D}$ is a Λ-PSS with $\Lambda = 1/(d_{\min}\kappa)$.*

The earlier result (Davis, 1954) corresponds to the limit $\kappa \to 0^+$ or $\Lambda \to \infty$.

Convex Constraints

Now, consider the constrained problem

$$\min_{\boldsymbol{x} \in \Omega} \; f(\boldsymbol{x}),$$

where $\Omega \subseteq \mathbb{R}^n$ is a convex set with nonempty interior (e.g. bounds, linear inequalities).

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One measure of first-order optimality for this problem is

$$\pi(\boldsymbol{x}) := \left| \min_{\substack{\boldsymbol{x}+\boldsymbol{v}\in\Omega \\ \|\boldsymbol{v}\|_2\leq 1}} \nabla f(\boldsymbol{x})^T \boldsymbol{v} \right| \qquad (\text{e.g. } \pi(\boldsymbol{x}) = \|\nabla f(\boldsymbol{x})\|_2 \text{ if } \Omega = \mathbb{R}^n)$$

We have: $\pi(\boldsymbol{x}) \geq 0$, with $\pi(\boldsymbol{x}) = 0$ if and only if $\boldsymbol{x}$ is first-order critical, and $\pi(\cdot)$ is continuous. e.g. [Cartis, Gould & Toint, 2012]

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Question: how to generalize $\mathrm{cm}(\mathcal{D})$ to the constrained setting?

Constrained Positive Spanning Sets

There is no natural generalization of $\text{cm}(\mathcal{D})$ to the constrained setting*, but there is for Λ-PSS.

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i.e. just ensure all relevant points are feasible.

*only for subsets of the constrained region (approximate tangent cone — discussed later).

Constrained Positive Spanning Sets

This enables a very simple worst-case complexity result.

Theorem (LR & Royer, 2026)

If f has Lipschitz continuous gradients, $\|\boldsymbol{d}\|_2 \leq d_{\max}\alpha_k$ for all $\boldsymbol{d} \in \mathcal{D}_k$ and $\mathcal{D}_k$ is a Λ-PSS for $B(\boldsymbol{x}_k, \alpha_k) \cap \Omega$ for all k, then $\pi(\boldsymbol{x}_k) \leq \epsilon$ after at most $\mathcal{O}(\Lambda^2\epsilon^{-2})$ iterations.

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Key new idea: by definition, $\pi(\boldsymbol{x}_k) = -\nabla f(\boldsymbol{x}_k)^T \boldsymbol{v}_k$ for some $\|\boldsymbol{v}_k\|_2 \leq 1$ with $\boldsymbol{x}_k + \boldsymbol{v}_k \in \Omega$, invoke Λ-PSS property (or $\alpha_k \boldsymbol{v}_k$ if $\alpha_k < 1$).

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This matches the unconstrained result with $\Lambda \sim 1/\kappa$, and derivative-based and interpolation-based DFO theory. [Cartis, Gould & Toint, 2012], [Hough & LR, 2022]

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If we have $\Omega = \{\boldsymbol{x} : \boldsymbol{x}^L \leq \boldsymbol{x} \leq \boldsymbol{x}^U\}$, then use $\pm$ coordinate directions, scaled to length α and feasibility:

$$\mathcal{D} = \cup_{i=1}^{n} \{\alpha_i \boldsymbol{e}_i, -\alpha_{-i} \boldsymbol{e}_i\}, \qquad \text{where, e.g. } \alpha_i = \min(\alpha, x_i^U - x_i)$$

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$\mathcal{D}$ is a Λ-PSS with $\sqrt{n} \leq \Lambda(\boldsymbol{x}, \alpha) \leq n$ (depending on $\#$ nearly active constraints).

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This leads to $\mathcal{O}(n^2\epsilon^{-2})$ iterations or $\mathcal{O}(n^3\epsilon^{-2})$ evaluations to achieve $\pi(\boldsymbol{x}_k) \leq \epsilon$ [note: $\mathcal{O}(n^3)$ is not optimal result, but better in practice]. [Gratton et al., 2019]

Linearly Constrained Problems

Now suppose our feasible set is a polytope, formed by $\boldsymbol{a}_j^T \boldsymbol{x} \leq b_j$ for $j = 1, \ldots, m$.

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At every iteration (with $\boldsymbol{x}_k$ feasible), look at the nearly active constraints:

$$j \in \mathcal{J}(\boldsymbol{x}_k, \alpha_k) \qquad \Longleftrightarrow \qquad b_j - \alpha_k \|\boldsymbol{a}_j\|_2^2 \le \boldsymbol{a}_j^T \boldsymbol{x}_k \le b_j$$

i.e. the constraints whose boundaries intersect with $B(\boldsymbol{x}_k, \alpha_k)$.

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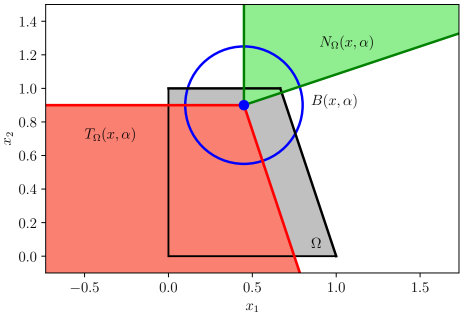
The approximate tangent cone is $T_\Omega(\boldsymbol{x}_k, \alpha_k)$ is its polar: $\boldsymbol{v}$ such that $\boldsymbol{v}^T \boldsymbol{a}_j \leq 0$ for all $j \in \mathcal{J}(\boldsymbol{x}_k, \alpha_k)$.

[Kolda, Lewis & Torczon, 2003 & 2007]

Example: Direct Search

Simple example: $x_1, x_2 \geq 0$, with $x_2 \leq 1$ and $3x_1 + x_2 \leq 3$ at $\boldsymbol{x} = [0.45, 0.9]$:



(a) $\alpha = 0.35$, nearly active constraints are $x_2 \leq 1$ and $3x_1 + x_2 \leq 3$

Modified from [Kolda, Lewis & Torczon, 2007]

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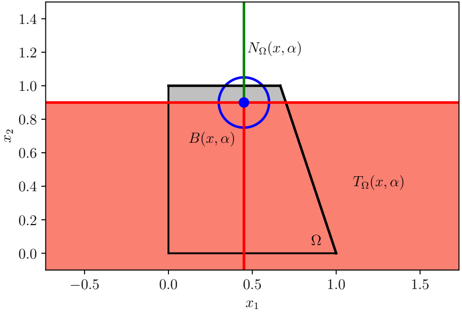

(b) $\alpha = 0.15$, nearly active constraint is $x_2 \leq 1$

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In existing theory, we choose the poll set such that

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such that

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For bound constraints, we can get $\kappa = 1/\sqrt{n}$, matching the unconstrained case.

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Why bother?

If we only need to use generators of $T_{\Omega}(\boldsymbol{x}_k, \alpha_k)$, why do we need Λ-PSS theory?

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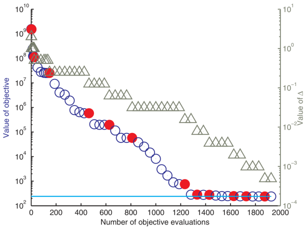
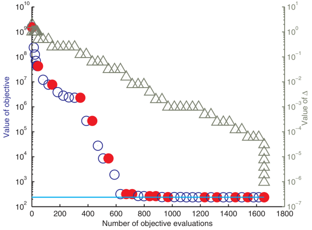
If we only need to use generators of $T_{\Omega}(\mathbf{x}_k, \alpha_k)$, why do we need Λ-PSS theory?

Adding directions outside the tangent cone is **practically successful without theoretical justification**—typically (scaled) normal vectors for nearly active constraints.



Tangent generators only



With normal directions

Figures from [Lewis, Shepherd & Torczon, 2007]

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Adding constraint normals

Is (generators of tangent cone) + (nearly active normal vectors) a Λ-PSS?

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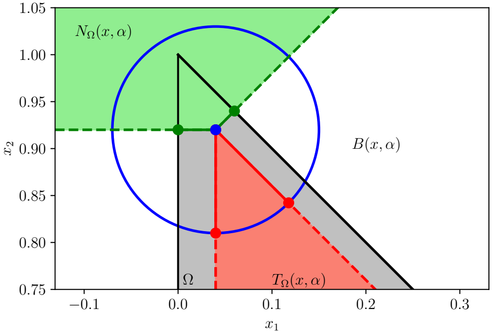
No!



Example: need (arbitrarily) large coefficients to reach v = top corner

PSS for Linear Constraints

Adding constraint normals

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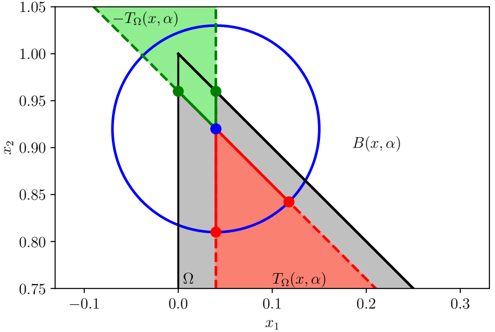
Use negatives of tangent generators (scaled to be feasible)!



Example: use negative of tangent cone generators

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If $\{\boldsymbol{a}_j : j \in \mathcal{J}(\boldsymbol{x}_k, \alpha_k)\}$ is linearly independent, then $\pm$ generators of tangent cone (scaled to be in $B(\boldsymbol{x}_k, \alpha_k) \cap \Omega$) is a Λ-PSS with $\Lambda = |\mathcal{J}|\,\kappa(A_{\mathcal{J}}) + \sqrt{n - |\mathcal{J}|}$, where $A_{\mathcal{J}}$ is the matrix with columns $\boldsymbol{a}_j$.

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It is not clear how to guarantee Λ-PSS in the general case, but in practice:

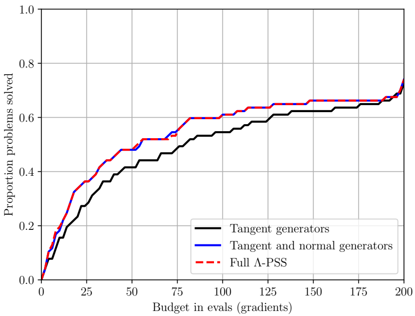
- If $A_{\mathcal{J}}$ not full rank, use same approach
  - Enumerating generators requires some care — e.g. [Fukuda & Prodon, 1996]
- If $T_{\Omega}(\boldsymbol{x}_k, \alpha_k) = \{\boldsymbol{0}\}$, use (scaled) nearly active normals (guaranteed to be a PSS)
- If $\pm$ generators of T_{Ω} do not (linearly) span $\mathbb{R}^n$, augment with poll set in the null space (recursively)

Numerical Results

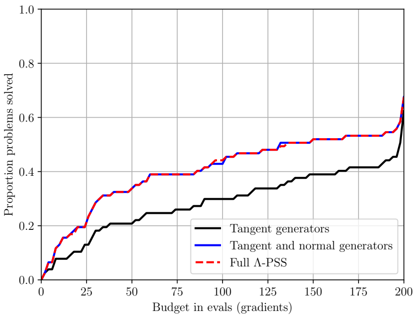
For our testing:

- Compare poll sets from:
  - Existing theory: tangent generators only
  - Existing heuristic approach: tangent generators + nearly active normals
  - Our approach: $\pm$ tangent generators
- Opportunistic polling (i.e. accept the first poll direction that achieves sufficient decrease)
- Only try extra poll directions if all tangent generators do not achieve sufficient decrease
- Test on 77 bound-constrained and 45 linear inequality constrained CUTEst problems (low dimension, $n \leq 51$) for up to $200(n+1)$ objective evaluations

Numerical Results — Bound Constraints



Low accuracy, $\tau = 10^{-3}$



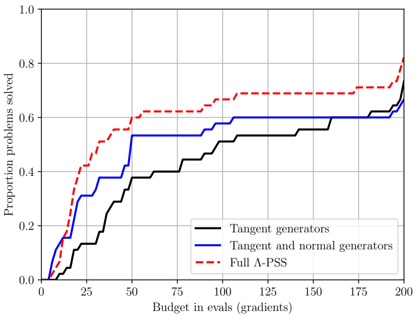
High accuracy, $\tau = 10^{-6}$

Bound-constrained problems

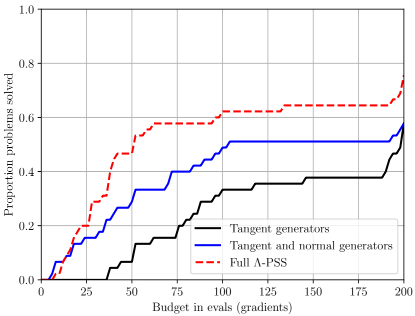
Data profiles: proportion of problems solved after given number of objective evaluations (units of $n+1$).

Higher is better.

Numerical Results — Linear Inequality Constraints



Low accuracy, $\tau = 10^{-3}$



High accuracy, $\tau = 10^{-6}$

Linear inequality constrained problems

Data profiles: proportion of problems solved after given number of objective evaluations (units of $n+1$). Higher is better.

Conclusions & Future Work

Conclusions

- Alternative poll set quality measure, Λ-PSS, generalizes naturally to constrained problems
- Can construct Λ-PSS for bound constraints and some general linear inequality constraints
- Provides some theoretical justification to long-standing practical observation
- Strong numerical performance

Future Work

- Full Λ-PSS theory for all possible linear constraints
- Extension to large-scale problems via random embeddings

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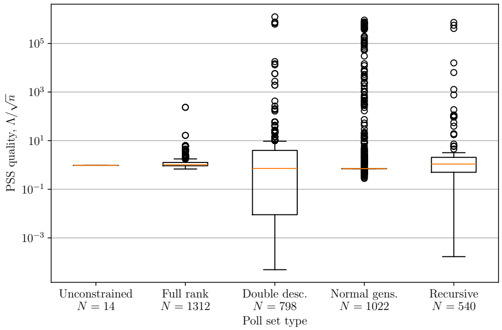
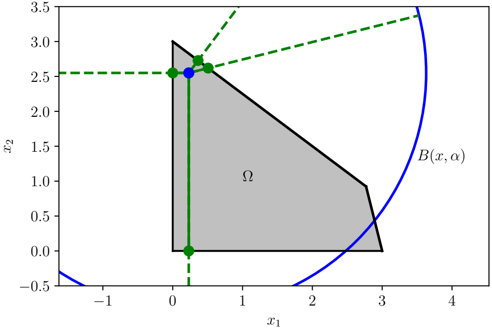
Practical Construction Quality



Distribution of realized Λ for linearly constrained problems

Practical Construction Quality



Example where practical approach can be improved ($T_\Omega = \{0\}$, using active normal directions)