MADS - Mesh Adaptive Direct Search for constrained optimization

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Outline

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- The GPS and MADS algorithm classes

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$$\text{subject to} \quad x \in \Omega,$$

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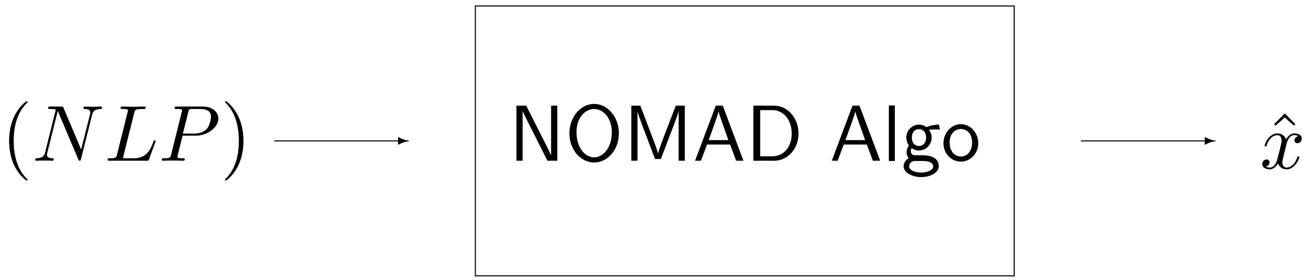
- accurate approximation of derivatives is problematic
- surrogate models $s \approx f$ and $P \approx X$ may be available

Goals – or validation of the method



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if f is convex	then $0 \in \underline{\partial} f(\hat{x})$
if f is Lipschitz near $\hat{x}$	then $0 \in \partial f(\hat{x})$

Clarke Calculus – for f Lipschitz near x

- Clarke generalized derivative at x in the direction v:

$$f^\circ(x;v) \;=\; \limsup_{y\to x,\ t\downarrow 0} \frac{f(y+tv)-f(y)}{t}.$$

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- $f^\circ(x;v)$ can be obtained from $\partial f(x)$:
$f^\circ(x;v)=\max\{v^T\zeta : \zeta\in\partial f(x)\}$.

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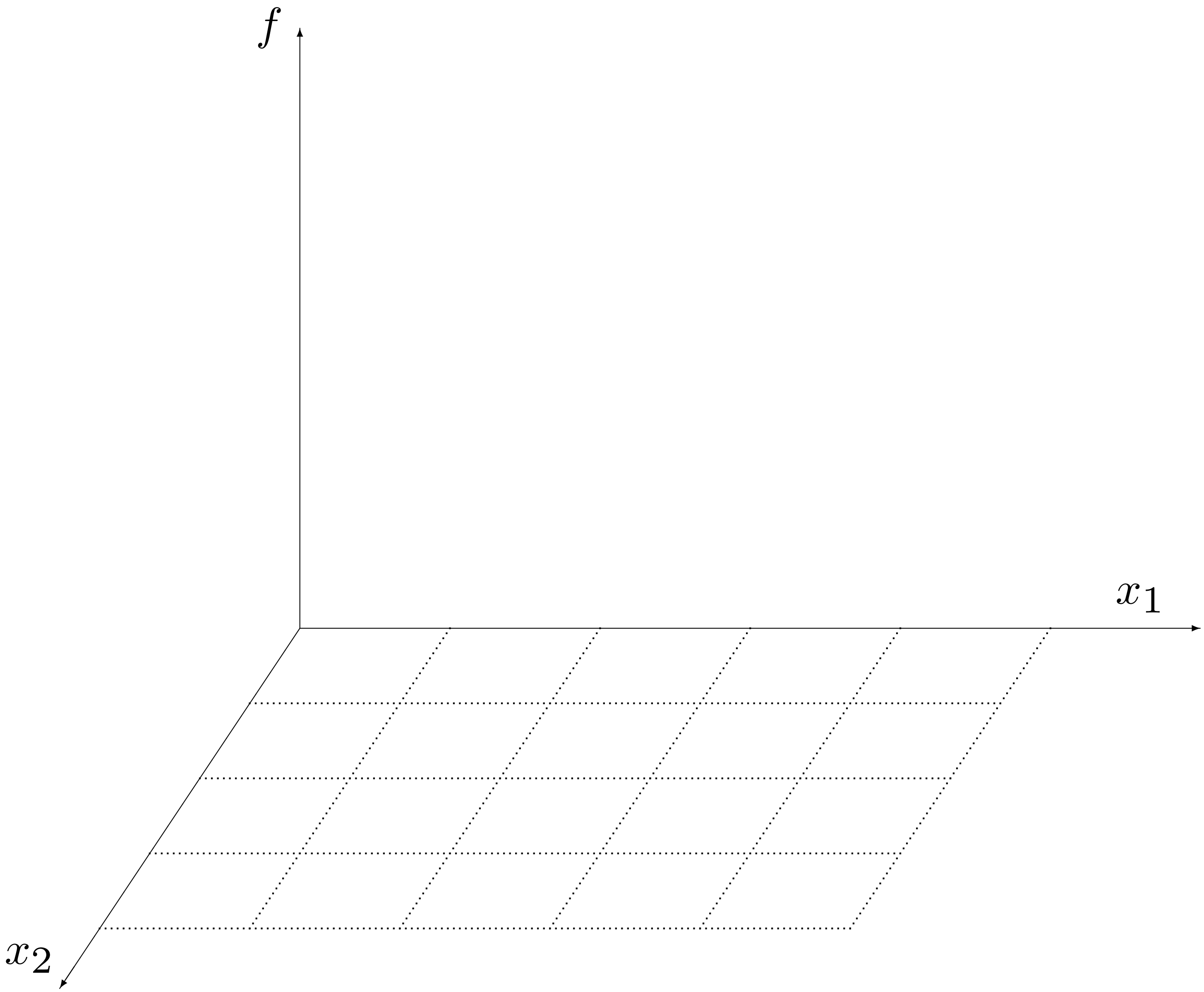
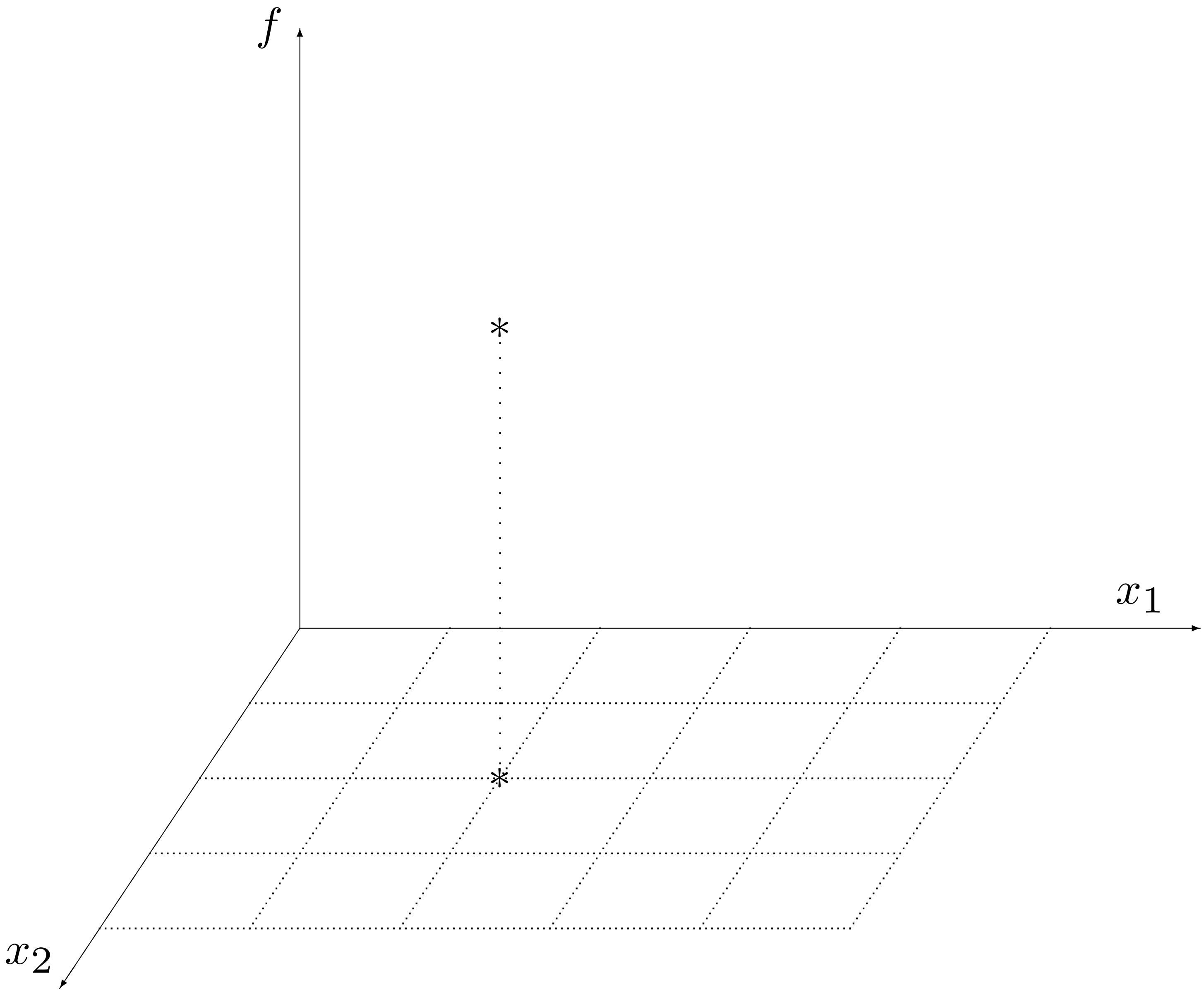
- The LOCAL POLL around the incumbent solution is more rigidly defined, but it ensures convergence to a point satisfying necessary first order optimality conditions.
- This talk focusses on the basic algorithm, and the convergence analysis. In the next talks, Alison, Mark and Gilles will talk about surrogates in the SEARCH.


f
x1
x2



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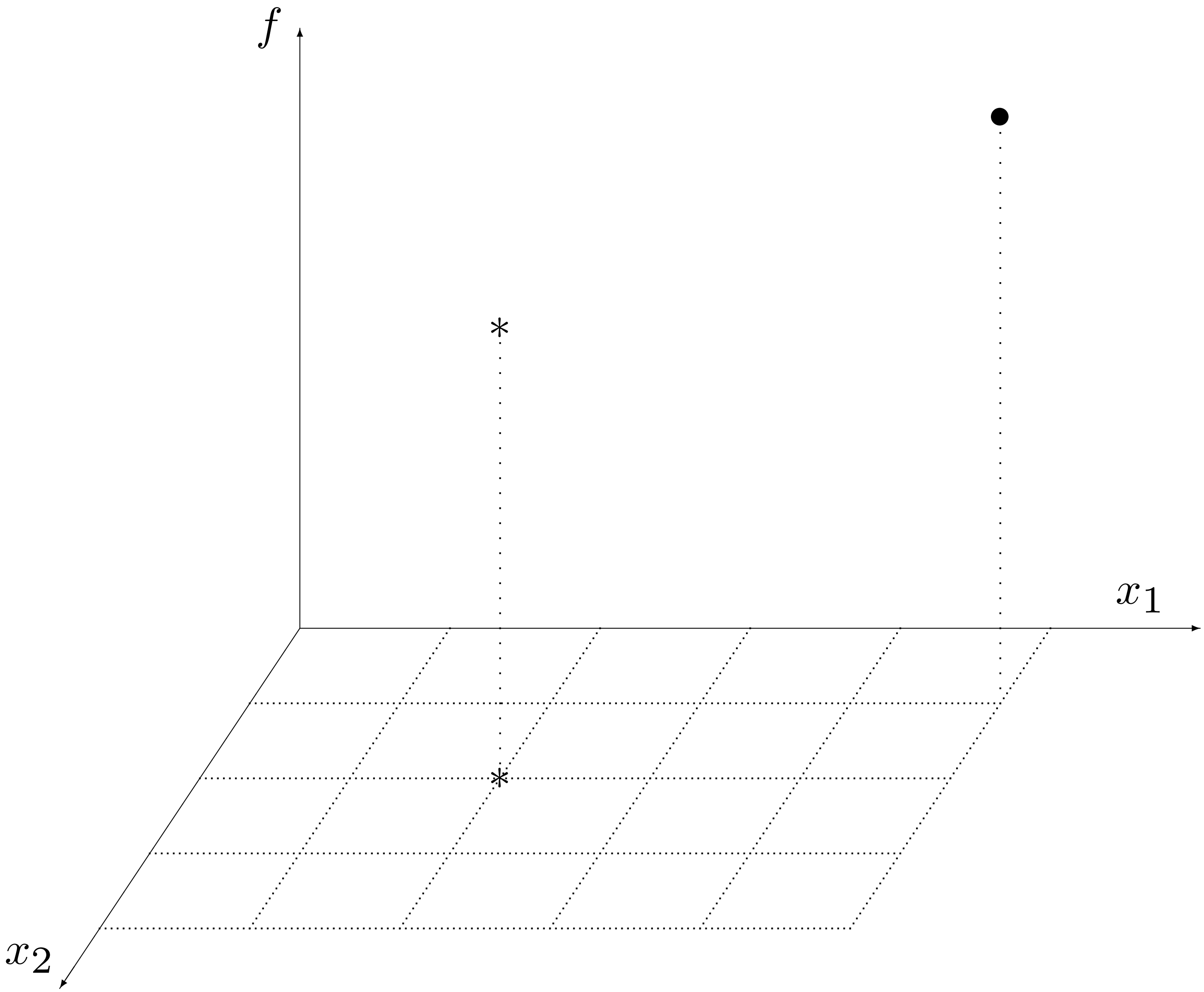

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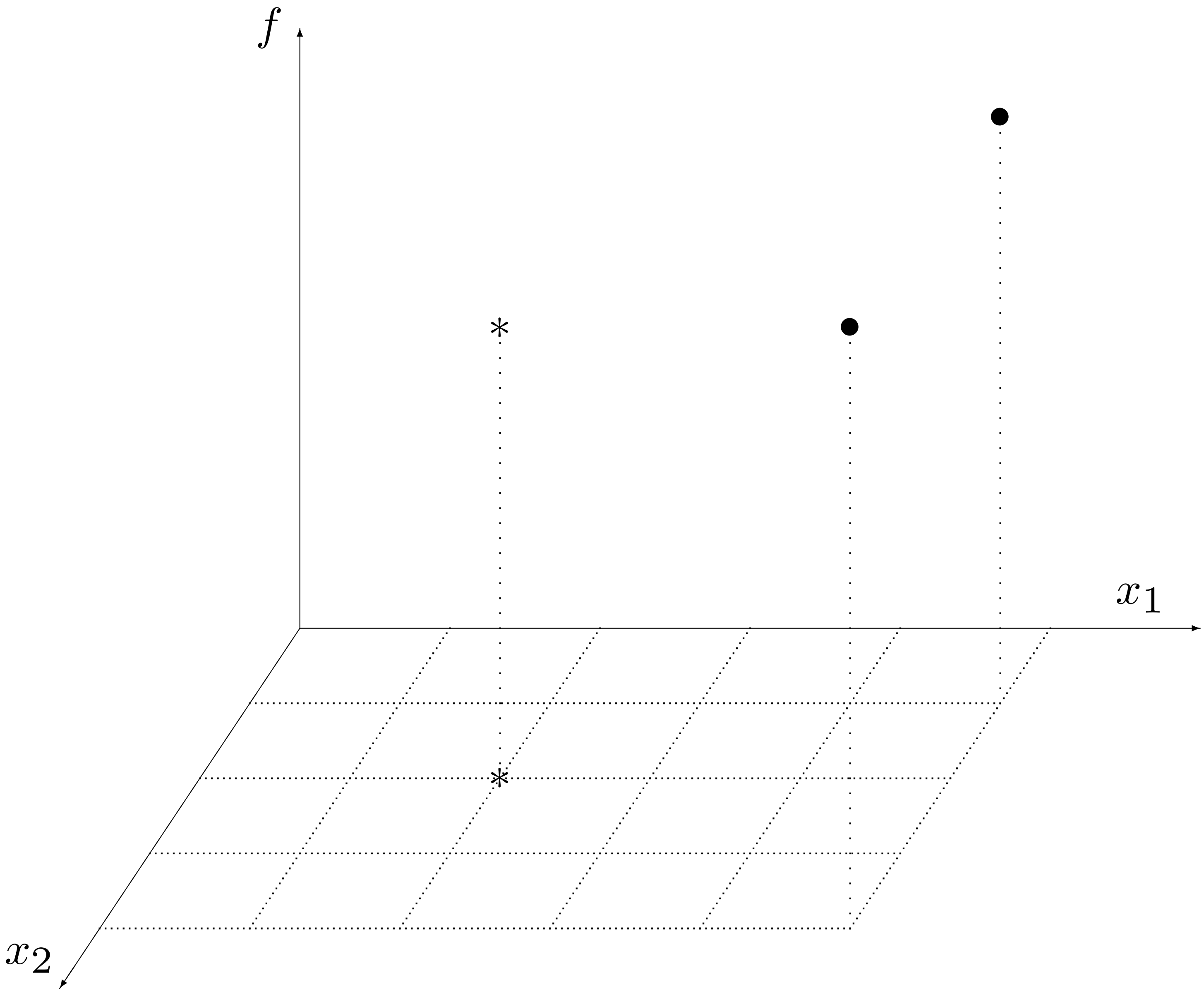

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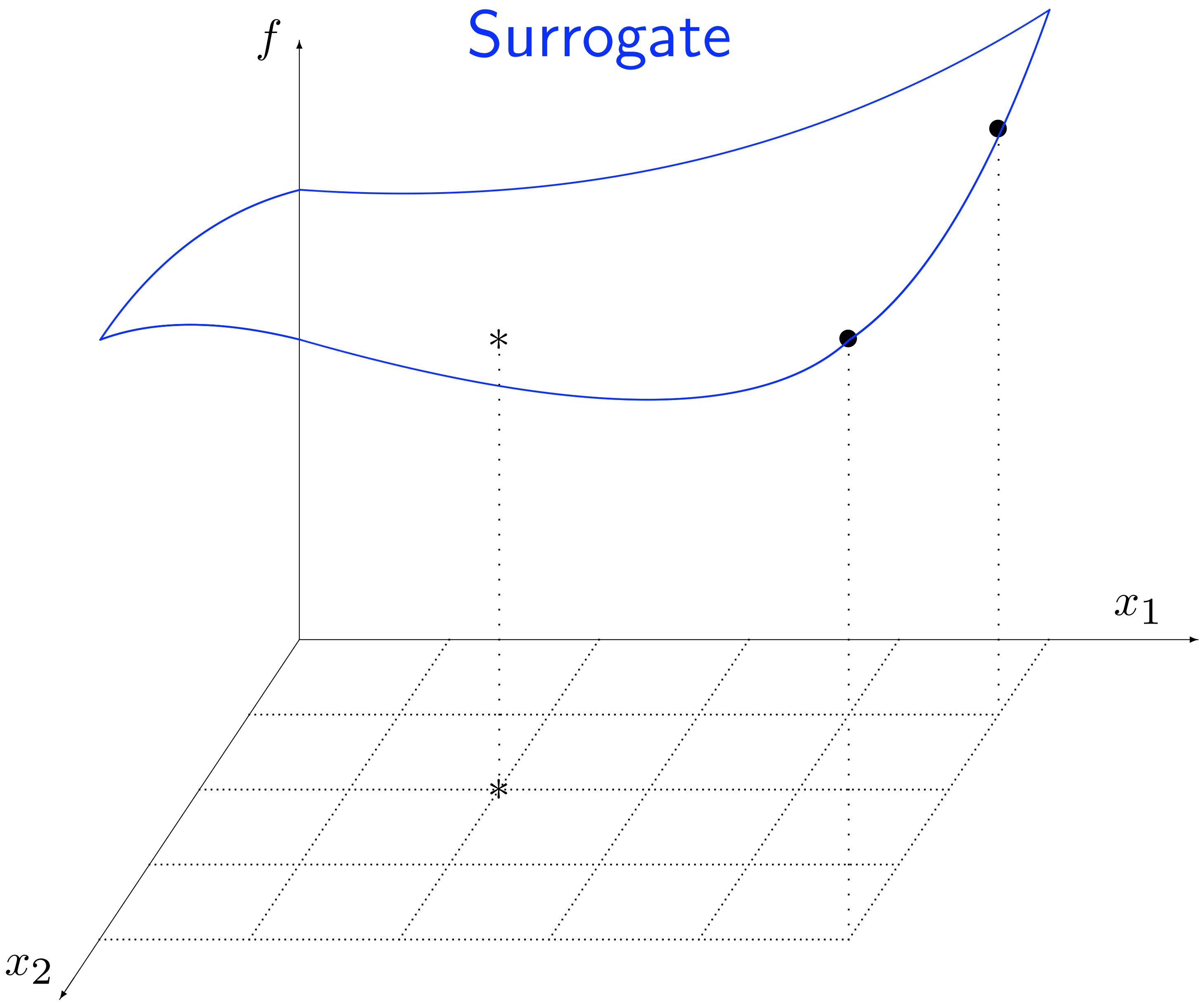

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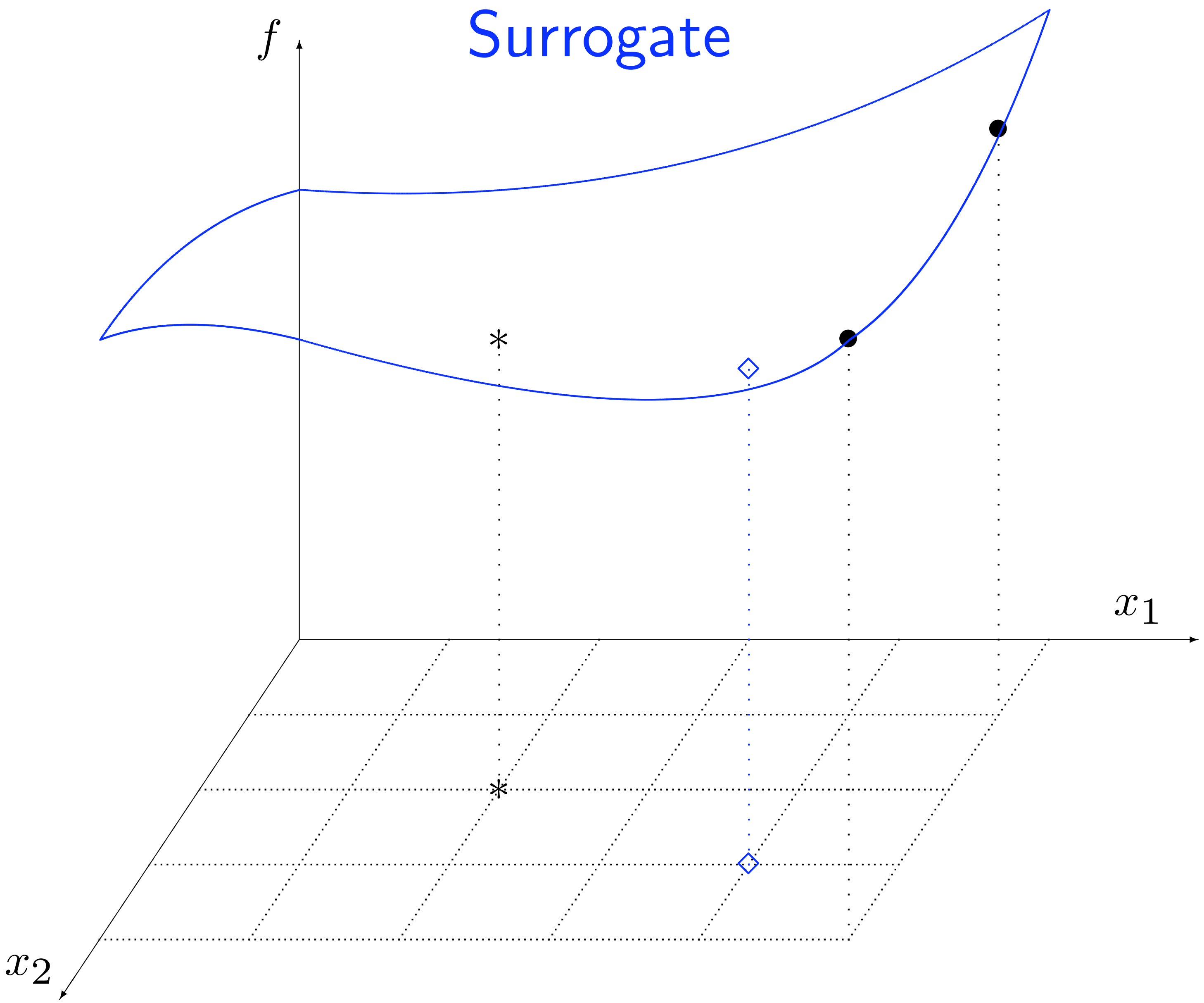

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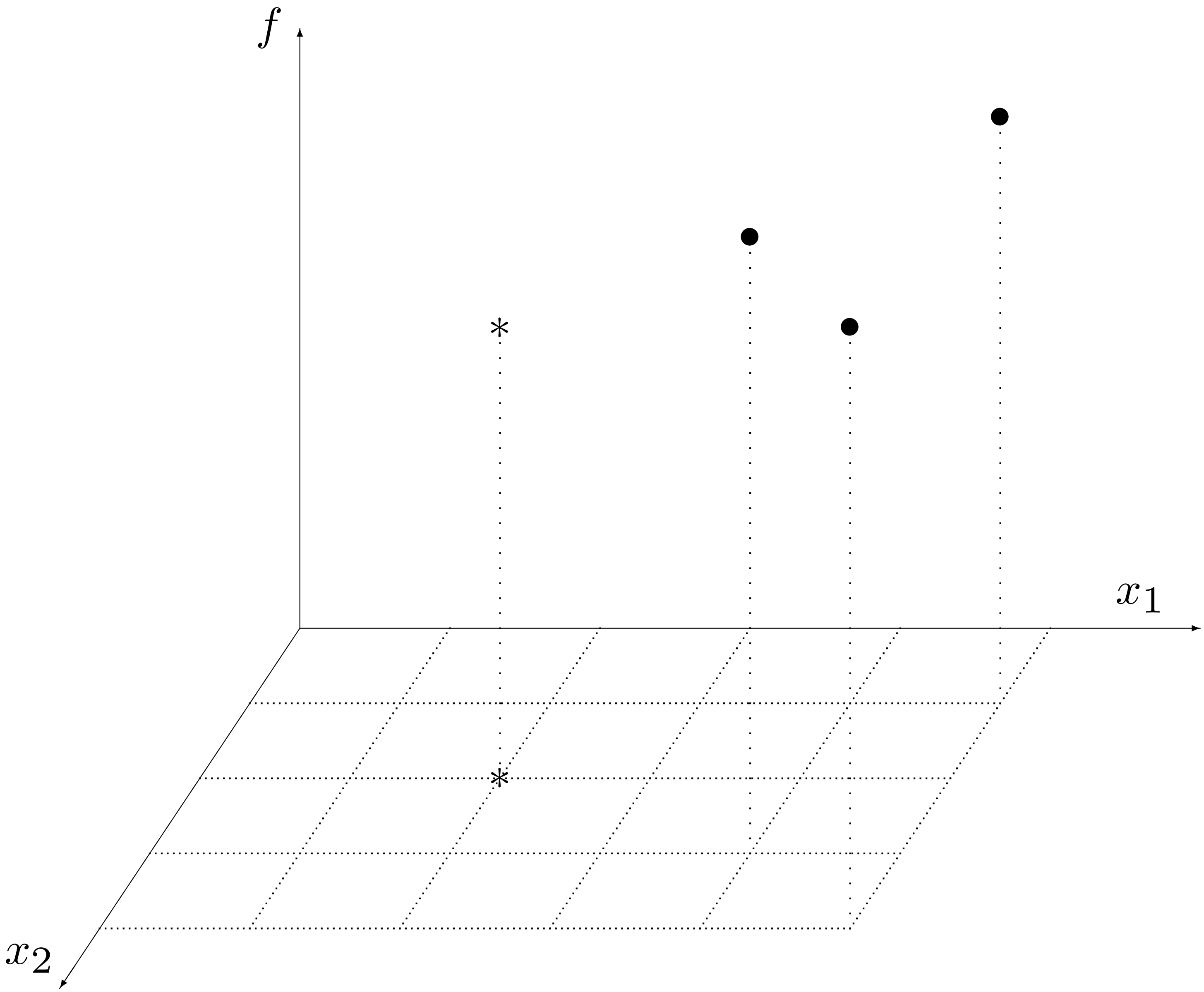

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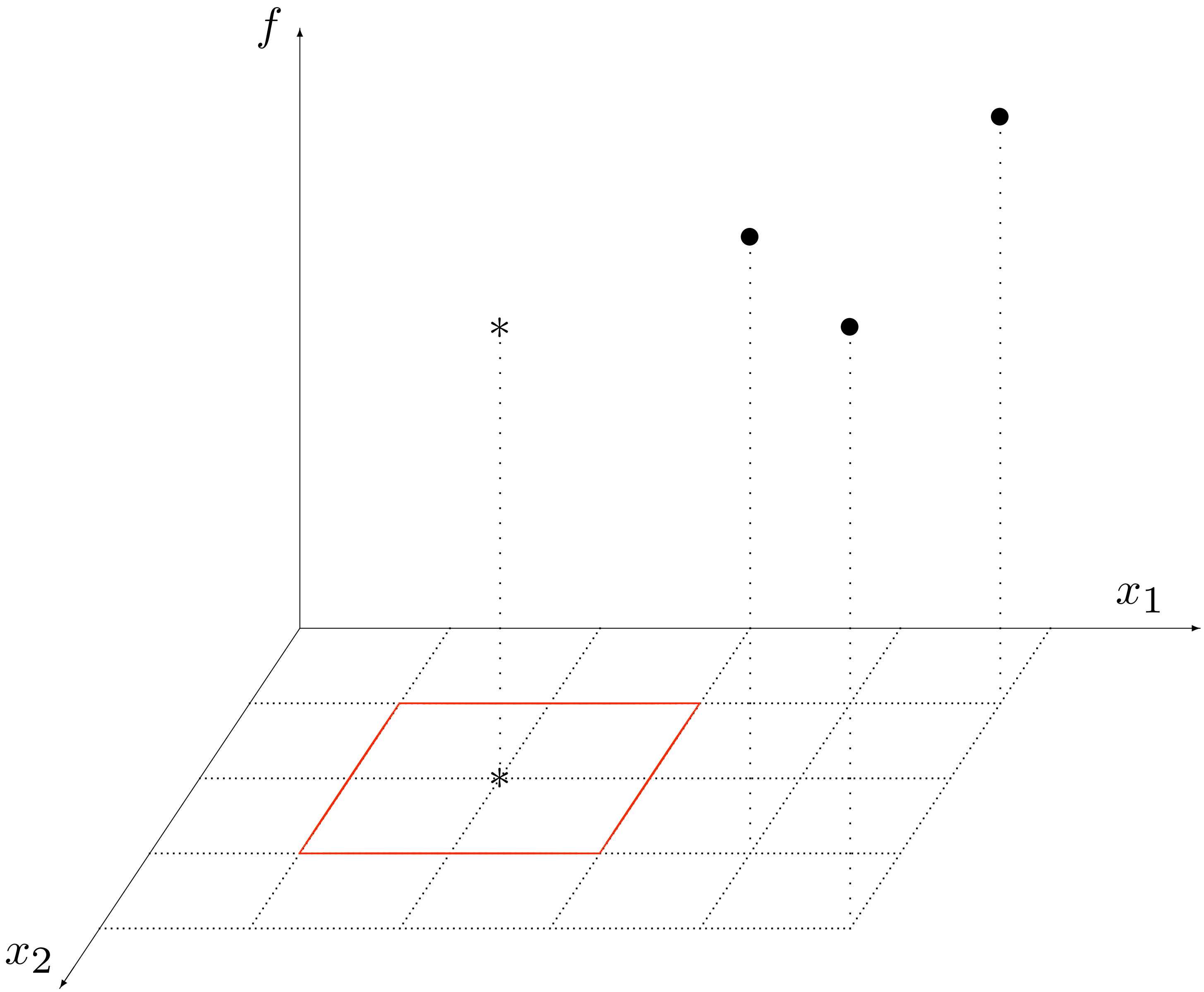

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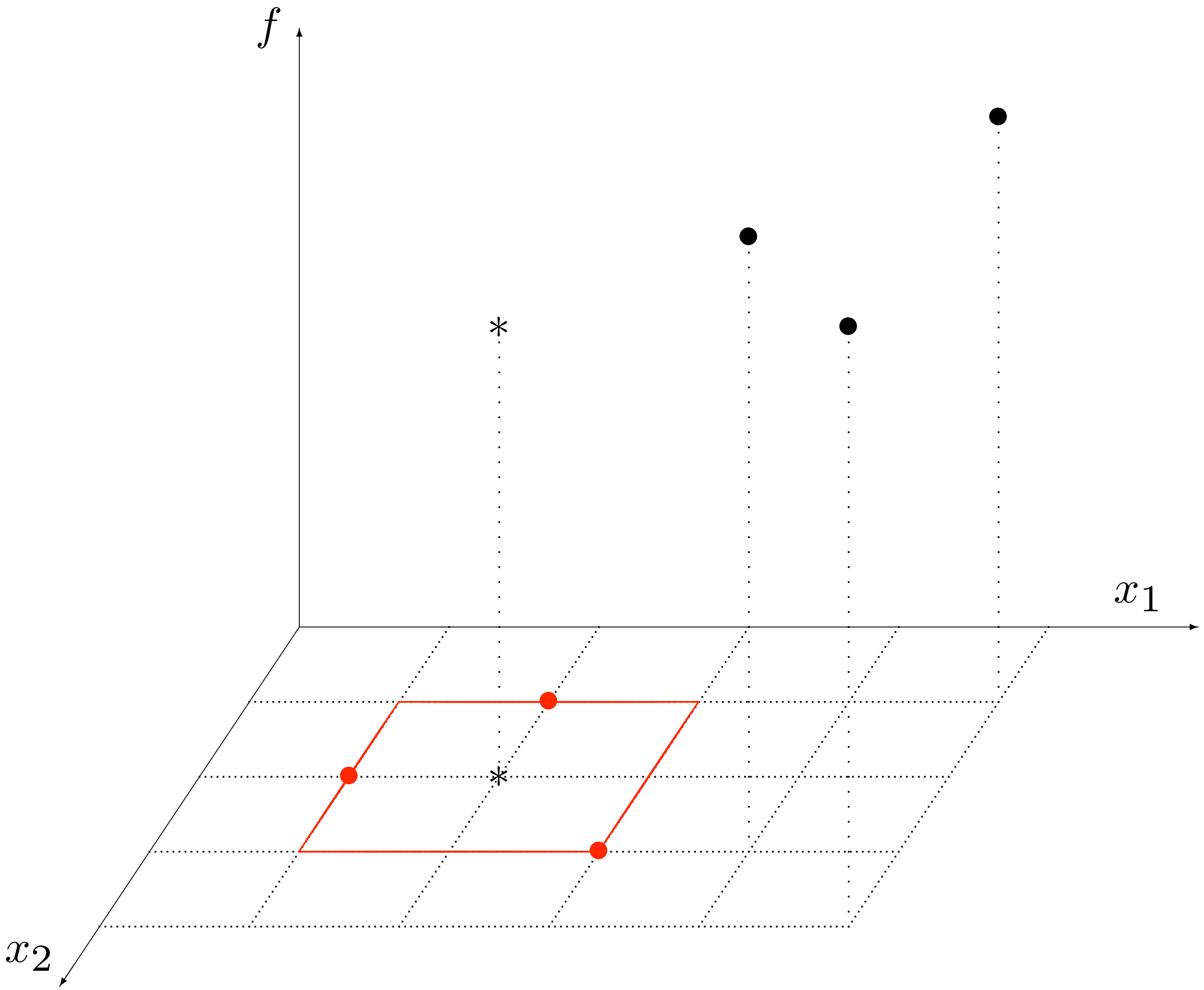

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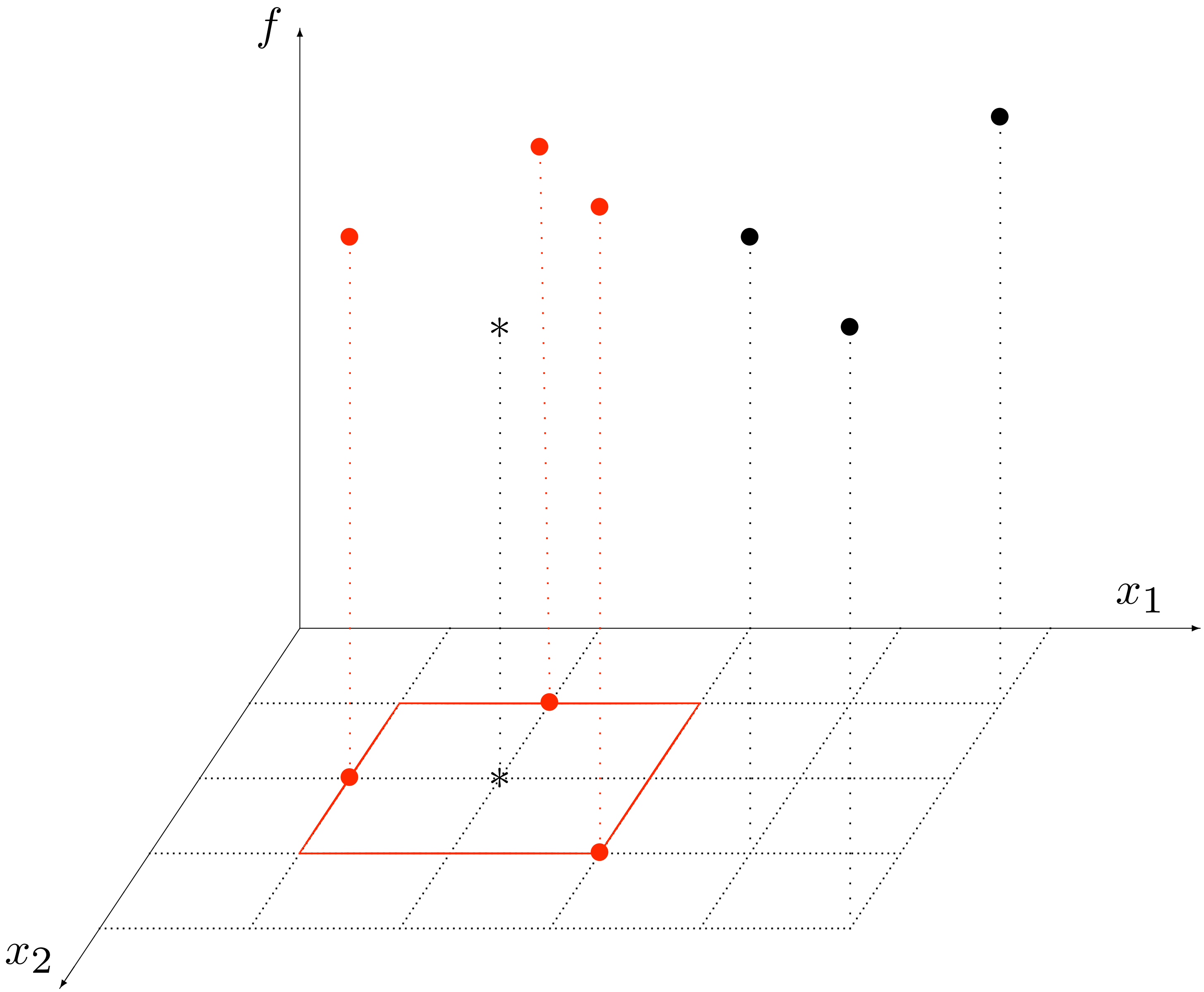

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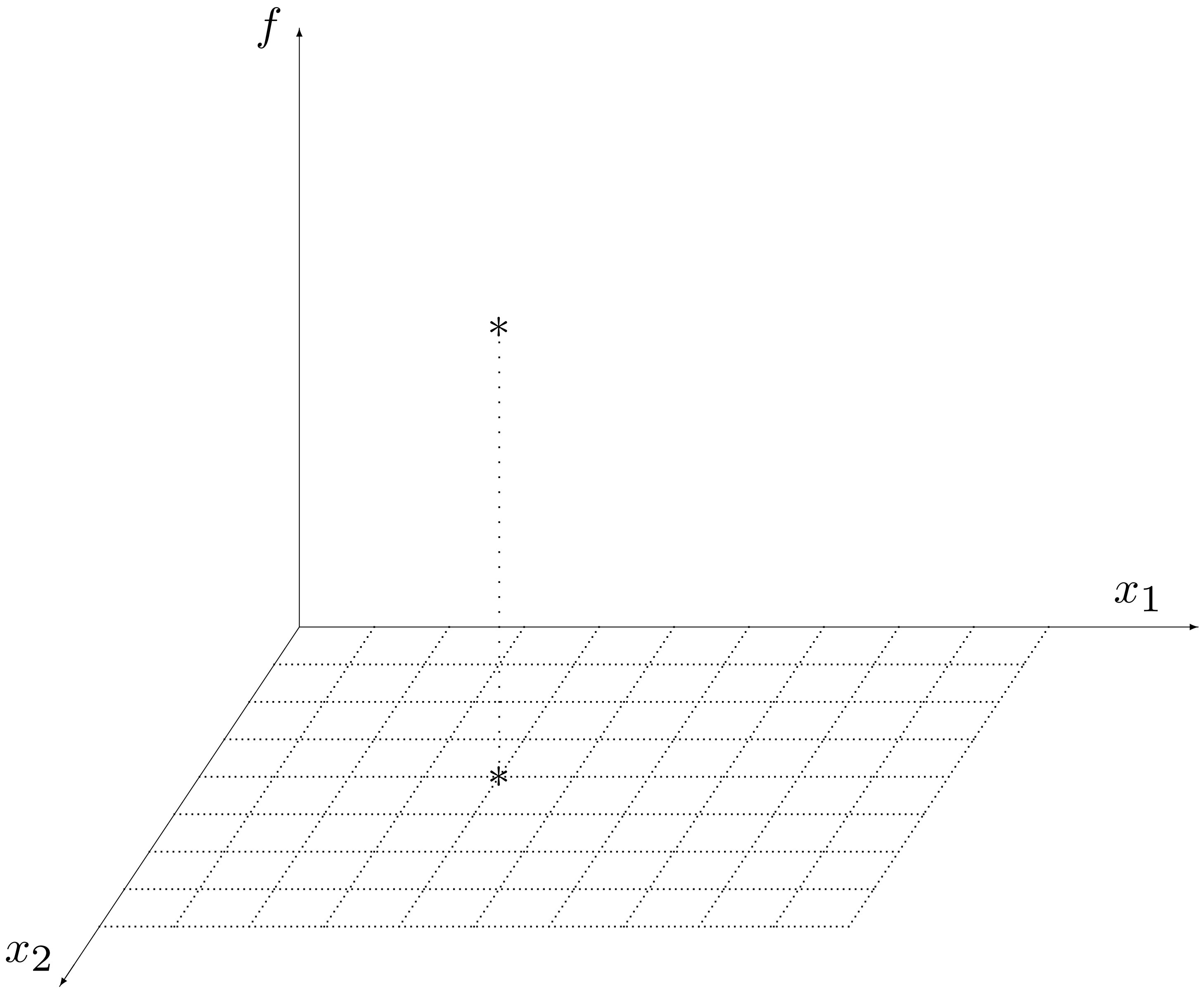

New iteration from the same incumbent solution, but on a finer mesh

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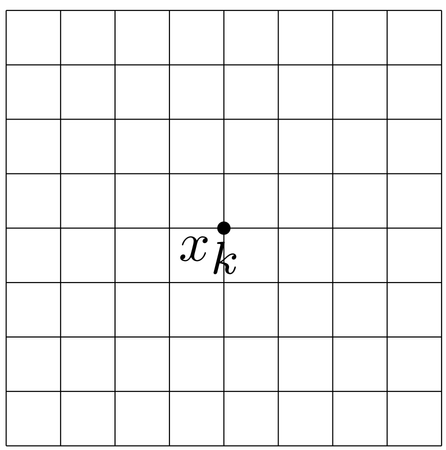

Ex: $D=[I; \ -I]$

Basic pattern search algorithm for unconstrained optimization

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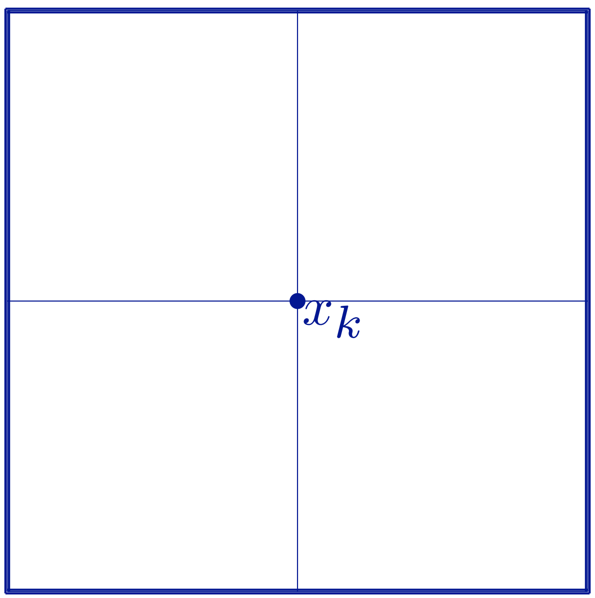
2. Else if x_k minimizes $f(x)$ for $x \in P_k$, then set $x_{k+1} = x_k$ and $\Delta_{k+1}^m = \Delta_k^m/2$ (x_k is called a *minimal frame center*).

The Coordinate Search (CS) frame P_k

$P_k = \{x_k + \Delta_k^m d : d \in [I; -I]\}$;
$2n$ points adjacent to x_k in M_k.

$\Delta_k^m = 1$



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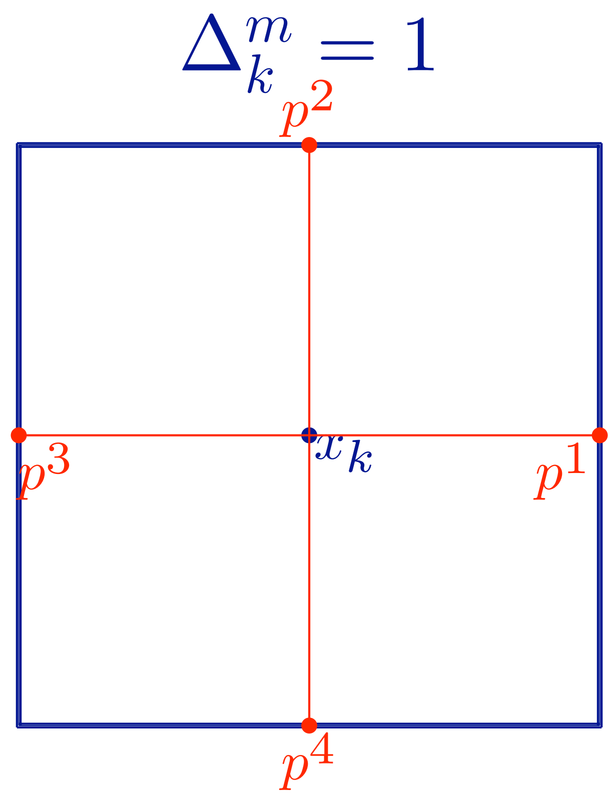

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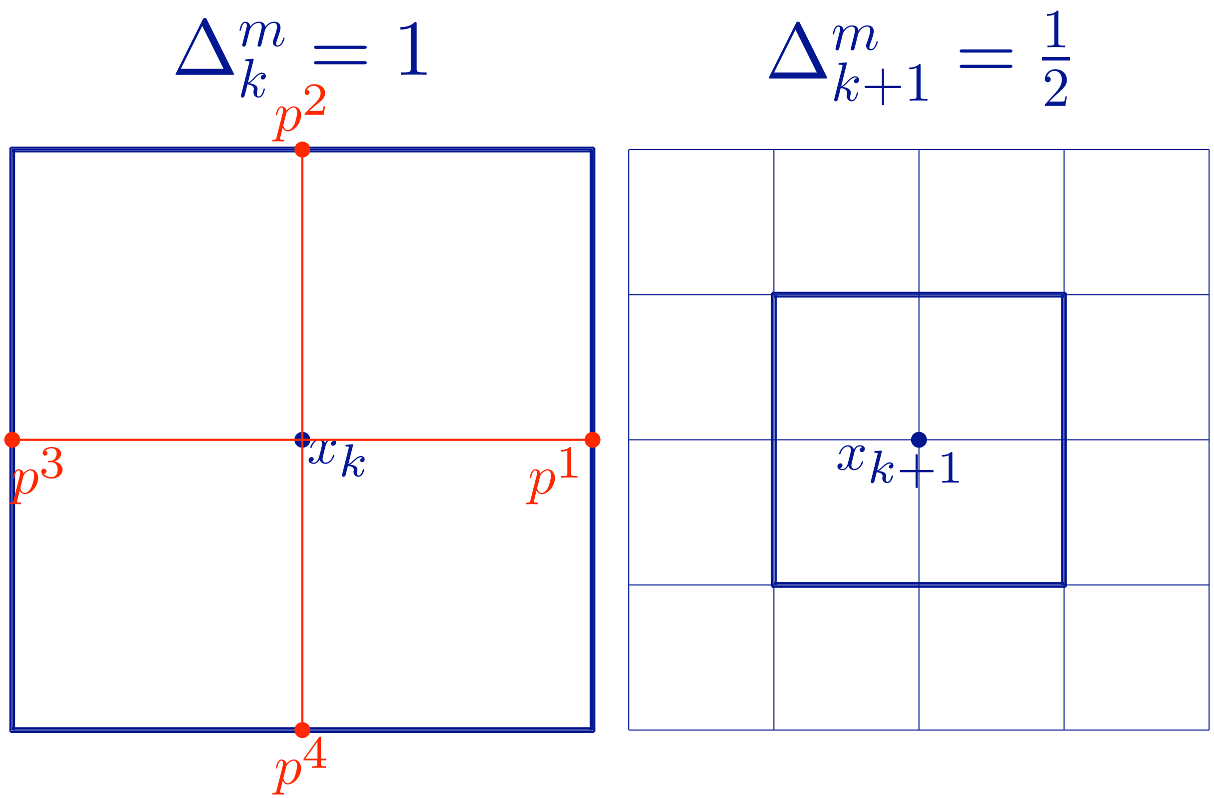

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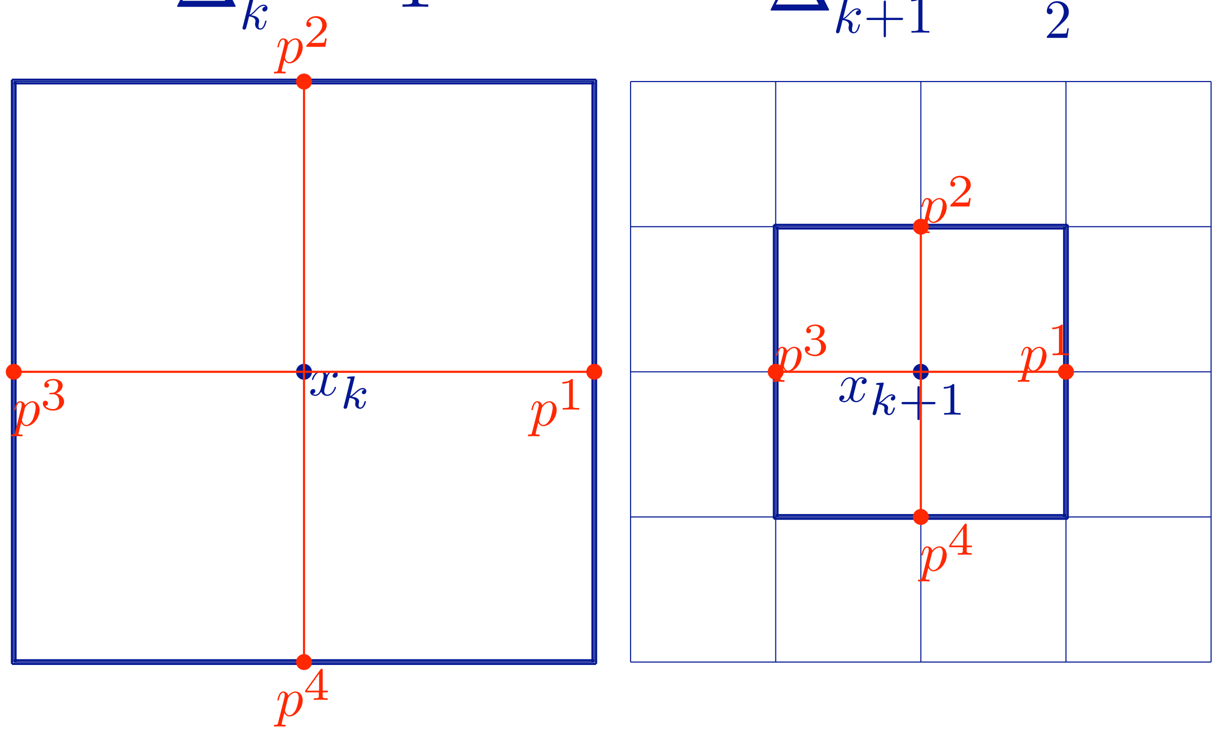

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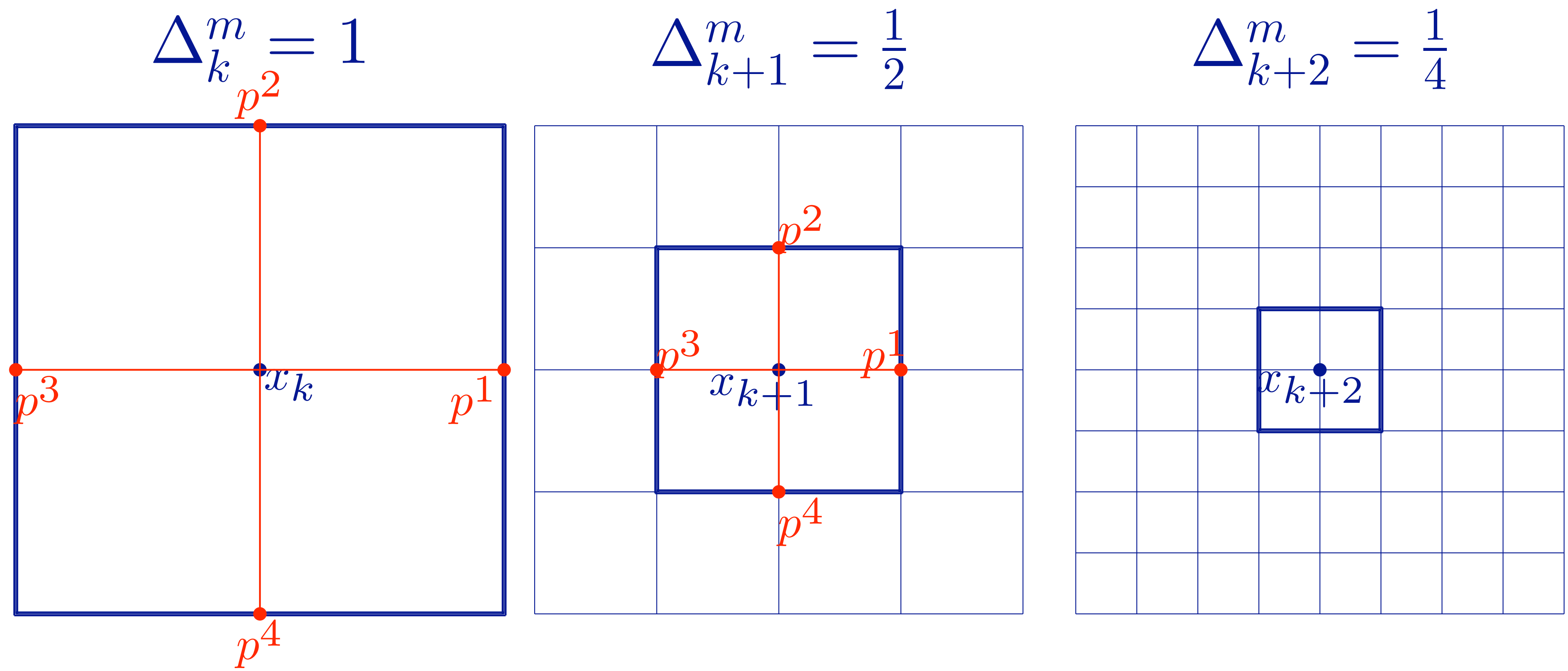

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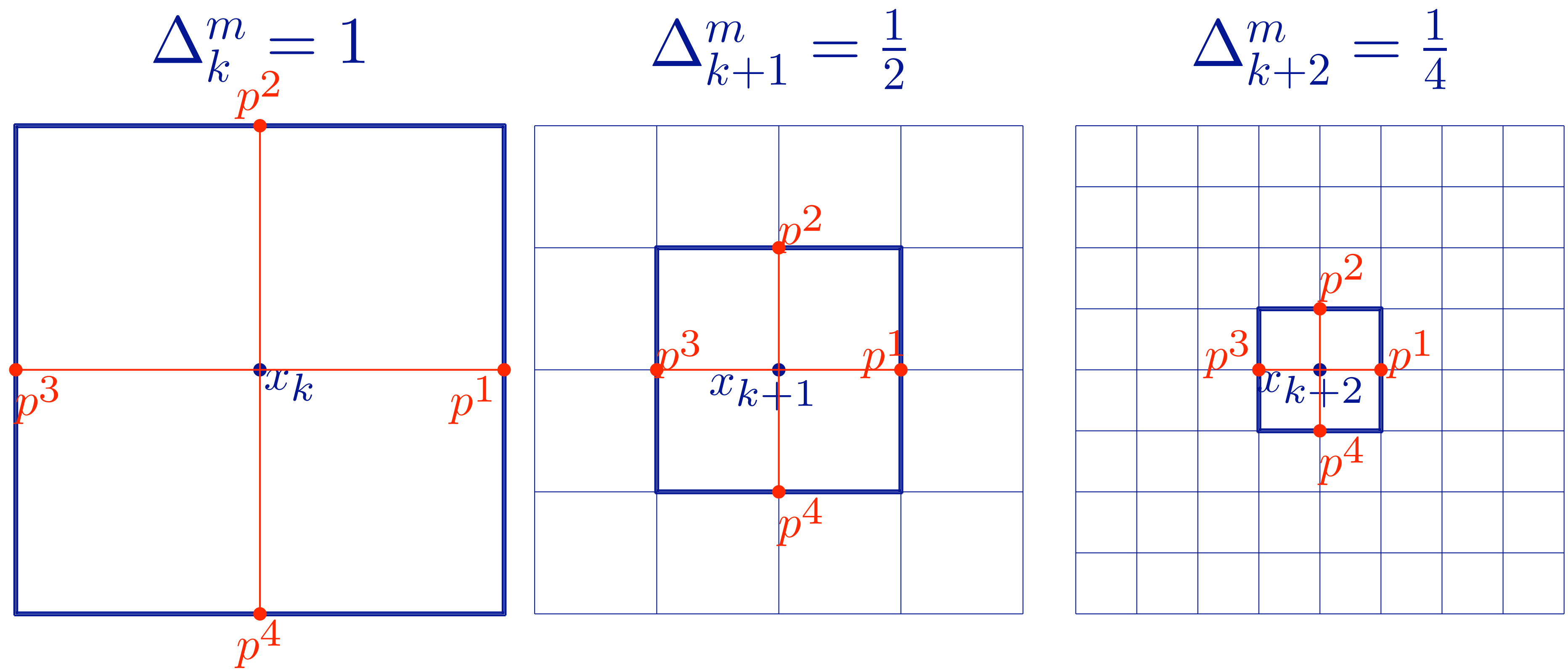

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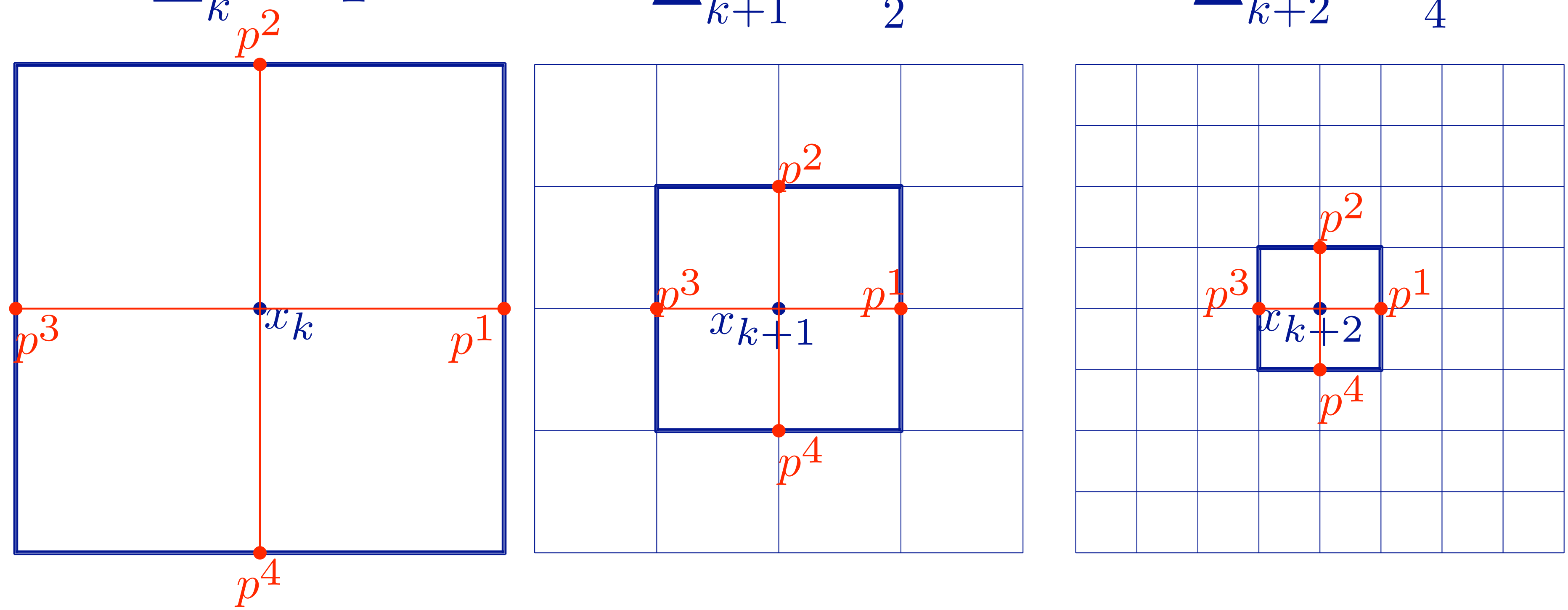

Always the same $2n = 4$ directions, regardless of Δ_k.

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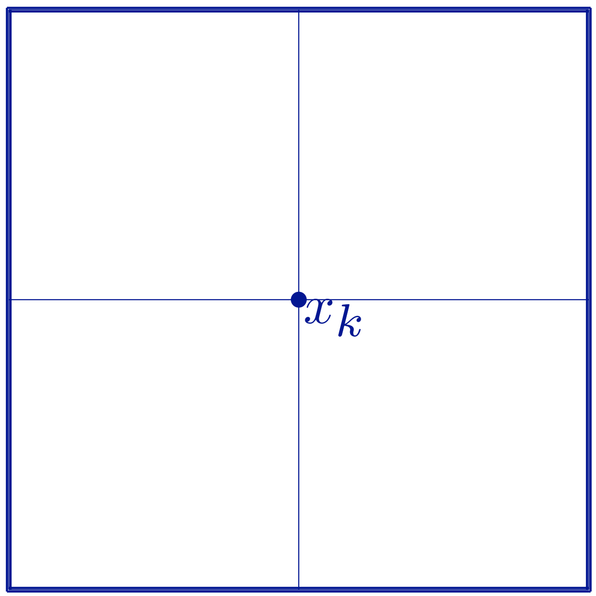

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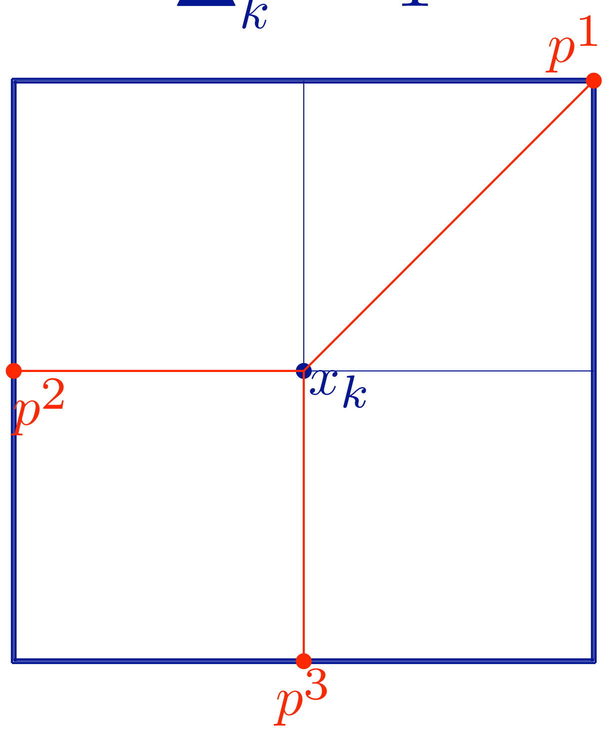

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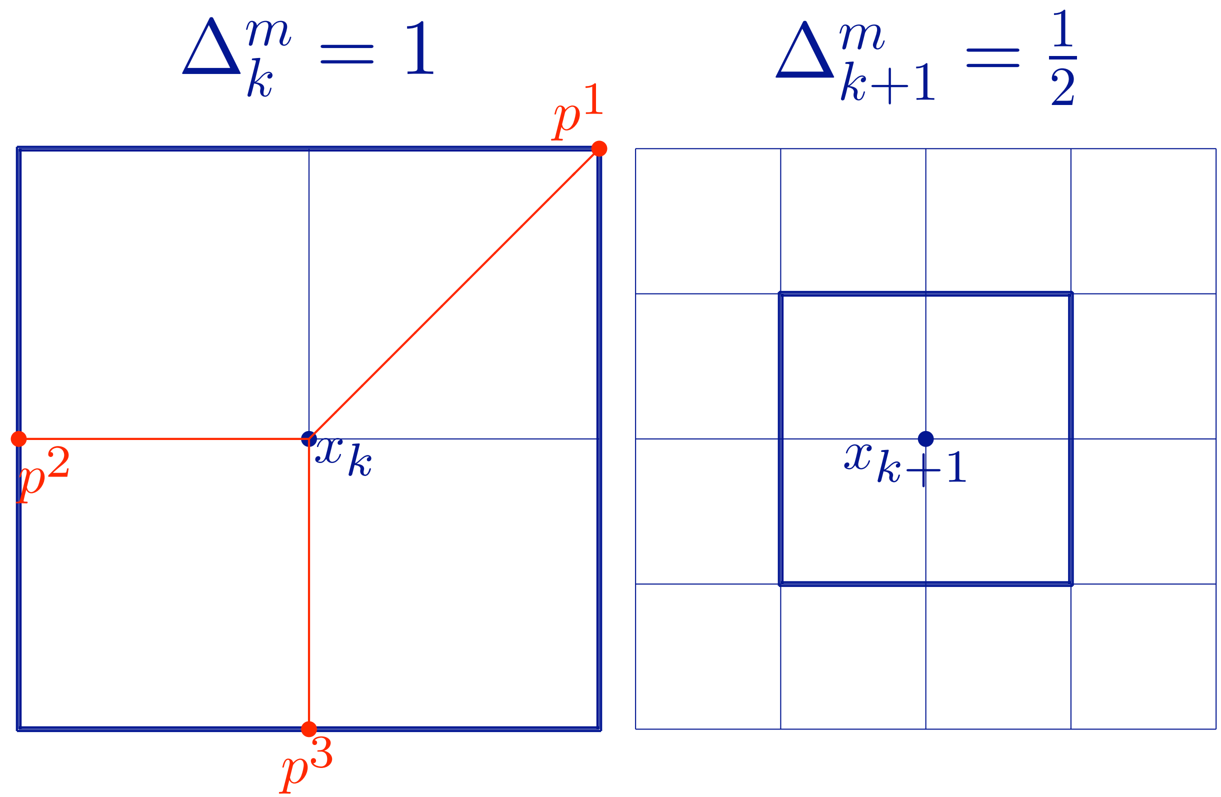

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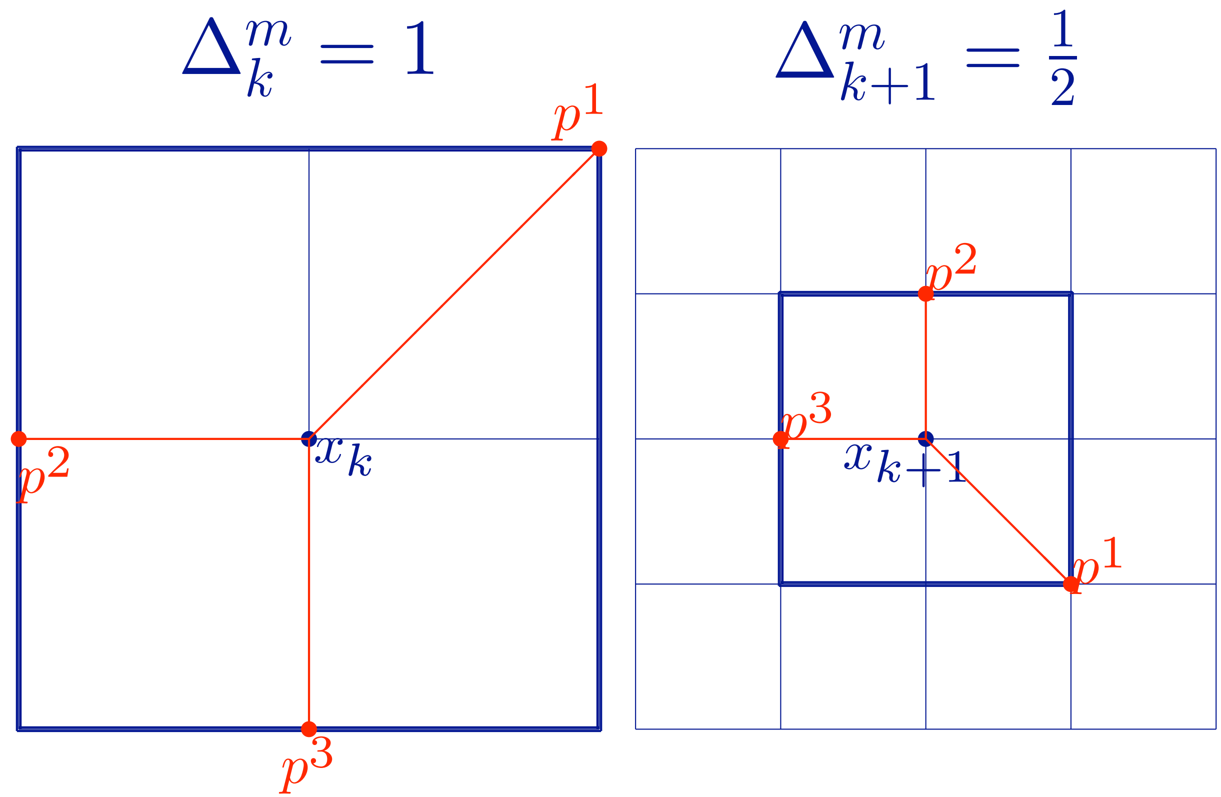

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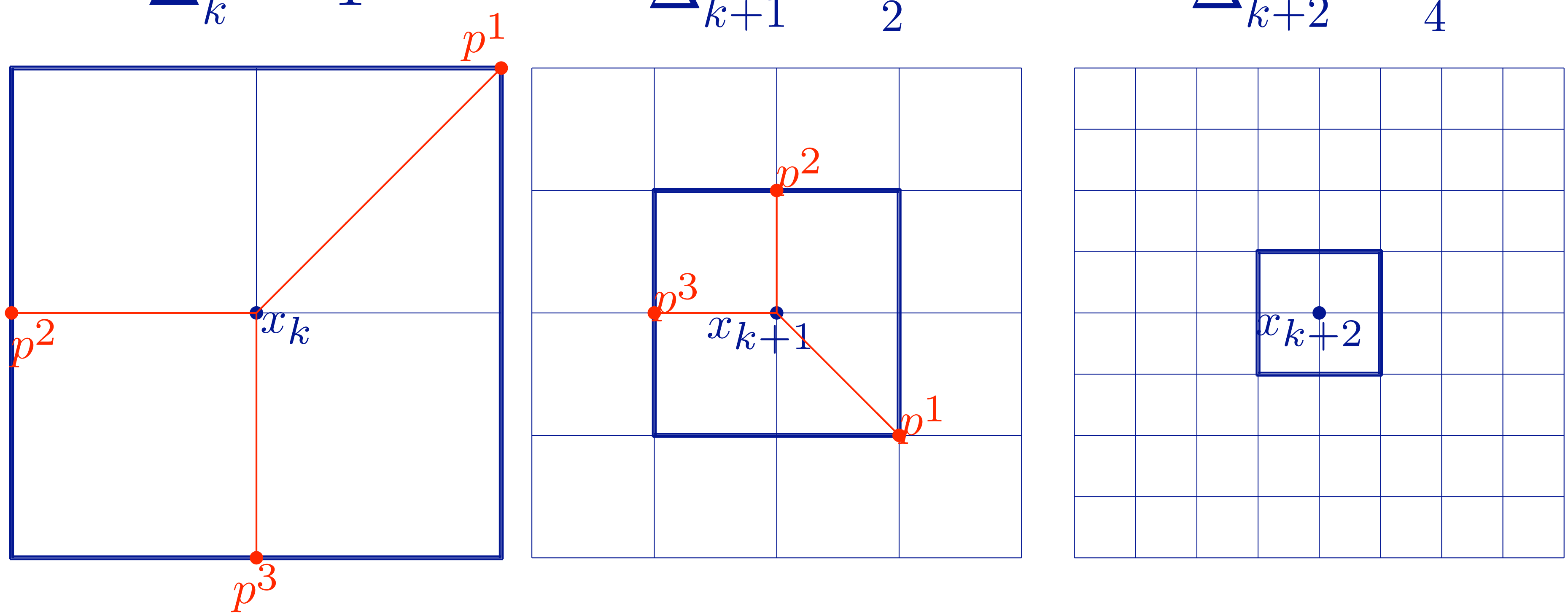

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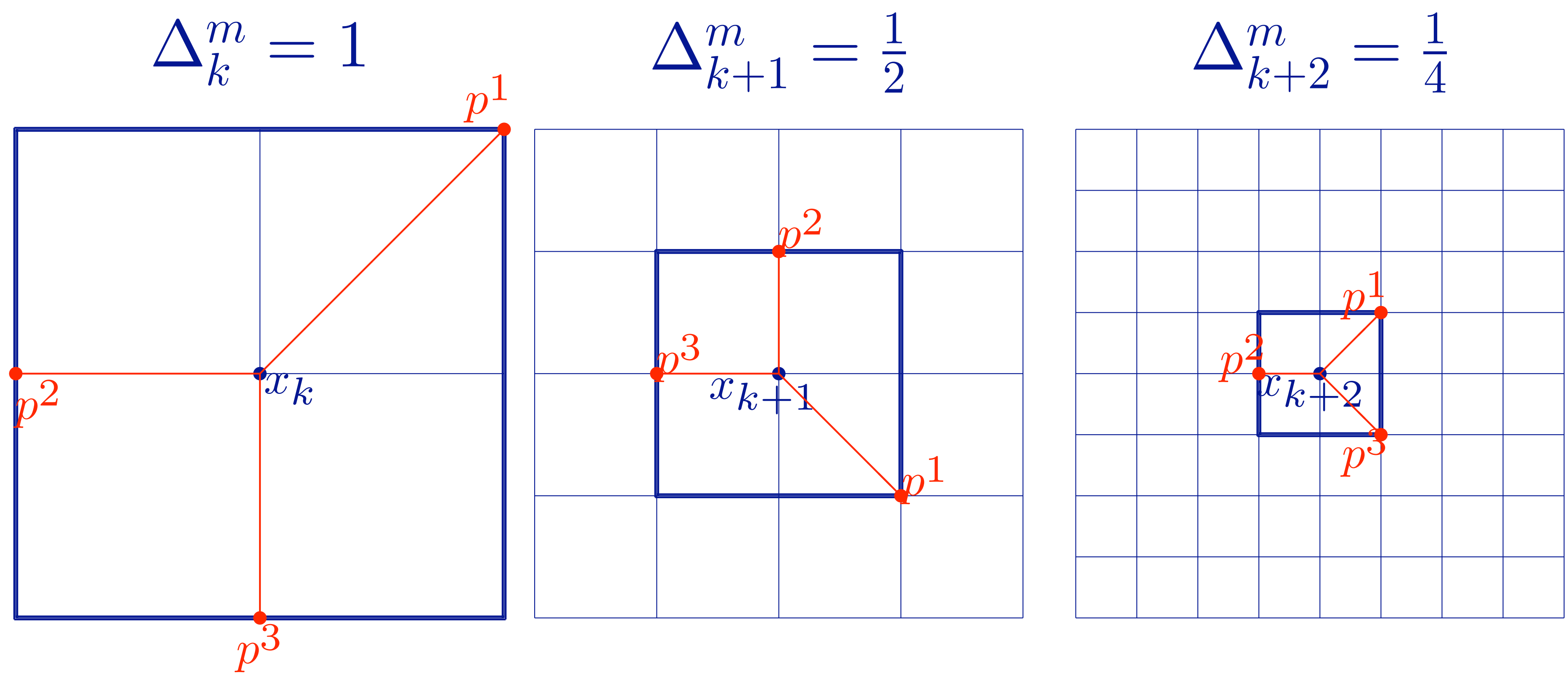

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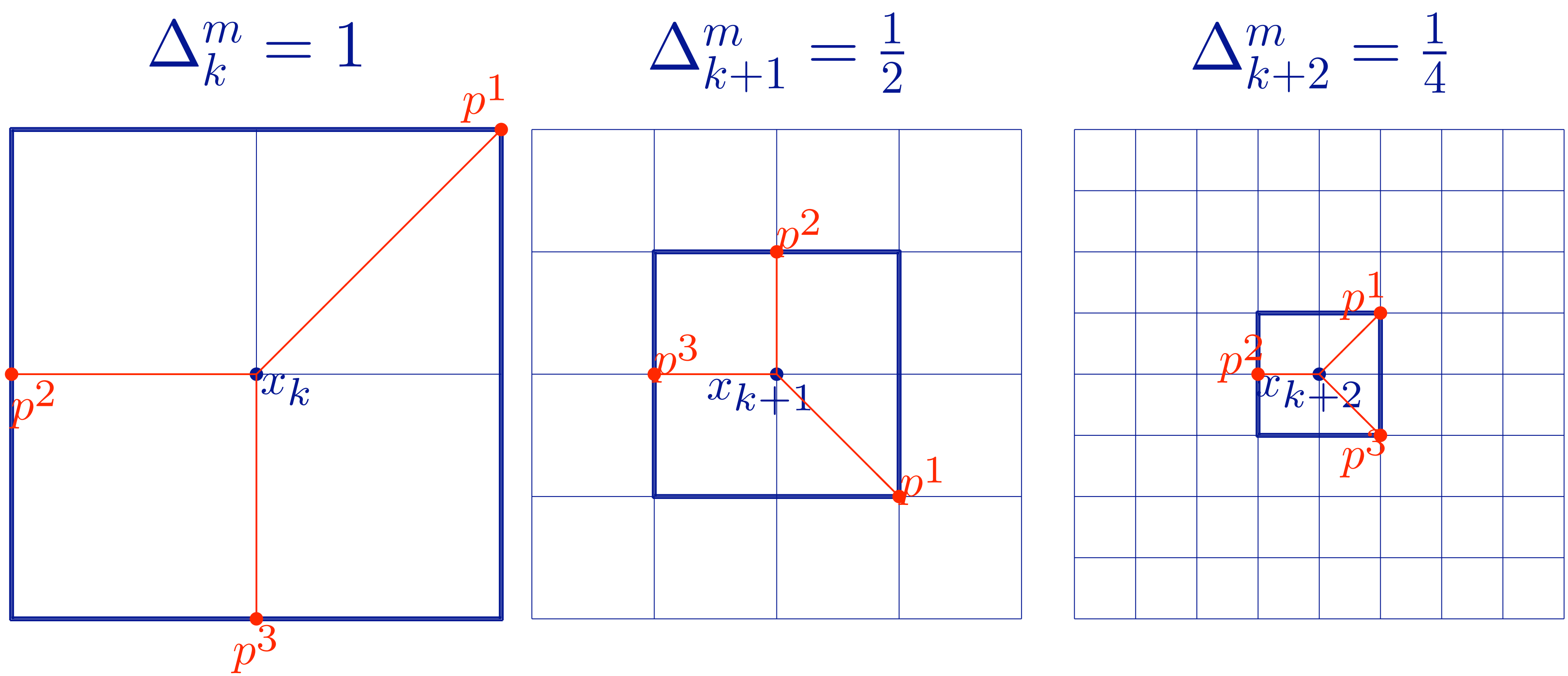

Here, only 14 different ways of selecting D_k, regardless of Δ_k.

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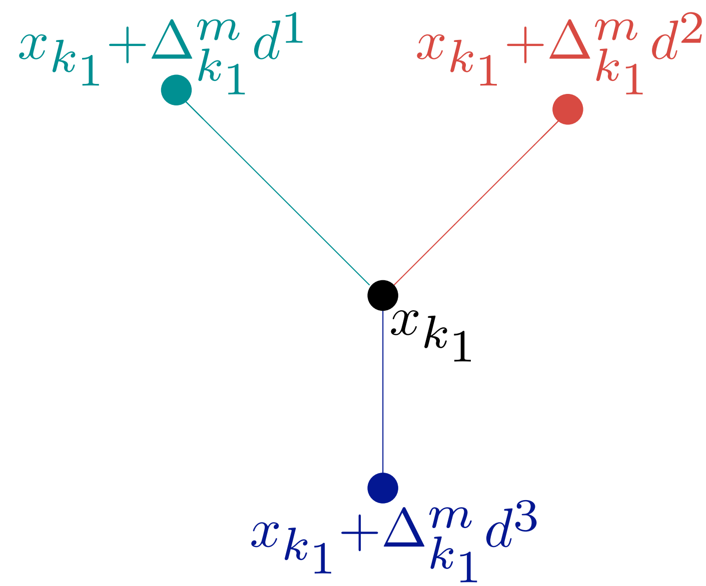
- $f(x_k) \leq f(x_k + \Delta_k^m d)\ \forall\ d \in D_k \subset D$ with $k \in K$.
  Let $\hat{D} \subseteq D$ be the set of POLL directions used infinitely often in the refining subsequence.
  $\hat{D}$ is the set of refining direction.

Set of refining directions $\hat{D}$



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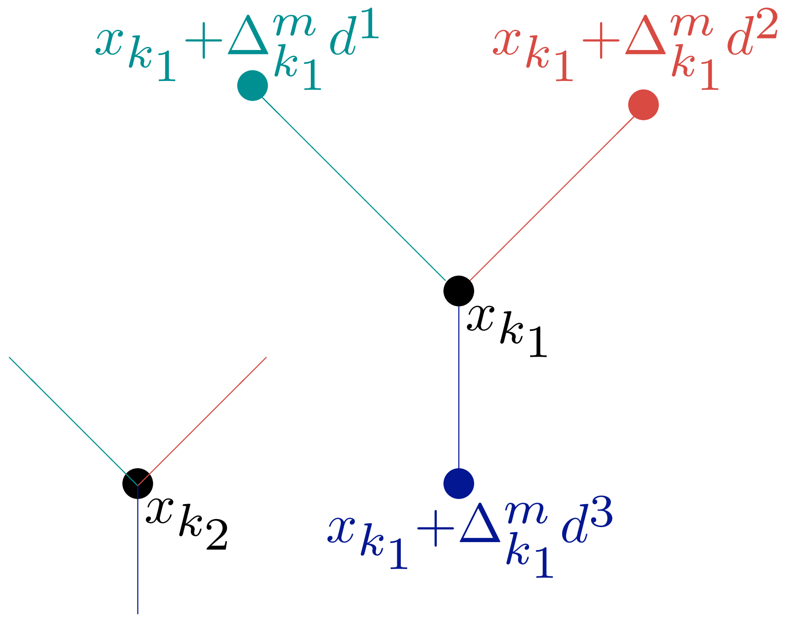

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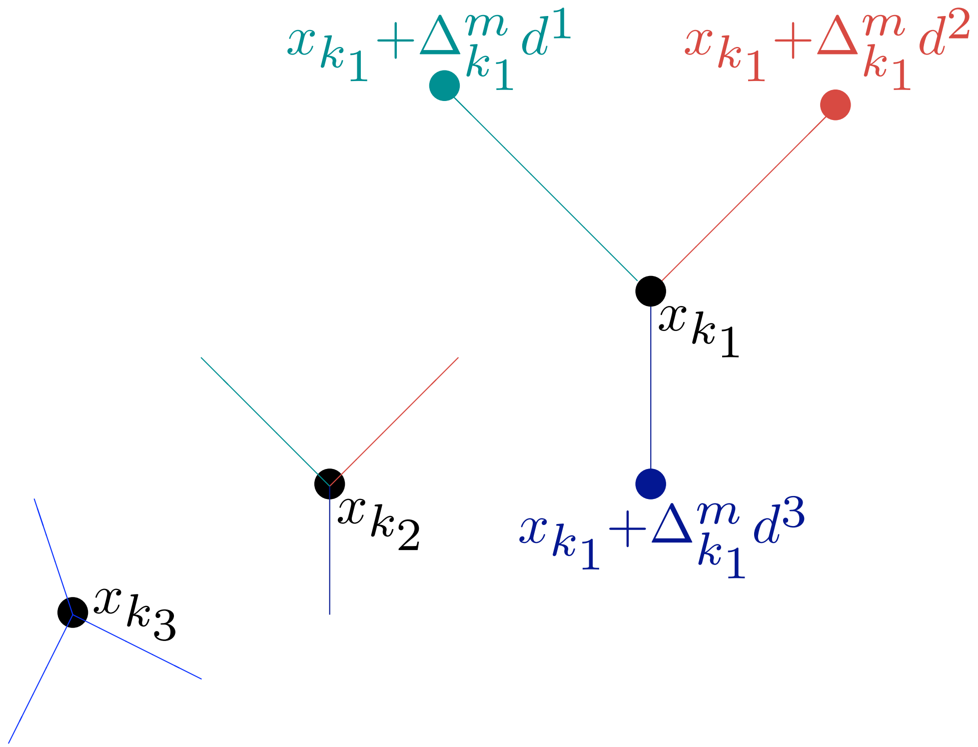

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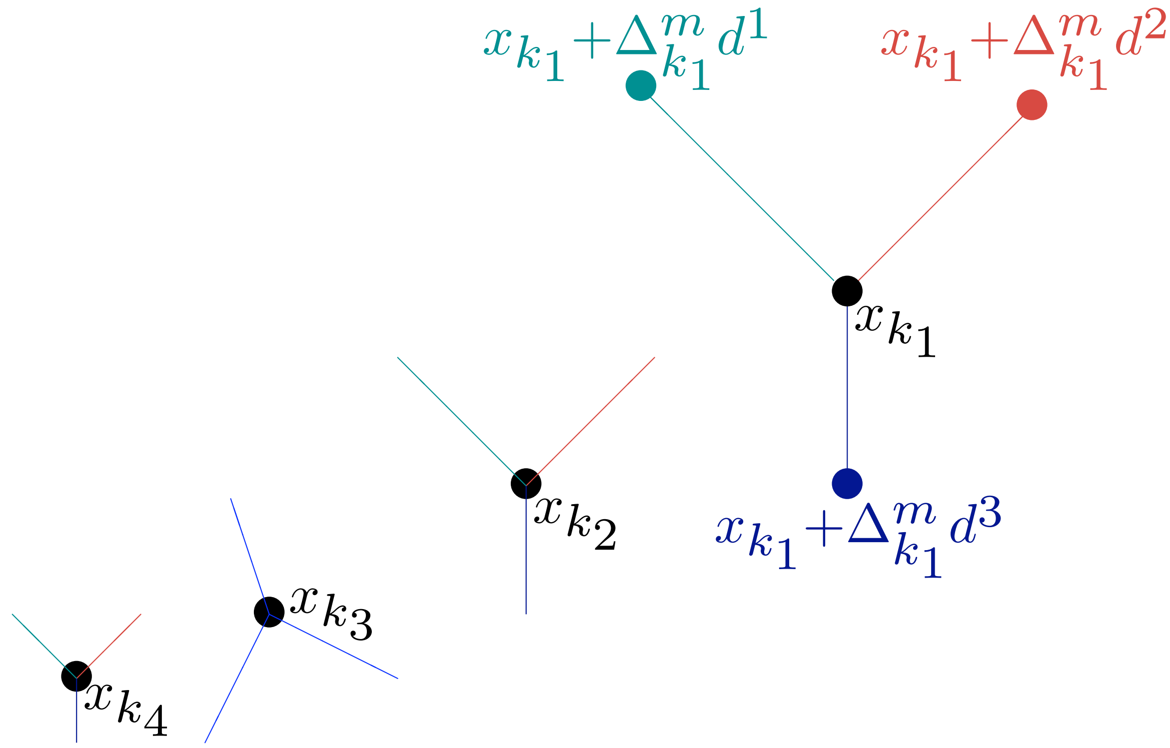

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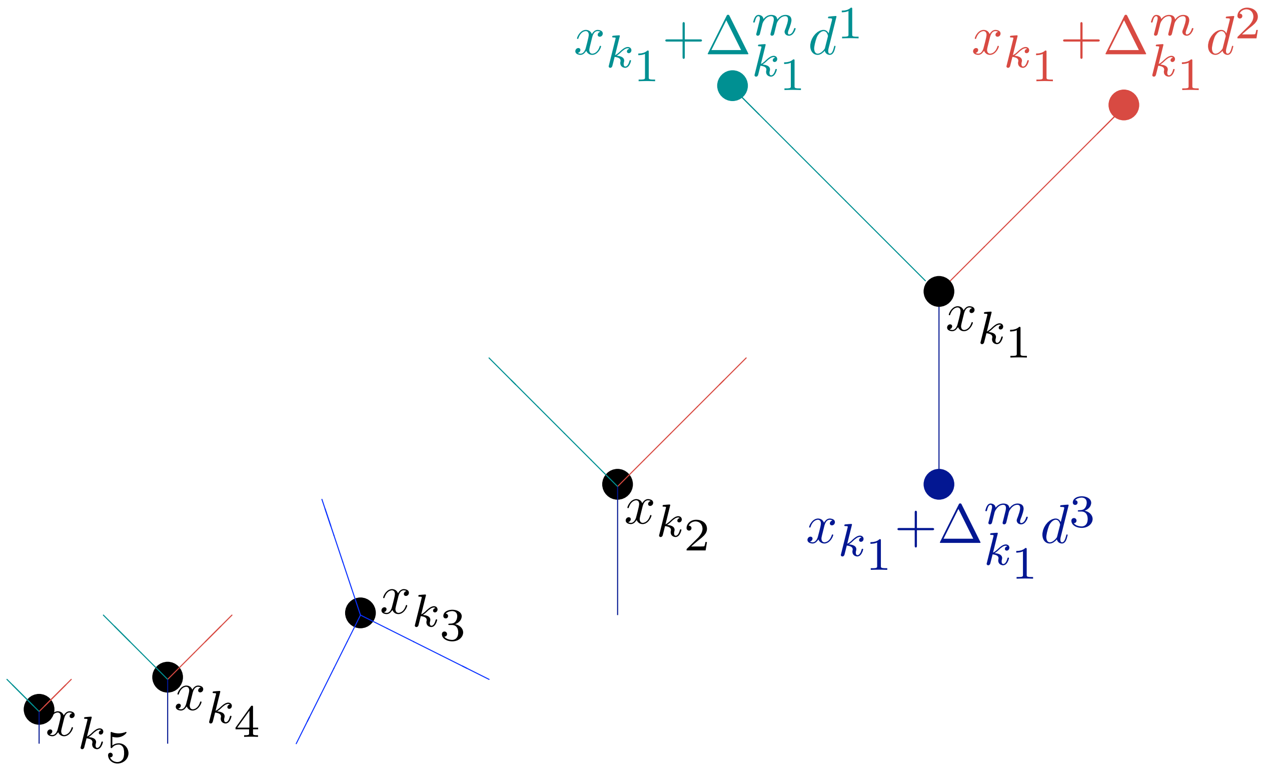

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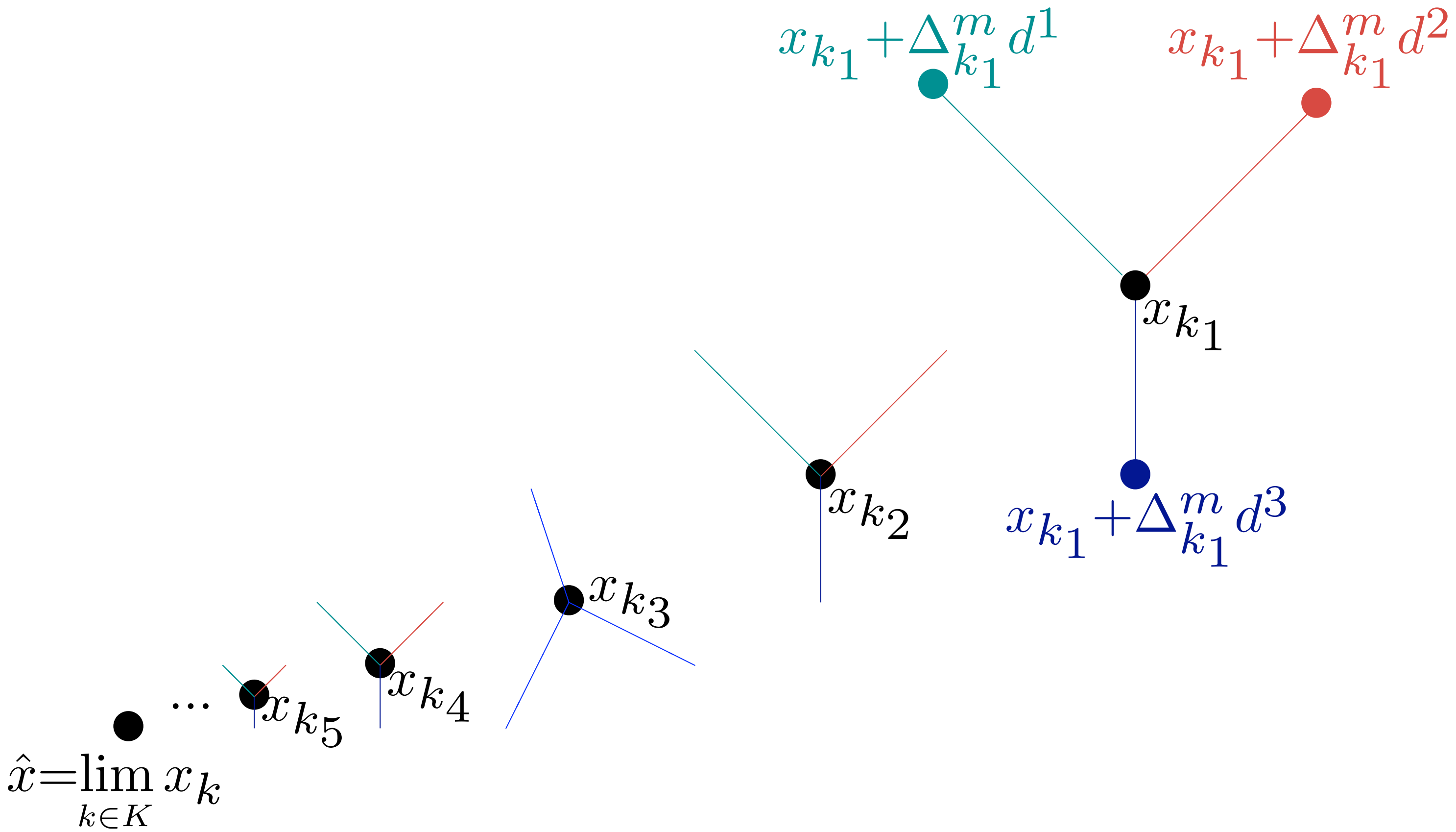

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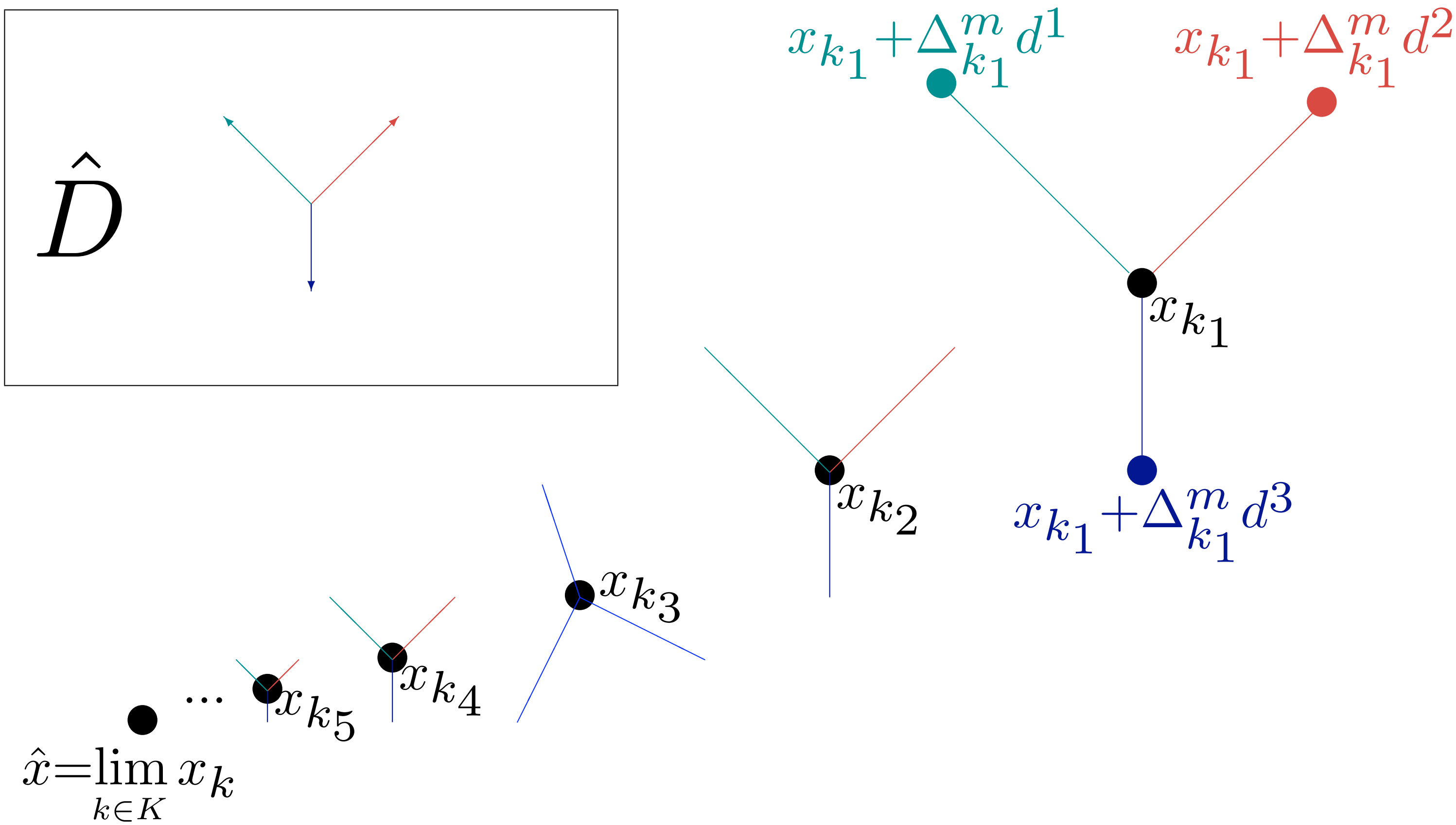

Convergence results – unconstrained GPS

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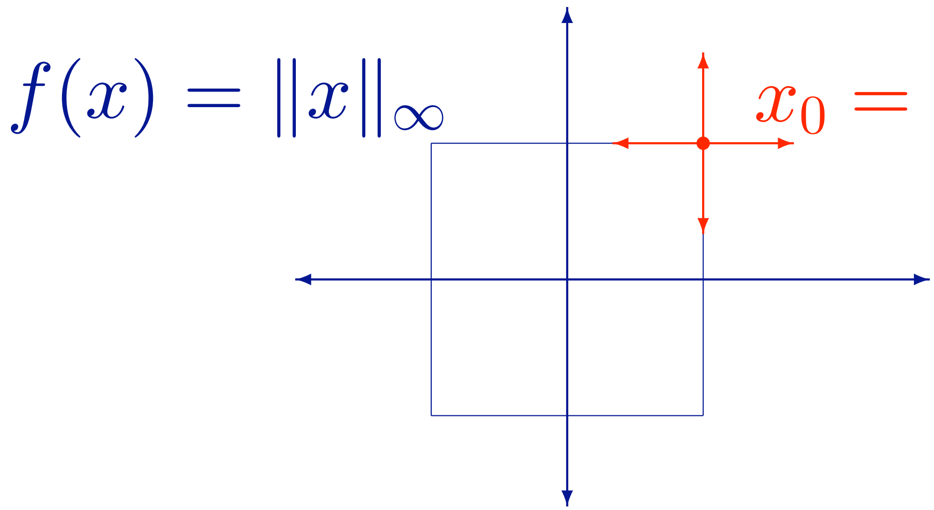

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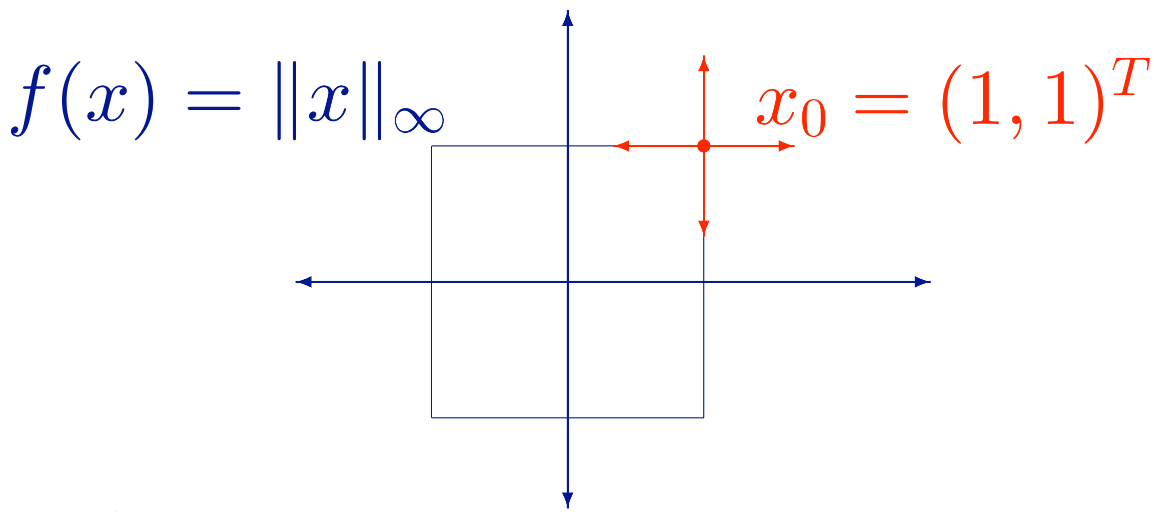
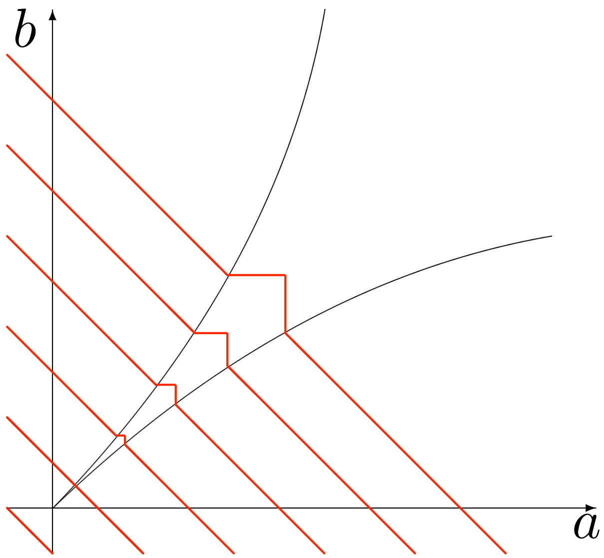


Even with a C^1 function, GPS may generate infinitely many limit points, some of them non-stationary.

GPS convergence to a bad solution

Level Sets



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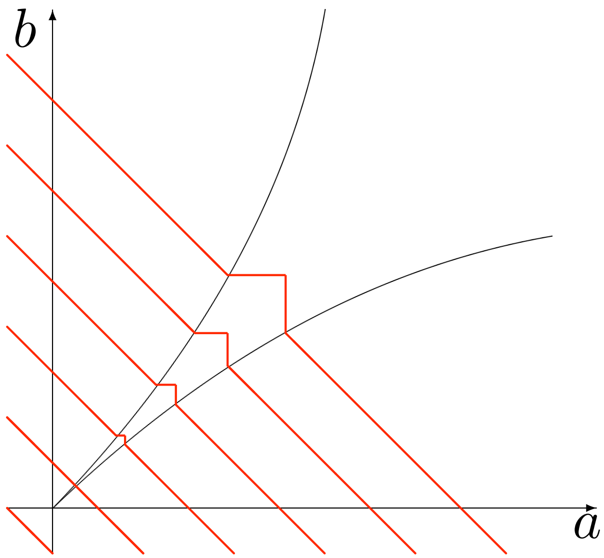
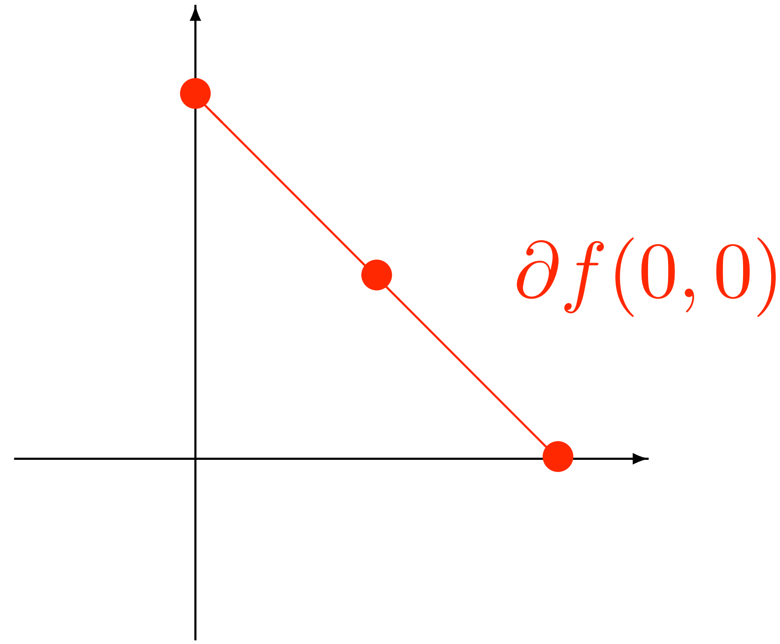


$(0,0) \notin \partial f(0,0)$



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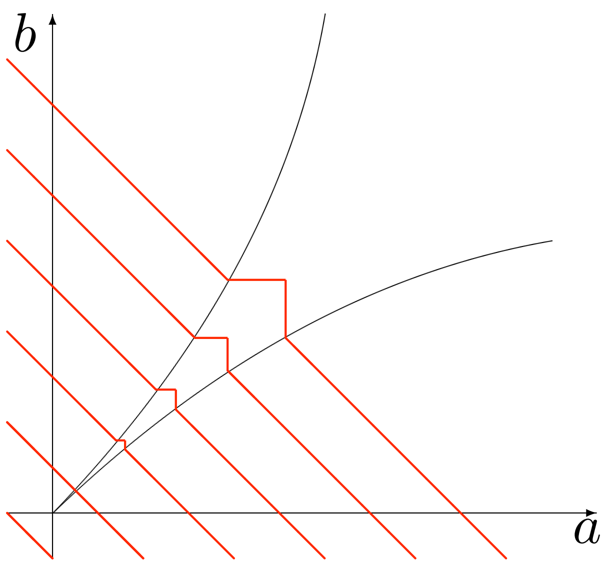

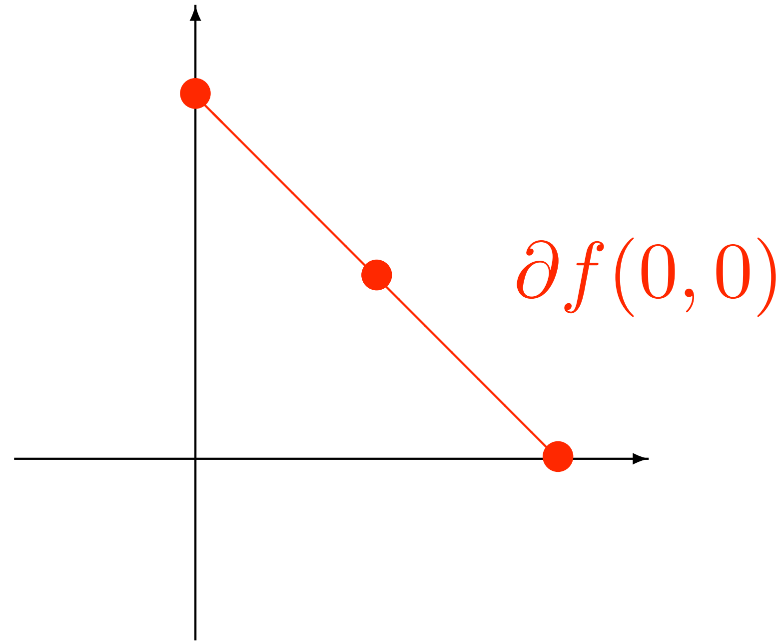

GPS iterates – with a bad strategy – converge to the origin, where the gradient exists and is nonzero (f is differentiable at $(0,0)$ but not strictly differentiable).

Outline

- Statement of the optimization problem
- The GPS and MADS algorithm classes
- GPS theory and limiting examples
- The MADS algorithm class
  - An implementable MADS instance
  - MADS theory
  - Numerical results
- Discussion

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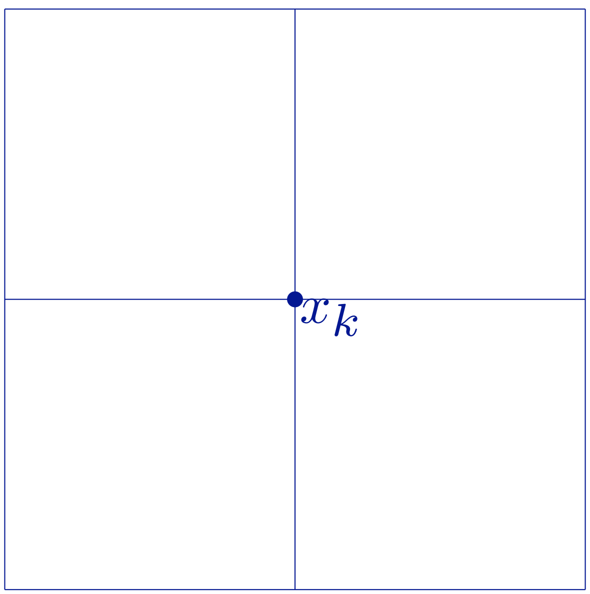

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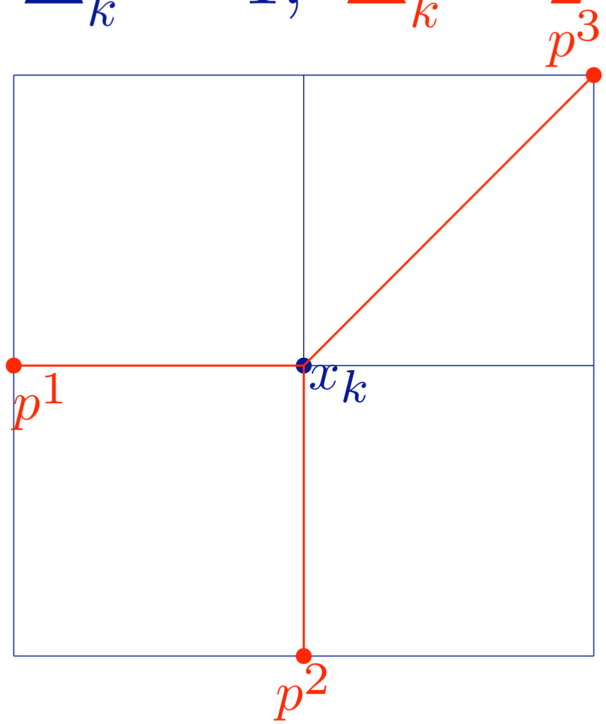

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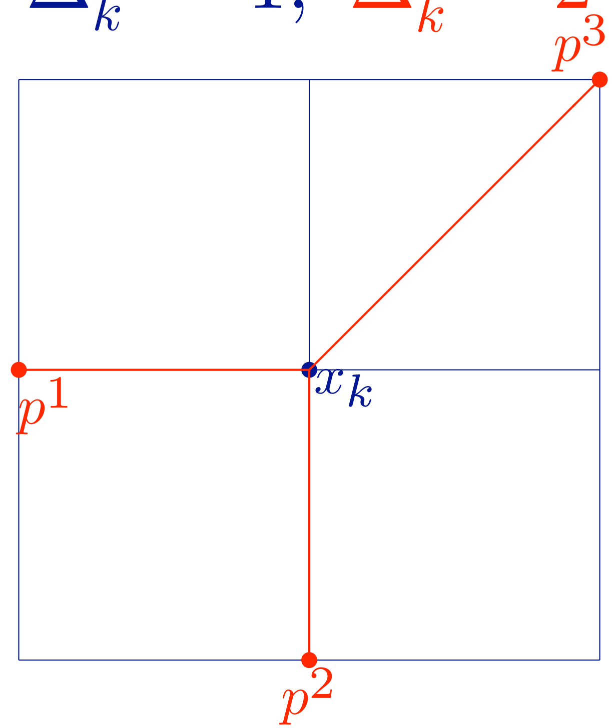

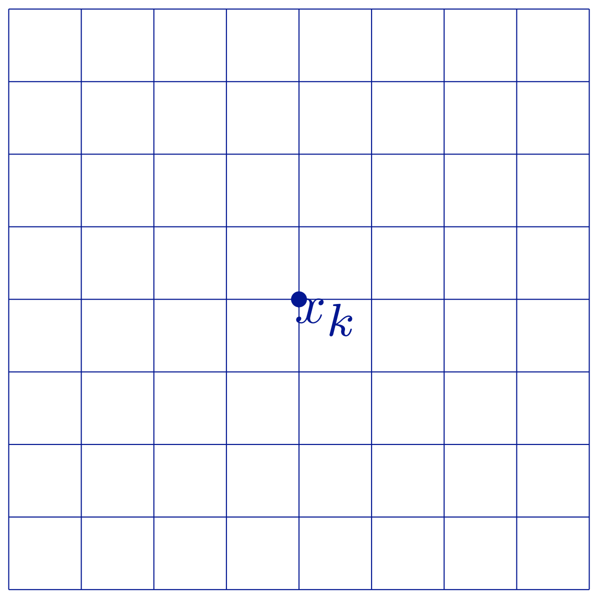

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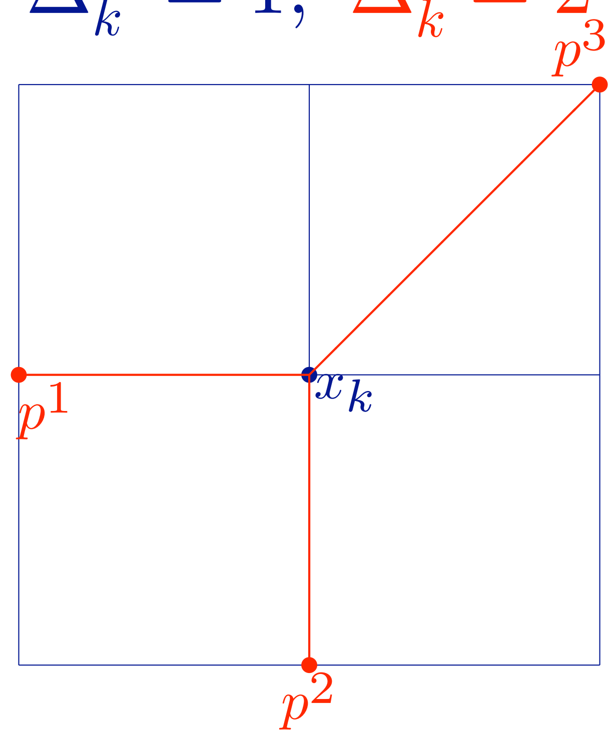

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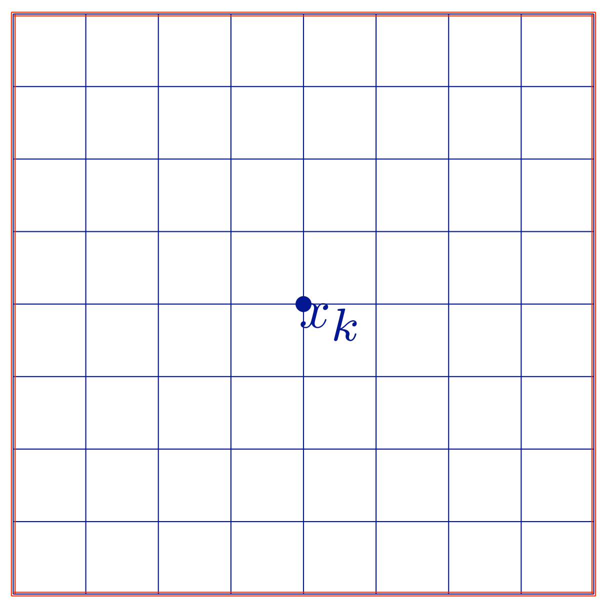

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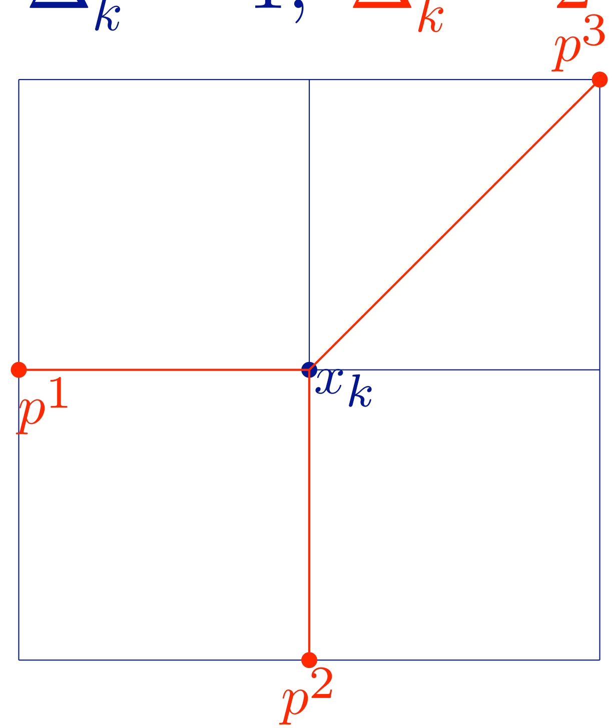

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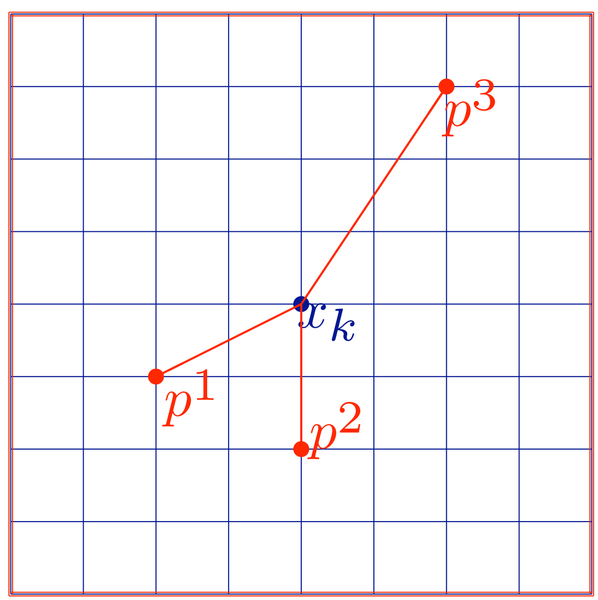

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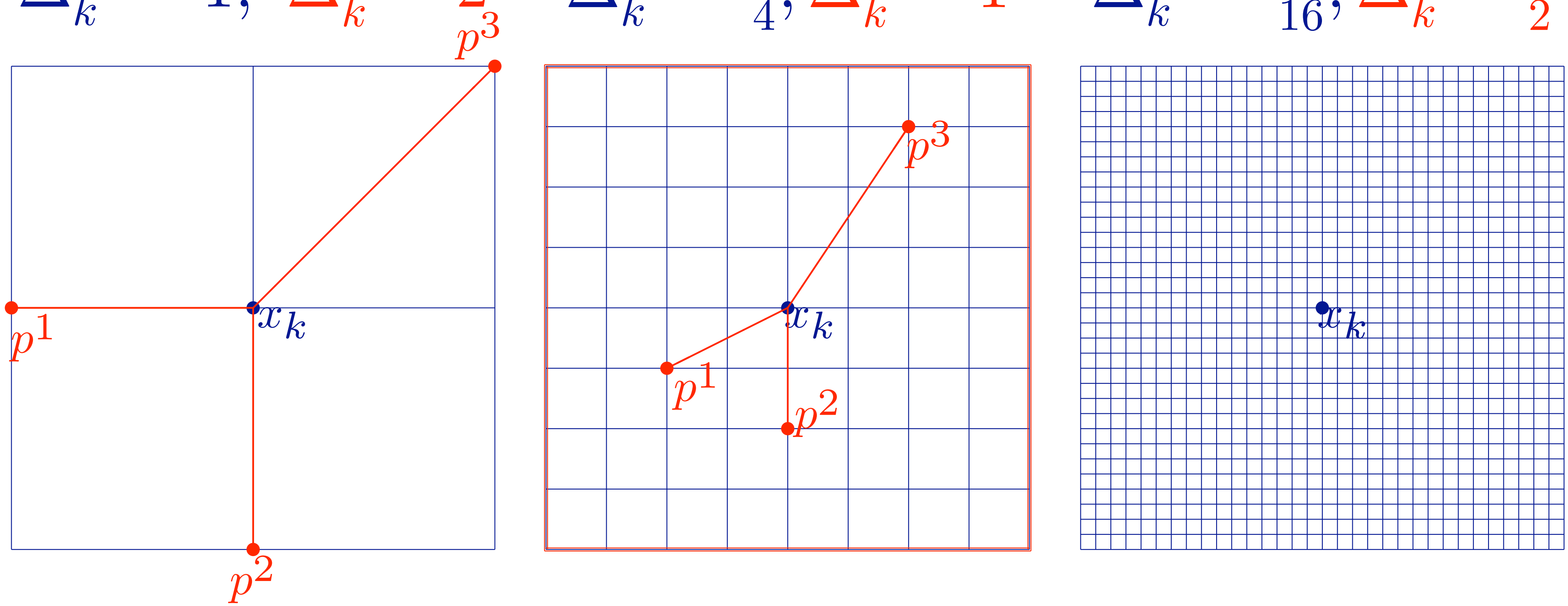

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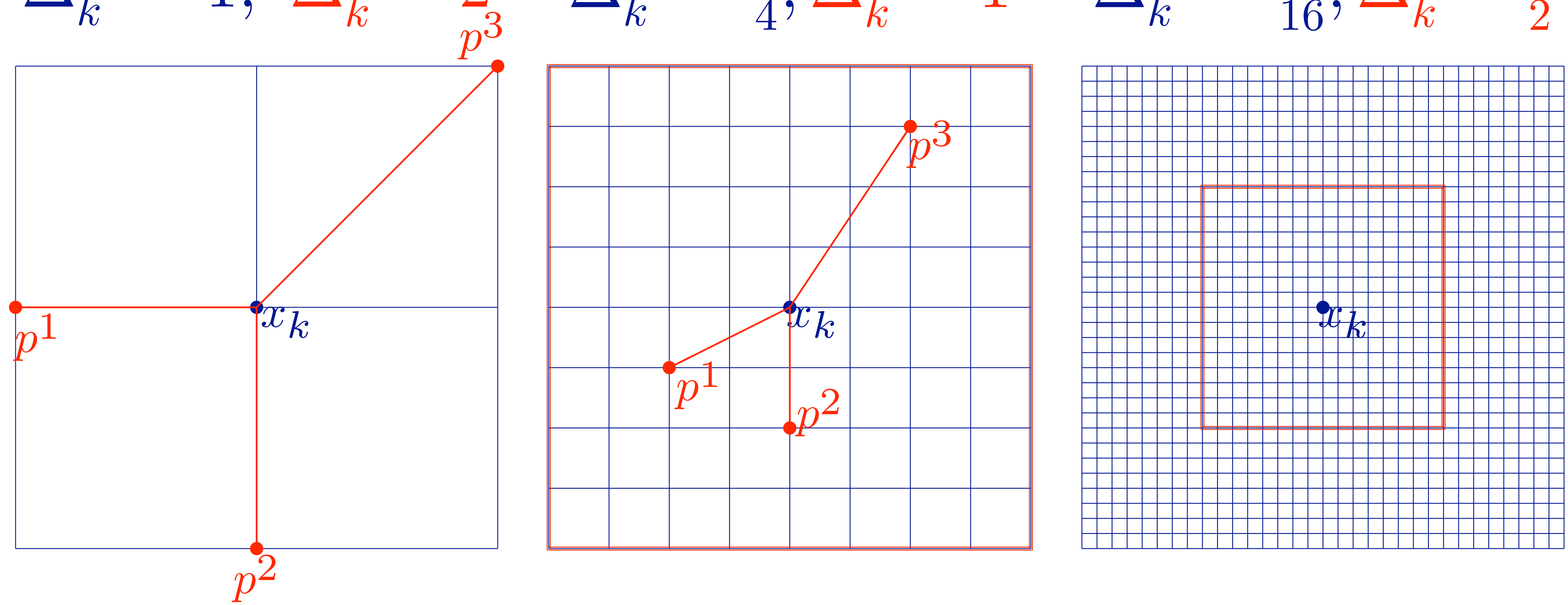

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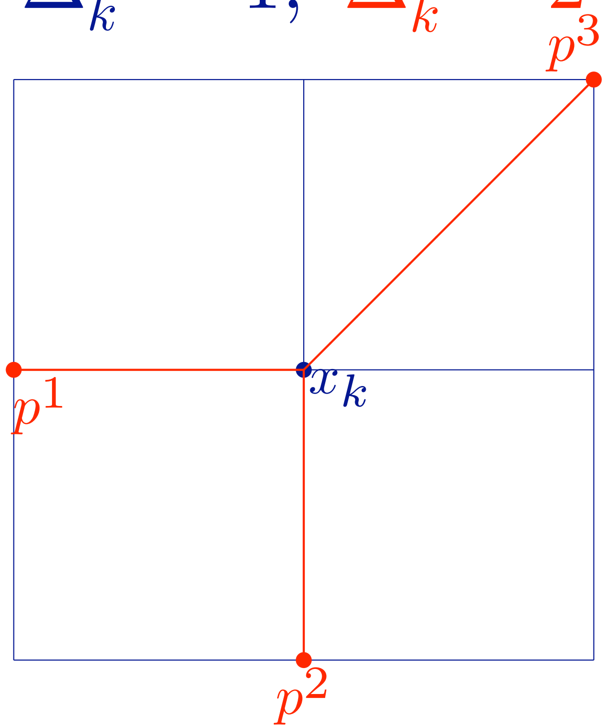

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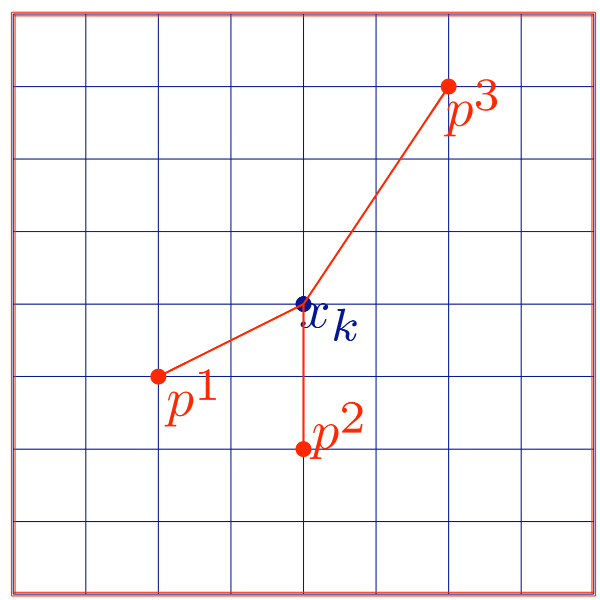

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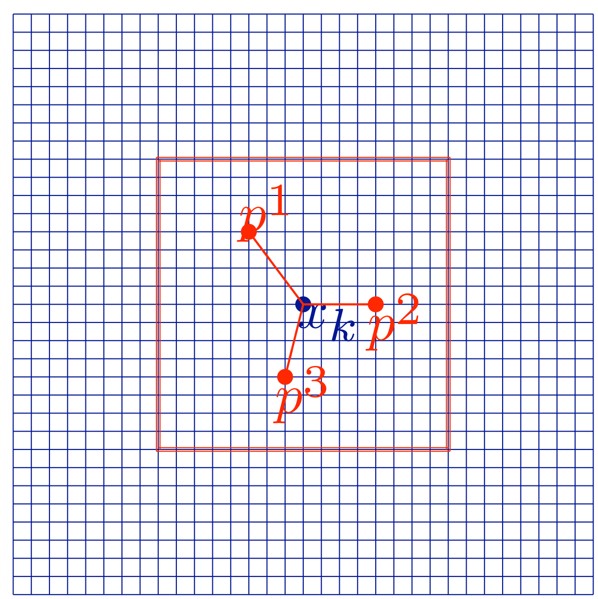

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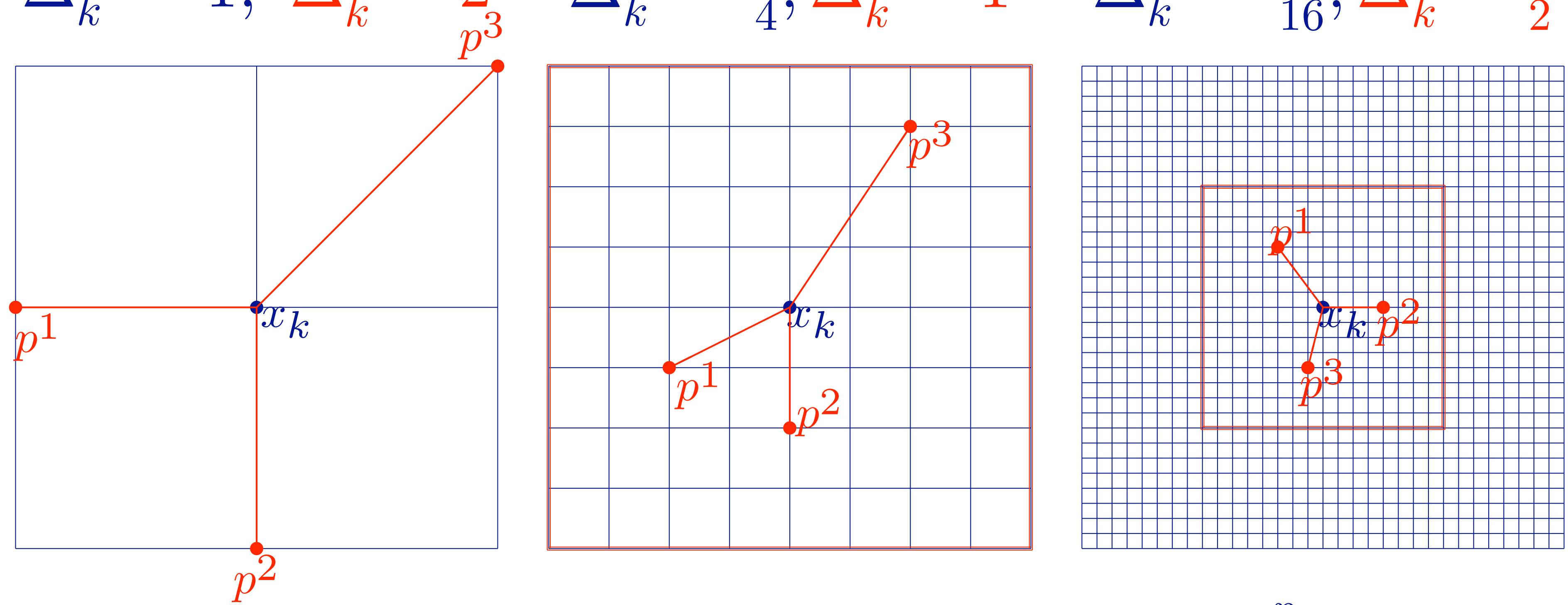

Number of ways of selecting D_k increases as Δ_k^p gets smaller.

Barrier approach to constraints

To enforce Ω constraints, replace f by a barrier objective

$$f_\Omega(x) \ := \ \begin{cases} f(x) & \text{if } x \in \Omega, \\ +\infty & \text{otherwise.} \end{cases}$$

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Quality of the limit solution depends the local smoothness of f, not of f_Ω.

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An implementable way to generate D_k:

- Let B be a lower triangular nonsingular random integer matrix.
- Randomly permute the lines of B
- Complete to a positive basis
  - $D_k = [B; \ -B]$ (maximal positive basis $2n$ directions). or
  - $D_k = [B; \ -\sum_{b \in B} b]$ (minimal positive basis $n+1$ directions).
  - Use Luis' talk to order the poll directions

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The ultimate goal is a way to be sure that the subset of refining directions $\hat{D}$ is dense.

Then the barrier approach to constraints promises strong optimality under weak assumptions - the existence of a hypertangent vector, e.g., a vector that makes a negative inner product with all the active constraint gradients.

MADS convergence results

Let f be Lipschitz near a limit $\hat{x}$ of a refining sequence.

Theorem 2. *Suppose that $\hat{D}$ is dense in Ω.*

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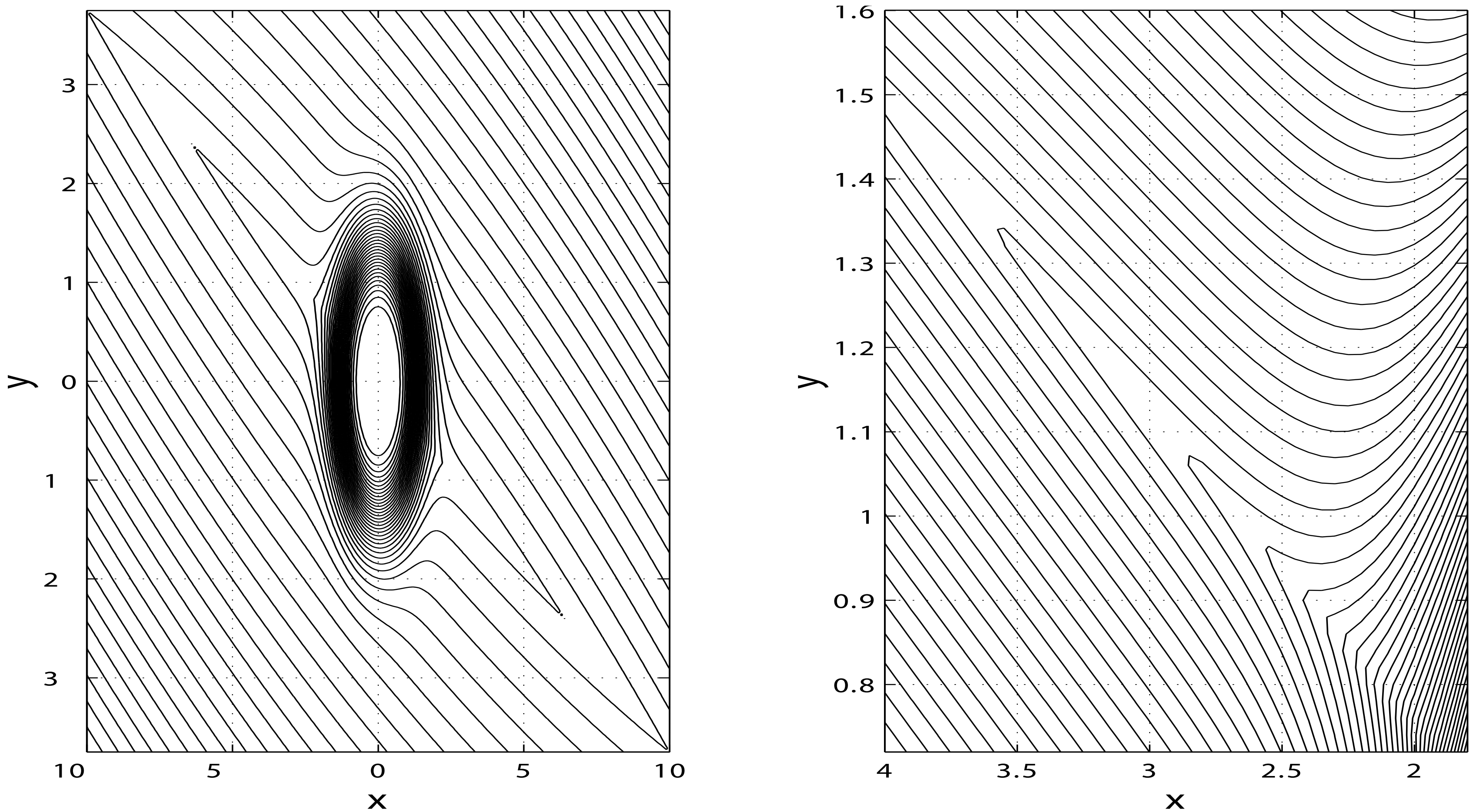
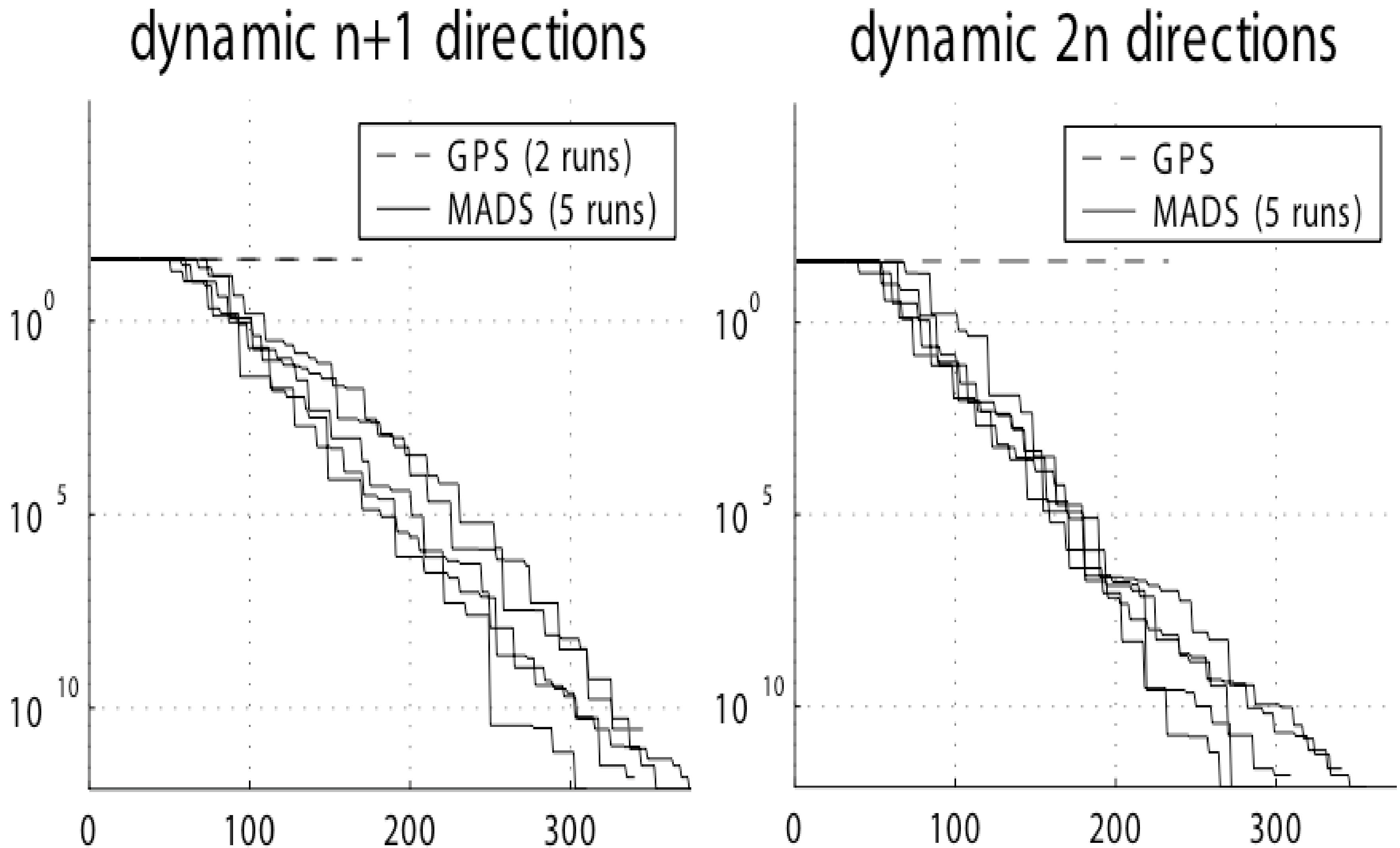
A problem for which GPS stagnates



Our results


dynamic n+1 directions
GPS (2 runs)
MADS (5 runs)
10^0
10^5
10^10
0
100
200
300
dynamic 2n directions
GPS
MADS (5 runs)
10^0
10^5
10^10
0
100
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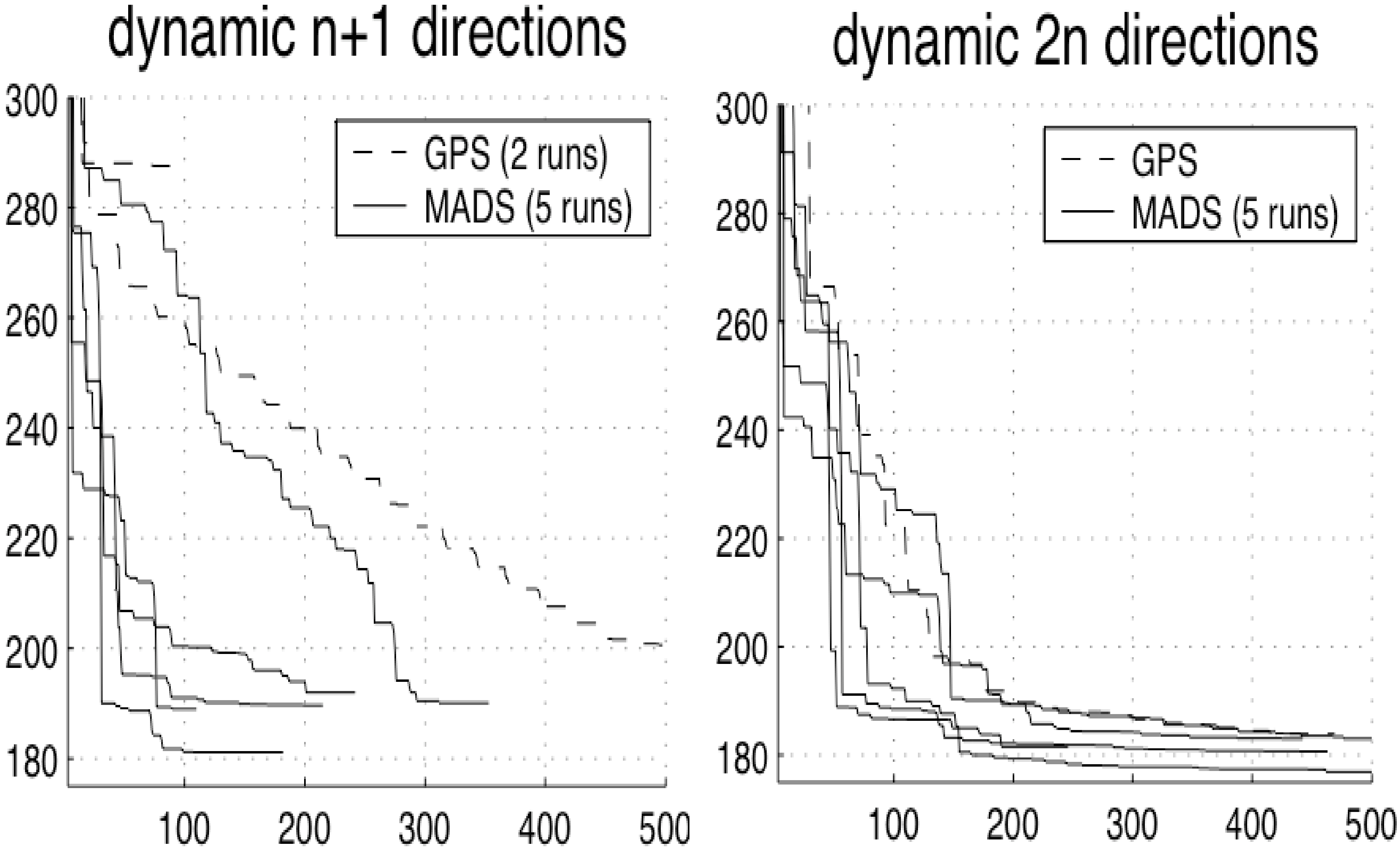
Results for a chemE pid problem



Constrained optimization

A disk constrained problem

$$\begin{aligned} \min_{x,y} \quad & x + y \\ \text{s.t.} \quad & x^2 + y^2 \leq 6 \end{aligned}$$

How hard can that be?

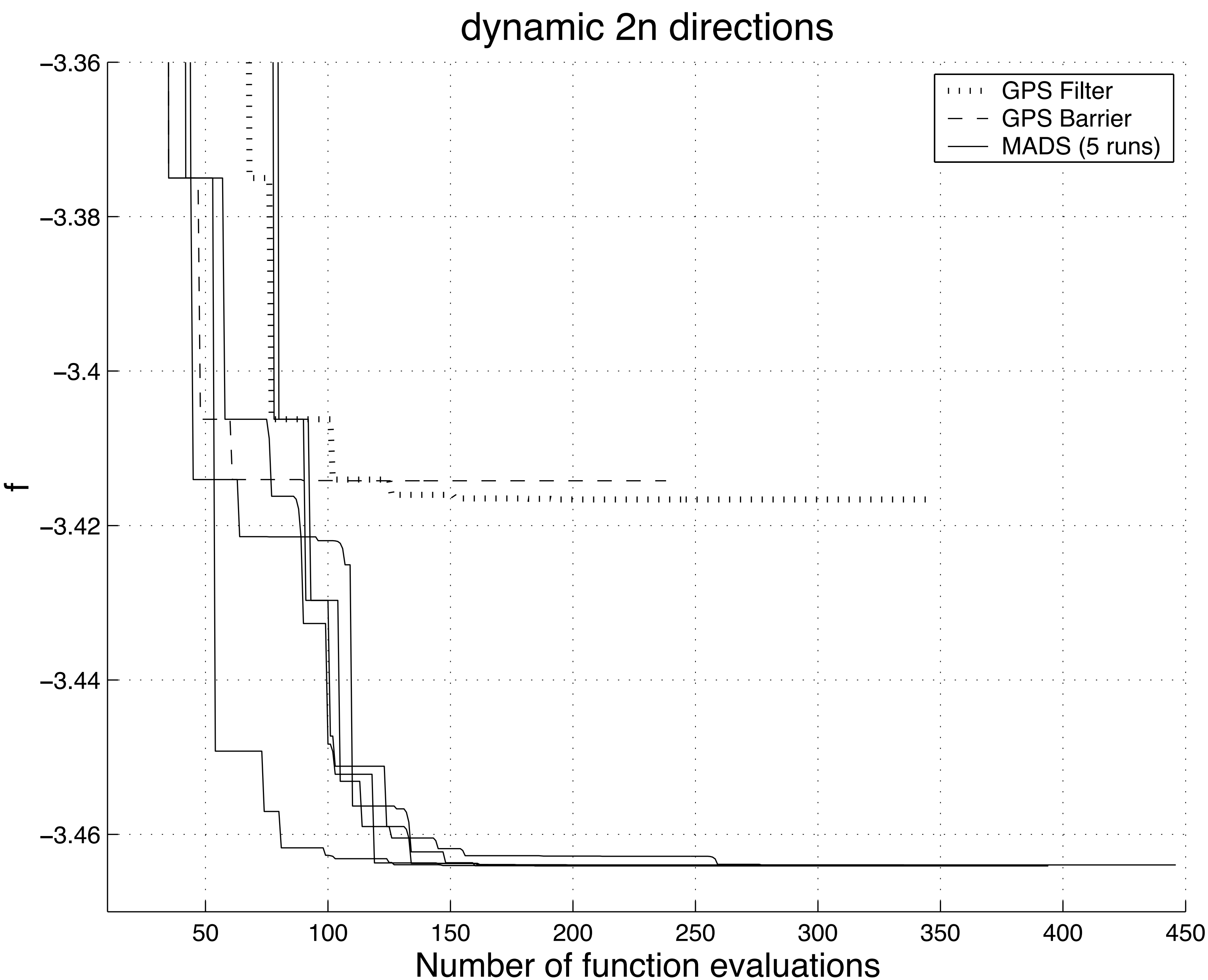
Constrained optimization

A disk constrained problem

$$\min_{x,y} \quad x + y$$
$$\text{s.t.} \quad x^2 + y^2 \leq 6$$

How hard can that be?

Very hard for GPS and filter-GPS with the standard 2n directions with an empty SEARCH


dynamic 2n directions
−3.36
−3.38
−3.4
−3.42
−3.44
−3.46
f
50
100
150
200
250
300
350
400
450
Number of function evaluations
GPS Filter
GPS Barrier
MADS (5 runs)

Parameter fit in a rheology problem

Rheology is a branch of mechanics that studies properties of materials which determine their response to mechanical force.

MODEL :

Viscosity η of a material can be modelled as a function of the shear rate $\dot{\gamma}_i$:

$$\eta(\dot{\gamma}) \;=\; \eta_0(1 + \lambda^2\dot{\gamma}^2)^{\frac{\beta-1}{2}}$$

A parameter fit problem.

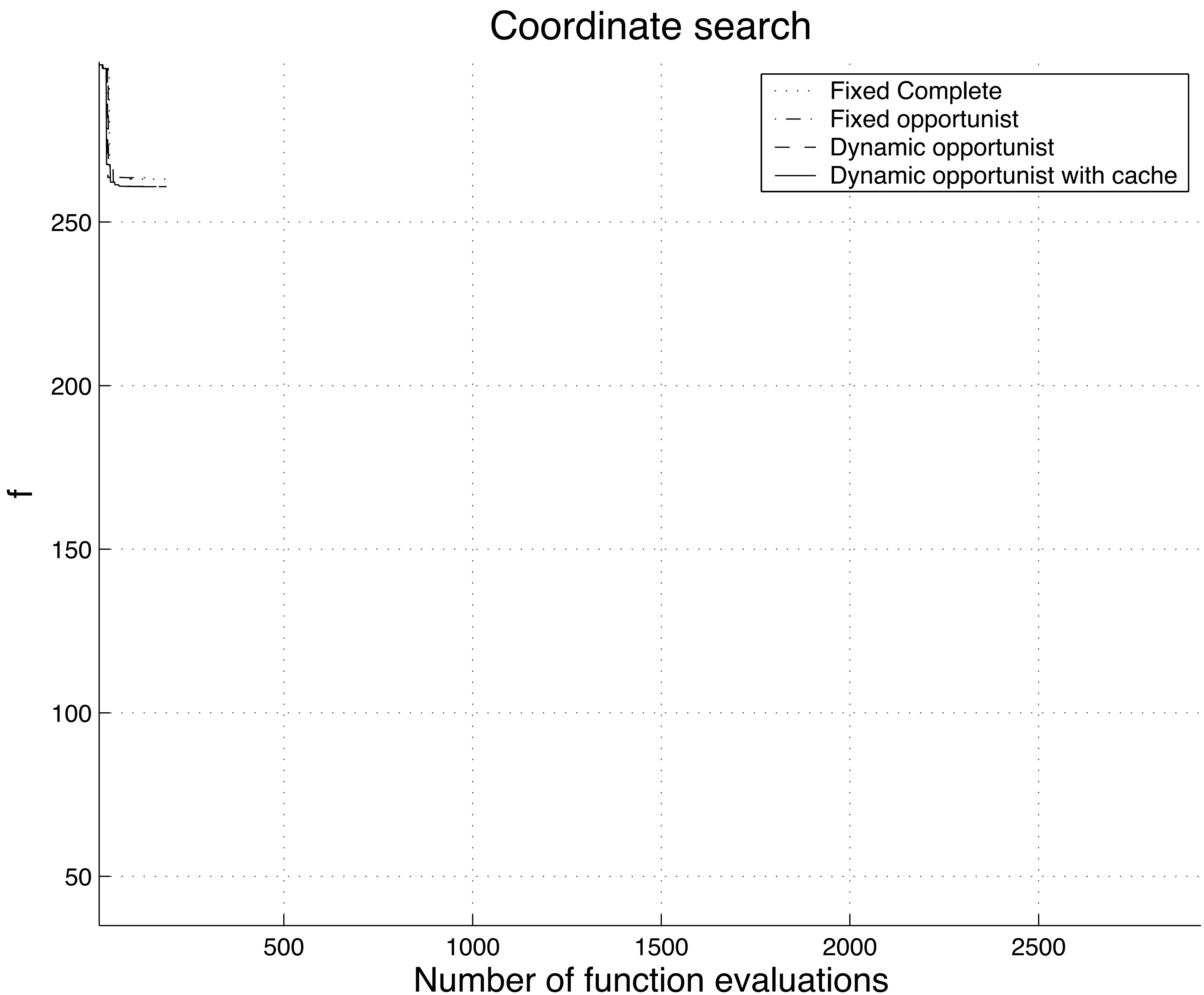
Observation i	Strain rate $\dot{\gamma}_i$ (s^{-1})	Viscosity η_i $(Pa \cdot s)$
1	0.0137	3220
2	0.0274	2190
3	0.0434	1640
4	0.0866	1050
5	0.137	766
6	0.274	490
7	0.434	348
8	0.866	223
9	1.37	163
10	2.74	104
11	4.34	76.7
12	5.46	68.1
13	6.88	58.2

The unconstrained optimization problem :

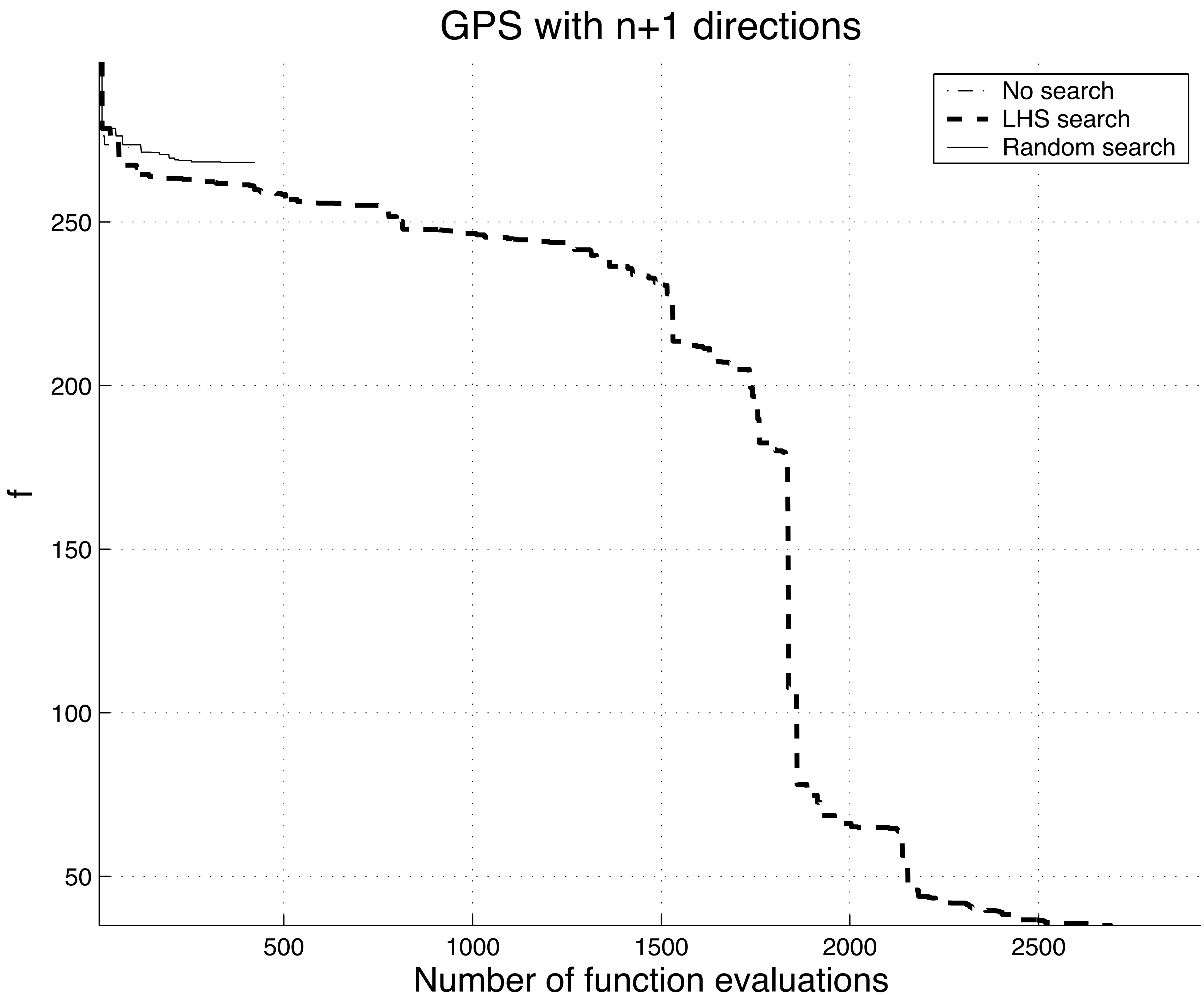
$$\min_{\eta_0,\lambda,\beta} \; g(\eta_0, \lambda, \beta)$$

with

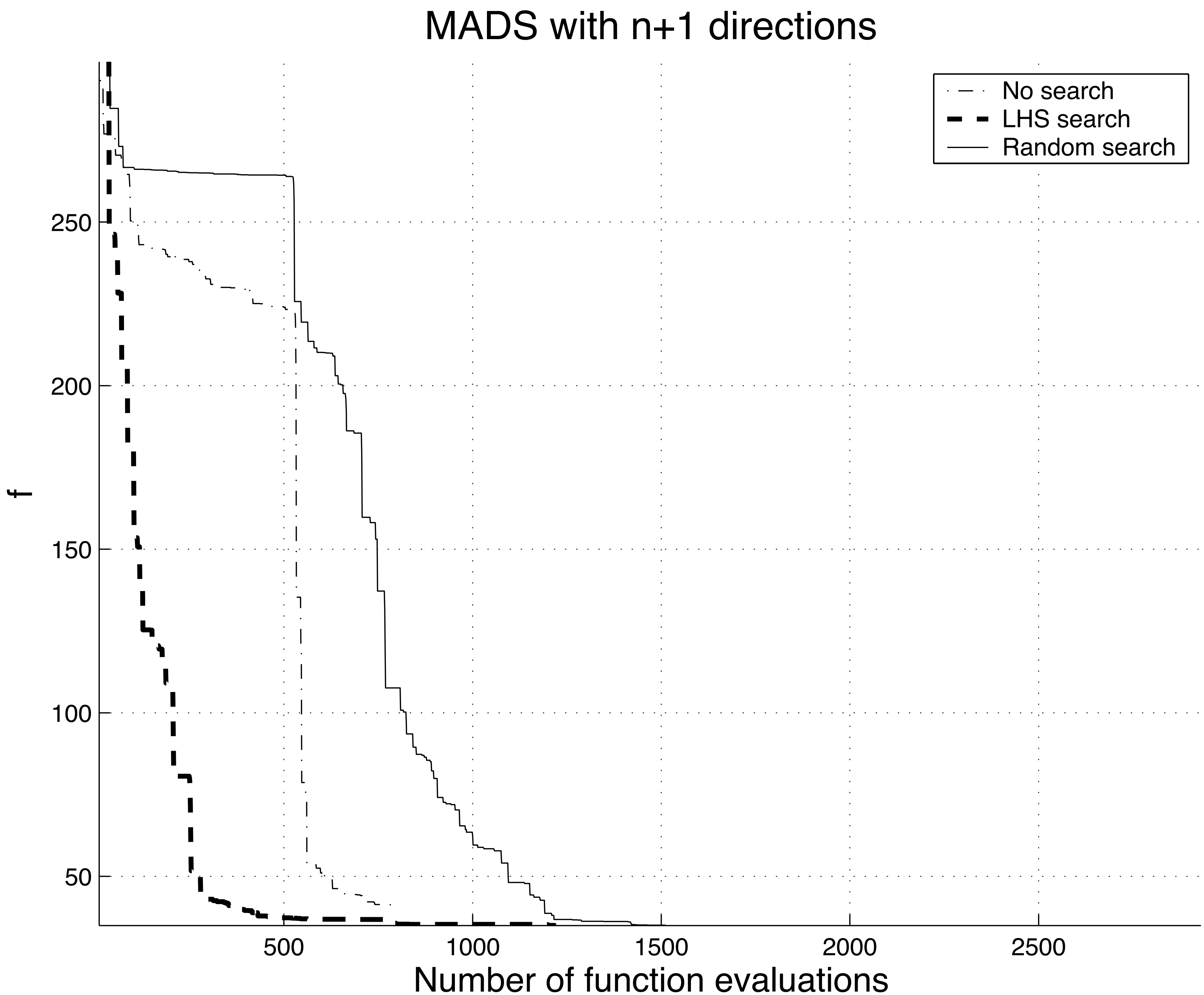
$$g = \sum_{i=1}^{13} |\eta(\dot{\gamma}) - \eta_i|$$


Coordinate search
Fixed Complete
Fixed opportunist
Dynamic opportunist
Dynamic opportunist with cache
250
200
150
100
50
f
500
1000
1500
2000
2500
Number of function evaluations

Rice 2004


GPS with n+1 directions
No search
LHS search
Random search
f
250
200
150
100
50
500
1000
1500
2000
2500
Number of function evaluations

Rice 2004


MADS with n+1 directions
No search
LHS search
Random search
f
250
200
150
100
50
500
1000
1500
2000
2500
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Rice 2004

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- Numerically, randomness is a blessing and a curse.
- MADS can handle oracular or yes/no constraints.
- The underlying mesh is finer in MADS than in GPS : Good for general searches and surrogates.
- MADS is the result of nonsmooth analysis pointing up the weaknesses in GPS.

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  Alison will present in the next talk the use of a surrogate in a specific mechanical engineering problem using GPS/MADS.

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- MADS replaces GPS in our NOMADm and NOMAD softwares. Gilles and Mark will present a demo of these sofwares after lunch.