A multistart multisplit direct search methodology for global optimization

Ismael Vaz (Univ. Minho)
Luis Nunes Vicente (Univ. Coimbra)

IPAM, Optimization and Optimal Control for Complex Energy and Property Landscapes

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Outline

1. LOCAL: Probabilistic direct search.

   Deterministic case first. Motivation, performance, complexity.

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   Deterministic case first. Motivation, performance, complexity.

2. GLOBAL: By multistarting & multispliting probabilistic DS.

   How to split and merge runs. Use of non-convex modelling.

Direct-search methods

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- *In the smooth and deterministic case, these points are defined by directions in positive spanning sets (PSS):*

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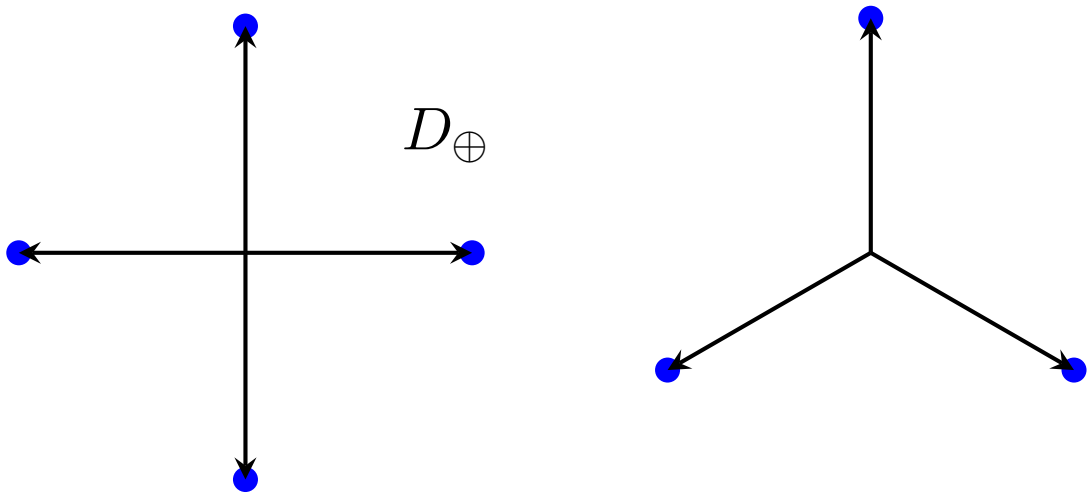
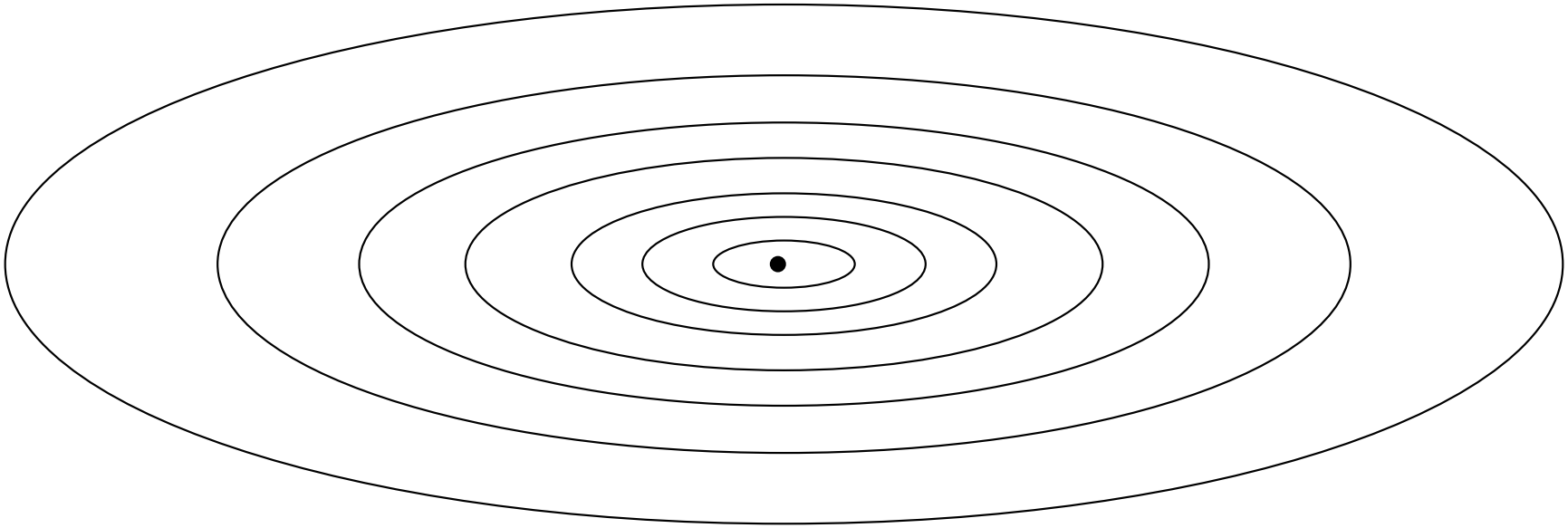


Coordinate search



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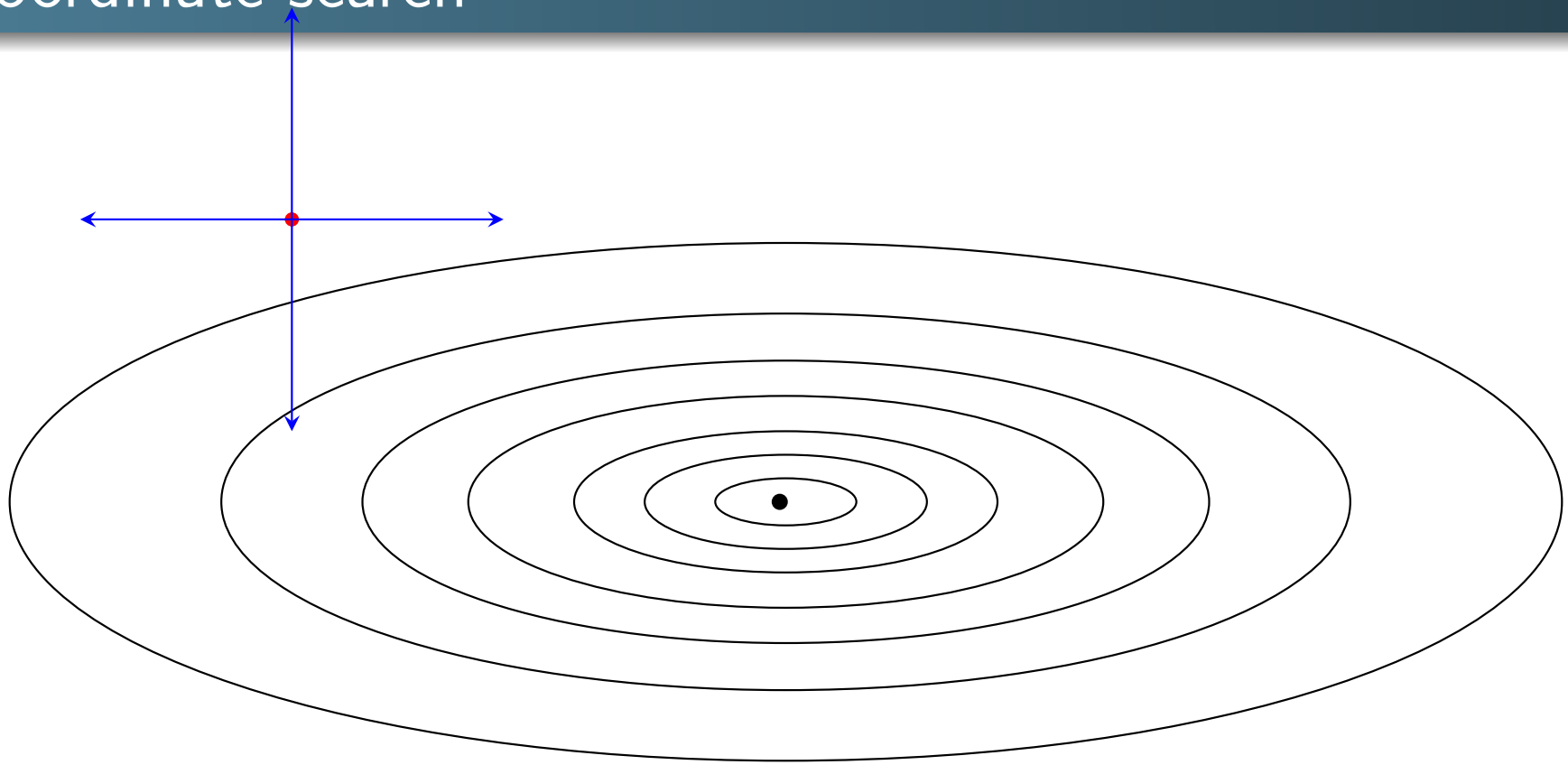

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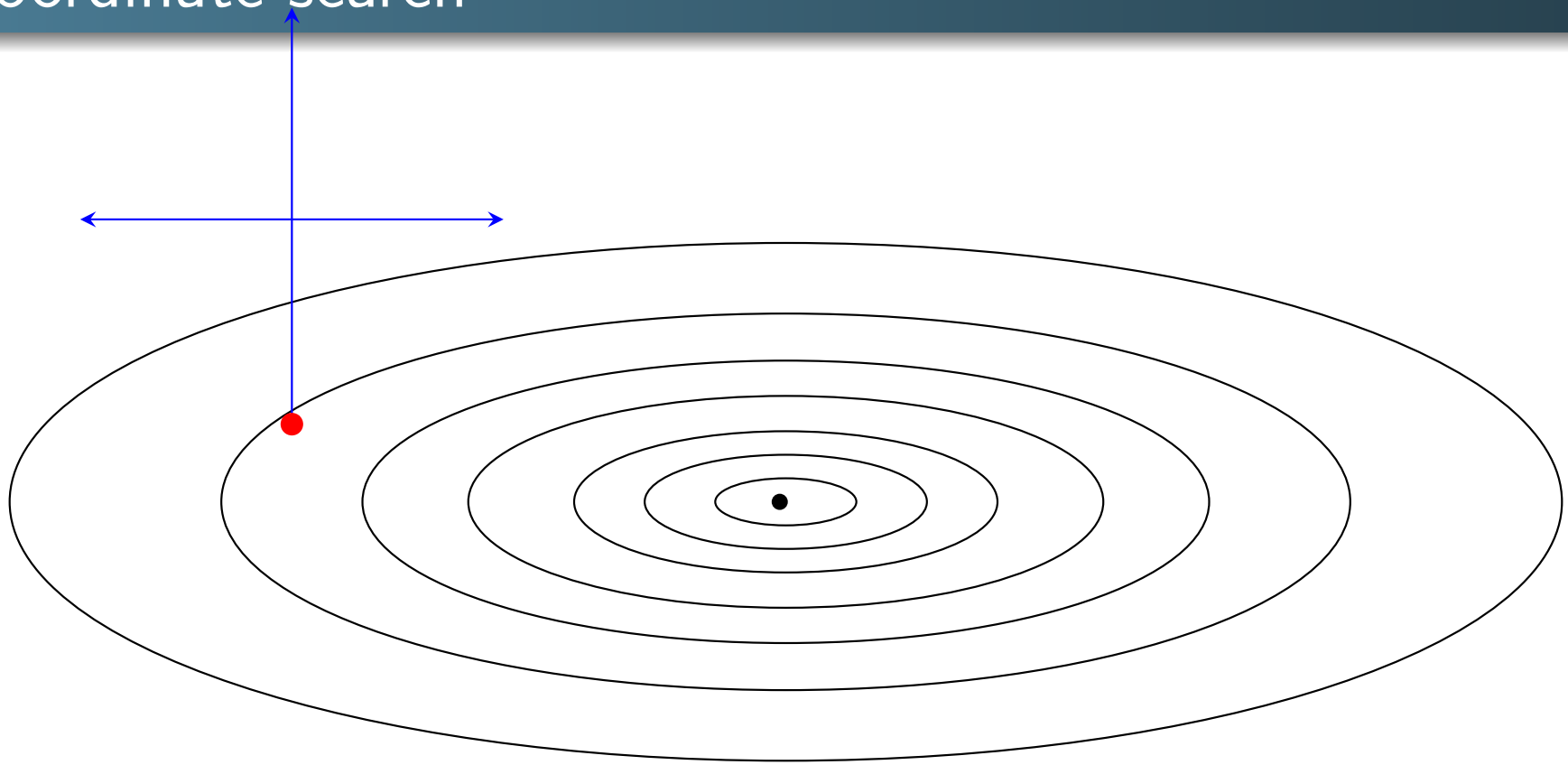

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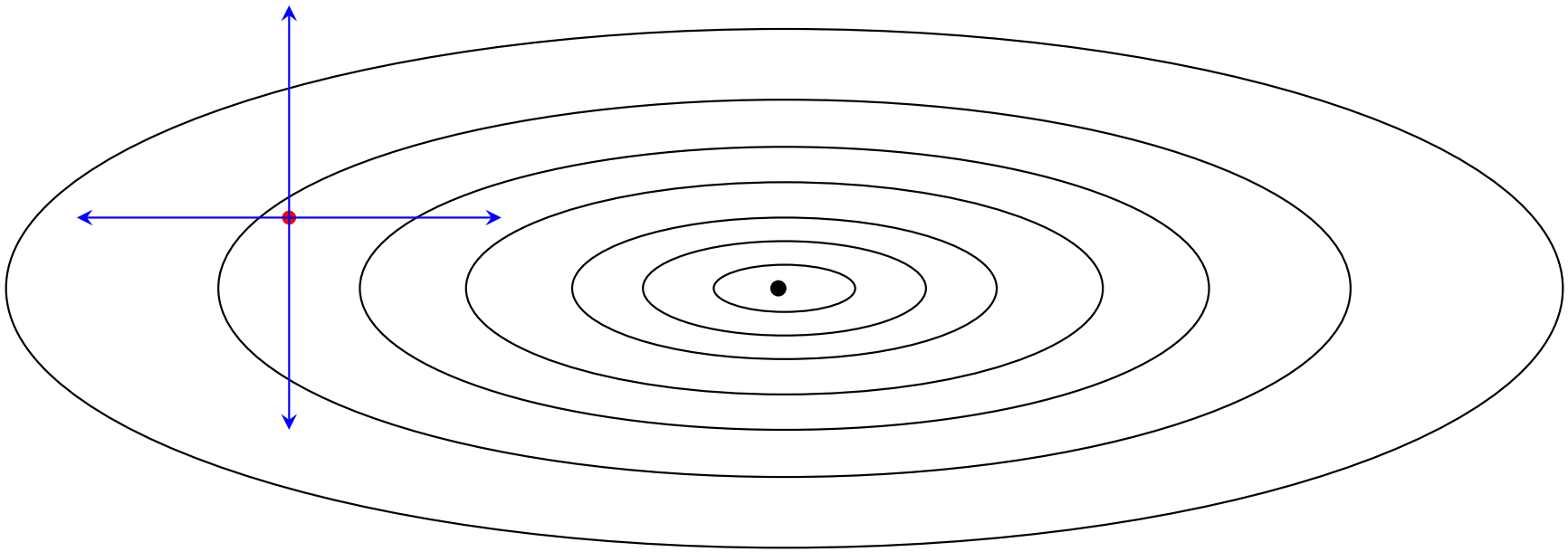

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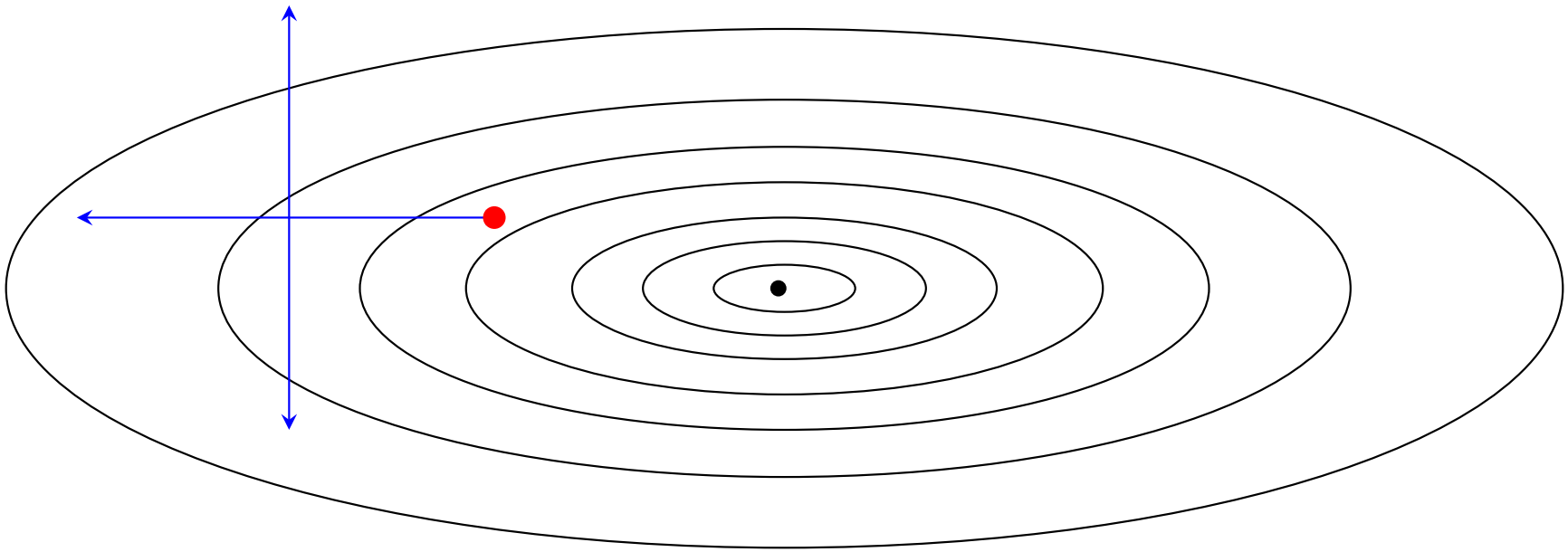

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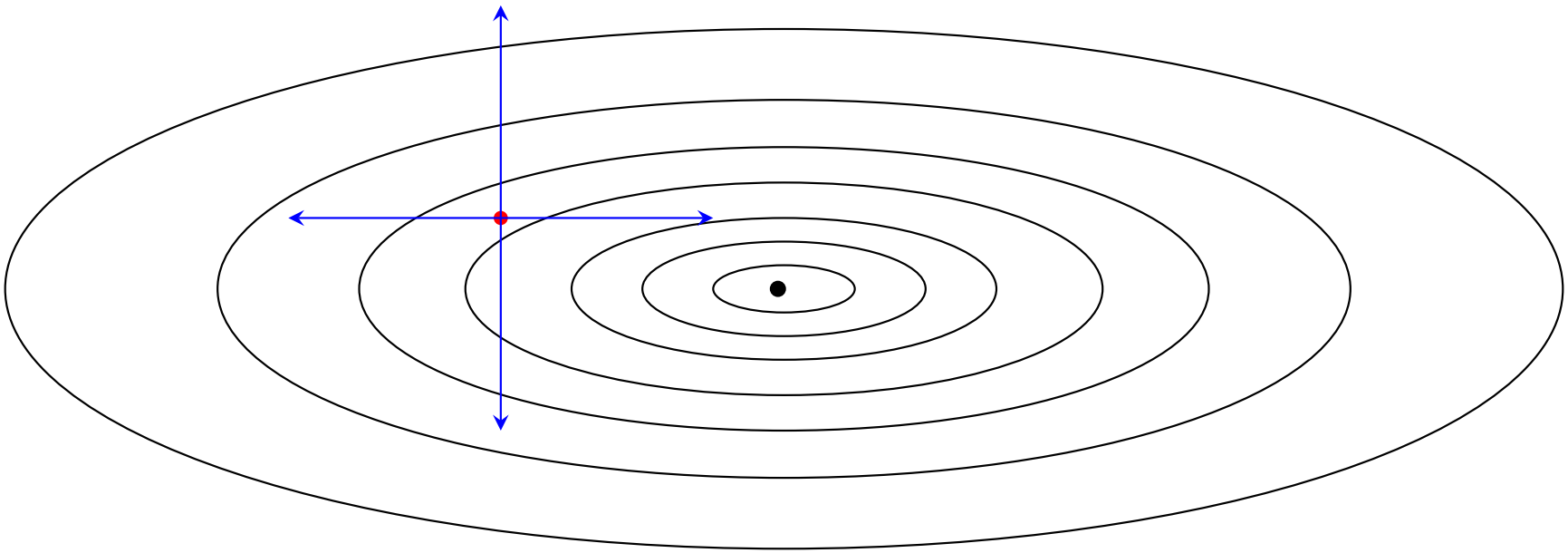

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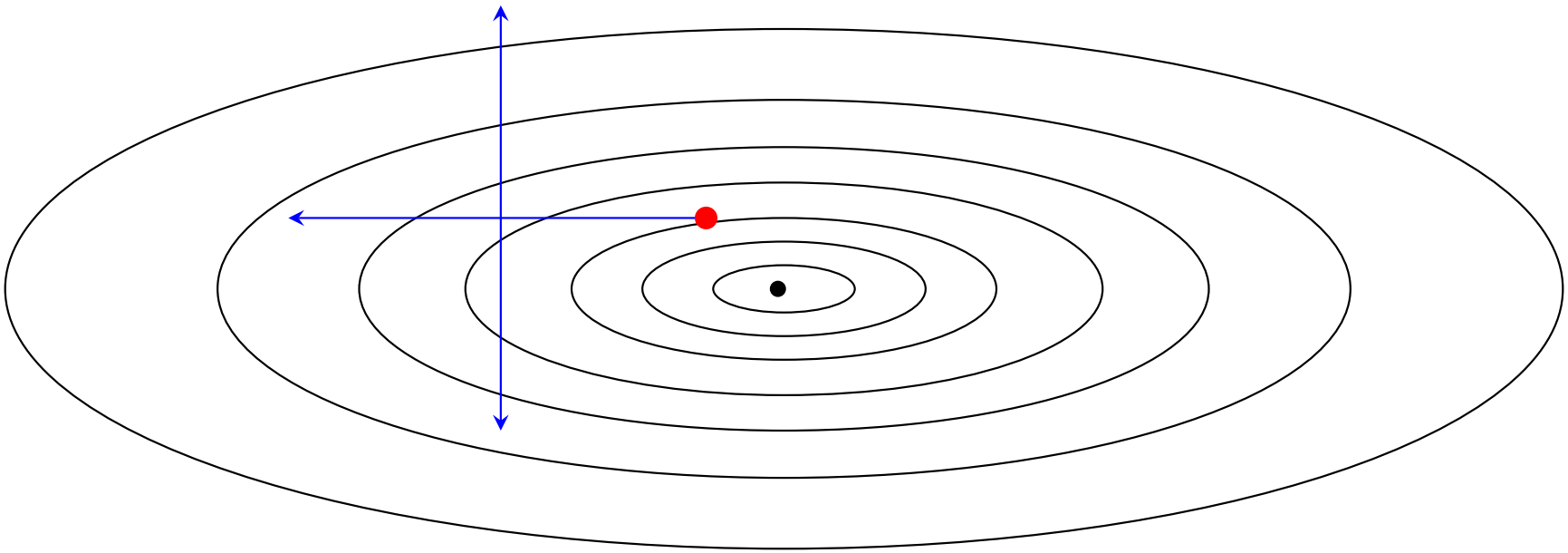

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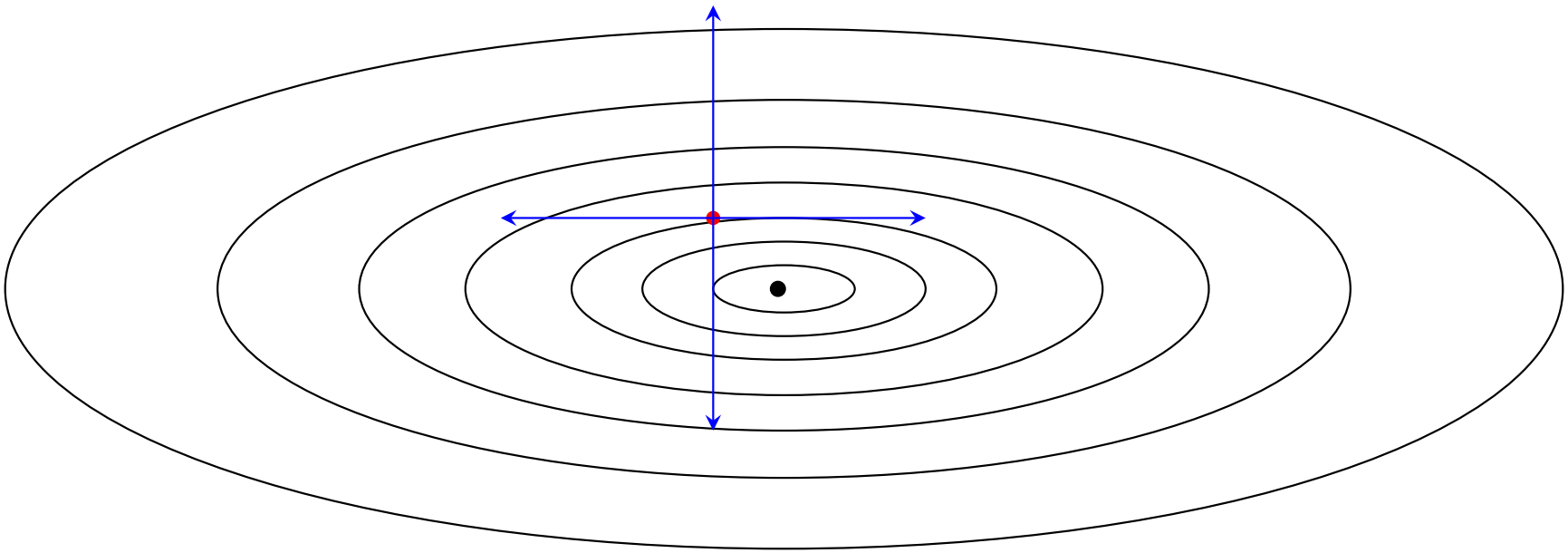

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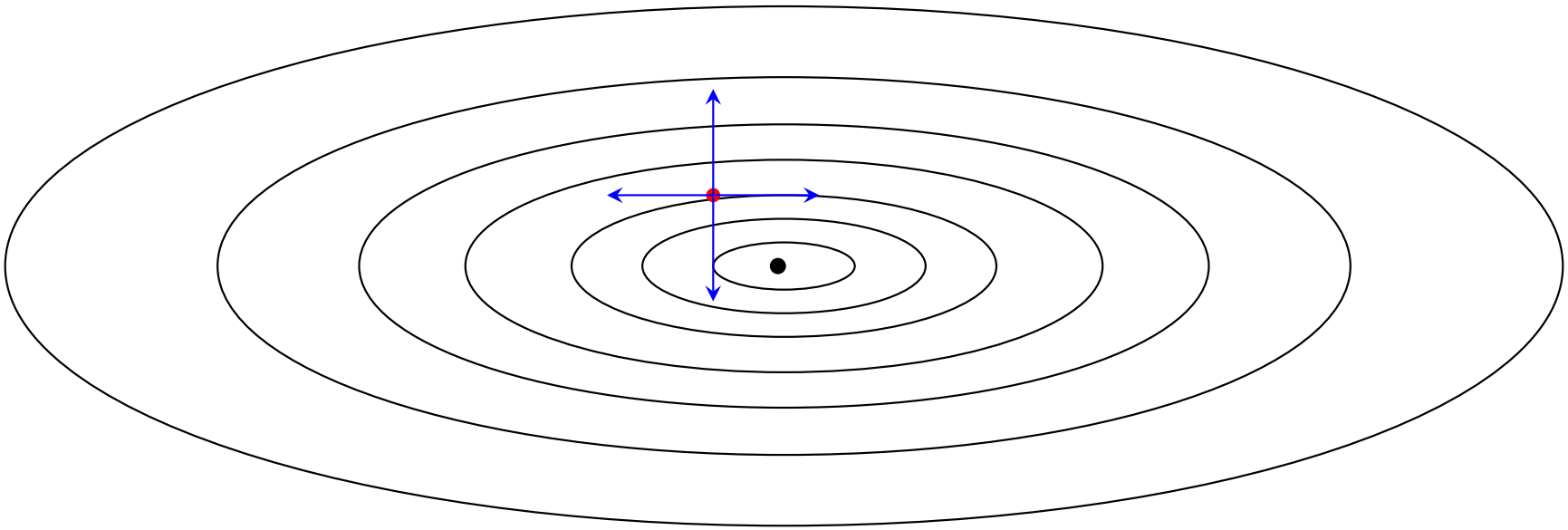

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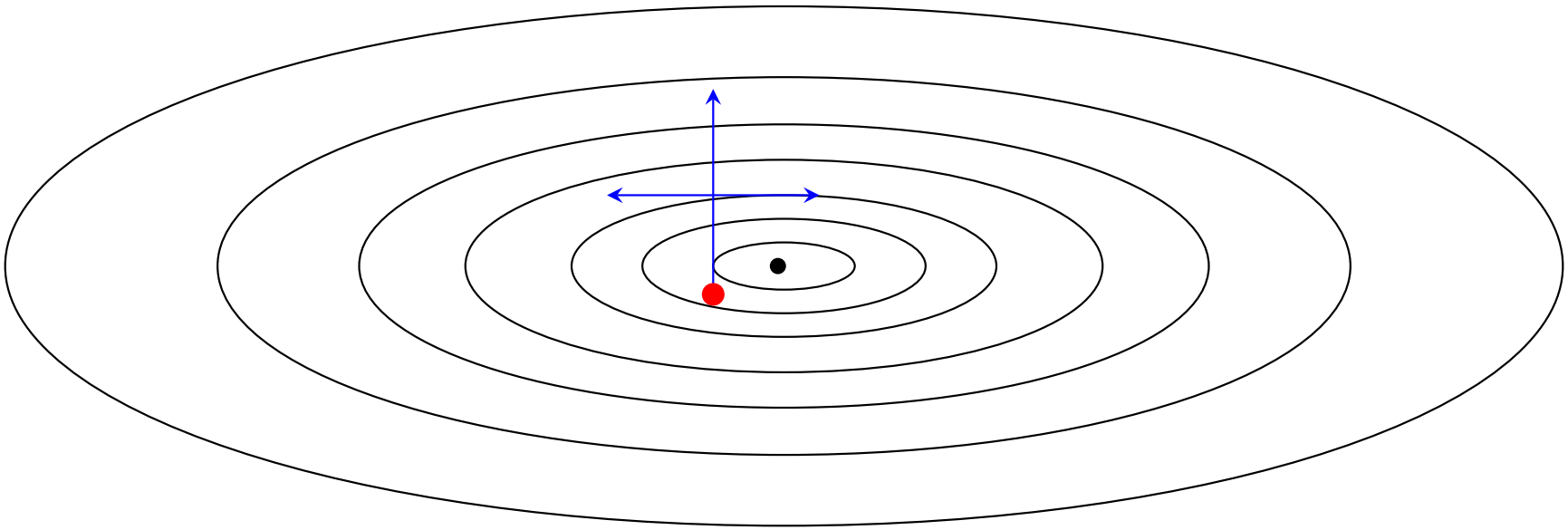

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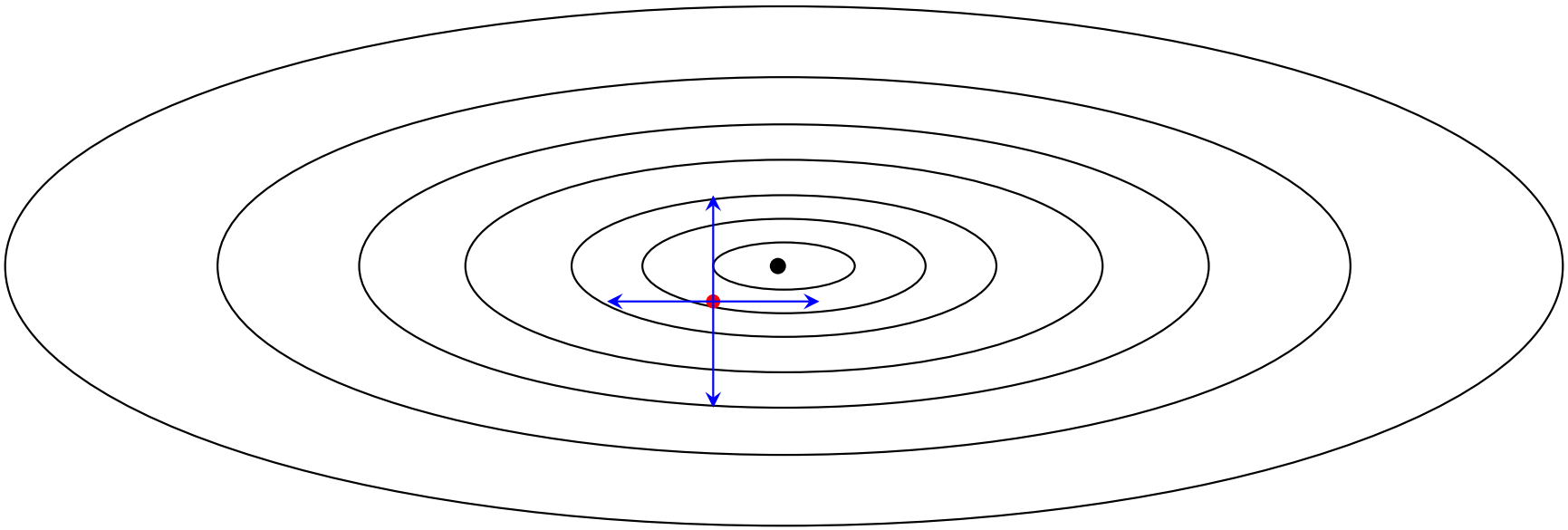

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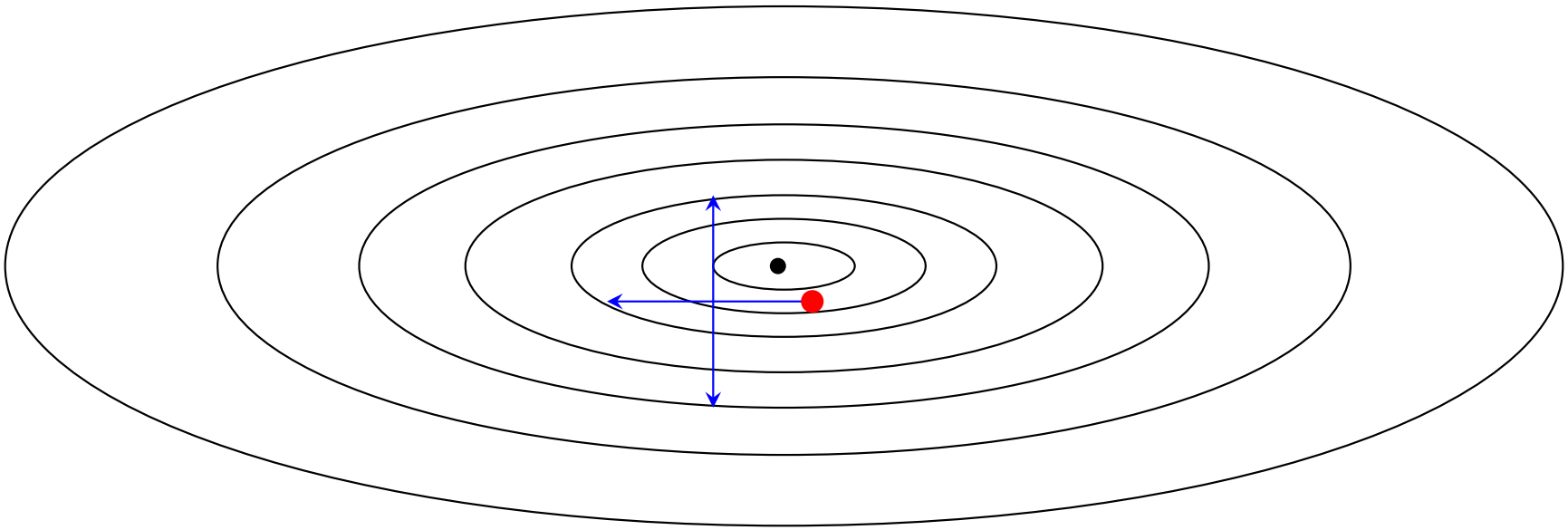

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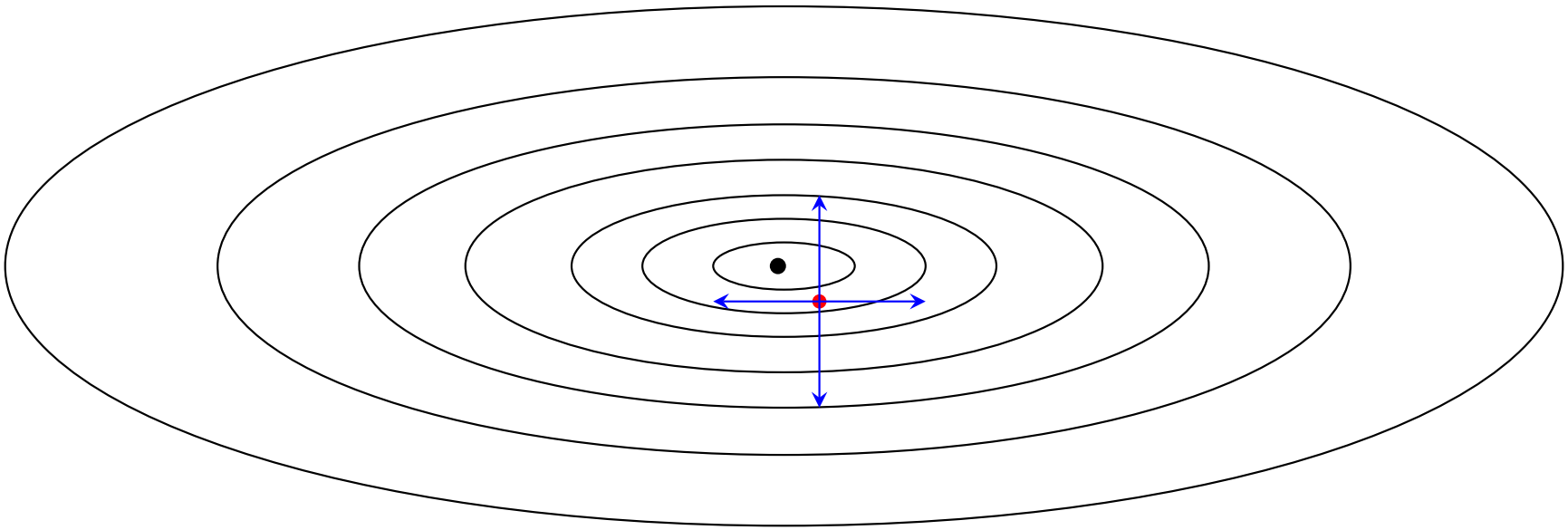

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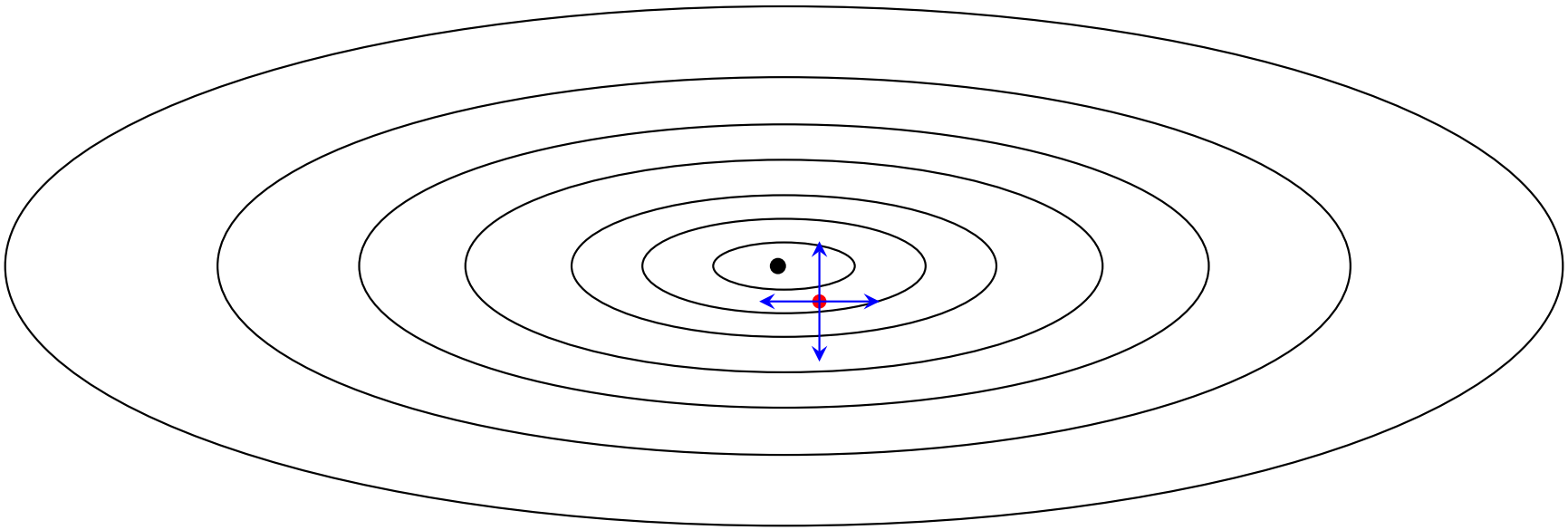

A class of DS methods

Choose: x_0 and α_0.

For $k = 0, 1, 2, \ldots$ (Until α_k is suff. small)

- **Search step (optional)**

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$$f(x_k + \alpha_k d_k) < f(x_k) - \rho(\alpha_k) \qquad \text{like } \rho(\alpha) = \alpha^2/2.$$

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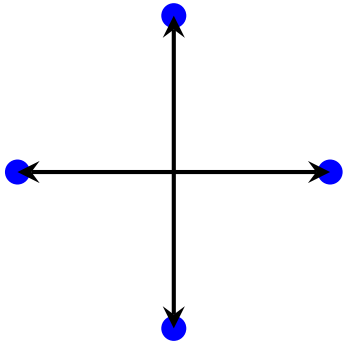
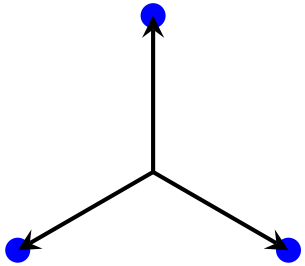
- **SUCCESS:** Move $x_{k+1} = x_k + \alpha_k d_k$ and possibly increase $\alpha_{k+1} = \gamma\, \alpha_k$ $(\gamma = 1 \text{ or } 2)$.
- **UNSUCCESS:** Stay $x_{k+1} = x_k$ and decrease $\alpha_{k+1} = \theta\, \alpha_k$ $(\theta = 1/2)$.

Deterministic approach

- Positive spanning set (PSS)





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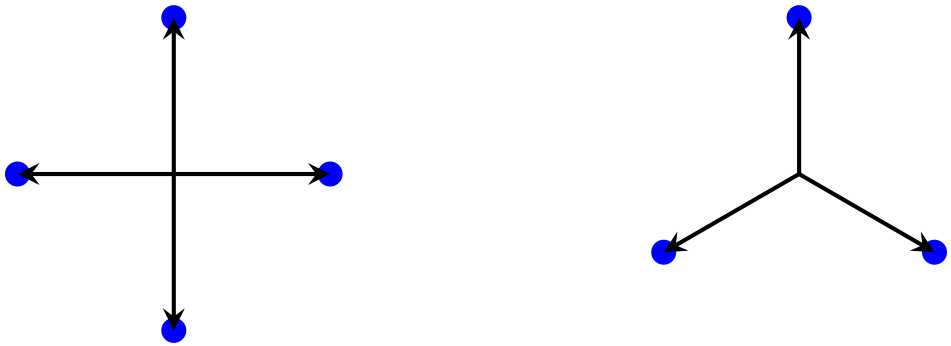

- Cosine measure of a PSS D

$$\mathrm{cm}(D) = \min_{0 \neq v \in \mathbb{R}^n} \max_{d \in D} \frac{d^\top v}{\|d\|\|v\|} > 0.$$

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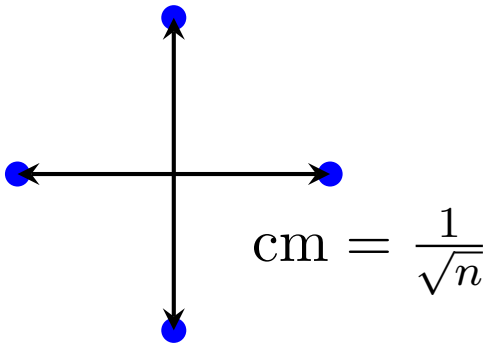

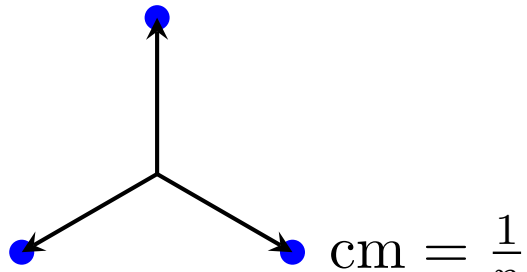

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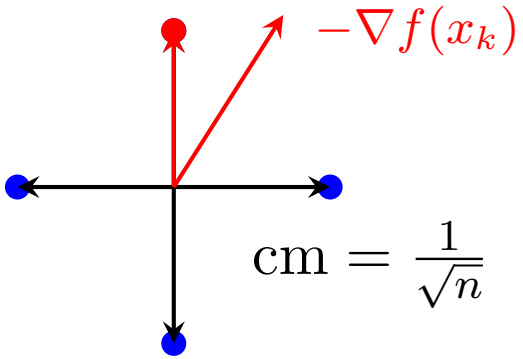

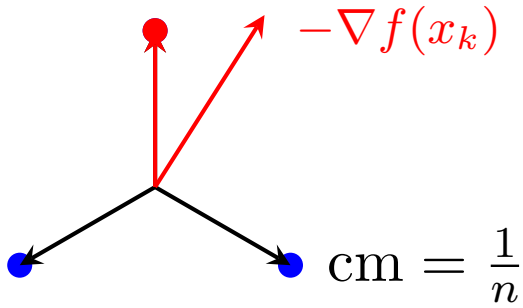

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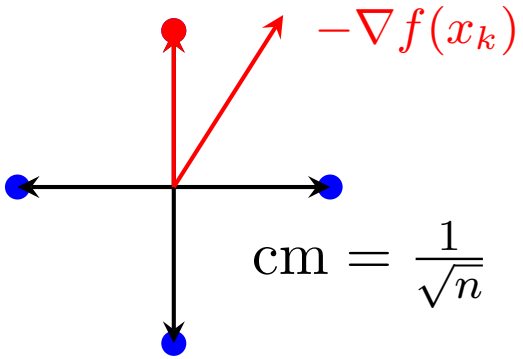

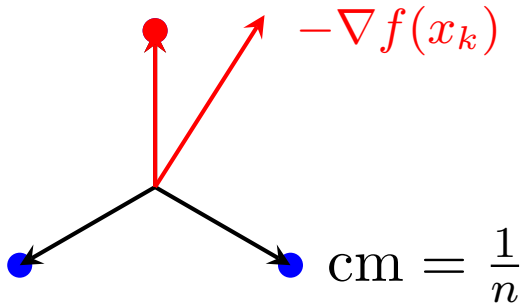

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  $\Longrightarrow$ α_k small leads to success!

WCC of DS (smooth case)

Insight: $\underbrace{(\text{decrease in } f) \geq \mathcal{O}(\alpha_k^2)}_{\text{success}} \geq \cdots \geq \underbrace{\mathcal{O}(\alpha_{k_u}^2) \geq \mathcal{O}(\|\nabla f(x_{k_u})\|^2)}_{\text{unsuccess}}$

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Theorem (LNV, 2013 EURO J. Comp. Optim.)

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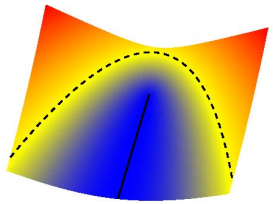
- Bounds depend on $L_{\nabla f}^2$ (instead of $L_{\nabla f}$ as in gradient method).

WCC of DS (smooth, convex case)

Ruling out cases where the supreme distance from the initial level set $L_f(x_0)$ to the solution set X_*^f is infinite...



Theorem (M. Dodangeh and LNV, 2016 Math. Program.)

Any such DS method generates a sequence $\{x_k\}_{k\geq 0}$ *such that:*

$$f(x_k) - f_* \;=\; \mathcal{O}(1/k) \qquad k_\epsilon \;\leq\; \mathcal{O}\left(n\,\epsilon^{-1}\right).$$

Again, the # of fevals must be multiplied by n*:* $\mathcal{O}\left(n^2\,\epsilon^{-1}\right)$.

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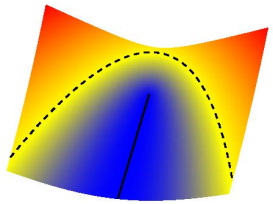

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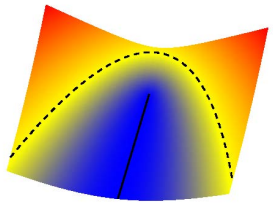

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The n^2 factor comes from $\frac{|D|}{\mathrm{cm}(D)^2}$. For $D = D_\oplus$ one obtains

$$\frac{2n}{(1/\sqrt{n})^2} \;=\; 2n^2. \qquad \text{Is this optimal?}$$

Optimality of the n^2 factor

Theorem (M. Dodangeh, LNV, and Z. Zhang, 2016 Optim. Lett.)

The factor n^2 is optimal since any PSS D in $\mathbb{R}^n$ satisfies

$$\frac{|D|}{\mathrm{cm}(D)^2} \geq \frac{1}{\zeta^2} n^2$$

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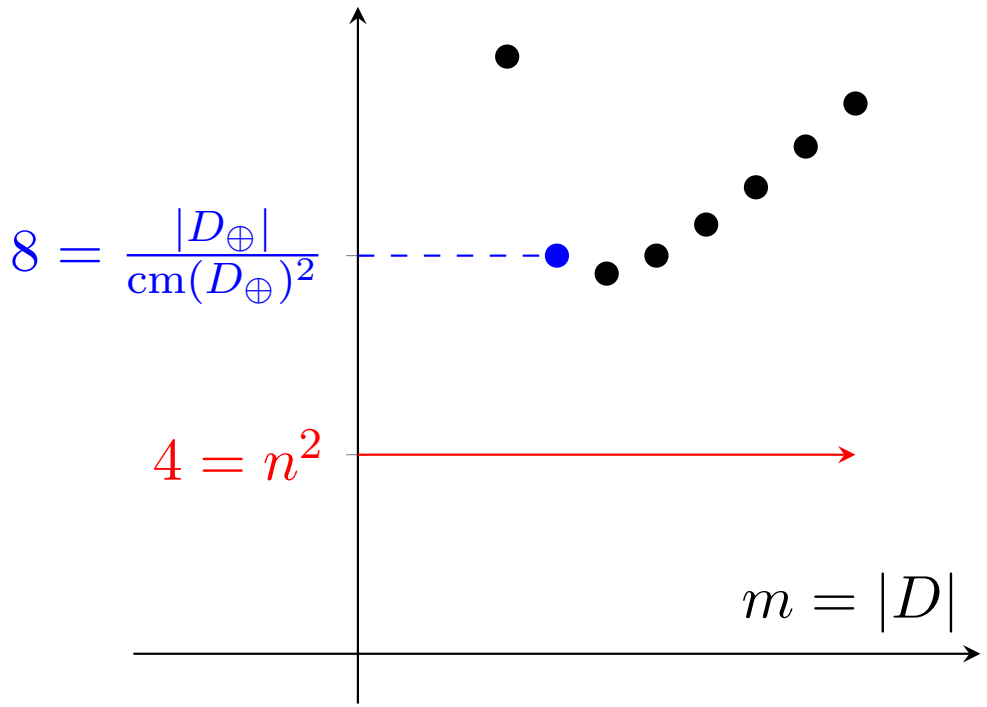

Plot of

$$\frac{|D|}{\mathrm{cm}(D)^2} \geq n^2.$$

for the case $n = 2$ and D's with uniform angles,

Global rate of DS (smooth, strongly convex case)

Theorem (M. Dodangeh and LNV, 2014 Math. Program.)

Any such DS method generates a sequence $\{x_k\}_{k\geq 0}$ *such that:*

$$f(x_k) - f_* \ < \ Cr^k,$$

where $r \in (0,1)$ *and* $C > 0$.

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- When f is SC (constant $\mu > 0$), one has (k_0 first unsucc.)

$$\|x_k - x_*\| \ \leq \ \sqrt{L_{\nabla f}/\mu}\, \|x_{k_0} - x_*\|.$$

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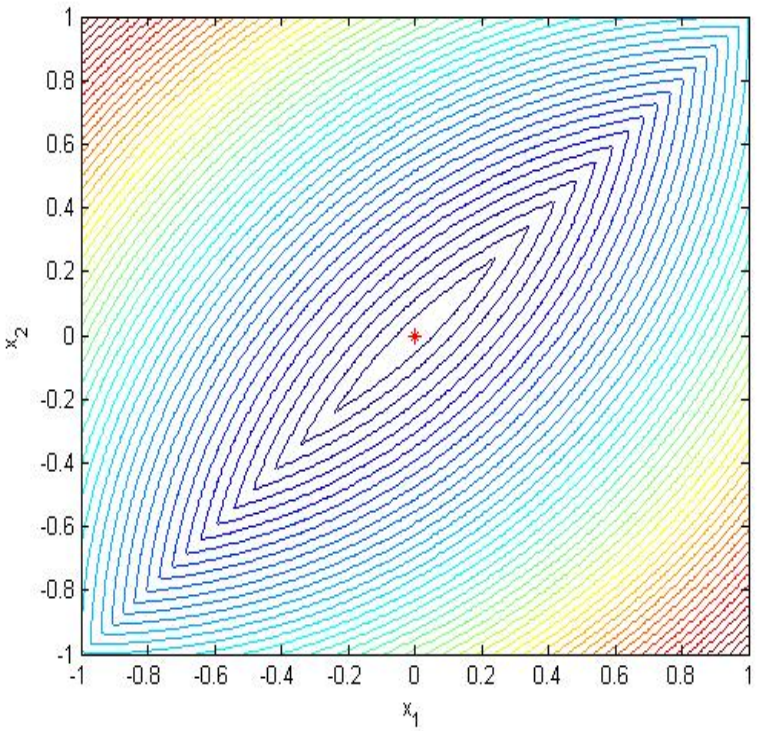
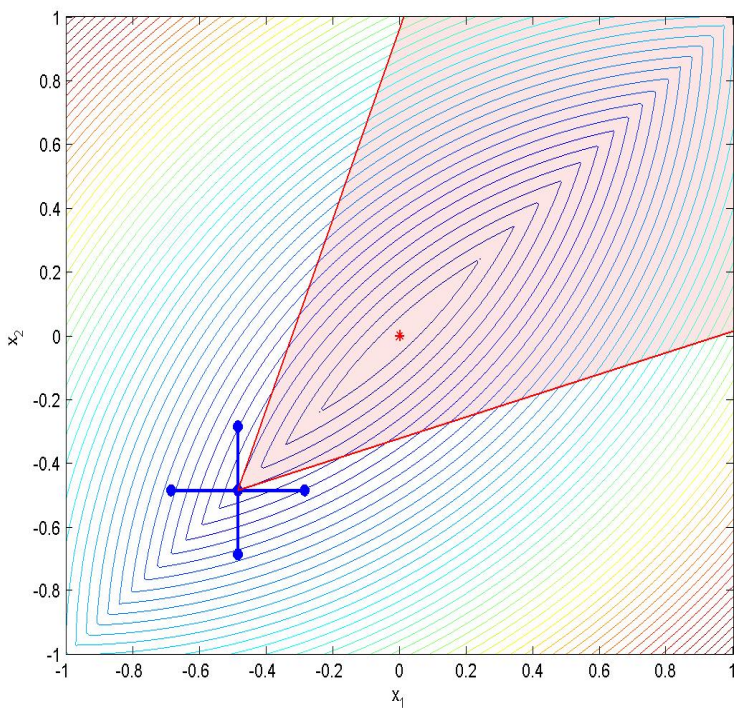
- A linear rate for the iterates can be derived from

$$\frac{1}{2}\mu\|x - x_*\|^2 \ \leq \ f(x) - f_*.$$

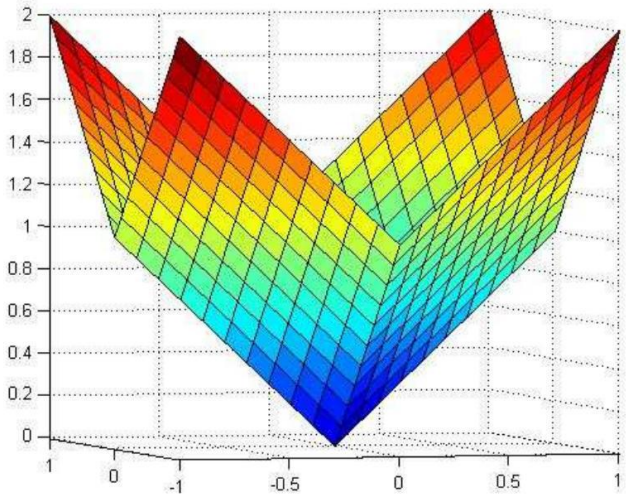
Difficulties in the nonsmooth case





The cone of descent directions at the poll center is shaded.

One possible fix: Combine DS with Smoothing



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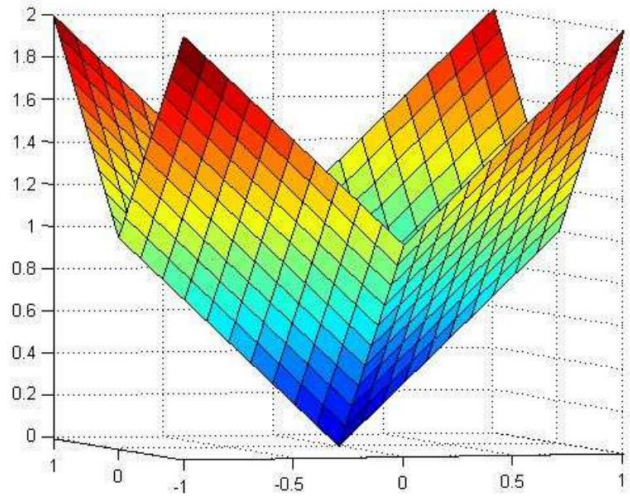

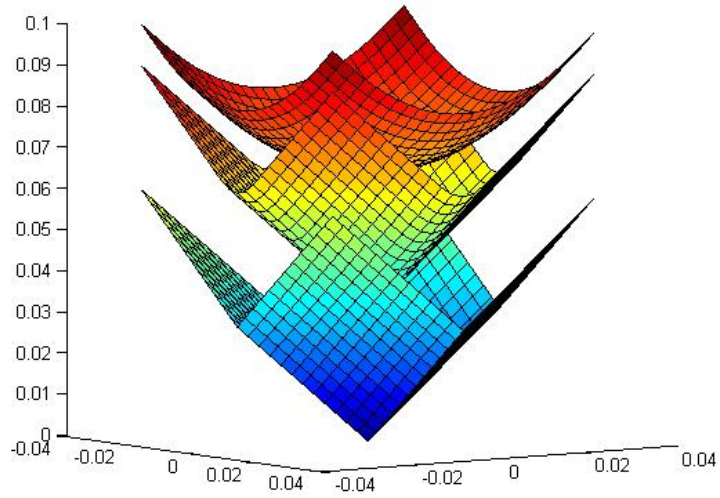

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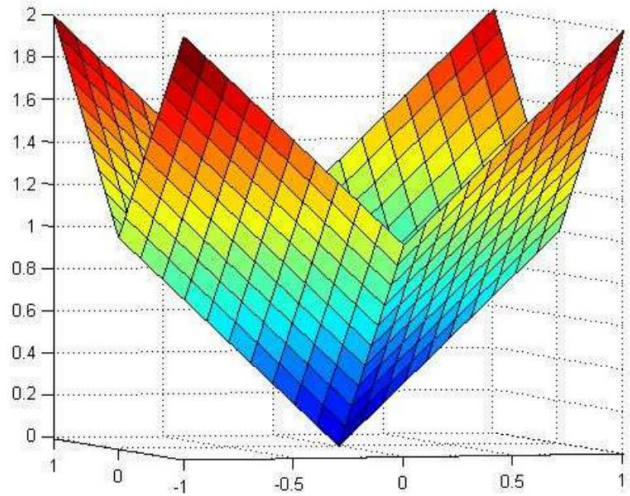

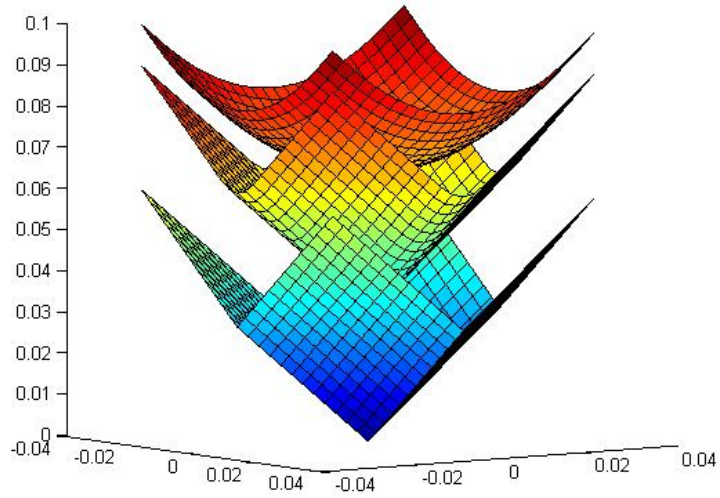

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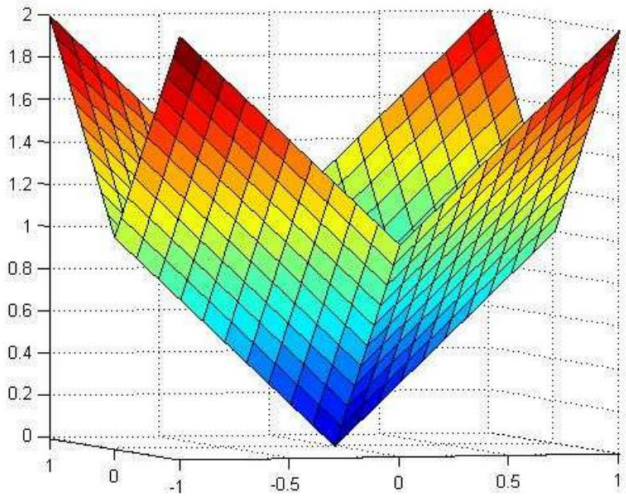

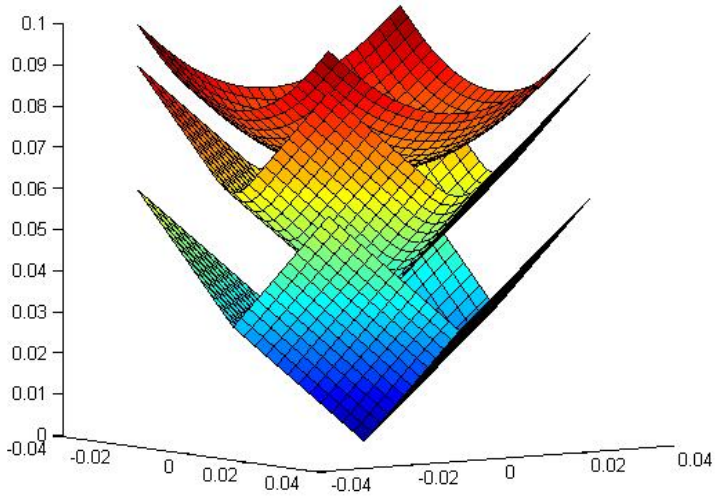

- Essentially the WCC cost increases from $\mathcal{O}\left(\epsilon^{-2}\right)$ to $\mathcal{O}\left(\epsilon^{-3}\right)$ [R. Garmanjani and LNV, 2013 IMA J. Numer. Anal.].
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- $\mathcal{O}(\epsilon^{-3})$ non-smooth, non-convex — (using smoothing techniques).

Descent condition and successful iterations

Assume the polling directions are normalized.

Lemma

If

$$\operatorname{cm}\left(D_k, -\nabla f(x_k)\right) \geq \kappa \quad \textit{and} \quad \alpha_k < \frac{2\kappa\|\nabla f(x_k)\|}{L_{\nabla f}+1},$$

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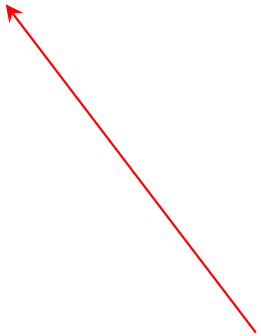
where $\mathrm{cm}(D,v)$ is the cosine measure of D given v, defined by

$$\mathrm{cm}(D,v) = \max_{d\in D} \frac{d^\top v}{\|d\|\|v\|}$$

and $L_{\nabla f}$ is a Lipschitz constant of ∇f.

Randomly generating ‘positive spanning sets’ ...

$-\nabla f(x_k)$



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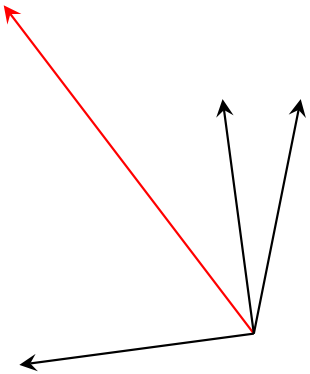

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in this case not a PSS

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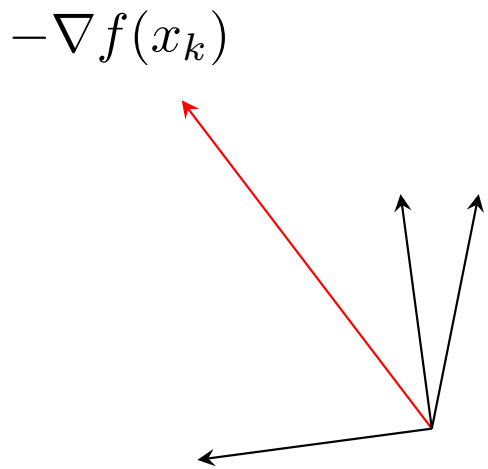

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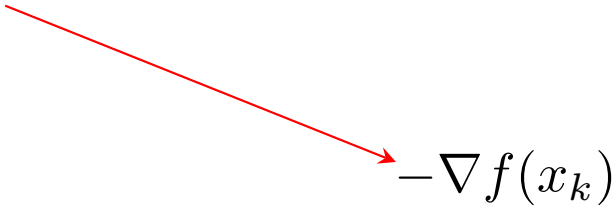

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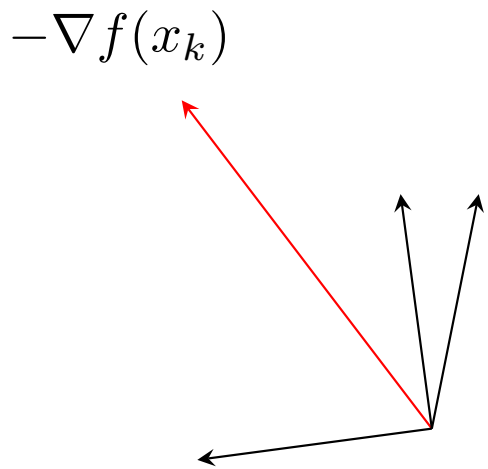

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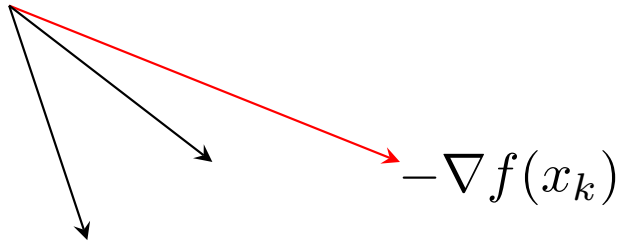

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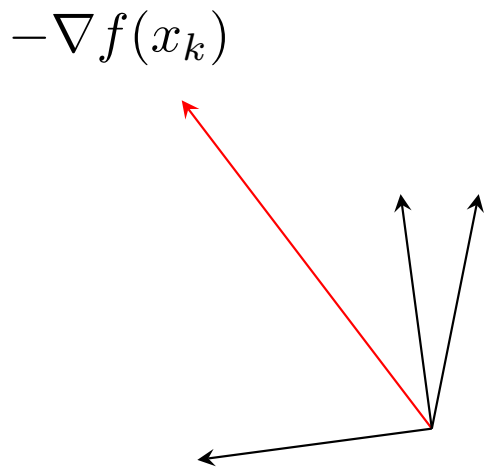

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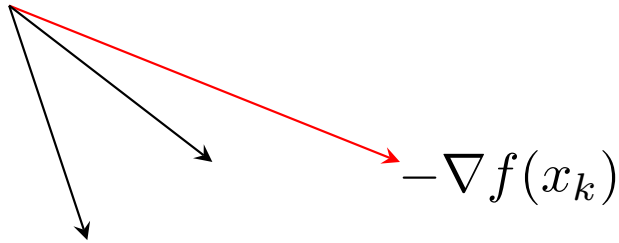

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$\mathrm{cm}\big(D_k, -\nabla f(x_k)\big) \geq \kappa$ can be satisfied 'probabilistically' ...

Numerical illustration

Relative performance for different sets of polling directions ($n = 40$).

	$[I \ -I]$	$[Q \ -Q]$	$2n$	$n+1$	$n/4$	2	1
arglina	3.42	8.44	10.30	6.01	1.88	1.00	–
arglinb	20.50	10.35	7.38	2.81	1.85	1.00	2.04
broydn3d	4.33	6.55	6.54	3.59	1.28	1.00	–
dqrtic	7.16	9.37	9.10	4.56	1.70	1.00	–
engval1	10.53	20.89	11.90	6.48	2.08	1.00	2.08
freuroth	56.00	6.33	1.00	1.67	1.67	1.00	4.00
integreq	16.04	16.29	12.44	6.76	2.04	1.00	–
nondquar	6.90	30.23	7.56	4.23	1.87	1.00	–
sinquad	–	–	1.65	2.01	1.00	1.55	–
vardim	1.00	3.80	1.80	2.40	1.80	1.80	4.30

Solution accuracy was 10^{-3}. Averages were taken over 10 independent runs.

Probabilistic descent

From the definition of probabilistic models (Bandeira, LNV, Scheinberg, 2014 SIOPT):

Definition

The sequence $\{\mathfrak{D}_k\}$ *is* (p, κ)*-probabilistically descent if, for each* $k \geq 0$,

$$\Pr\left(\mathrm{cm}(\mathfrak{D}_k, -\nabla f(X_k)) \geq \kappa \mid \mathfrak{D}_0, \ldots, \mathfrak{D}_{k-1}\right) \geq p,$$

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Let Z_k be the indicator function of $\left\{\mathrm{cm}\left(\mathfrak{D}_k, -\nabla f(X_k)\right) \geq \kappa\right\}$, and

$$p_0 \;=\; \frac{\ln \theta}{\ln(\gamma^{-1}\theta)} \;=\; \frac{1}{2} \qquad \theta = 1/2,\ \gamma = 2.$$

Global rate: Counting descent

For each realization of the DS algorithm, define

- $\tilde{g}_k$: the gradient with minimum norm among $\nabla f(x_0), \ldots, \nabla f(x_k)$,

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Let z_ℓ denote the realization of $Z_\ell = \left\{\mathrm{cm}\big(\mathfrak{D}_\ell, -\nabla f(X_\ell)\big) \geq \kappa\right\}$ $(\ell \geq 0)$.

Intuition: If $\|\tilde{g}_k\|$ is 'big', then $\sum_{\ell=0}^{k-1} z_\ell$ is probably 'small'.

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In fact, one can prove

$$\sum_{\ell=0}^{k-1} z_\ell \;\leq\; \mathcal{O}\left(\frac{1}{\|\tilde{g}_k\|^2}\right) + p_0 k.$$

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Hence

$$\Pr\left(\|\tilde{G}_k\| \leq \epsilon\right) \;=\; 1 - \Pr\left(\|\tilde{G}_k\| > \epsilon\right) \;\geq\; 1 - \underbrace{\Pr\left(\sum_{\ell=0}^{k-1} Z_\ell \leq \lambda\, k\right)}_{\text{apply Chernoff \& Submartingale Theory}}.$$

Global rate and WCC bound

Theorem (Gratton, Royer, LNV, and Zhang, 2015 SIOPT)

Suppose that $\{\mathfrak{D}_k\}$ *is* (p, κ)*-probabilistically descent with* $p > p_0$*. Then*

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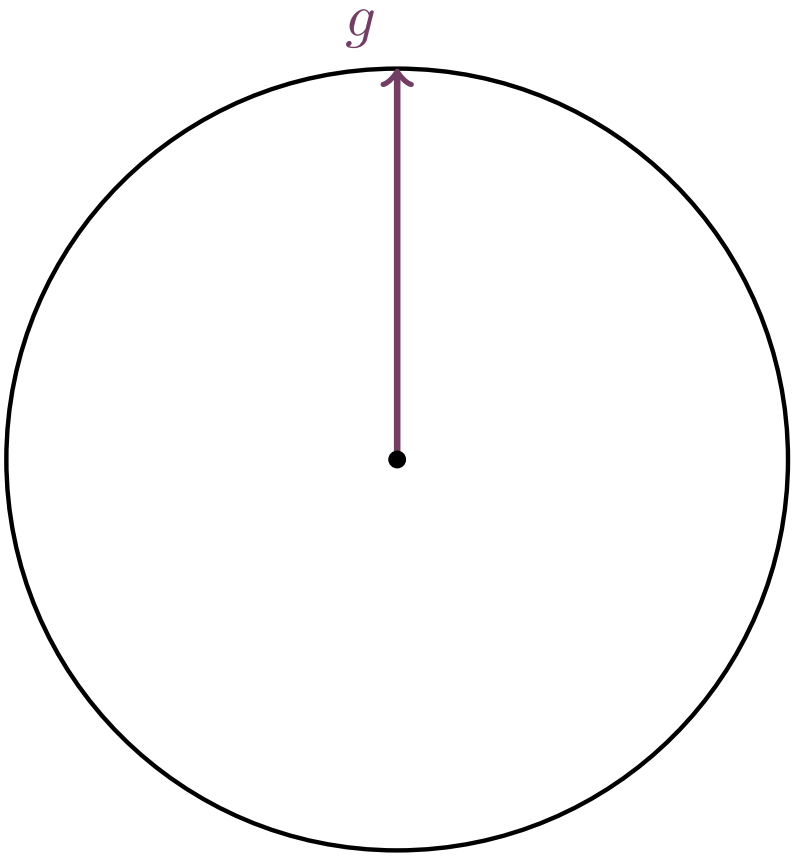
$\longrightarrow \mathcal{O}(\epsilon^{-2})$ bound for # of iter. with overwhelmingly high probability.

Two uniform directions are enough, one is not



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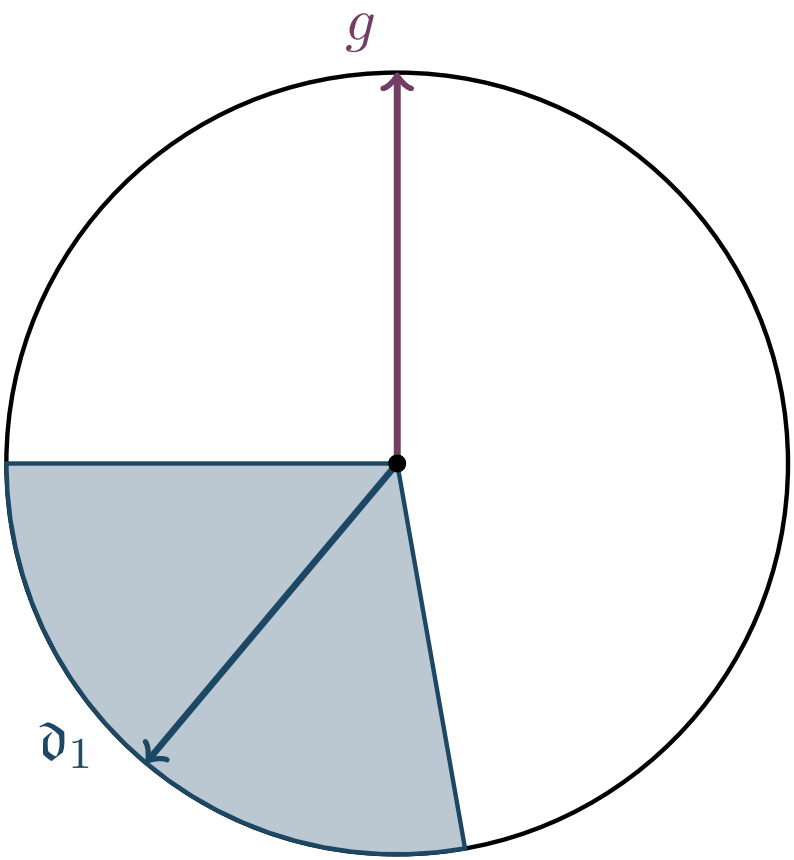

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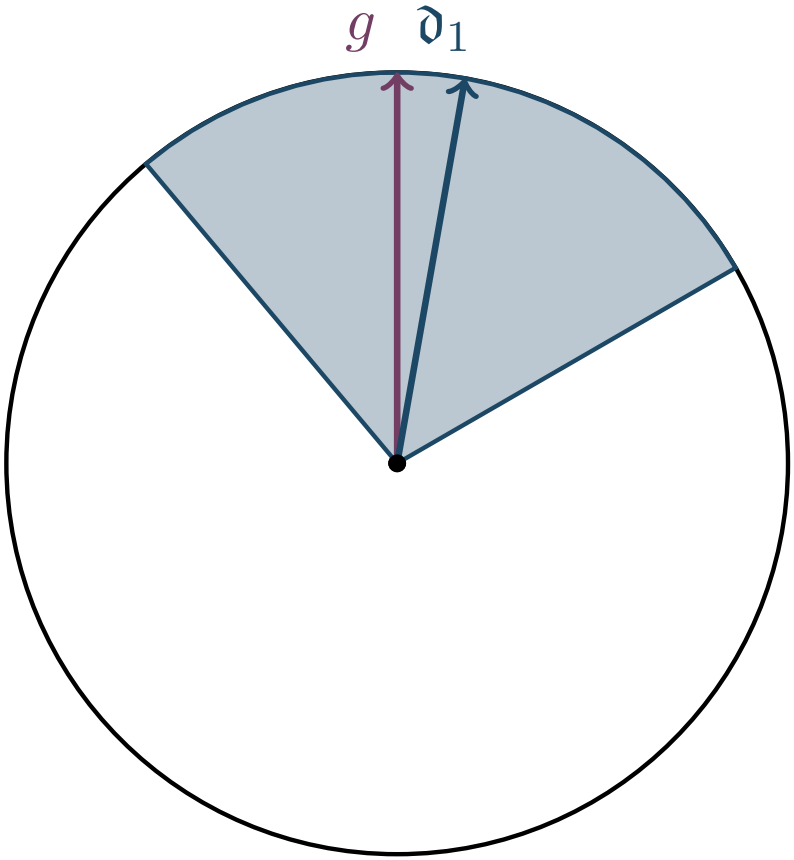

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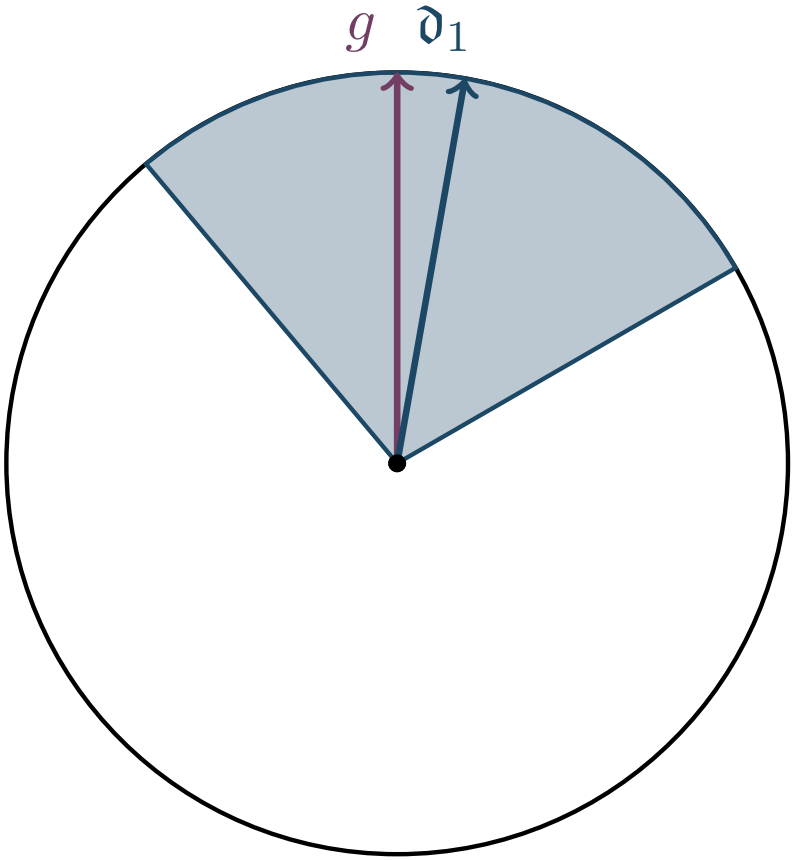

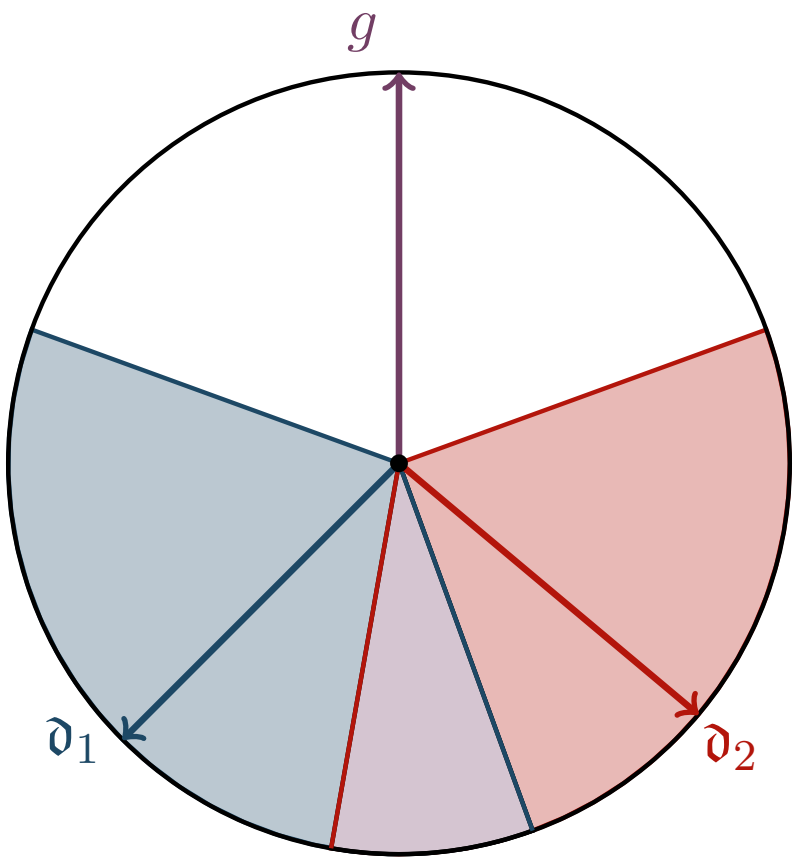

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$$\mathfrak{d}_1, \mathfrak{d}_2 \sim \mathcal{U}(\mathbb{S}^1) \Rightarrow \exists \kappa^* \in (0,1), \quad \Pr\left(\mathrm{cm}\left(\{\mathfrak{d}_1, \mathfrak{d}_2\}, g\right) \geq \kappa^*\right) > 1/2.$$

Worst case complexity: Dependence on the dimension

Then, when $r = |D| > 1$, $\{\mathfrak{D}_k\}$ is p-probabilistically $(1/\sqrt{n})$-descent for some $p > p_0 = 1/2$ independent of n.

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WCC (number of function evaluations)

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Theory admits $r = 2$, leading to

$$\mathcal{O}(n\epsilon^{-2}) \quad !!!$$

A more detailed look at the numerical experiments

Relative performance for different sets of polling directions ($n = 40$).

	$[I \ -I]$	$[Q \ -Q]$	2 ($\gamma = 2$)	4 ($\gamma = 1.1$)
arglina	1.00	3.17	5.86	6.73
arglinb	34.12	5.34	1.00	2.02
broydn3d	1.00	1.91	2.04	3.47
dqrtic	1.18	1.36	1.00	1.48
engval1	1.05	1.00	2.29	2.89
freuroth	17.74	7.39	1.35	1.00
integreq	1.54	1.49	1.00	1.34
nondquar	1.00	2.82	1.37	1.73
sinquad	–	1.26	1.00	–
vardim	20.31	11.02	1.00	1.84

Now $\gamma = 1$ for $[I \ -I]$ and $[Q \ -Q]$.

A more detailed look at the numerical experiments

Relative performance for different sets of polling directions ($n = 100$).

	$[I \ -I]$	$[Q \ -Q]$	2 ($\gamma = 2$)	4 ($\gamma = 1.1$)
arglina	1.00	3.86	5.86	7.58
arglinb	138.28	107.32	1.00	1.99
broydn3d	1.00	2.57	1.92	3.21
dqrtic	3.01	3.25	1.00	1.46
engval1	1.04	1.00	2.06	2.84
freuroth	31.94	17.72	1.36	1.00
integreq	1.83	1.66	1.00	1.22
nondquar	1.18	2.83	1.00	1.17
sinquad	–	–	–	–
vardim	112.22	19.72	1.00	2.36

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$$\Pr\left(\operatorname{cm}(\mathfrak{D}_k, v) \geq \kappa\right) = \Pr\left(\mathfrak{d}^\top v \geq \kappa\right) + \Pr\left(-\mathfrak{d}^\top v \geq \kappa\right) = 2\varrho.$$

with $\varrho = \Pr\left(\{\mathfrak{d}^\top v \geq \kappa\}\right)$.

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with $\varrho = \Pr\big(\{\mathfrak{d}^\top v \geq \kappa\}\big)$.

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In addition, for any $\mathfrak{D} = \{\mathfrak{d}_1, \mathfrak{d}_2\}$ u.d. in the unit sphere,

$$\Pr\big(\operatorname{cm}(\mathfrak{D}, v) \geq \kappa\big) \;=\; 2\varrho - \Pr\big(\{\mathfrak{d}_1^\top v \geq \kappa\} \cap \{\mathfrak{d}_2^\top v \geq \kappa\}\big) \leq \; 2\varrho.$$

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What we obtain is a global rate of $\mathcal{O}(1/\sqrt{k})$, with overwhelmingly high probability.

Examples of application

This technique has also been applied to:

- Trust-region methods based on probabilistic models [Gratton, Royer, LNV, and Zhang, 2017 IMAJNA].

  When models are built iteratively in some random fashion and exhibit good accuracy with sufficiently high probability.

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- Trust-region methods based on probabilistic models [Gratton, Royer, LNV, and Zhang, 2017 IMAJNA].

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- Problems with linear constraints [Gratton, Royer, LNV, and Zhang, 2017].

  Random generation can be efficiently done in subspaces identified within approximate tangent cones.

Global Optimization part of the talk

Our goal is now to develop a solver for a global optimization problem of the type

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- Taking advantage of parallel computing.
- Having an approach capable of identifying several global or local minimizers of interest.

REMEMBER: Probabilistic DS (polling with 2 directions)

Choose: x_0 and α_0.

For $k = 0, 1, 2, \ldots$ (Until α_k is suff. small)

- **Search step (optional)**
- **Poll step:** Select $D_k = [d, -d]$ RANDOMLY and find $x_k + \alpha_k d_k$ ($d_k \in D_k$):

$$f(x_k + \alpha_k d_k) < f(x_k) - \rho(\alpha_k) \qquad \text{like } \rho(\alpha) = \alpha^2/2.$$

- **SUCCESS:** Move $x_{k+1} = x_k + \alpha_k d_k$ and increase $\alpha_{k+1} = \gamma\, \alpha_k$ $(\gamma = 2)$.
- **UNSUCCESS:** Stay $x_{k+1} = x_k$ and decrease $\alpha_{k+1} = \theta\, \alpha_k$ $(\theta = 1/2)$.

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- We allow MULTISTART runs and SPLITTING/MERGING of runs.

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MULTISTART: Select initial points for R_0 DS runs: $x_j^0, j = 1, \ldots, R_0$ (and initial step sizes $\alpha_j^0, j = 1, \ldots, R_0$).

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- INNER ITERATIONS:
  - Perform (in parallel) a certain number of iterations for all the $R_{\ell+1}$ DS runs, starting from $x_j^{\ell+1}, j = 1, \ldots, R_{\ell+1}$.

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- Using space clustering.
- Using nonconvex models built from previous function values.

The space clustering approach

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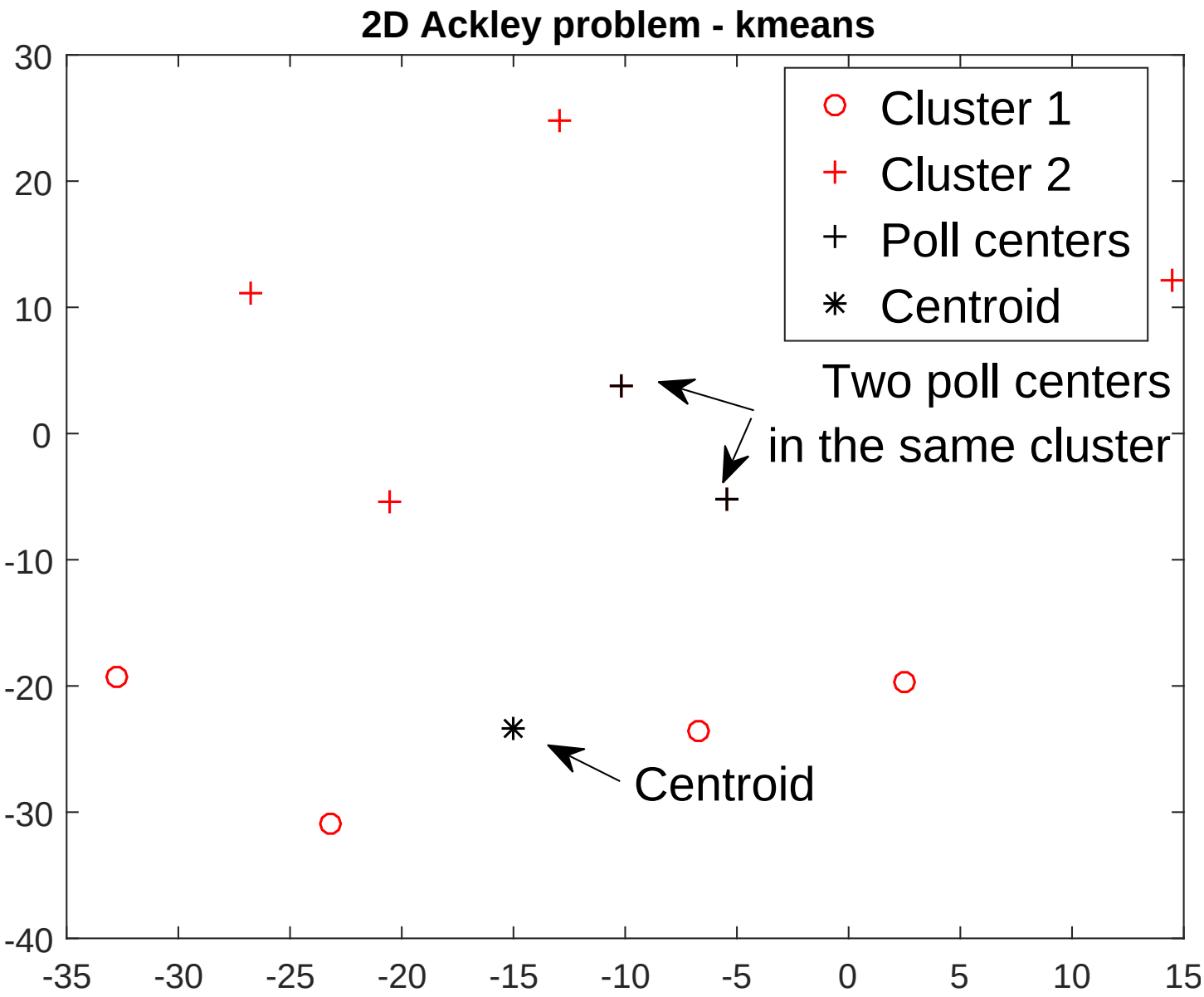
POSSIBLE DRAWBACK: The kmeans approach does not take into account the previous objective function values (clustering is done in the variables space).

The space clustering approach (example)



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$$q(p; y) \;=\; \min_{1 \leq i \leq n_q} \left\{ a_i + c_i^\top y + \frac{1}{2} y^\top H_i y \;=\; q_i(y) \right\},$$

and where the H_i's must be assured symmetric and PD.

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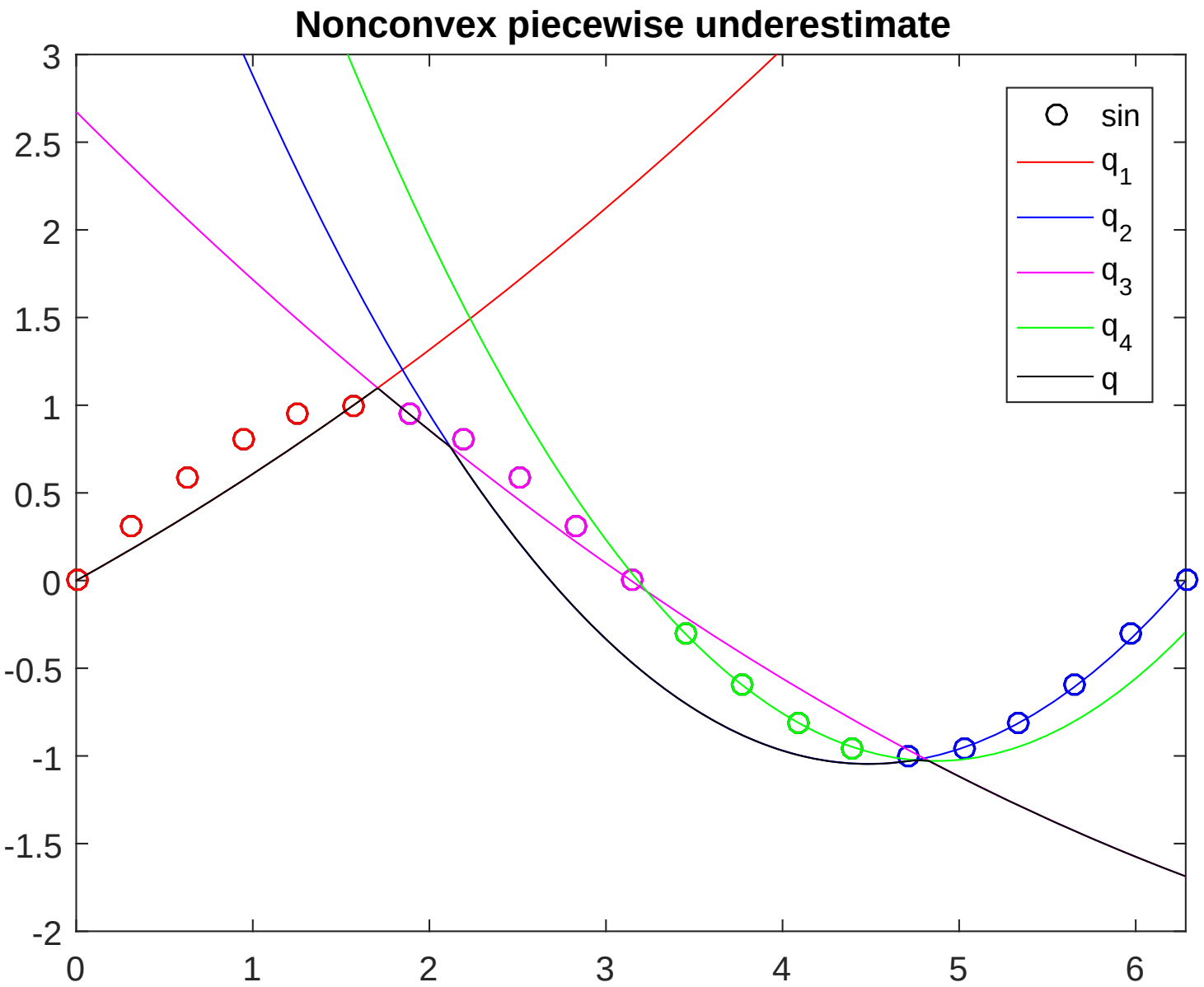

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The # of variables reduces to $\overline{n_p}$ (# of auxiliary variables) + $(n+1)(n+2)/2$ (one quadratic).

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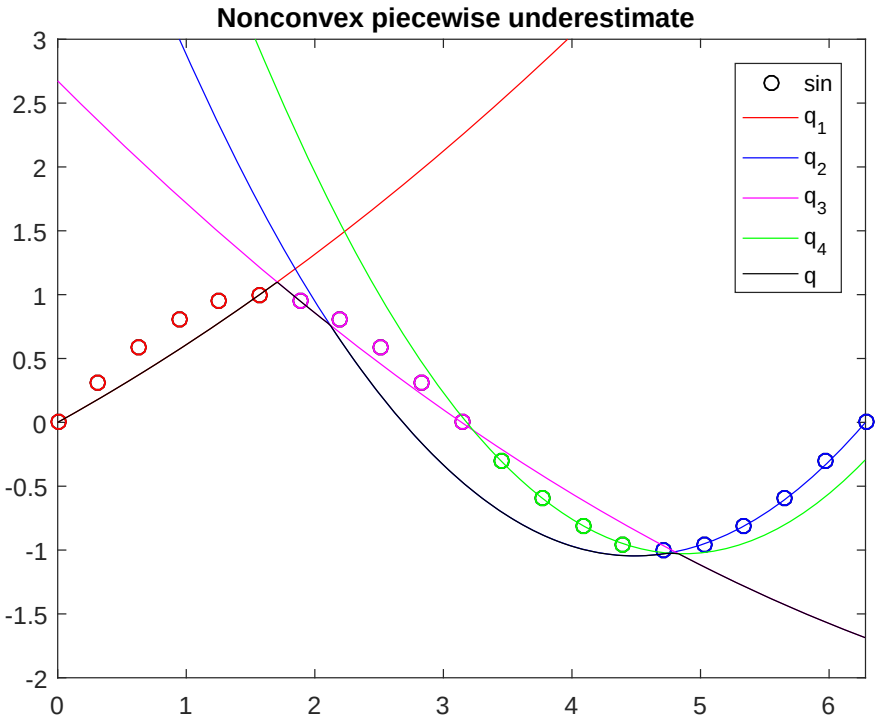
  - In addition, if $\theta_{i,j}$, $i \neq j$, is small, then merge DS runs i and j, using the poll center with lowest objective value.

The nonconvex modeling approach (example)



$\theta_{i,j}$ values:

	clusters or runs			
q_1	0.2068	433.1825	22.4790	75.9993
q_2	168.5406	0.0019	1.1115	0.4049
q_3	36.9686	12.3333	0.0441	0.1387
q_4	394.8617	0.5690	2.1869	0.0000

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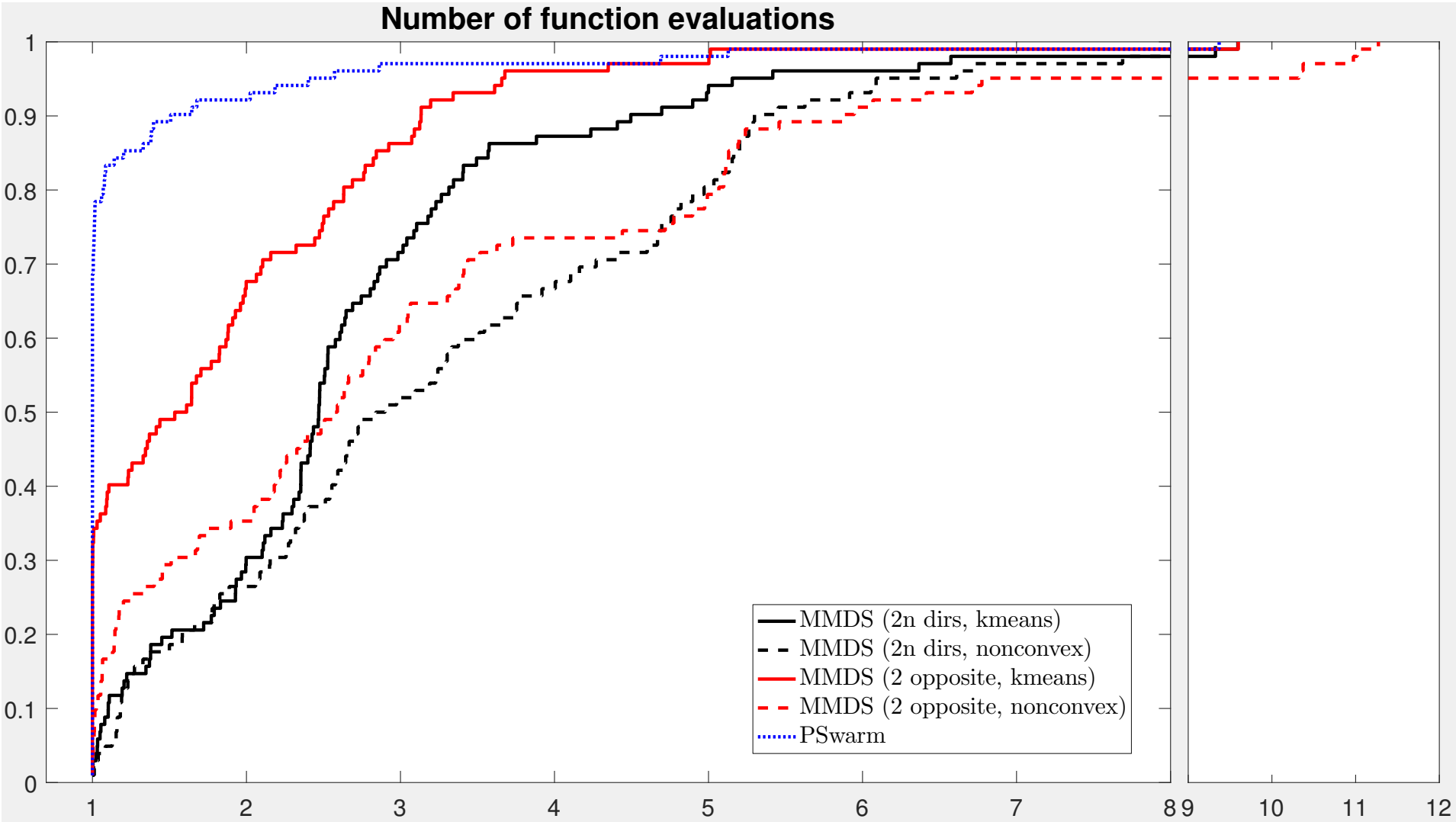
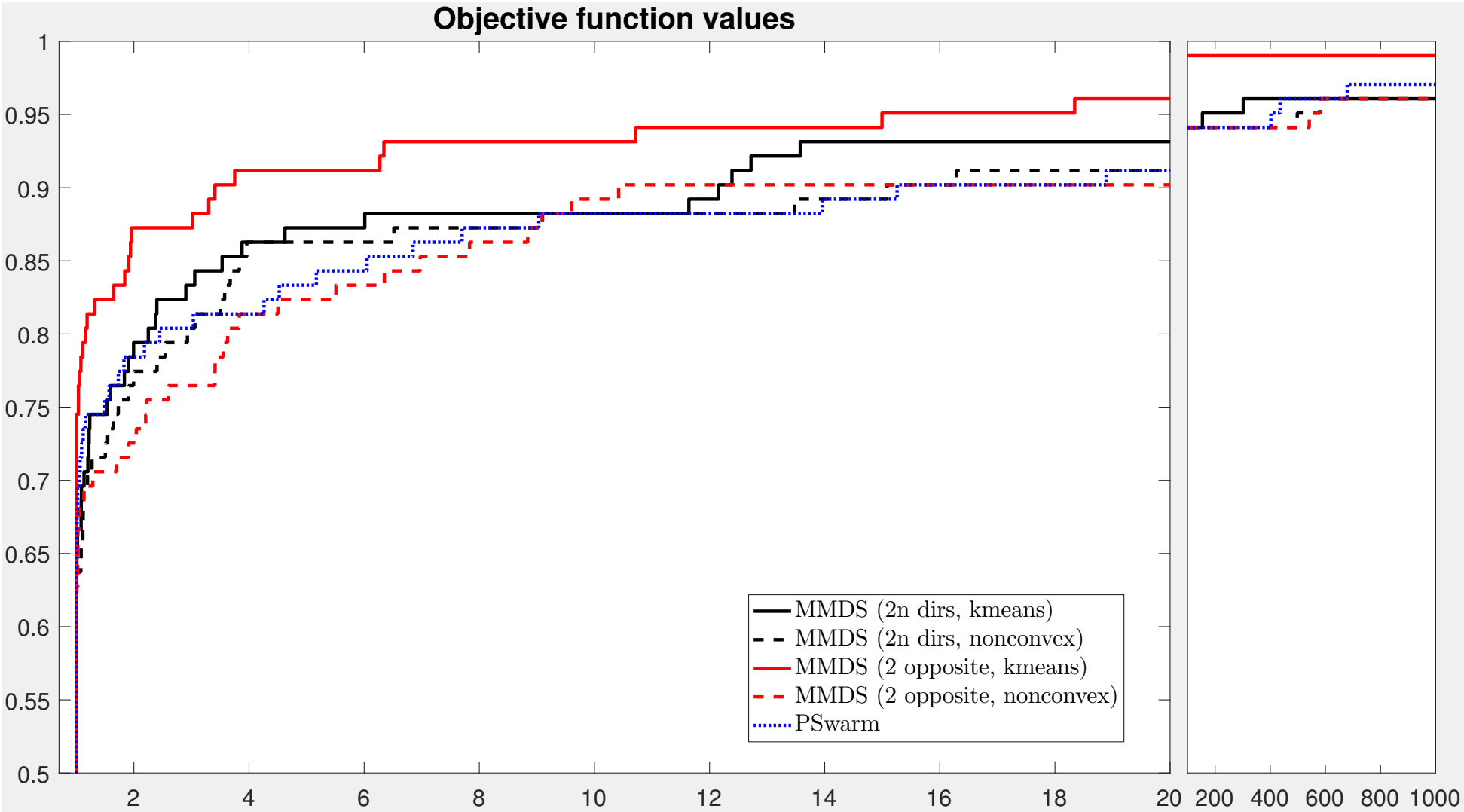
A comparison is made with PSwarm (a direct search solver that uses a particle swarm heuristic as a search step).

Performance profiles (# function evaluations)



Performance profiles (quality of final f)



Numerical results (application problem)

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$$\min_{(\theta_x,\theta_y)} \sum_j \begin{cases} \frac{h^2 A_j |d.n_j|}{2} & \text{if } |d.n_j| \neq 1, \\ 0 & \text{otherwise,} \end{cases}$$

where h is the slicing thickness, A_j is the area of the j–triangle, d is the slicing direction, and n_j is the j–triangle normal.

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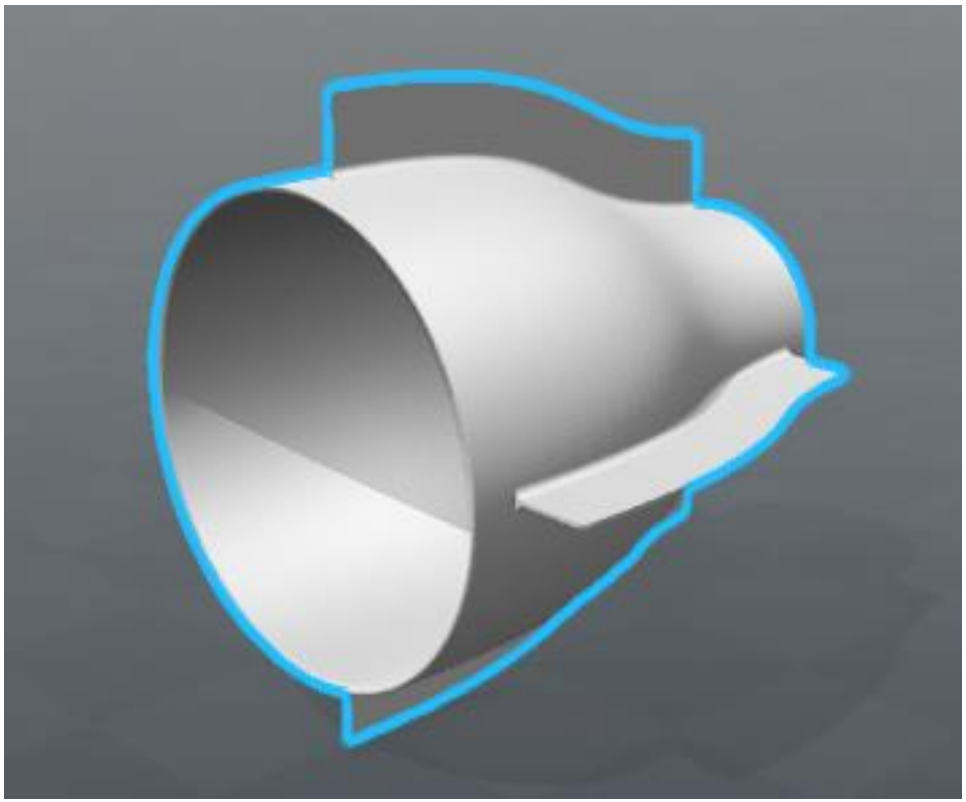
This is a 2D problem where $(\theta_x, \theta_y) \in [0, 180]^2$ are the rotation degrees along the x-axis and y-axis, respectively, in a three dimension space.

A used part

We consider an aerospace complex part for numerical testing.

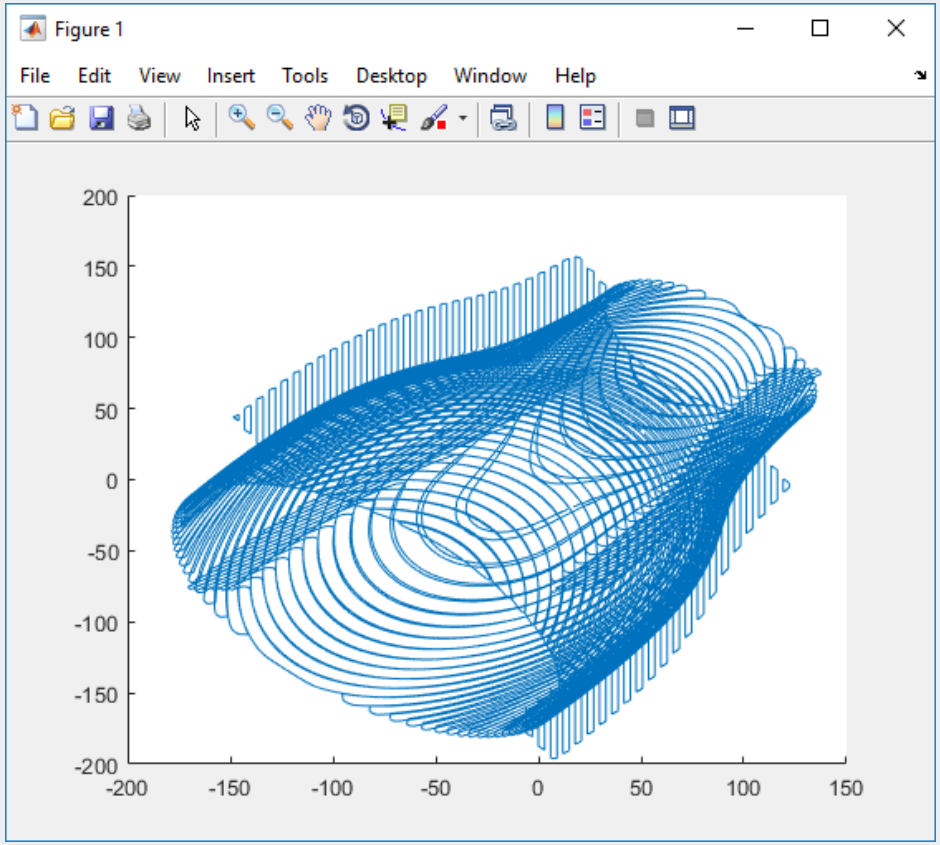


Nearly 80000 triangles are needed to define the part.

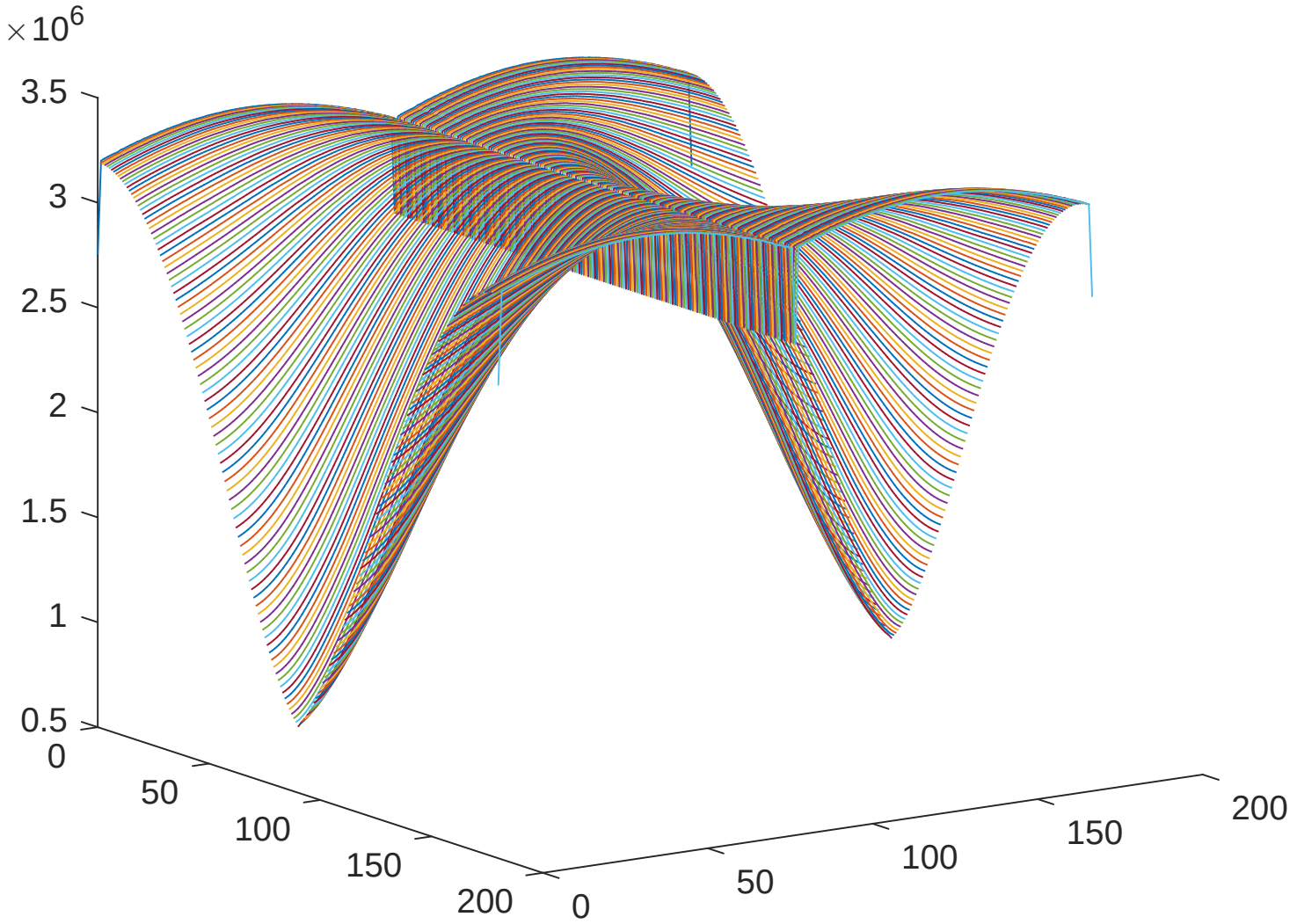
The part/object to be considered

Slices are taken along the z axis with 5mm high, resulting in 64 slices.

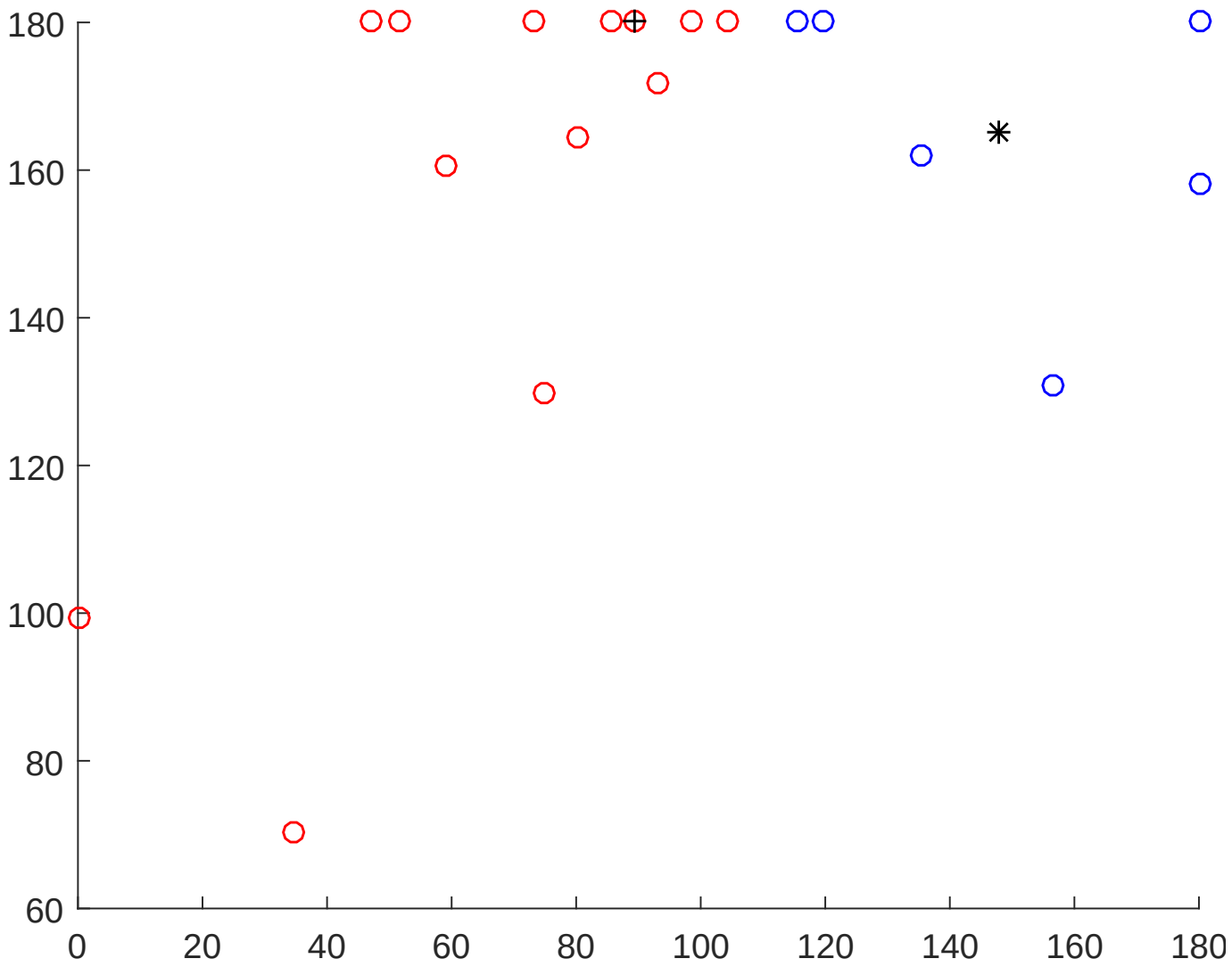
Before optimization



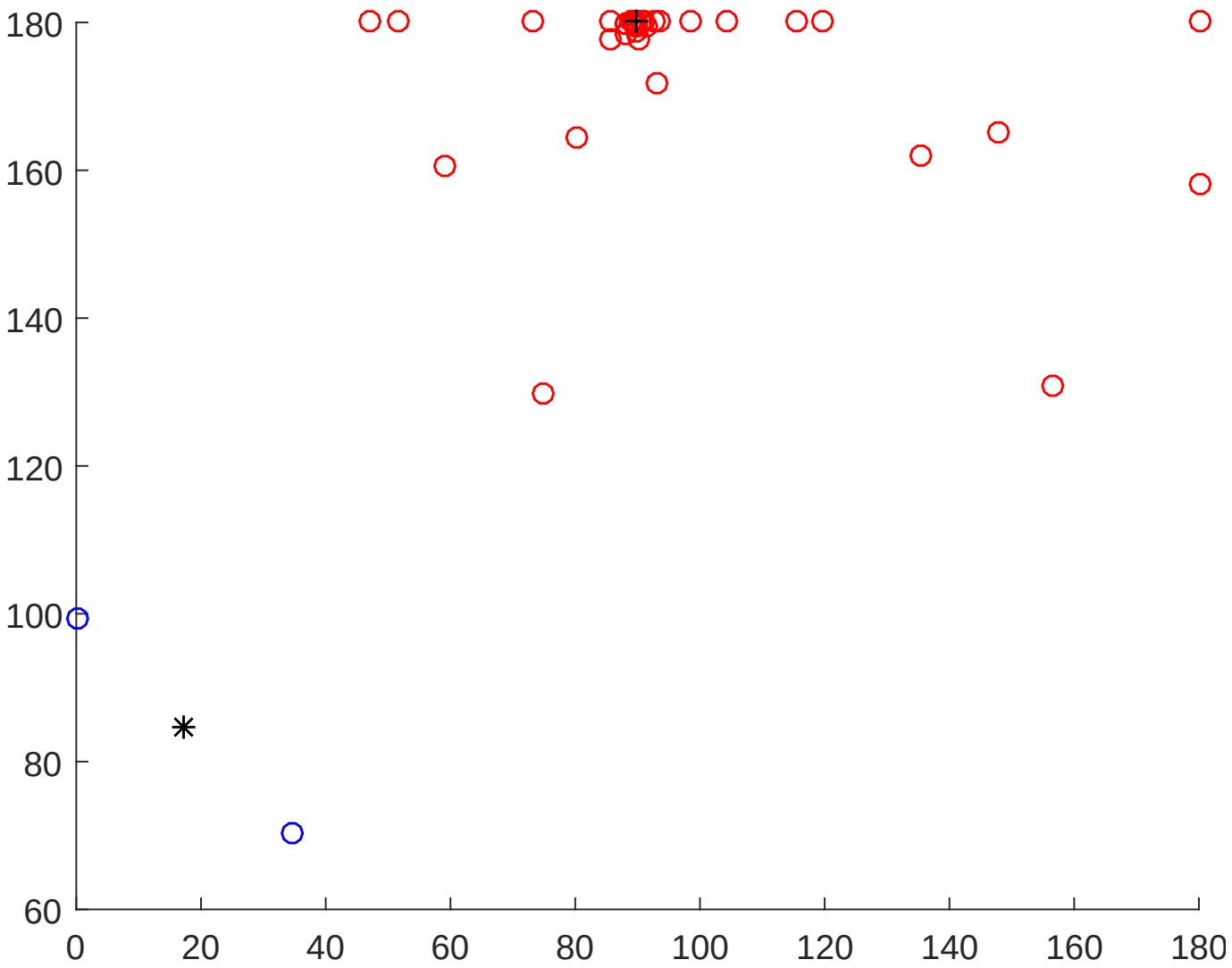
Objective function landscape



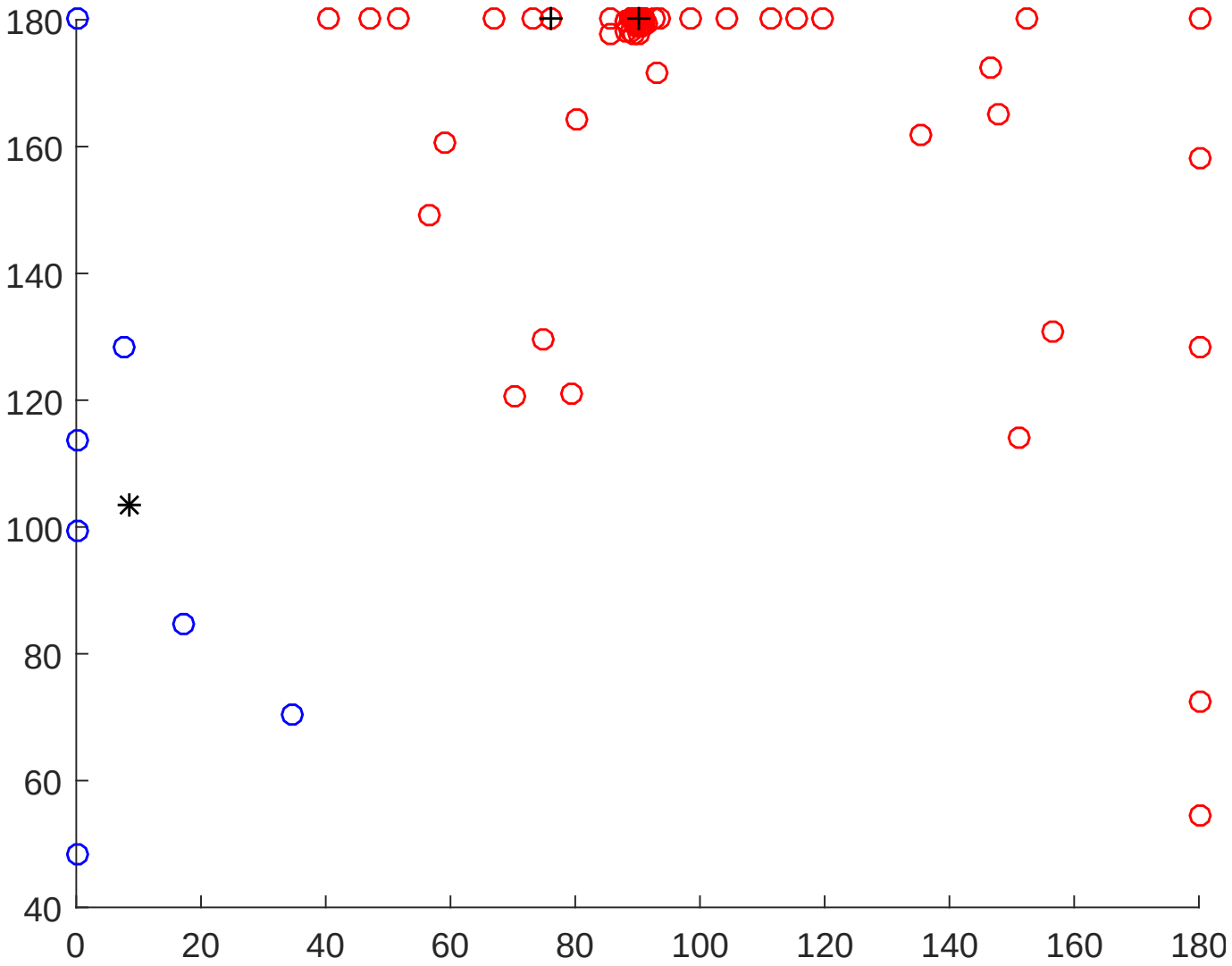
Numerical results (space clustering)



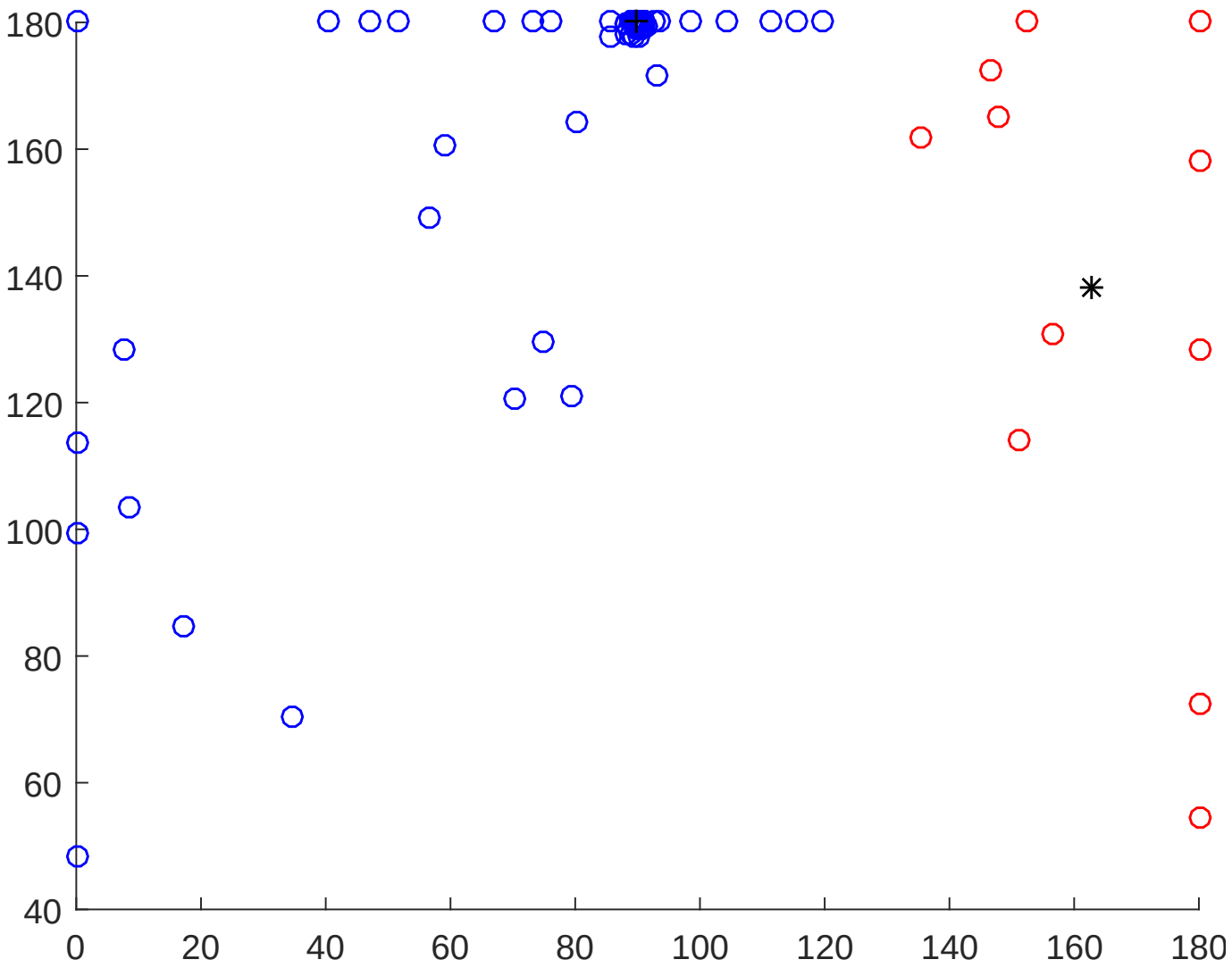
Numerical results (space clustering)



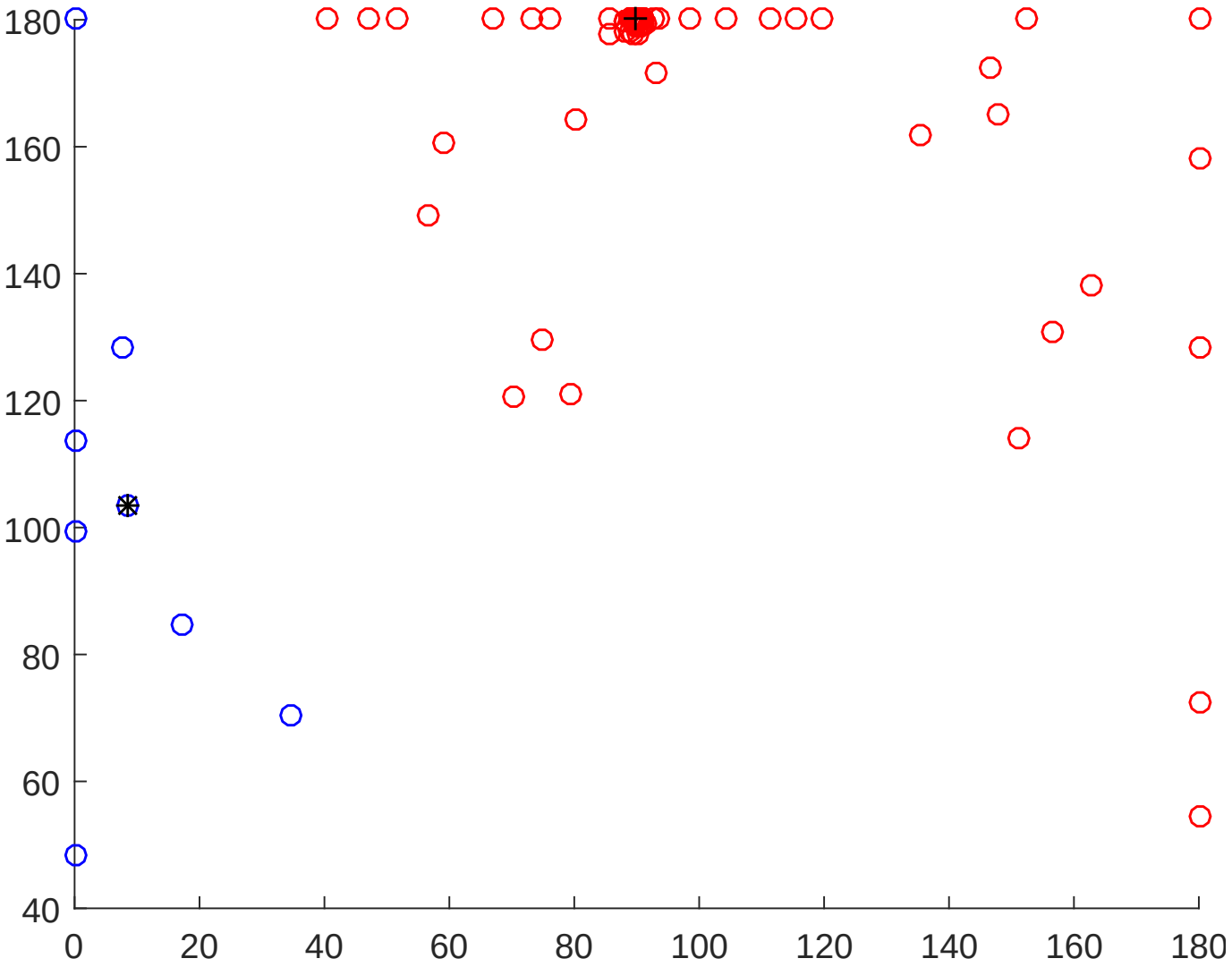
Numerical results (space clustering)



Numerical results (space clustering)



Numerical results (space clustering)



Numerical results (space clustering)

The solver stops at

$$(\theta_x, \theta_y) = (90, 180), \quad \text{with } f^* = 8.1404e + 05,$$

taking 124 function evaluations.

Numerical results (space clustering)

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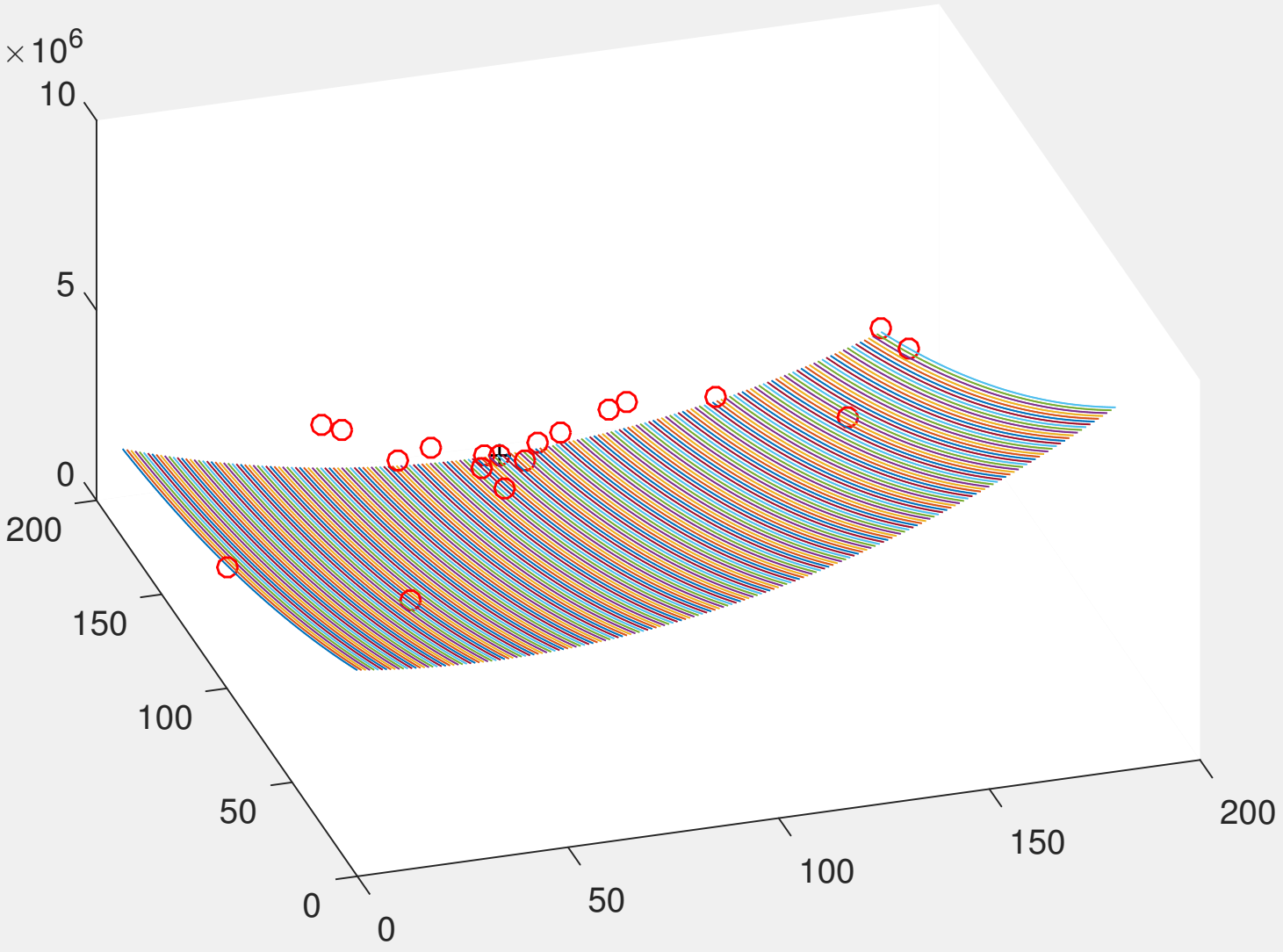
$$(\theta_x, \theta_y) = (90, 180), \quad \text{with } f^* = 8.1404e + 05,$$

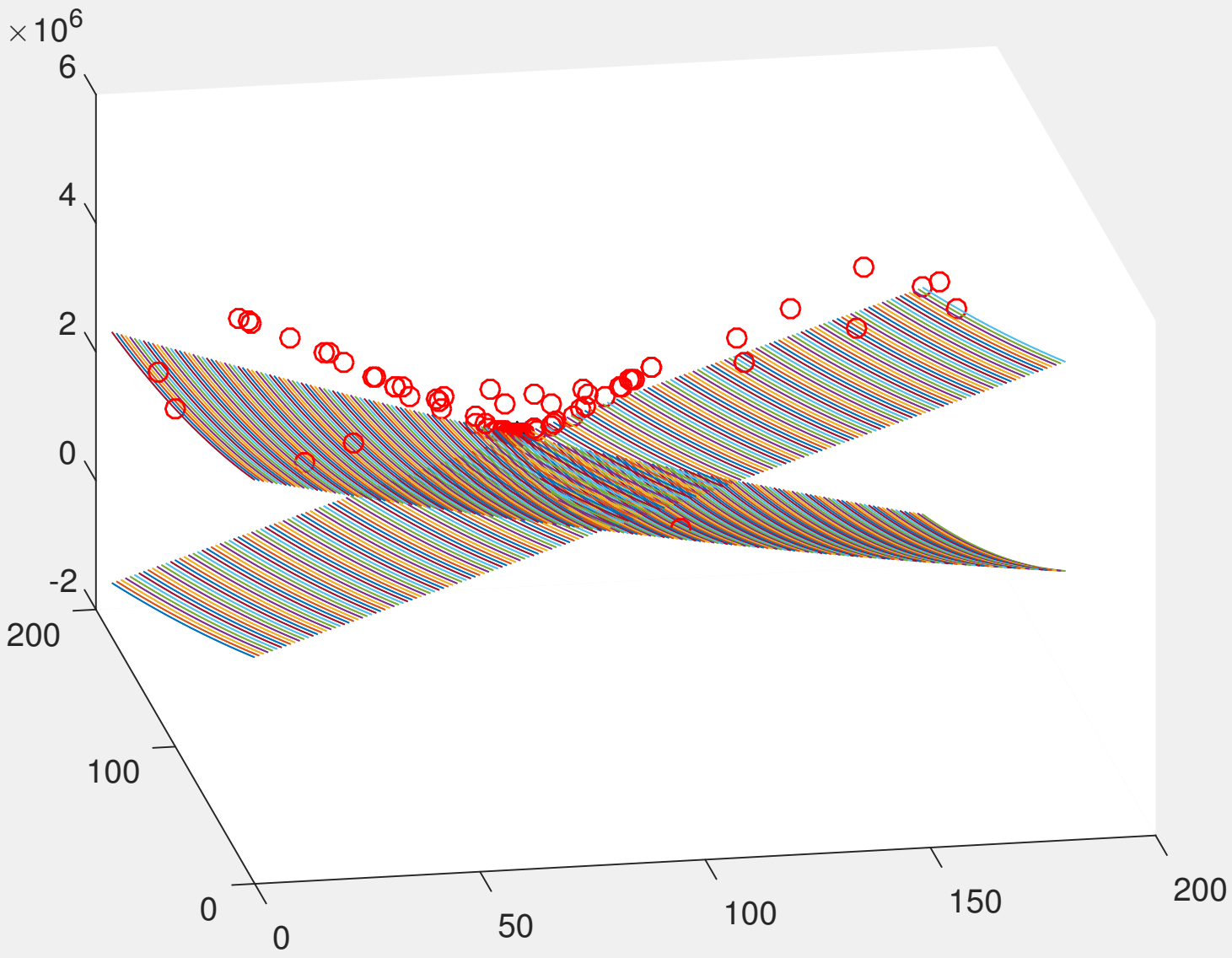
taking 124 function evaluations.

The space clustering approach determined only one of the global minimizers!

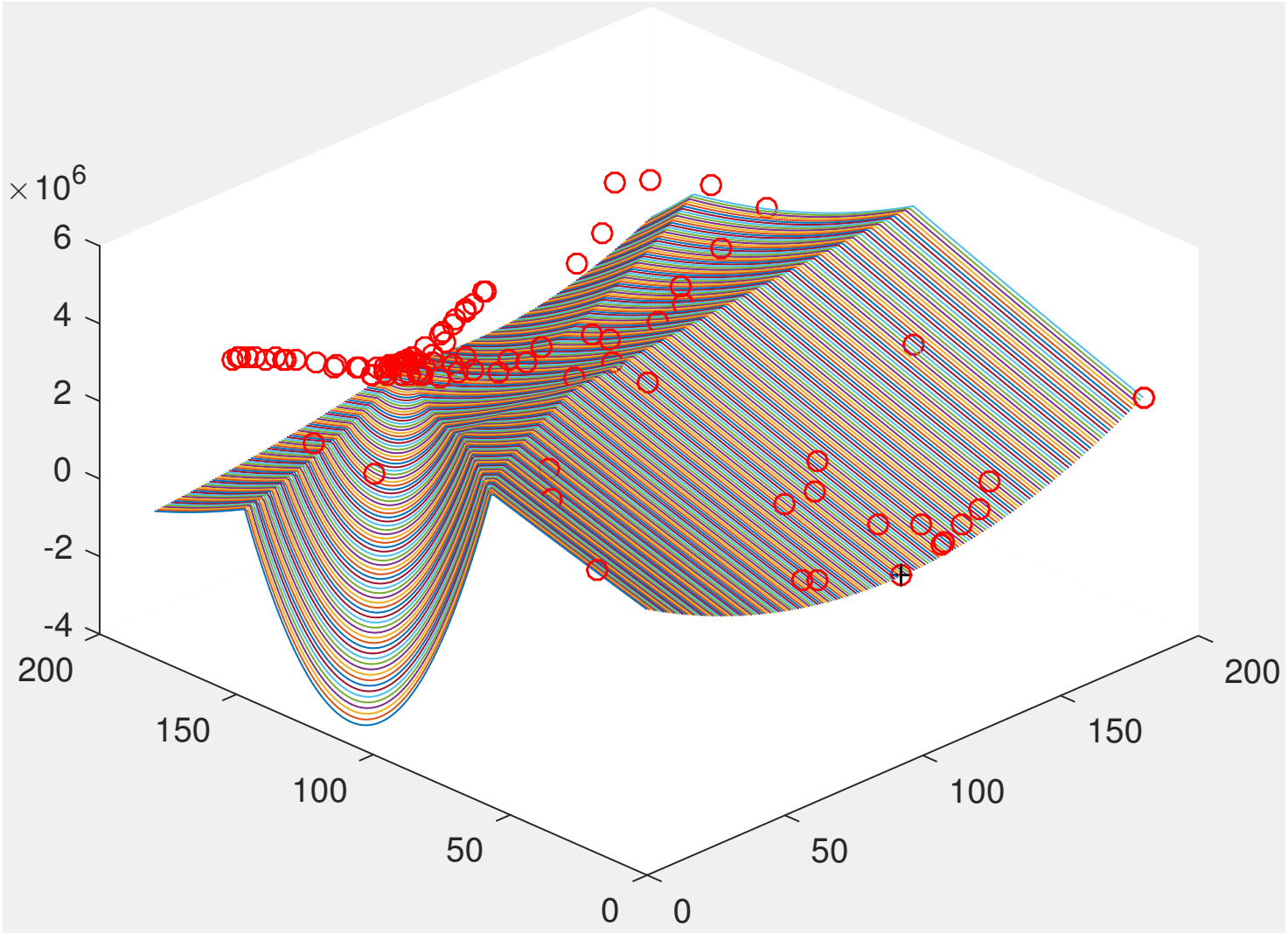
Numerical results (nonconvex modeling) — q_1



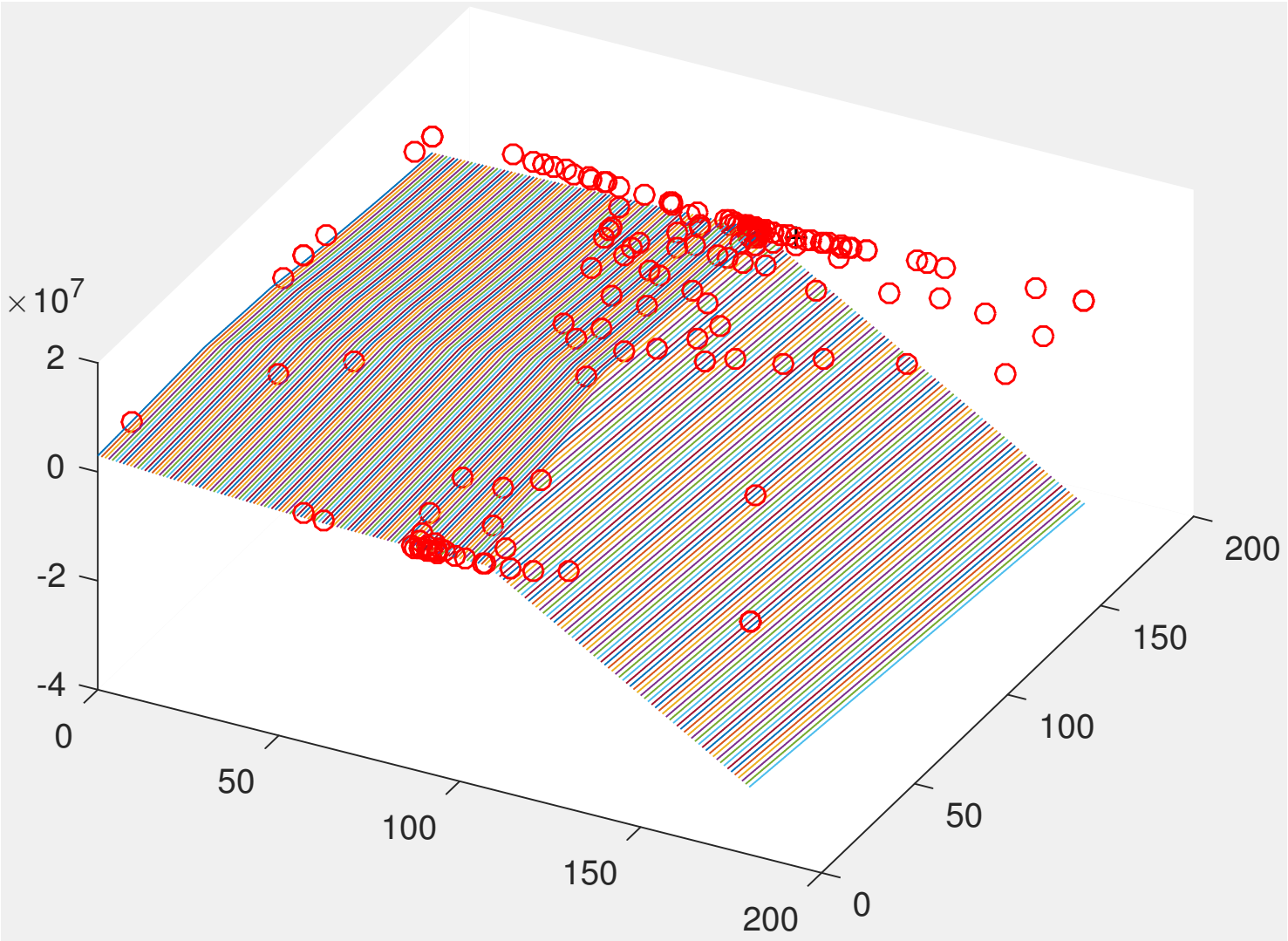
Numerical results (nonconvex modeling) — q_1,q_2



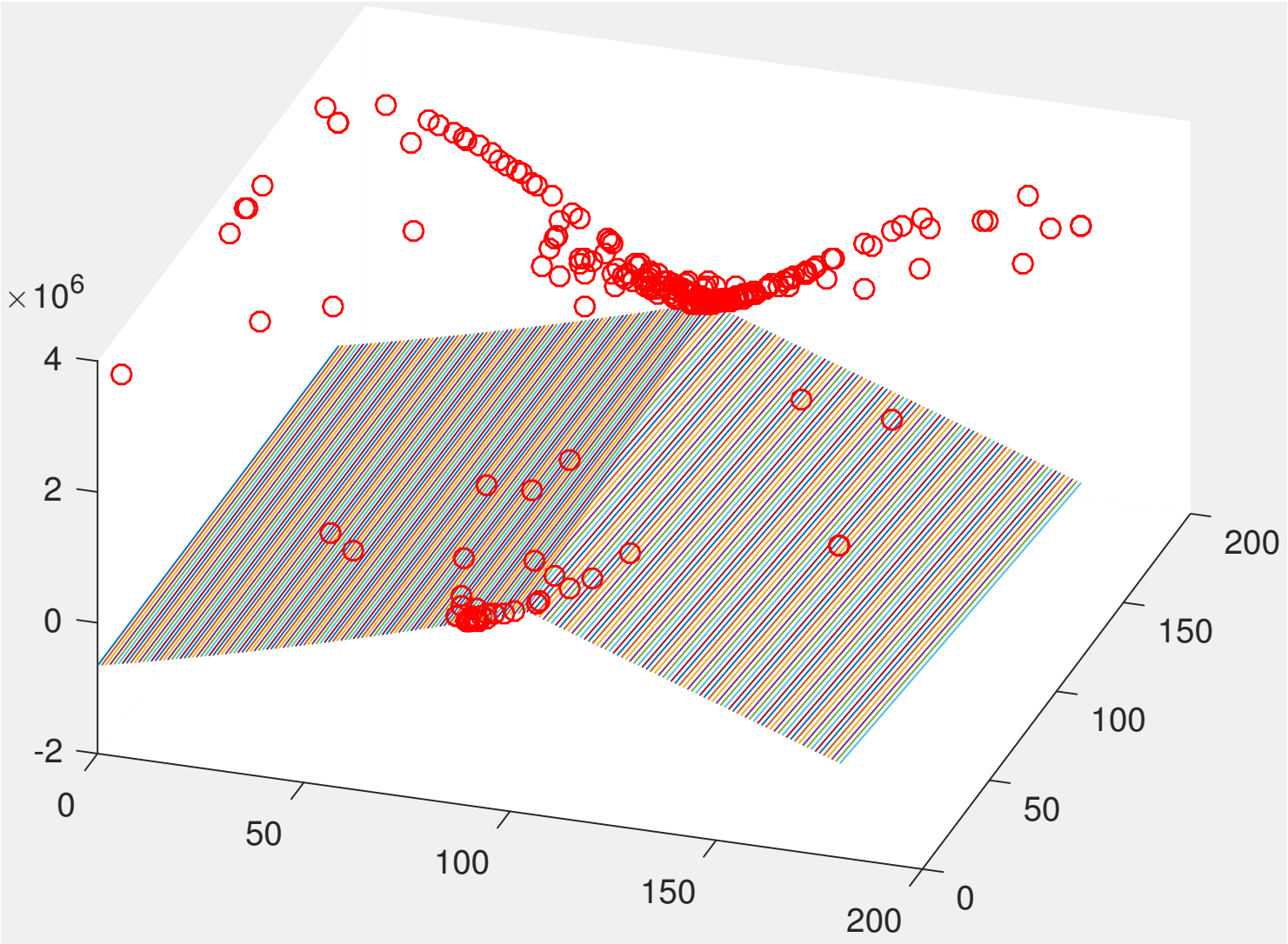
Numerical results (nonconvex modeling) — min of q's



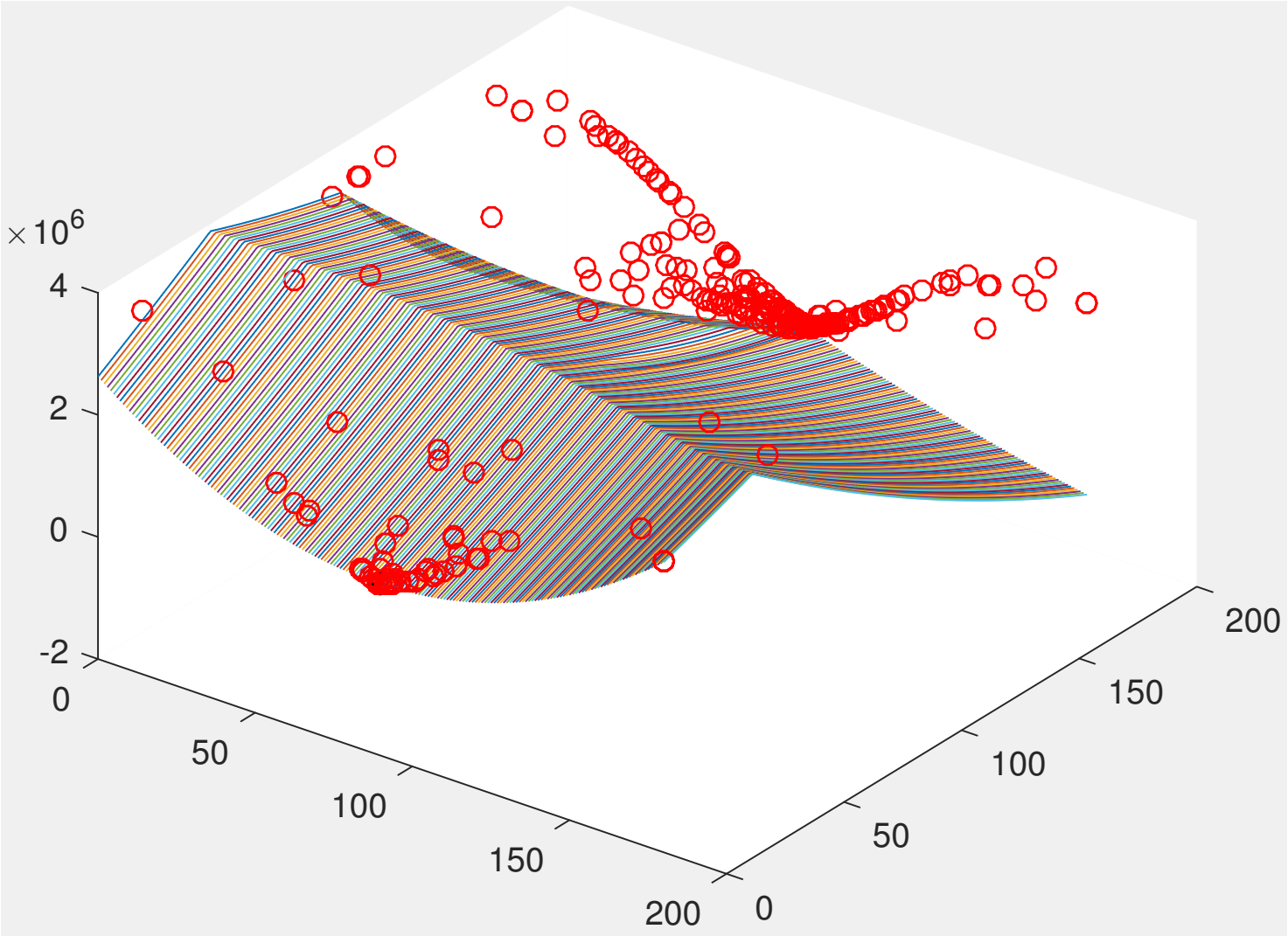
Numerical results (nonconvex modeling) — min of q's



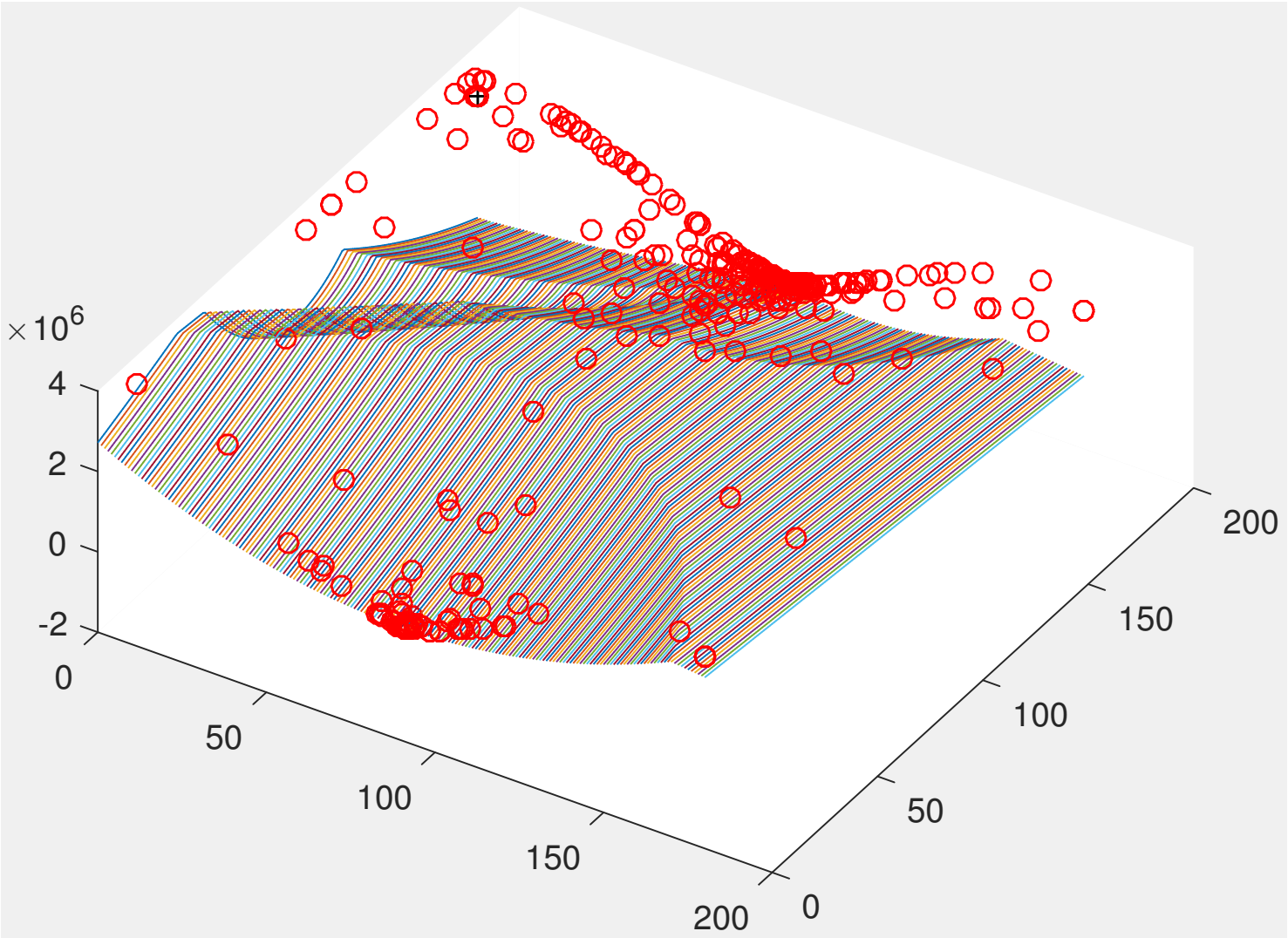
Numerical results (nonconvex modeling) — min of q's



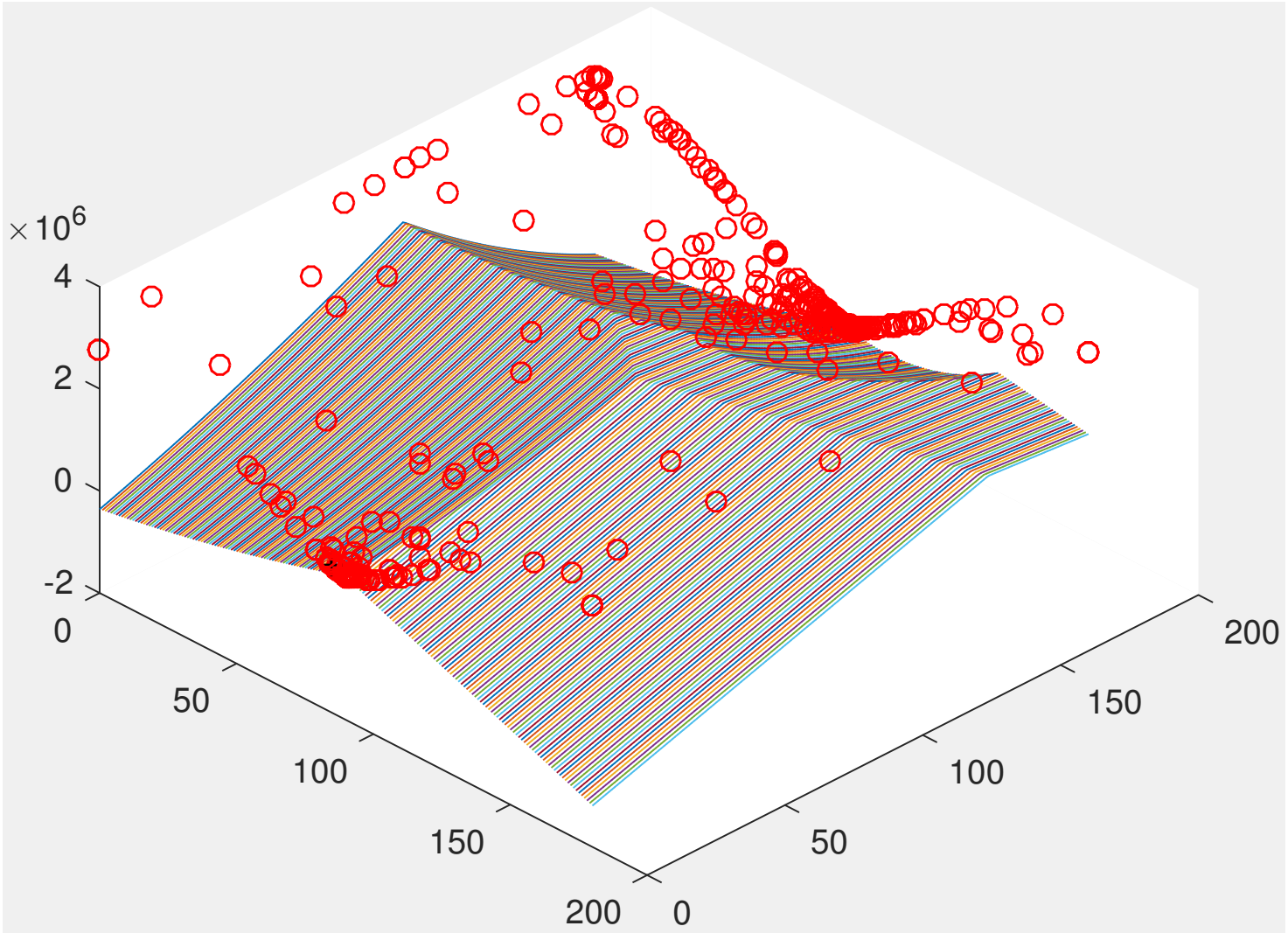
Numerical results (nonconvex modeling) — min of q's



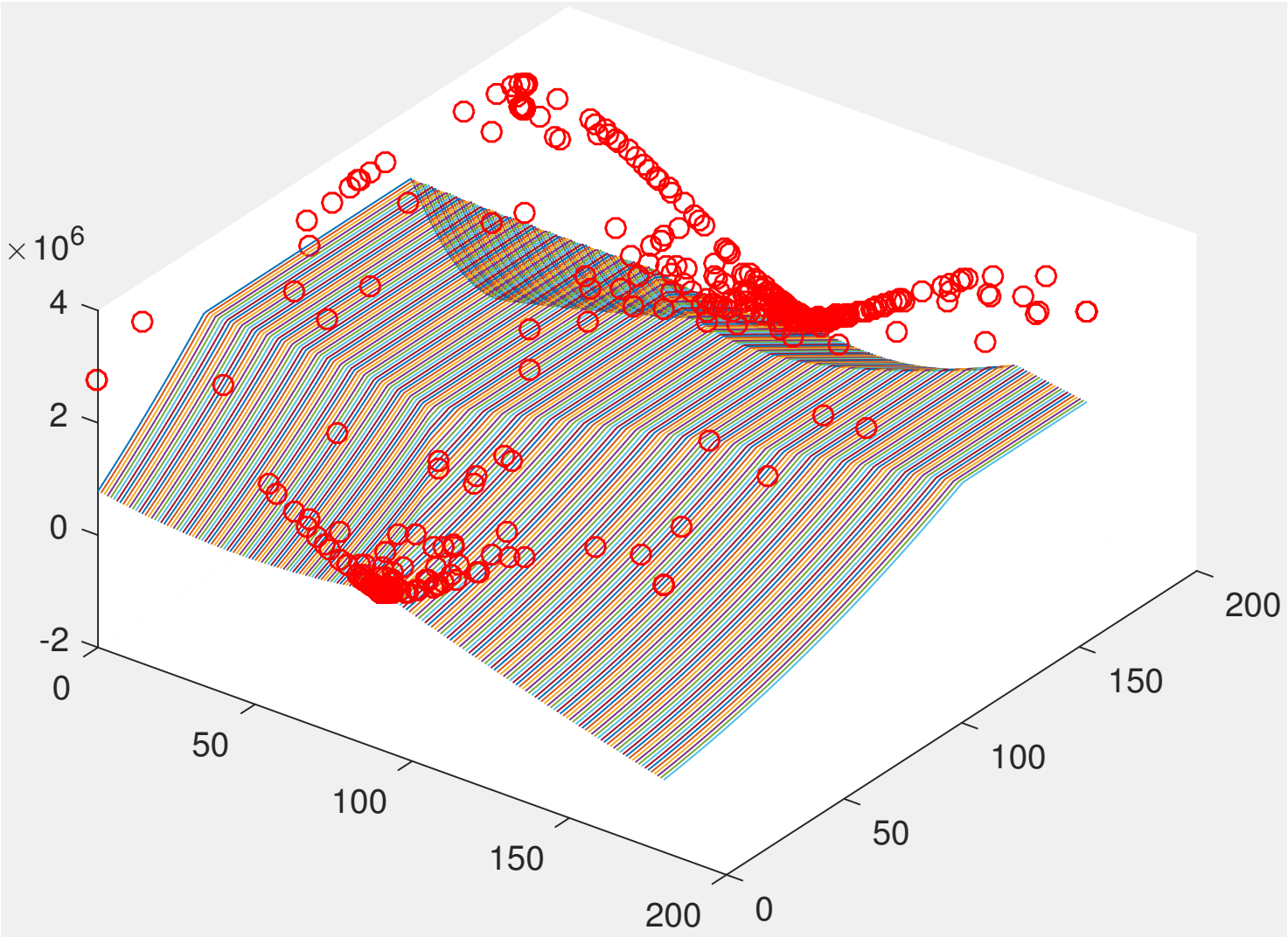
Numerical results (nonconvex modeling) — min of q's



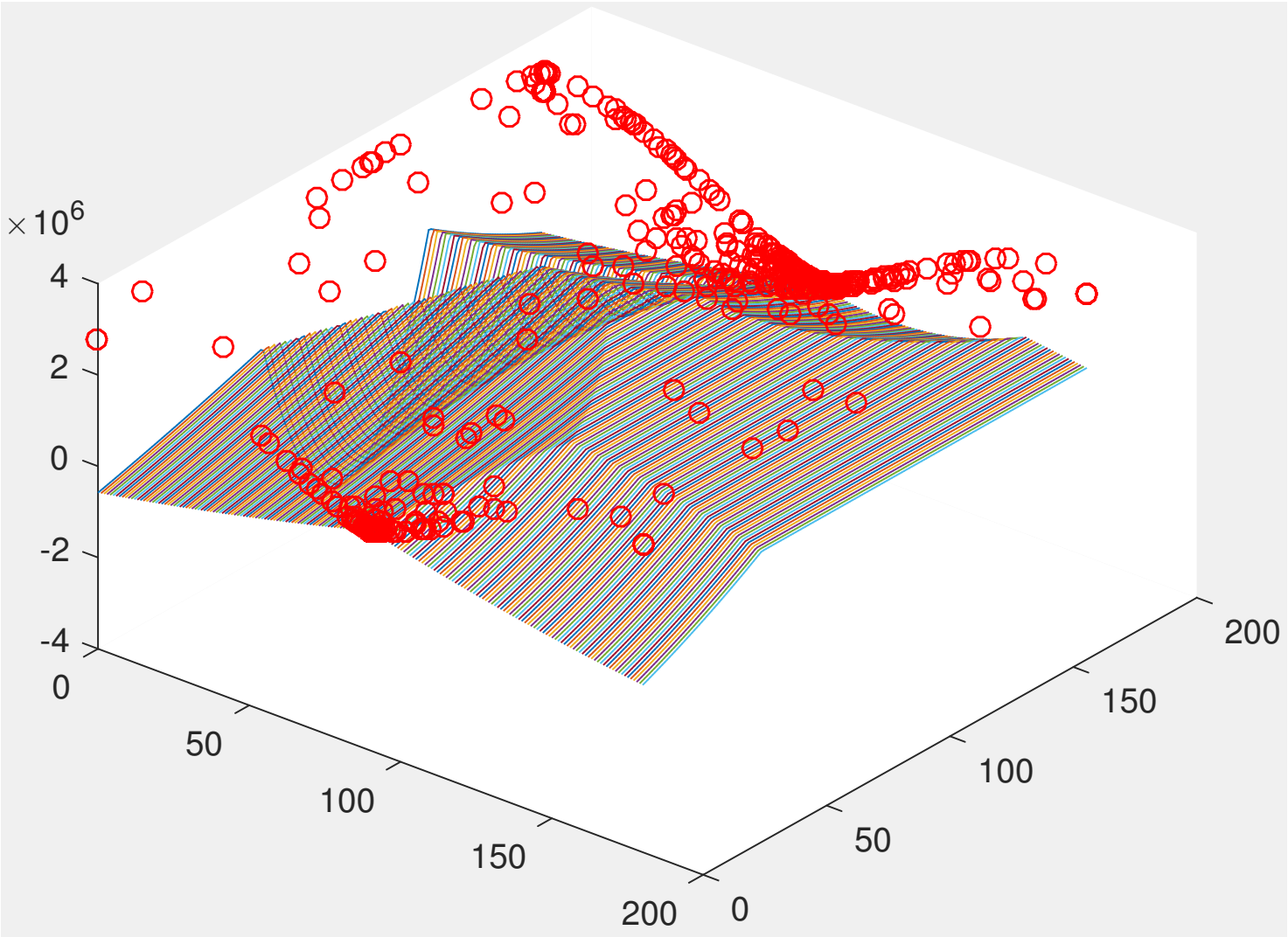
Numerical results (nonconvex modeling) — min of q's



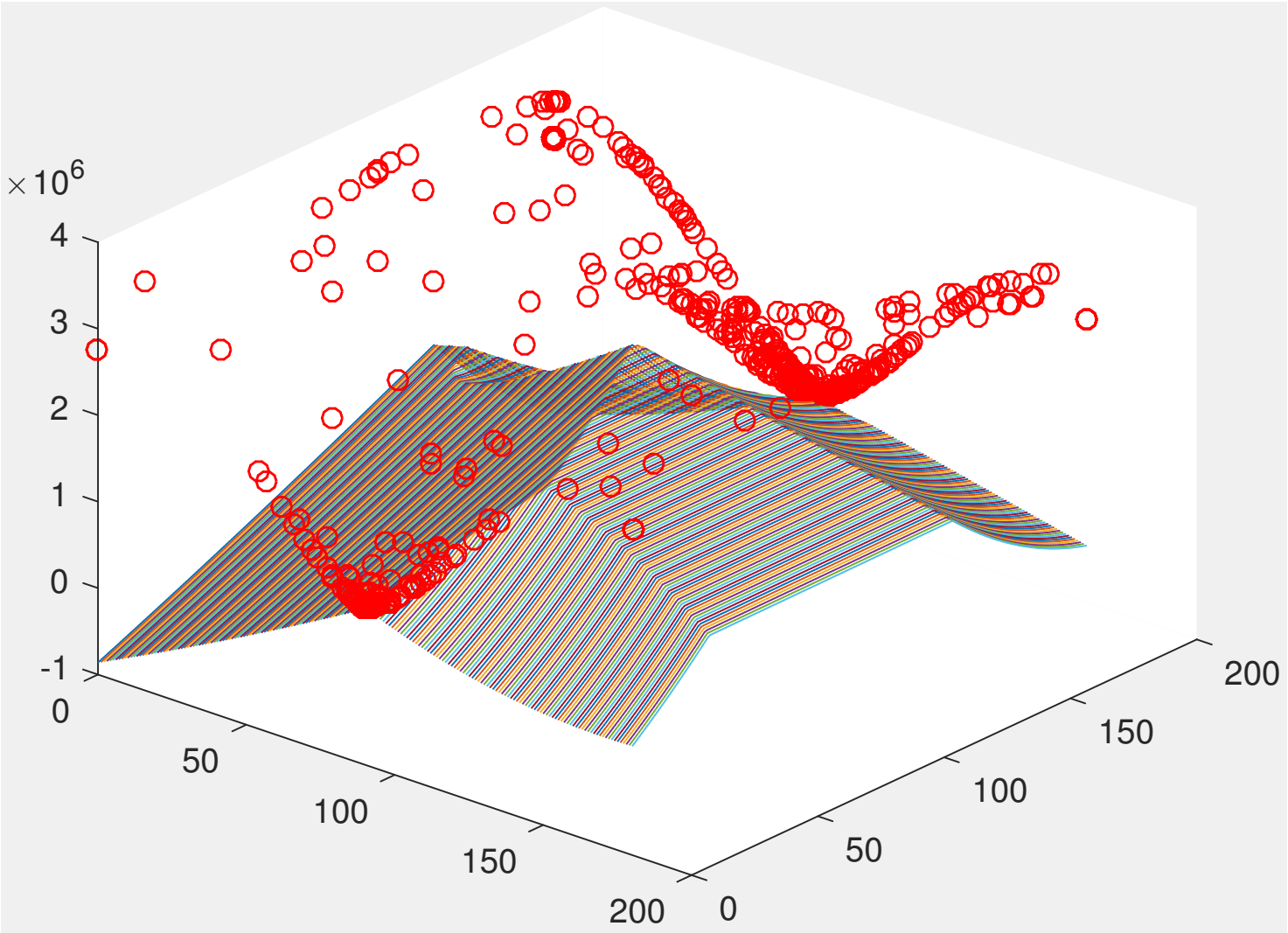
Numerical results (nonconvex modeling) — min of q's



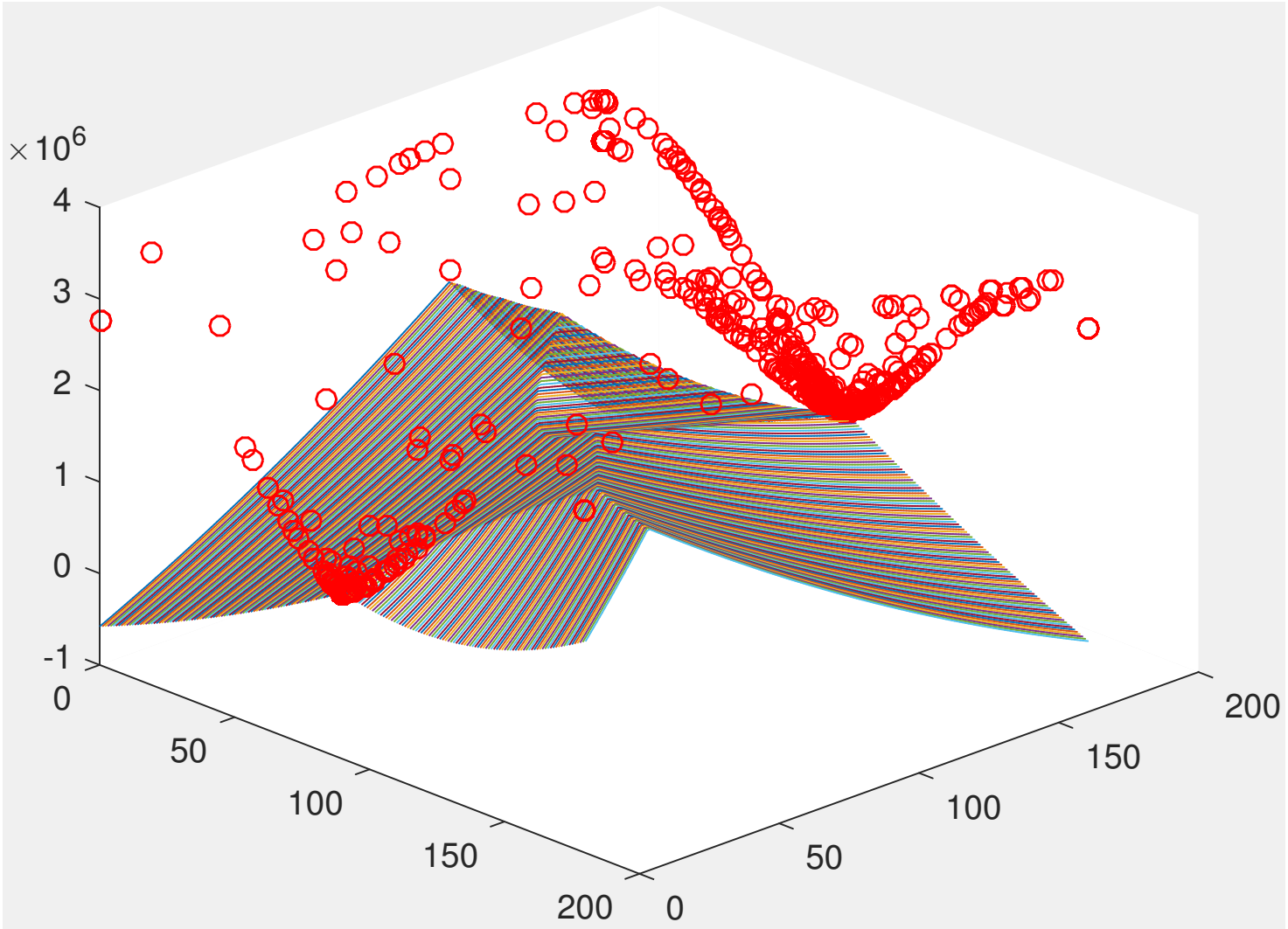
Numerical results (nonconvex modeling) — min of q's



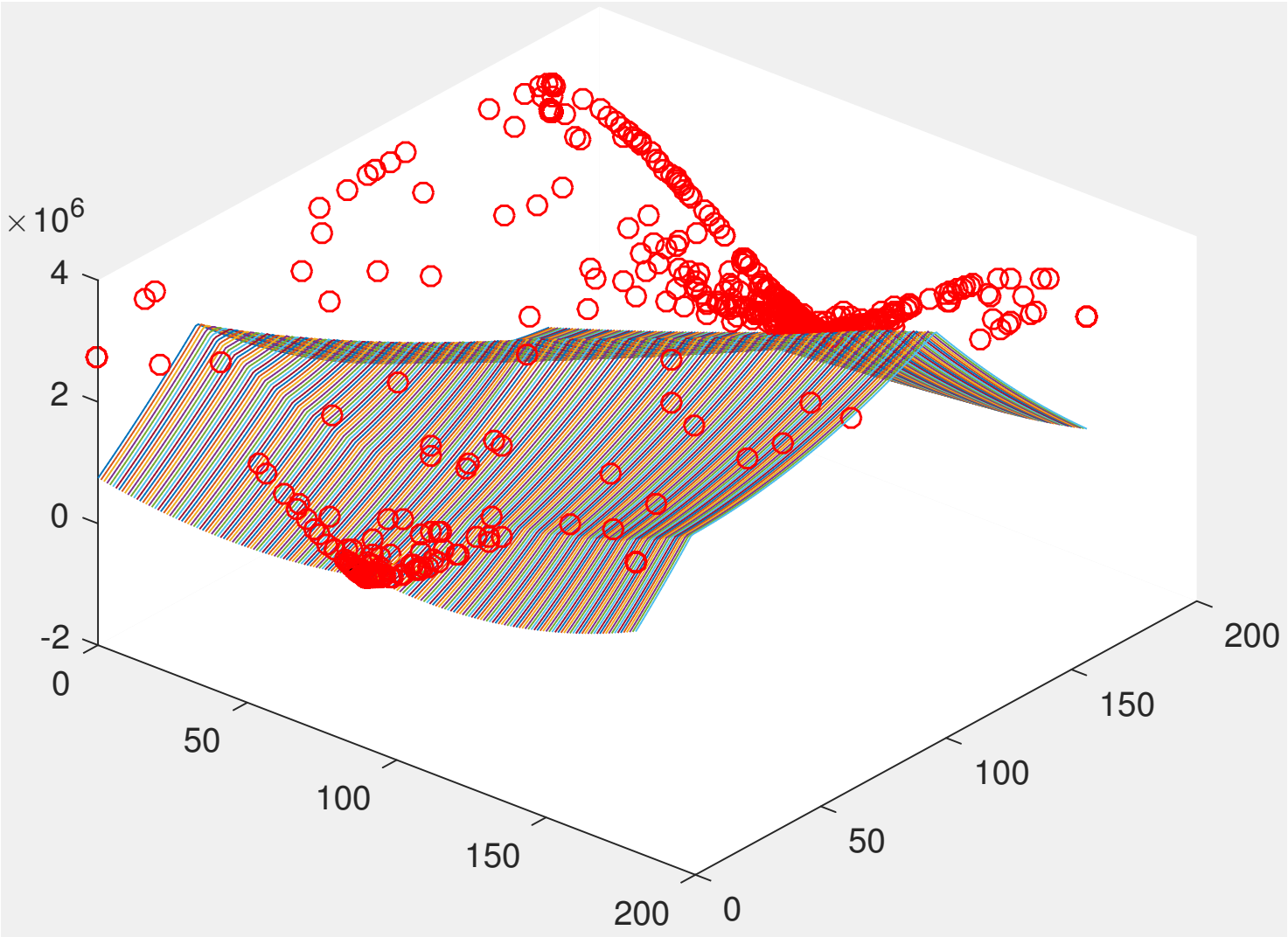
Numerical results (nonconvex modeling) — min of q's



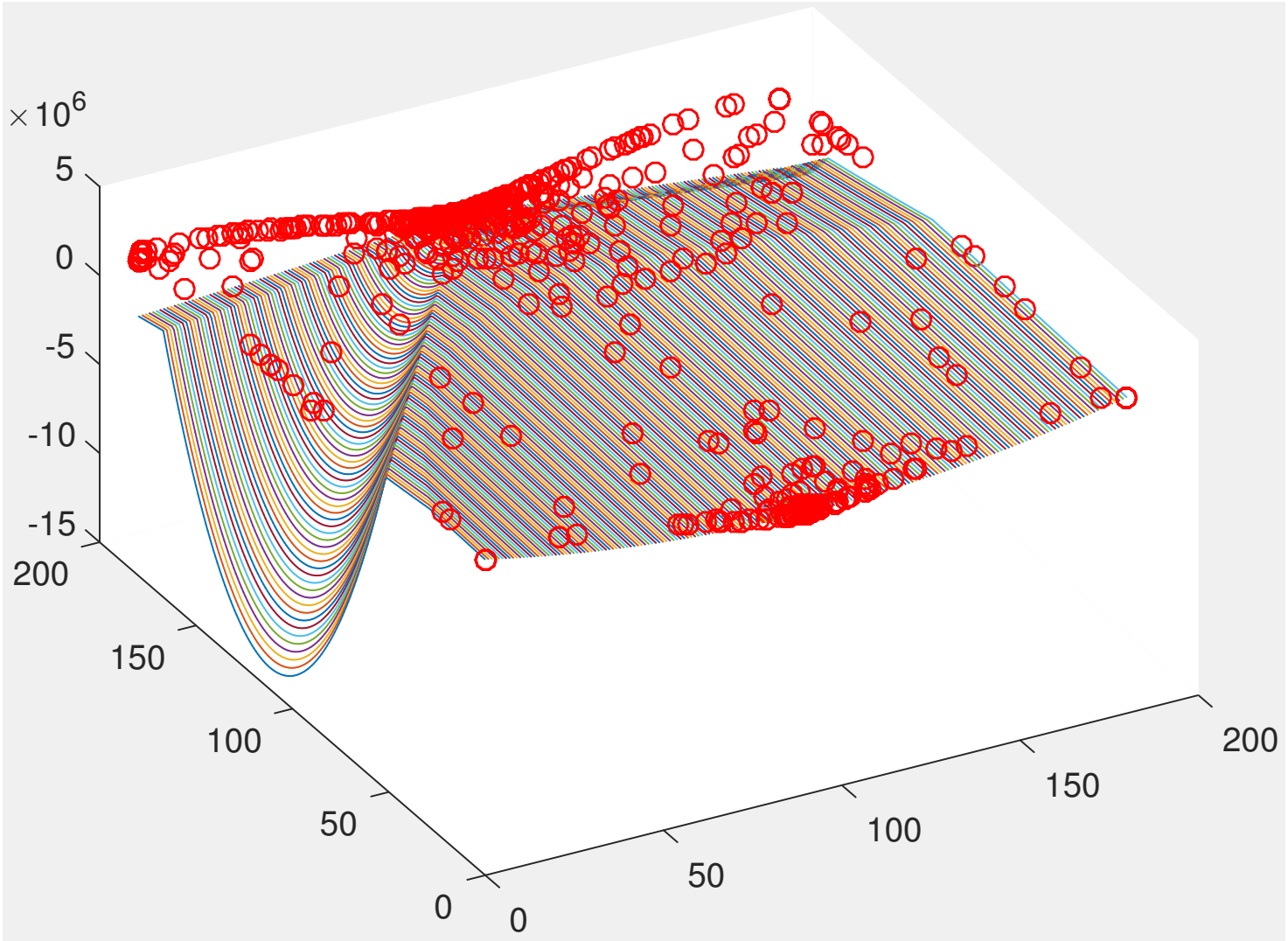
Numerical results (nonconvex modeling) — min of q's



Numerical results (nonconvex modeling) — min of q's



Numerical results (nonconvex modeling) — min of q's



Numerical results (nonconvex modeling)

The solver stops now at

$(\theta_x, \theta_y) = (90, 180)$ and $(\theta_x, \theta_y) = (90, 0)$, both with $f^* = 8.1404e + 05$,

taking 2152 function evaluations.

Numerical results (nonconvex modeling)

The solver stops now at

$(\theta_x, \theta_y) = (90, 180)$ and $(\theta_x, \theta_y) = (90, 0)$, both with $f^* = 8.1404e + 05$,

taking 2152 function evaluations.

The nonconvex modeling approach determined both global minimizers of the problem!

The result of Optimization

Slices are taken along the z axis with 5mm high.

After optimization