Trends in Real-Parameter Optimization

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What is this talk about?
Black-Box Optimization
Local Search
Local Search Demo
Box Method
Rosenbrock's Optimization Algorithm
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What is this talk about?

About my personal (subjective) view on

- ✔ the important "historical" algorithms,
- ✔ their important features, and on
- ✔ the promising recent algorithms.

Outline:

1. Motivation
   - ✔ several classical optimization techniques
2. Optimization algorithm framework
   - ✔ lessons learned
   - ✔ various opt. techniques
3. State-of-the-art techniques
4. Comparison

Black-Box Optimization

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Optimization problem

$$\mathbf{x}^* = \arg\min_{\mathbf{x}\in\mathcal{S}} f(\mathbf{x})$$

- ✔ $\mathbf{x}$ is the object representation,
- ✔ $\mathcal{S}$, $x \in \mathcal{S}$, is the search space of all candidate objects,
- ✔ f is the objective function to be minimized.

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Black-box optimization problem: Nothing is known about f, it can be

- ✔ non-convex, non-differentiable
- ✔ multimodal,
- ✔ time-dependent, noisy,
- ✔ ...

Optimizers are based on direct sampling of the search space. They require only

1. *representation* of candidate solution, and
2. *objective function* (fitness) to evaluate the solution domain.

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Real-parameter black-box optimization problem

- ✔ $\mathcal{S} = \mathcal{R}^D$ where D is the dimensionality of the search space

Local Search

Local search with *first improving strategy*:

Algorithm 1: Hill-Climbing

```
begin
    x ← Initialize()
    while not TerminationCondition() do
        y ← Perturb(x)
        if BetterThan(y, x) then
            x ← y
end
```

Local search with *first improving strategy*:

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Neighborhood used in `Perturb()`:

- ✔ deterministic (pattern) vs. stochastic
- ✔ static vs. time-dependent vs. adaptive

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DEMO:

- ✔ `Perturb` uses isotropic Gaussian distribution with static parameters

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Local search with *best improving strategy*:

- ✔ complete search of the neighborhood in discrete spaces (impossible in $\mathcal{R}^{\mathcal{D}}$)
- ✔ knowledge of derivatives in the neighborhood would help (gradient algorithm), but we face black-box
- ✔ could be approximated by creating more candidates from the neighborhood and selecting the best one

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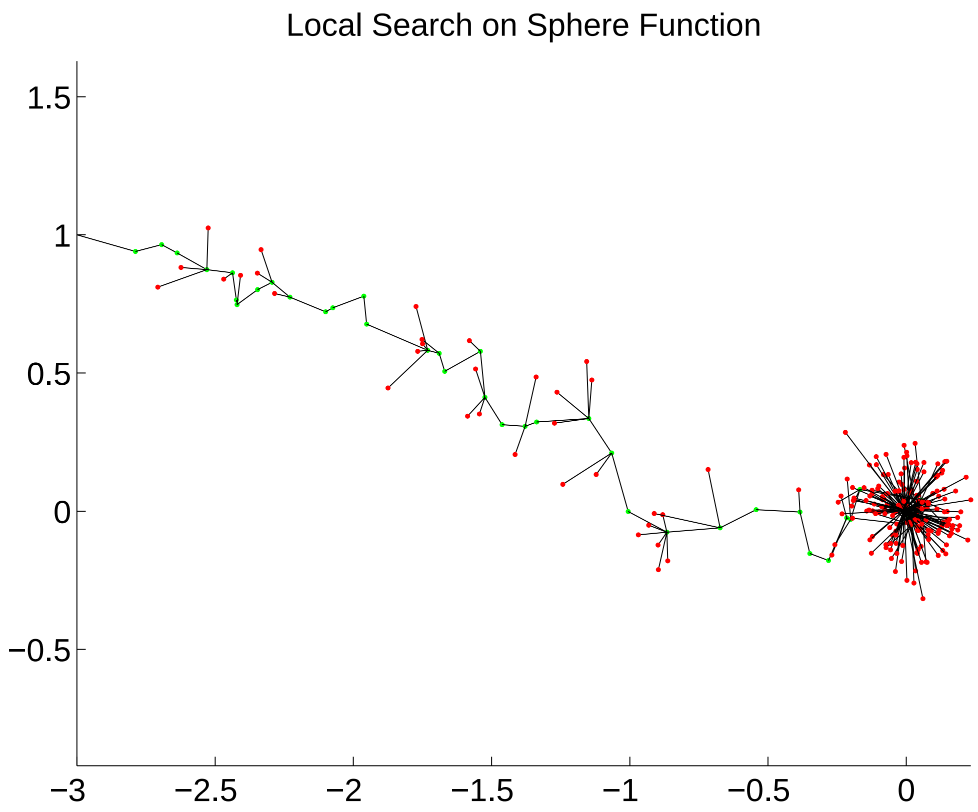
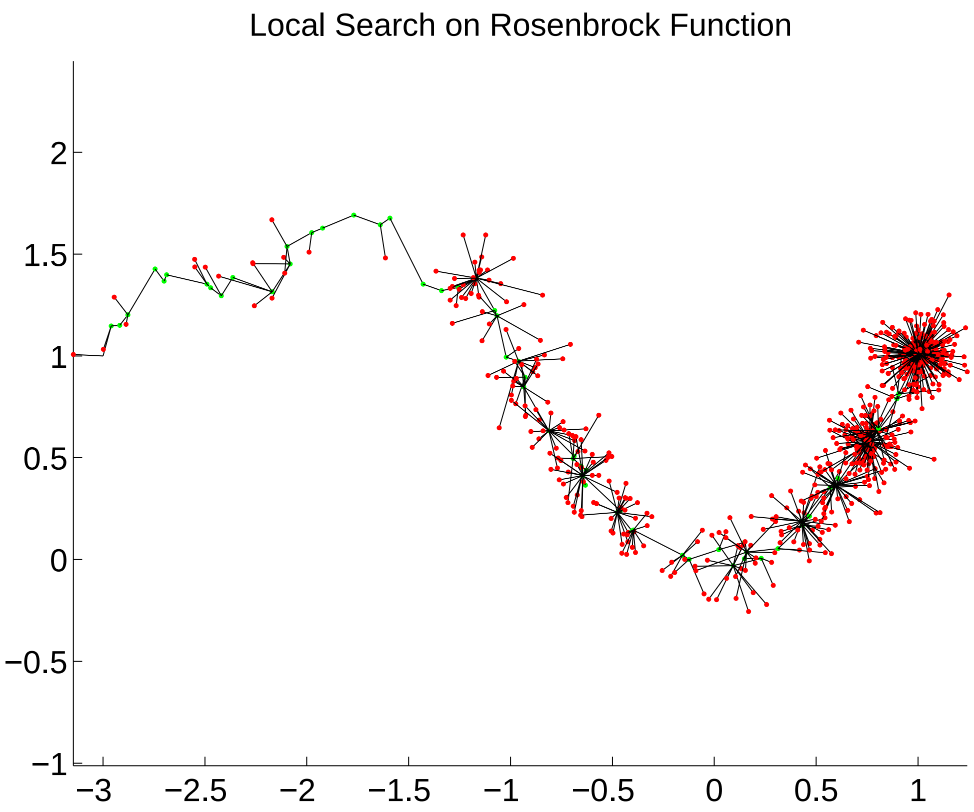
Parallel local search:

- ✔ equivalent to restarted local search
- ✔ uses a set of points $\mathbf{x}$

Local Search Demo





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Box Method

Evolutionary operation [Box57]:

Algorithm 2: Box's Evolutionary Operation

```
begin
    x ← Initialize()
    while not TerminationCondition() do
        𝒴 ← CornersOfBoxAround(x)
        x ← BestOf(𝒴)
end
```

Features:

- ✔ iterative application of 2-level full-factorial design of experiment
- ✔ 2^D candidates generated each iteration
- ✔ neighborhood in the form of a pattern
- ✔ static neighborhood parameters

Possible improvements:

- ✔ adaptive box size, e.g.
  - ✘ increase box size, if one of the corners improves solution, decrease box size, if no improvement found.

[Box57] G.E.P. Box. Evolutionary operation: Method for increasing industrial productivity. *Appl Stat*, 6(2):81–101, 1957.

Rosenbrock's Optimization Algorithm

Described in [Ros60]:

Algorithm 3: Rosenbrock's Algorithm

Input: $\alpha > 1$, $\beta \in (0,1)$

begin
    $\mathbf{x} \leftarrow$ `Initialize()`; $\mathbf{x}_o \leftarrow \mathbf{x}$
    $\{\mathbf{e}_1, \dots, \mathbf{e}_D\} \leftarrow$ `InitOrtBasis()`
    $\{d_1, \dots, d_D\} \leftarrow$ `InitMultipliers()`
    while not `TerminationCondition()` **do**
        for i=$1 \dots D$ **do**
            $\mathbf{y} \leftarrow \mathbf{x} + d_i \mathbf{e}_i$
            if `BetterThan(`y,x`)` **then**
                $\mathbf{x} \leftarrow \mathbf{y}$
                $d_i \leftarrow \alpha \cdot d_i$
            else
                $d_i \leftarrow -\beta \cdot d_i$
        if `AtLeastOneSuccInAllDirs()` **and** `AtLeastOneFailInAllDirs()` **then**
            $\{\mathbf{e}_1, \dots, \mathbf{e}_D\} \leftarrow$ `UpdOrtBasis(`$\mathbf{x} - \mathbf{x}_o$`)`
            $\mathbf{x}_o \leftarrow \mathbf{x}$
end

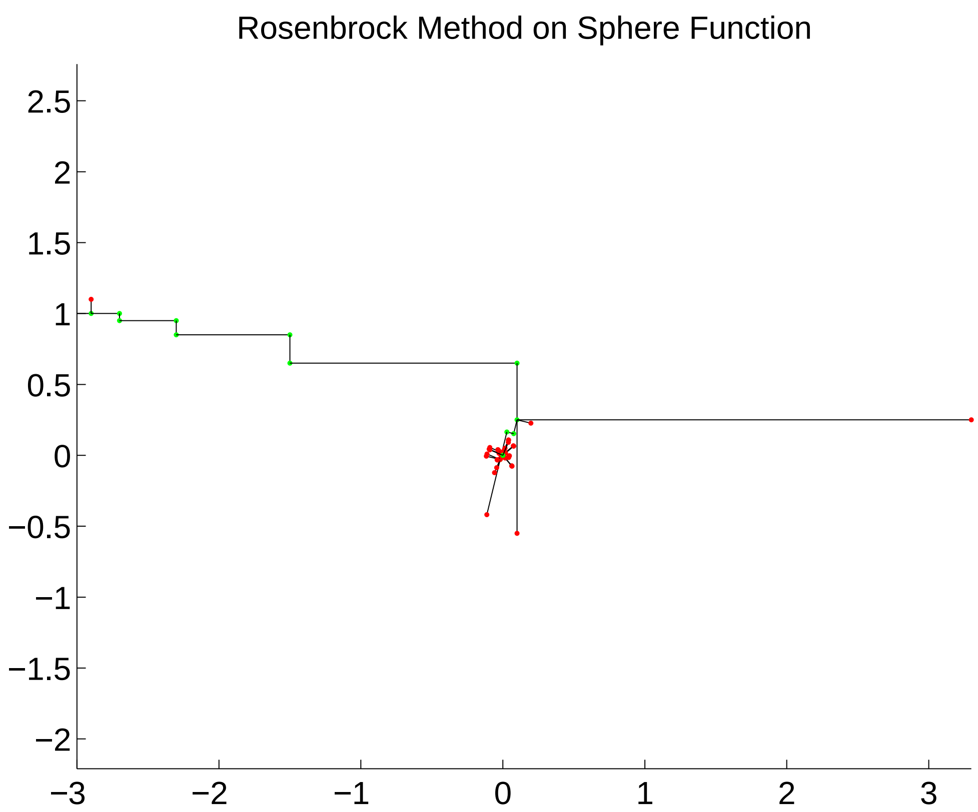
Features:

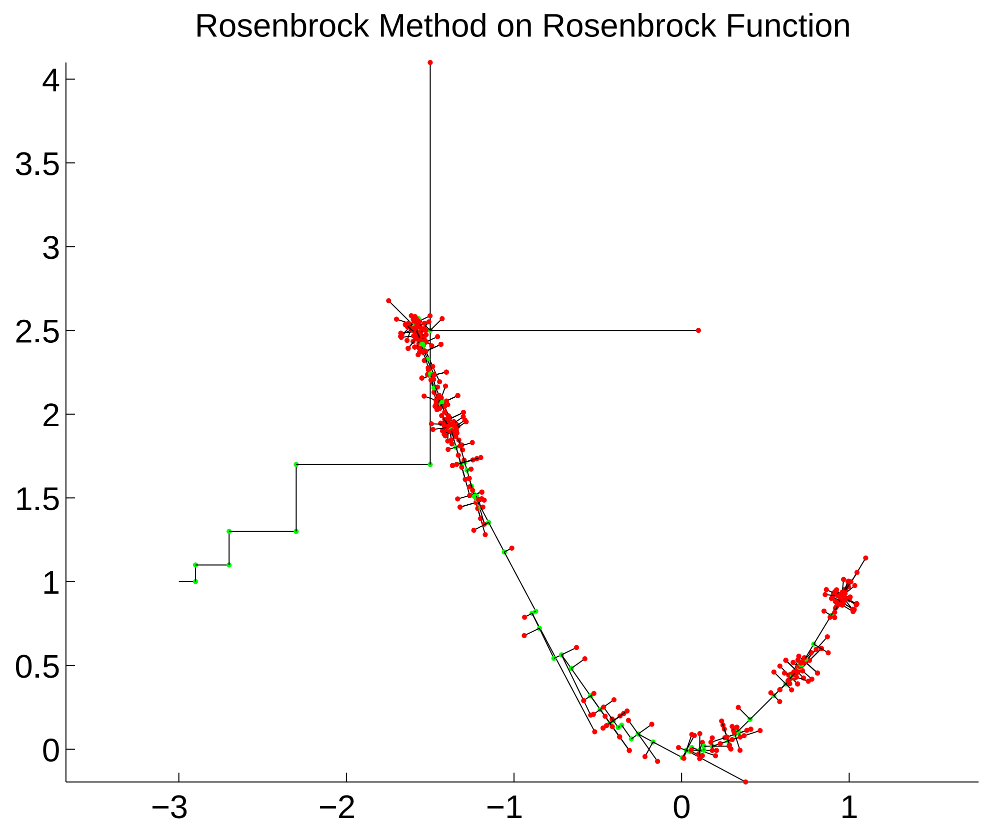
- ✔ D candidates generated each iteration
- ✔ neighborhood in the form of a pattern
- ✔ adaptive neighborhood parameters
  - ✘ distances
  - ✘ directions

DEMO

[Ros60] H.H. Rosenbrock. An automatic method for findong the greatest or least value of a function. *The Computer Journal*, 3:175–184, 1960.

Rosenbrock's Algorithm Demo



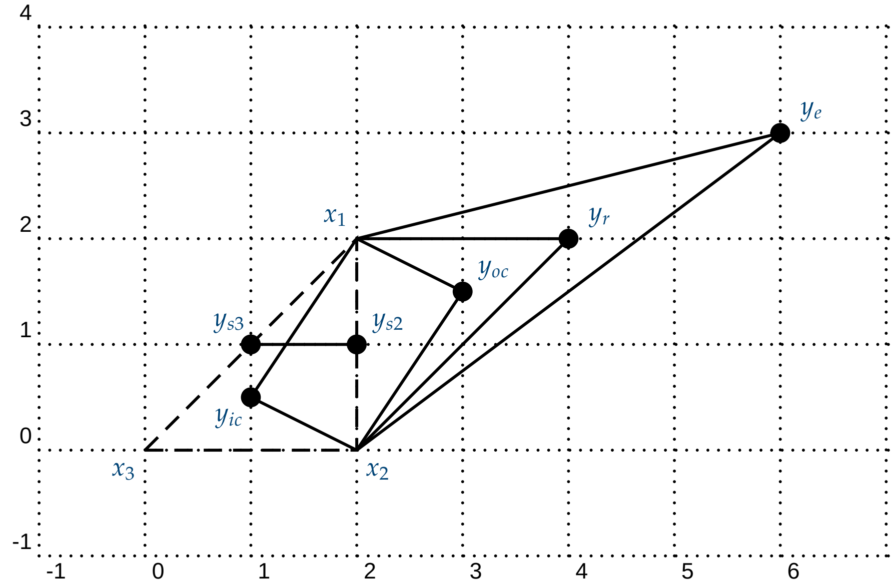


Nelder-Mead Simplex Search

Simplex downhill search (amoeba) [NM65]:

Algorithm 4: Nelder-Mead Simplex Algorithm

begin
    $(\mathbf{x}_1, \ldots, \mathbf{x}_{D+1}) \leftarrow$ `InitSimplex()`
    `so that` $f(x_1) \leq f(x_2) \leq \ldots \leq f(x_{D+1})$
    while not `TerminationCondition()` **do**
        $\bar{\mathbf{x}} \leftarrow \frac{1}{D} \sum_{d=1}^{D} \mathbf{x}_d$
        $\mathbf{y}_r \leftarrow \bar{\mathbf{x}} + \rho(\bar{\mathbf{x}} - \mathbf{x}_{D+1})$
        if `BetterThan`$(\mathbf{y}_r, \mathbf{x}_D)$ **then** $\mathbf{x}_{D+1} \leftarrow \mathbf{y}_r$
        if `BetterThan`$(\mathbf{y}_r, \mathbf{x}_1)$ **then**
            $\mathbf{y}_e \leftarrow \bar{\mathbf{x}} + \chi(\mathbf{x}_r - \bar{\mathbf{x}})$
            if `BetterThan`$(\mathbf{y}_e, \mathbf{y}_r)$ **then** $\mathbf{x}_{D+1} \leftarrow \mathbf{y}_e$;
            `Continue`
        if not `BetterThan`$(\mathbf{y}_r, \mathbf{x}_D)$ **then**
            if `BetterThan`$(\mathbf{y}_r, \mathbf{x}_{D+1})$ **then**
                $\mathbf{y}_{oc} \leftarrow \bar{\mathbf{x}} + \gamma(\mathbf{x}_r - \bar{\mathbf{x}})$
                if `BetterThan`$(\mathbf{y}_{oc}, \mathbf{y}_r)$ **then**
                $\mathbf{x}_{D+1} \leftarrow \mathbf{y}_{oc}$; `Continue`
            else
                $\mathbf{y}_{ic} \leftarrow \bar{\mathbf{x}} - \gamma(\bar{\mathbf{x}} - \mathbf{x}_{D+1})$
                if `BetterThan`$(\mathbf{y}_{ic}, \mathbf{x}_{D+1})$ **then**
                $\mathbf{x}_{D+1} \leftarrow \mathbf{y}_{ic}$; `Continue`
        $\mathbf{y}_{si} \leftarrow \mathbf{x}_1 + \sigma(\mathbf{x}_i - \mathbf{x}_1), \quad i \in 2, \ldots, D+1$
        `MakeSimplex`$(\mathbf{x}_1, \mathbf{y}_{s2}, \ldots, \mathbf{y}_{s(D+1)})$
end



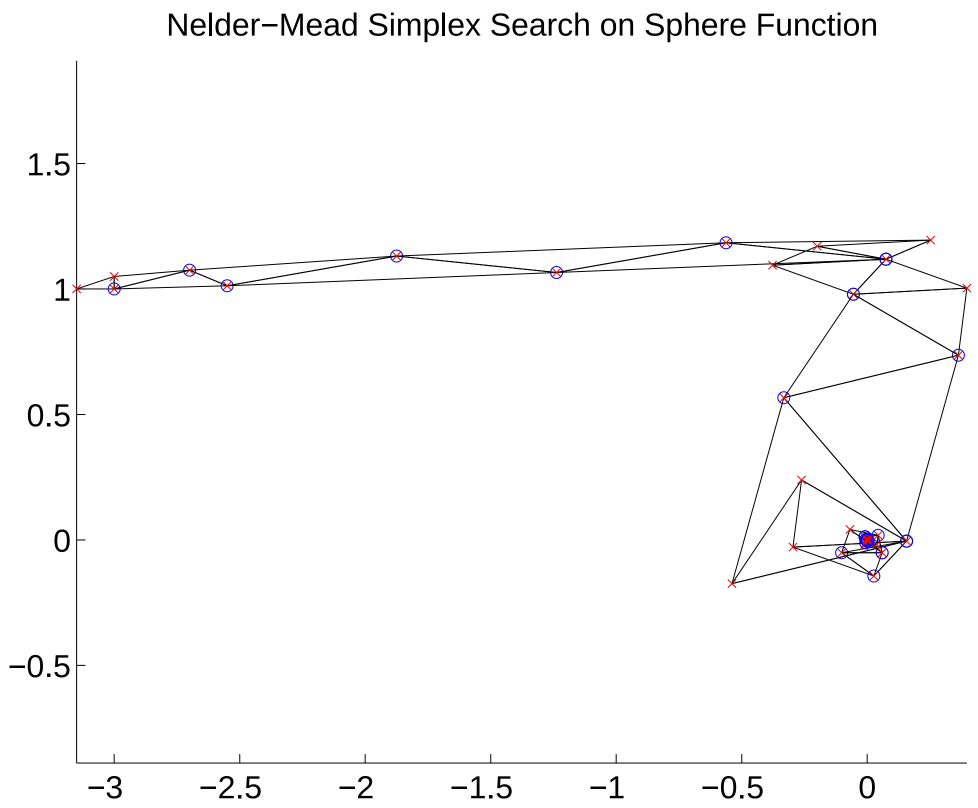
Features:

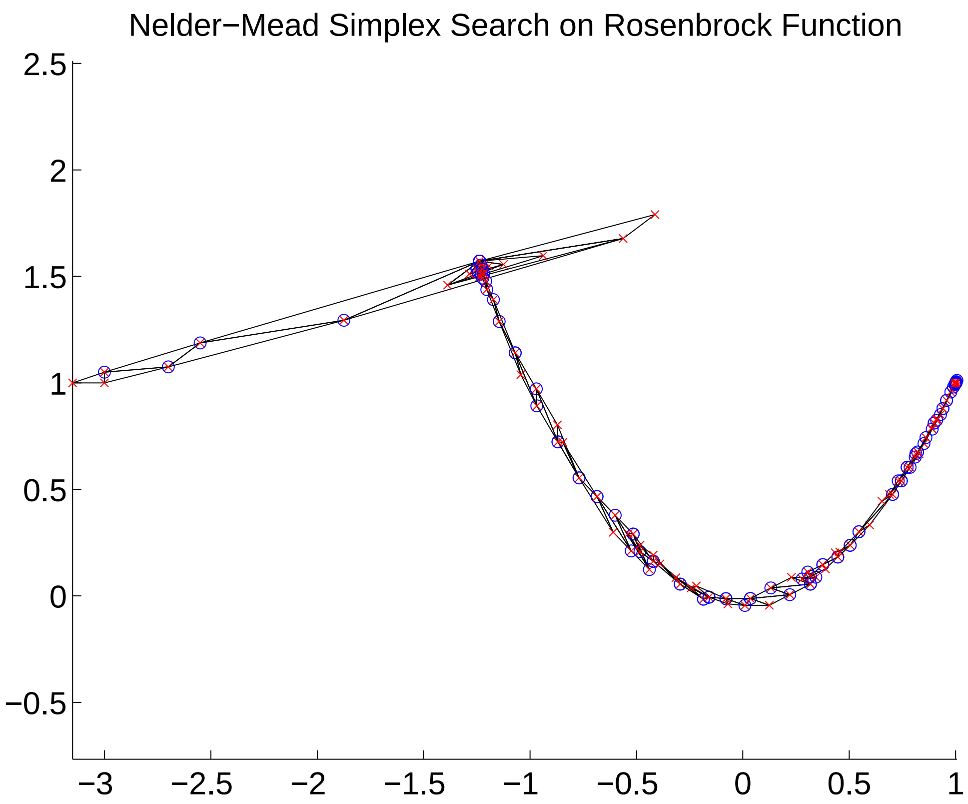
- ✔ $1 \ldots D+1$ candidates generated each iteration
- ✔ neighborhood in the form of a pattern
- ✔ static neighborhood parameters!
- ✔ adaptivity caused by changing relationships among solution vectors!

DEMO

[NM65] J.A. Nelder and R. Mead. A simplex method for function minimization. *The Computer Journal*, 7(4):308–313, 1965.

Nelder-Mead Simplex Demo





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- ✔ To *search for the optimum*, the algorithm must *maintain at least one base solution* (fullfiled by all algorithms).

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Lessons Learned

- ✔ To *search for the optimum*, the algorithm must *maintain at least one base solution* (fullfiled by all algorithms).
- ✔ To *adapt to the environmental changes* during the search (primarily not to changes of the fitness function itself, but to the changing position of the local neighborhood), the algorithm must either
  - ✘ *adapt the neighborhood (model)* structure or parameters (as done in Rosenbrock method), or
  - ✘ *adapt more than 1 base solutions* (as done in Nelder-Mead method), or
  - ✘ both of them.

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- ✔ The neighborhood
  - ✘ can be *finite*, have a form of a *pattern*, or
  - ✘ can be *infinite*, have a form of a *probabilistic distribution*.

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- ✔ The neighborhood
  - ✘ can be *finite*, have a form of a *pattern*, or
  - ✘ can be *infinite*, have a form of a *probabilistic distribution*.
- ✔ Candidate solutions can be generated from the neighborhood of
  - ✘ one base vector (LS, Box, Rosenbrock), or
  - ✘ all base vectors (Nelder-Mead), or
  - ✘ some of the base vectors (requires *selection* operator).

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Optimizer Description Framework

1. Initialize model, $\mathcal{M}$.
2. Initialize base solution set, $\mathcal{B}$.
3. Select parent solution set, $\mathcal{P}$, from $\mathcal{B}$.
4. Update $\mathcal{M}$ based on $\mathcal{B}$ and $\mathcal{P}$.
5. Generate candidate solution set, $\mathcal{C}$, using $\mathcal{M}$, $\mathcal{B}$, and $\mathcal{P}$.
6. Update $\mathcal{B}$ based on $\mathcal{B}$, $\mathcal{P}$ and $\mathcal{C}$.

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Presented algorithms described in the framework:

Algorithm	$\|\mathcal{B}\|$	$\|\mathcal{P}\|$	$\|\mathcal{C}\|$	Neighb. type	Neighb. adaptivity
LS, first impr.	1	1	1	PDF	none
LS, “best impr.”	1	1	>1	PDF	none
LS, parallel	>1	$\|\mathcal{B}\|$	$\|\mathcal{B}\|$	PDF	none
Box	1	1	2^D	pattern	none
Rosenbrock	1	1	1	pattern	model
Nelder-Mead	D+1	D+1	1 or D	pattern	population

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Evolution Strategies

Representation: $(\mathbf{x}, \sigma)$

- ✔ neigborhood parameters are part of the solution representation
- ✔ neighborhood is different for all parents

Select $\mathcal{P}$:

- ✔ select the whole $\mathcal{B}$ as $\mathcal{P}$

Model update:

$$\sigma \leftarrow \sigma \cdot e^{\tau z}, \quad z \sim \mathcal{N}(0,1)$$

Generate $\mathcal{C}$:

$$\mathbf{y} \leftarrow \mathbf{x} + \sigma \mathbf{z}, \quad \mathbf{z} \sim \mathcal{N}(0, \mathbf{I})$$

Population update:

- ✔ (μ, λ)-ES: select $\mathcal{B}_{new}$ from $\mathcal{C}$
- ✔ $(\mu + \lambda)$-ES: select $\mathcal{B}_{new}$ from $\mathcal{C}$ and $\mathcal{P}$

Summary in ODF:

- ✔ $|\mathcal{B}| = \mu$, $|\mathcal{P}| = \mu$, $|\mathcal{C}| = \lambda$
- ✔ Neighb. type: PDF (normal kernels)
- ✔ Neighb. adaptativity: population, model self-adaptation

[Rec65] Ingo Rechenberg. Cybernetic solution path of an experimental problem. Translation 1122, Royal Aircraft Establishment Library, 1965.

[Sch65] Hans-Paul Schwefel. Kybernetische evolution als strategie der experimentellen forschung in der strömungstechnik. Dipl.-ing. thesis, Technical University of Berlin, 1965.

[Sch95] Hans-Paul Schwefel. *Evolution and Optimum Seeking*. Wiley, New York, 1995.

Select $\mathcal{P}$:

- ✔ select 4 vectors from $\mathcal{B}$ uniformly as $\mathcal{P}$
- ✔ DE/rand: $\mathbf{x}_1$ is a random member of $\mathcal{B}$
- ✔ DE/best: $\mathbf{x}_1$ is the best member of $\mathcal{B}$

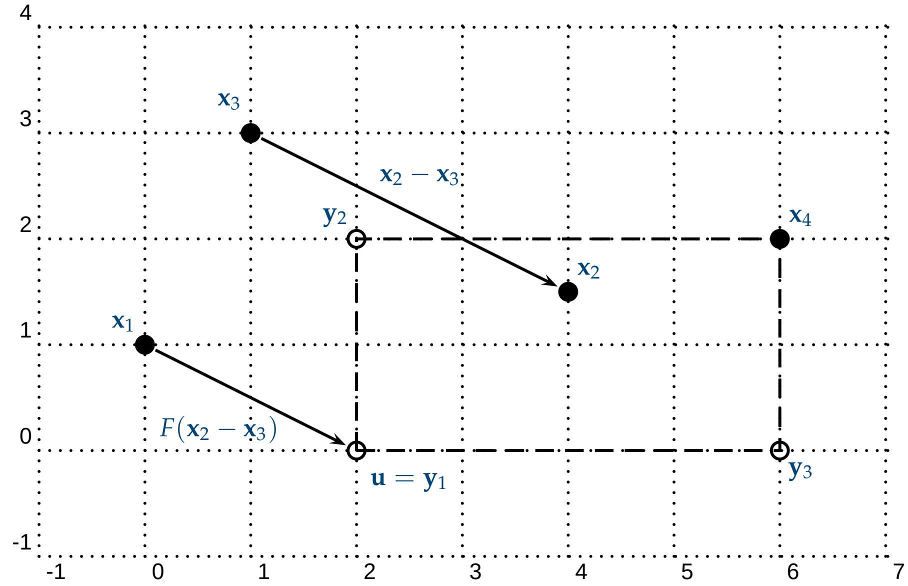
Model update: none

Generate $\mathcal{C}$:

$$\mathbf{u} \leftarrow \mathbf{x}_1 + F(\mathbf{x}_2 - \mathbf{x}_3), \quad F \in (0, 2)$$

$$y_d \leftarrow \begin{cases} u_d & \text{iff } \text{rand}_d \leq CR \text{ or } d = I_{\text{rand}} \\ x_{4,d} & \text{iff } \text{rand}_d > CR \text{ and } d \neq I_{\text{rand}} \end{cases}$$

- ✔ $\text{rand}_d \sim \mathcal{U}(0, 1)$, different for each dimension
- ✔ I_{rand} is a random index of the dimension that is always copied from $\mathbf{u}$
- ✔ $2^D - 1$ possible candidate points $\mathbf{y}$



Population update:

- ✔ if $\mathbf{y}$ is better than $\mathbf{x}_4$, replace $\mathbf{x}_4$ with $\mathbf{y}$ in $\mathcal{B}$

Summary in ODF:

- ✔ usually $|\mathcal{B}| > 1$, $|\mathcal{P}| = 4$, $|\mathcal{C}| = 1$
- ✔ Neighb. type: pattern! (PDF by randomization of F)
- ✔ Neighb. adaptativity: population

[SP95] Rainer Storn and Kenneth Price. Differential evolution - a simple and efficient adaptive scheme for global optimization over continuous spaces. Technical Report TR-95-012, ICSI, March 1995.

Particle Swarm Optimization

Initialize model:

- ✔ initialize particle velocities $\mathbf{v}_i$
- ✔ initialize personal best locations $\mathbf{x}_i^b$
- ✔ initialize global best location $\mathbf{x}^g$

Select $\mathcal{P}$:

- ✔ select the whole $\mathcal{B}$ as $\mathcal{P}$

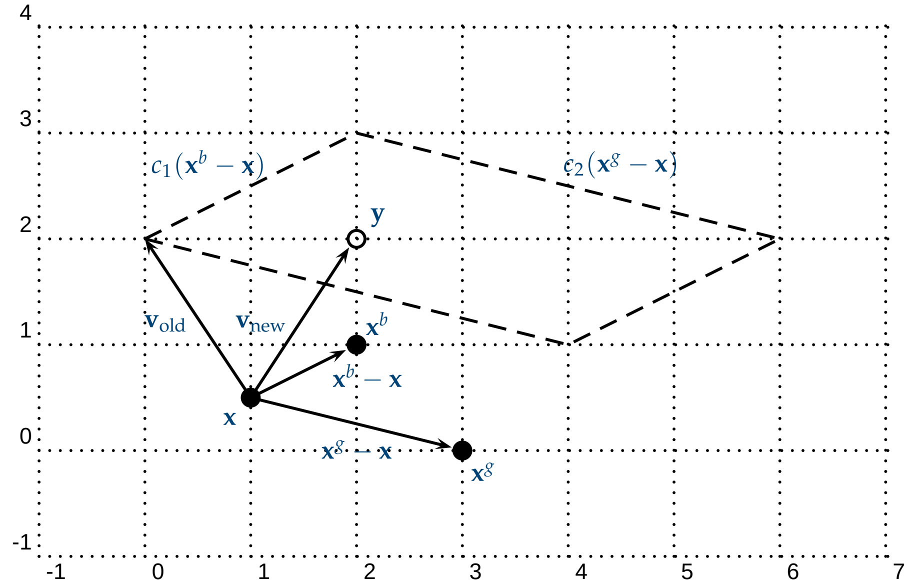
Model update:

$$\mathbf{v} \leftarrow \mathbf{v} + c_1 r_1 (\mathbf{x}^b - \mathbf{x}) + c_2 r_2 (\mathbf{x}^g - \mathbf{x})$$

- ✔ $r_1, r_2 \sim \mathcal{U}(0,1)$
- ✔ $c_1, c_2 \in (0,4)$, usually $c_1 = c_2 = 2$
- ✔ velocity vector $\mathbf{v}$ is updated to point to personal and global best solutions

Generate $\mathcal{C}$: $\mathbf{y} \leftarrow \mathbf{x} + \mathbf{v}$

- ✔ each particle i makes a step in the direction of $\mathbf{v}_i$



Population update: generational

- ✔ $\mathcal{B}_{new} = \mathcal{C}$

Summary in ODF:

- ✔ $|\mathcal{B}| > 1$, $|\mathcal{P}| = |\mathcal{B}|$, $|\mathcal{C}| = |\mathcal{B}|$
- ✔ Neighb. type: PDF
- ✔ Neighb. adaptativity: population, model

[EK95] Russel C. Eberhart and James Kennedy. A new optimizer using particle swarm theory. In *Proceedings of the Sixth International Symposium on Micromachine and Human Science*, pages 39–43, Nagoya, Japan, 1995.

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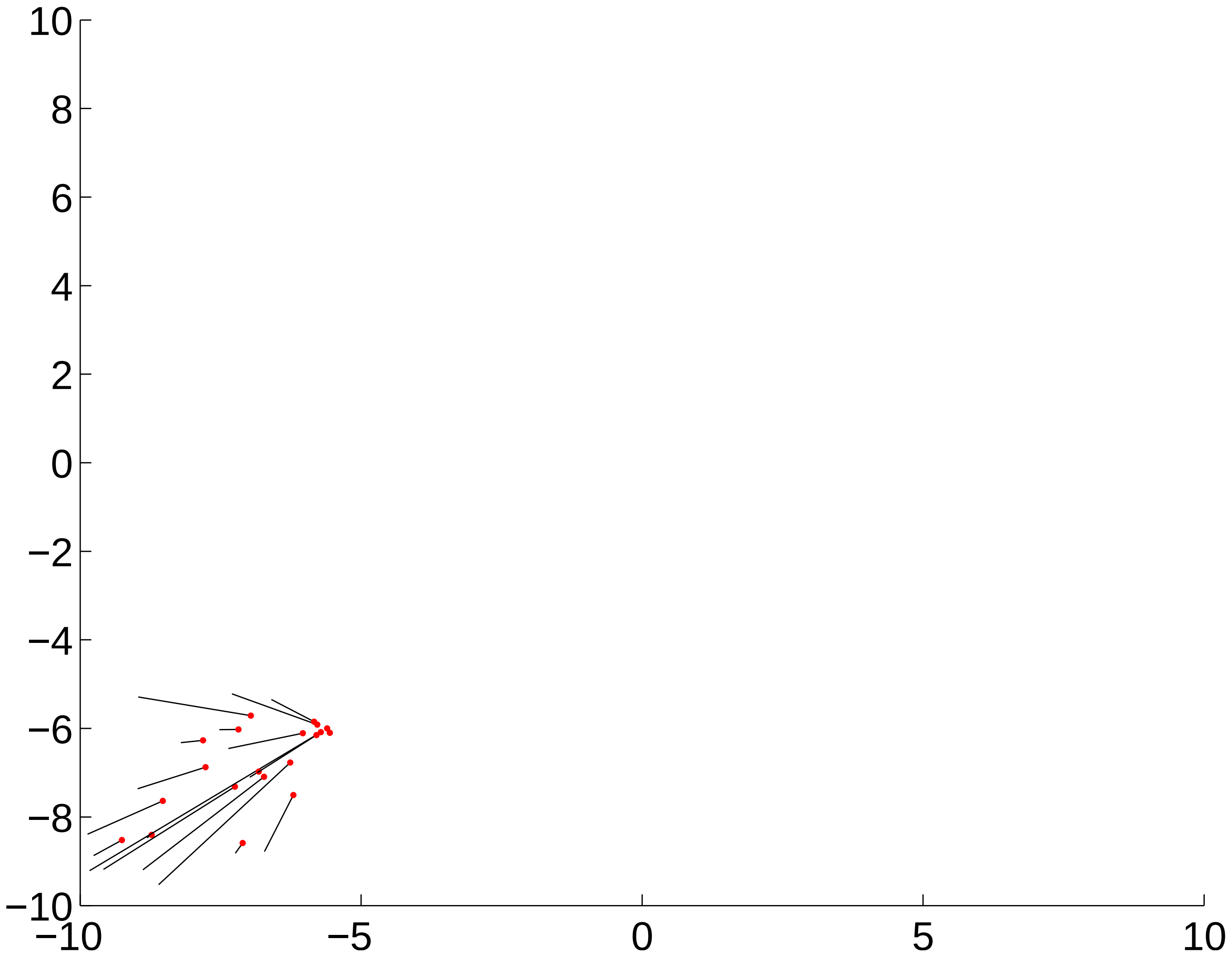
PSO on the sphere function:



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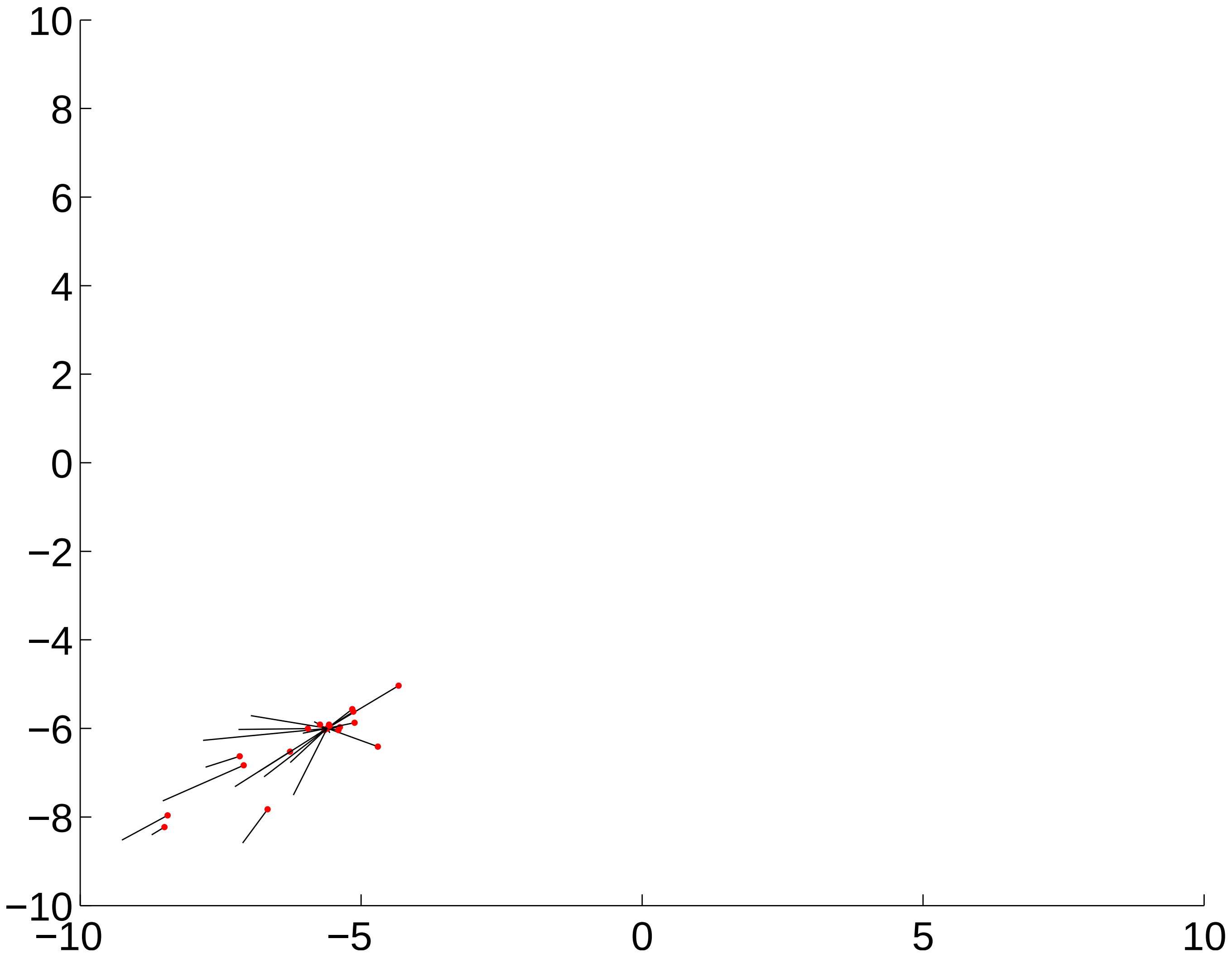

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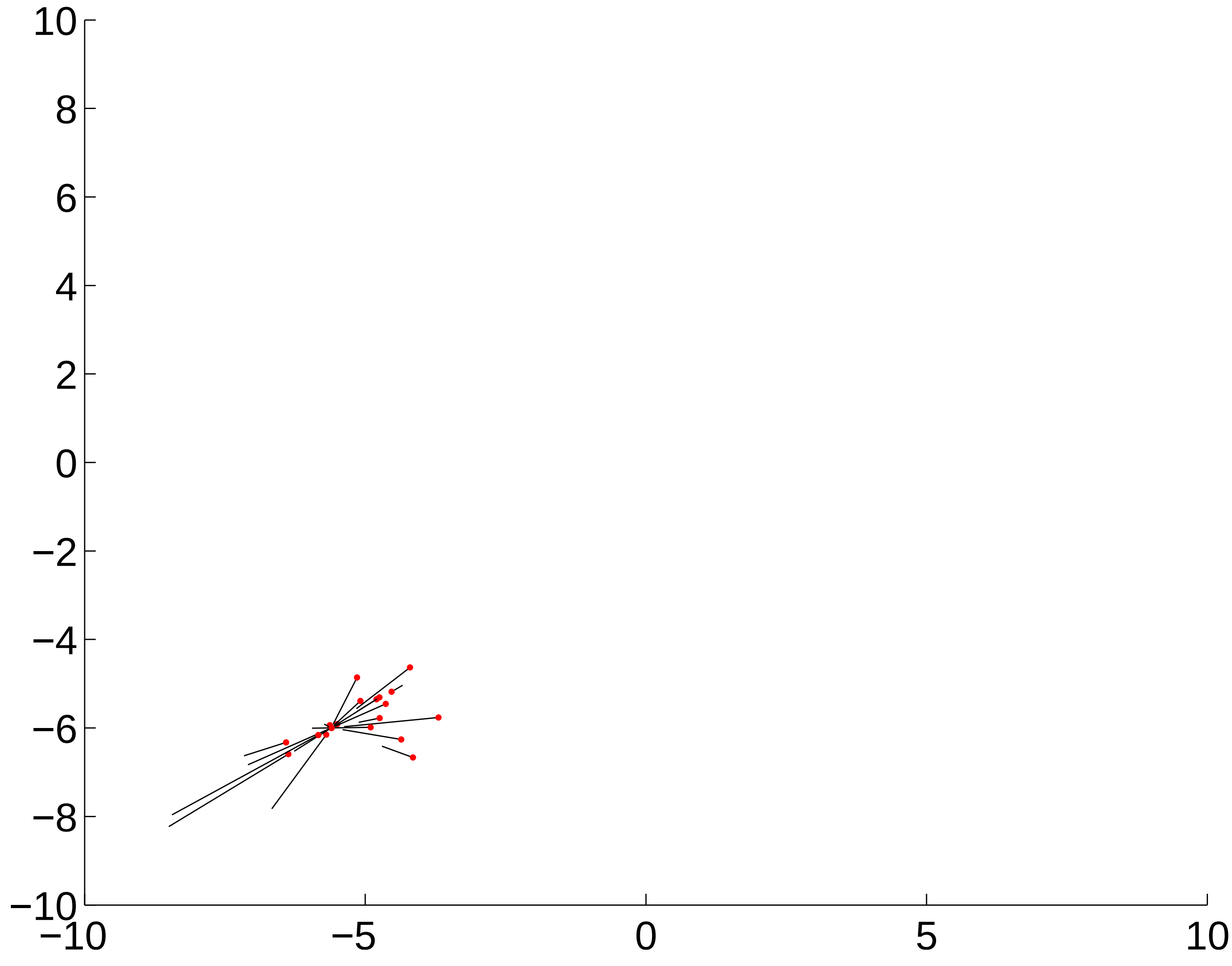

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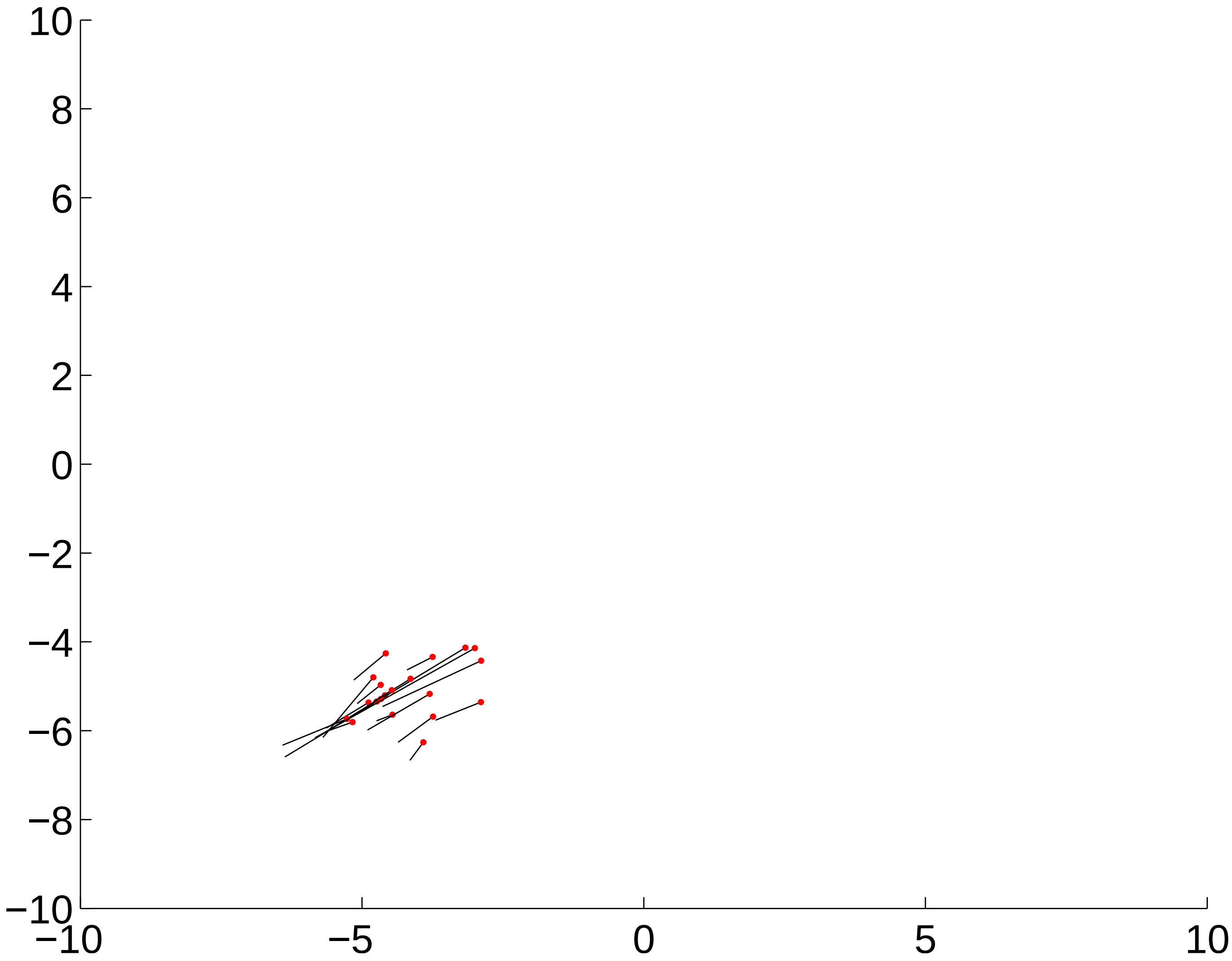
PSO on the sphere function:



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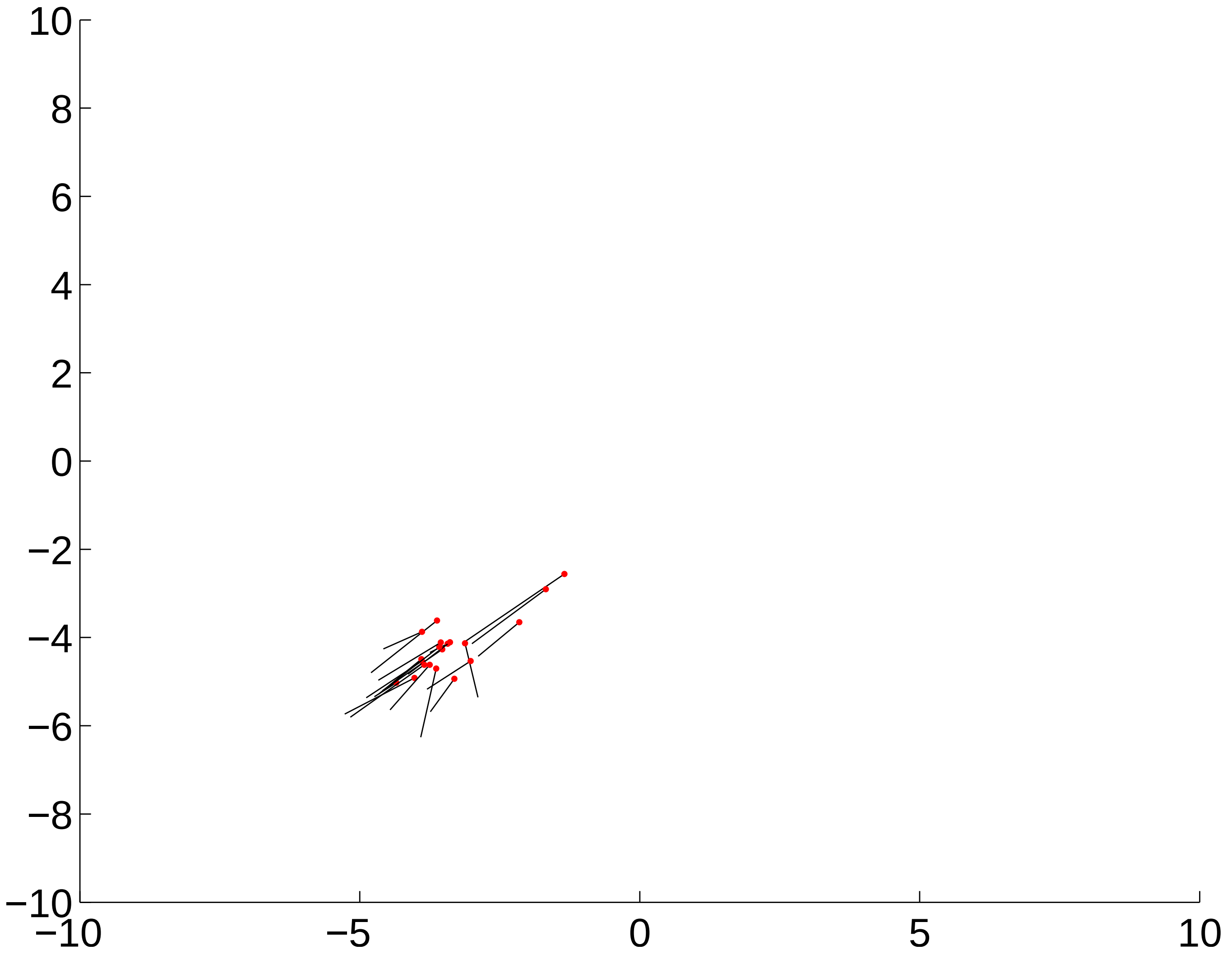

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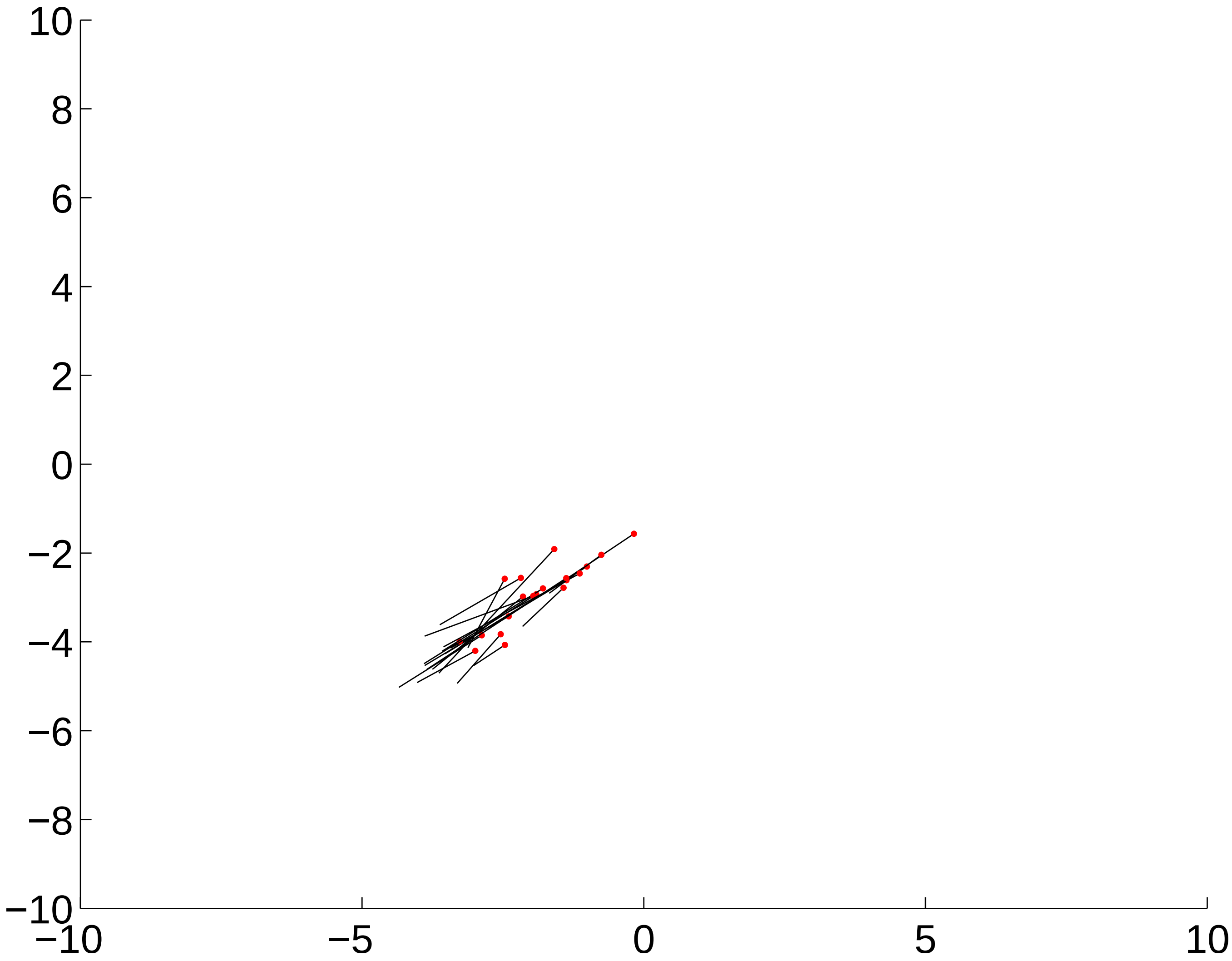

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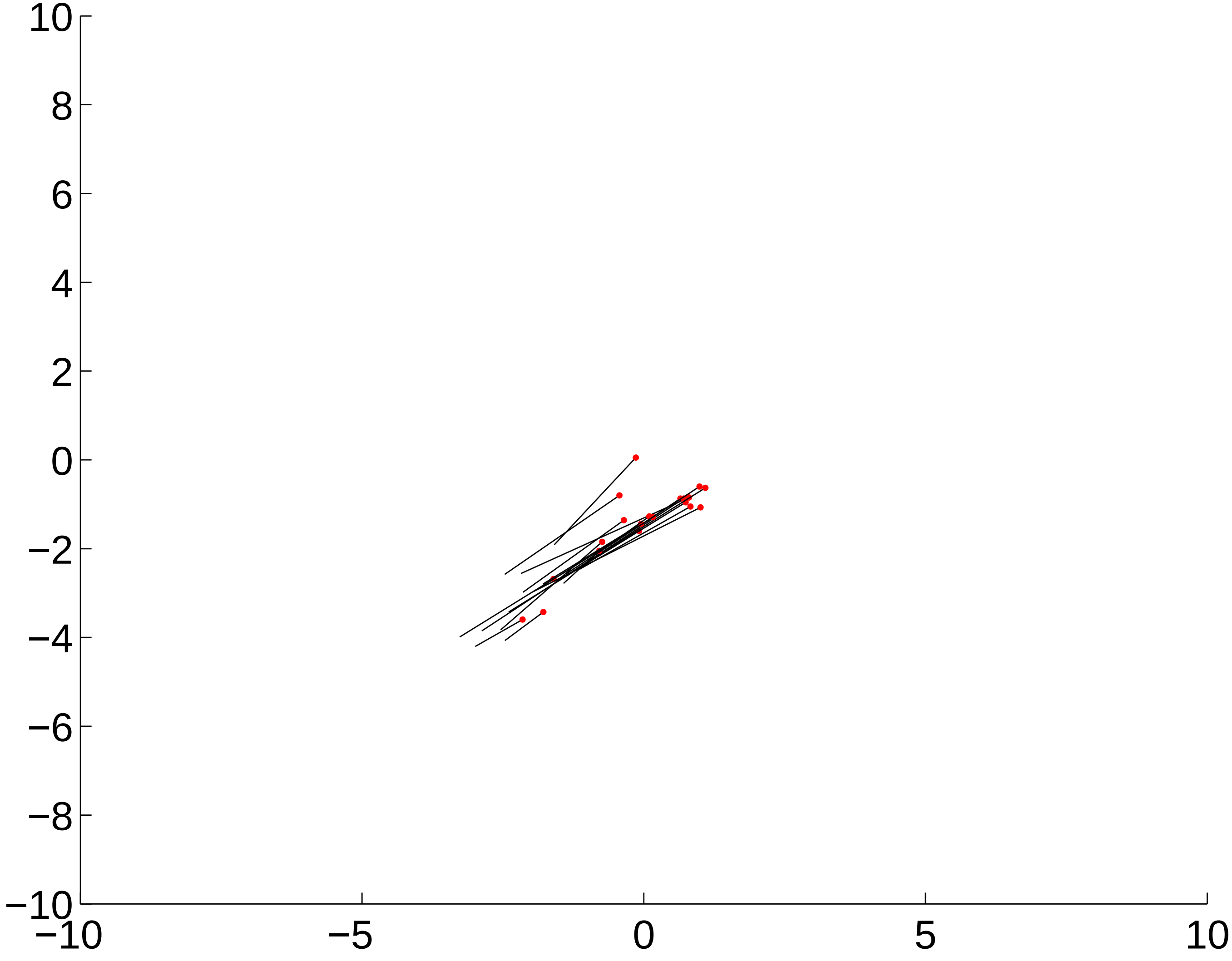

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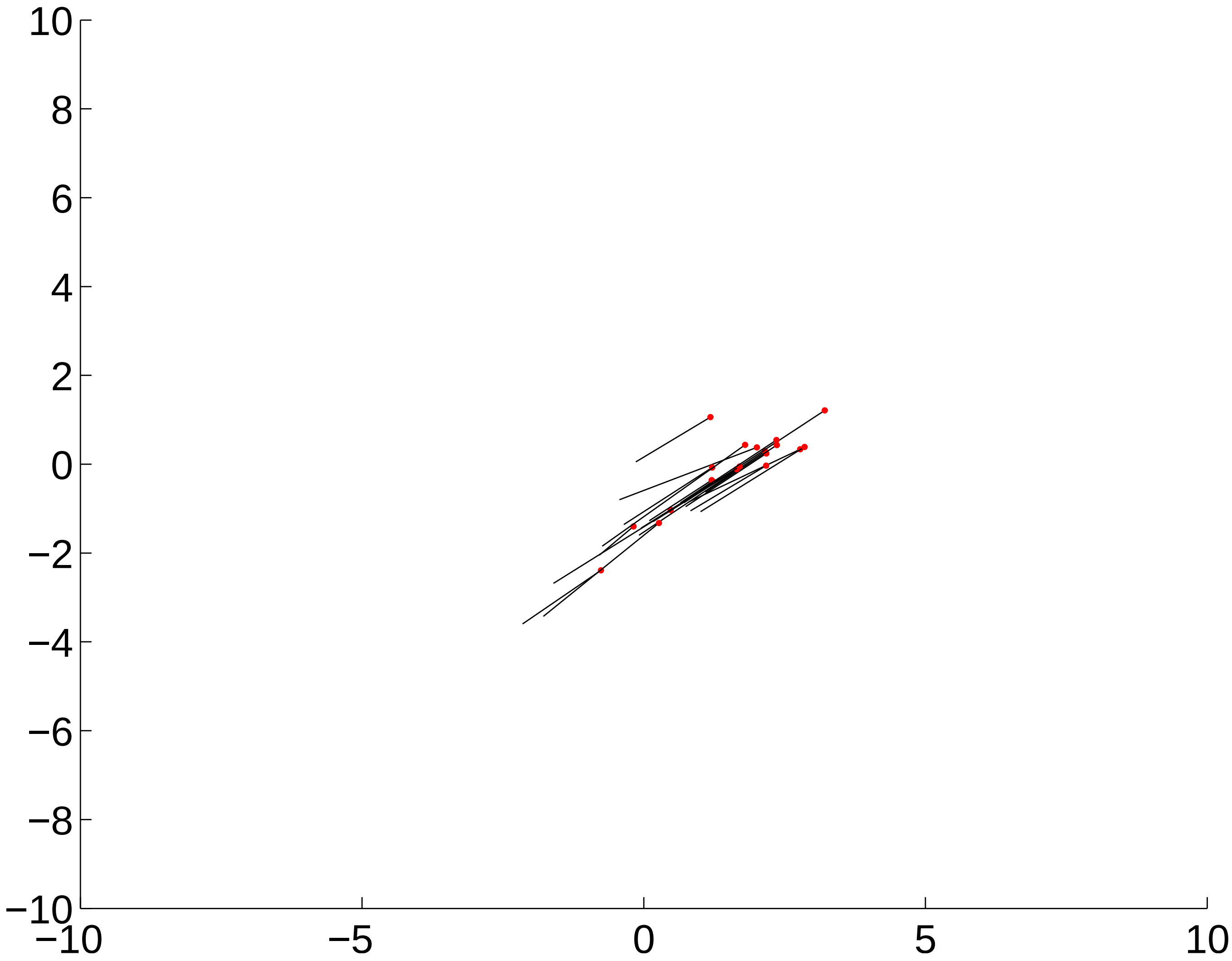

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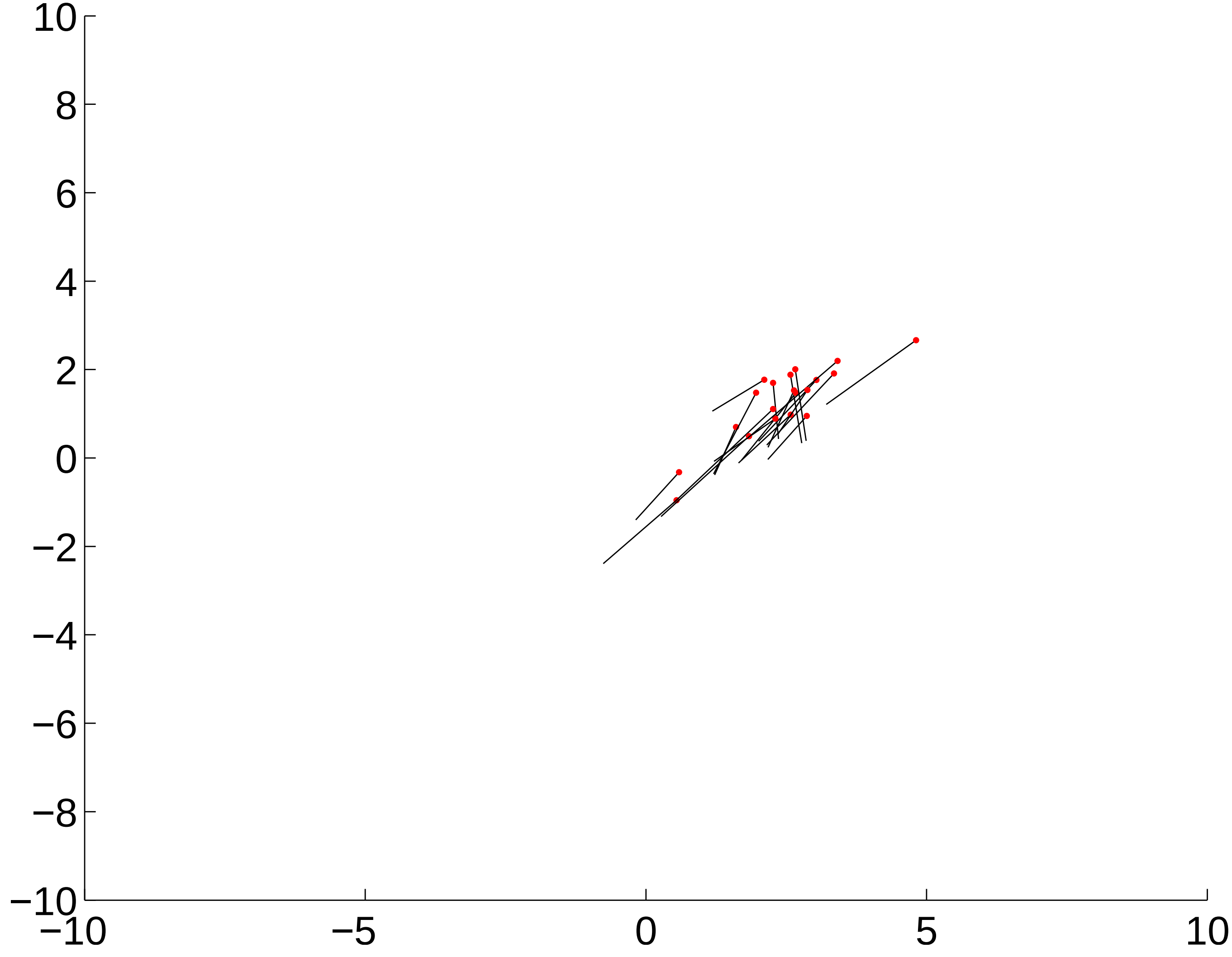

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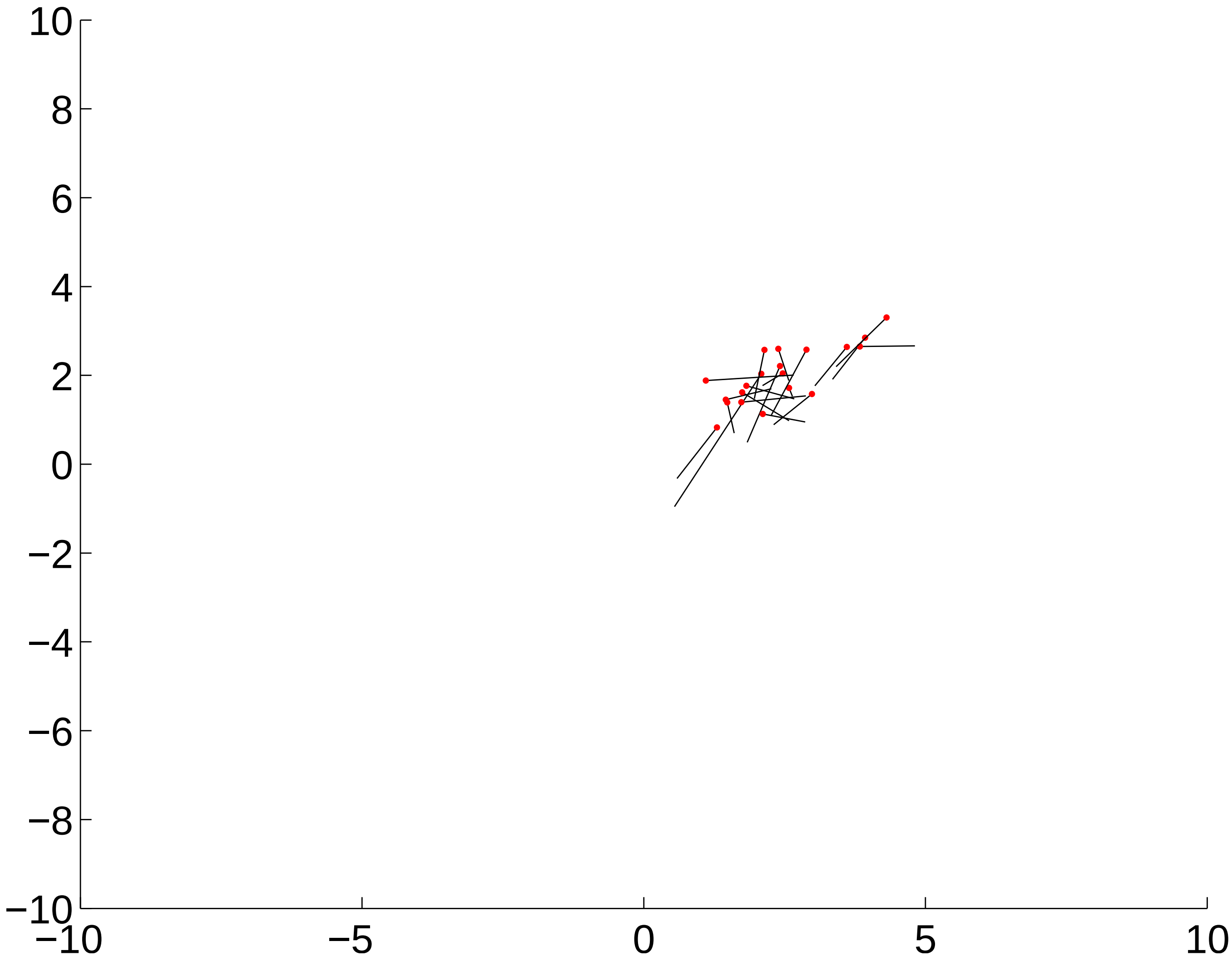

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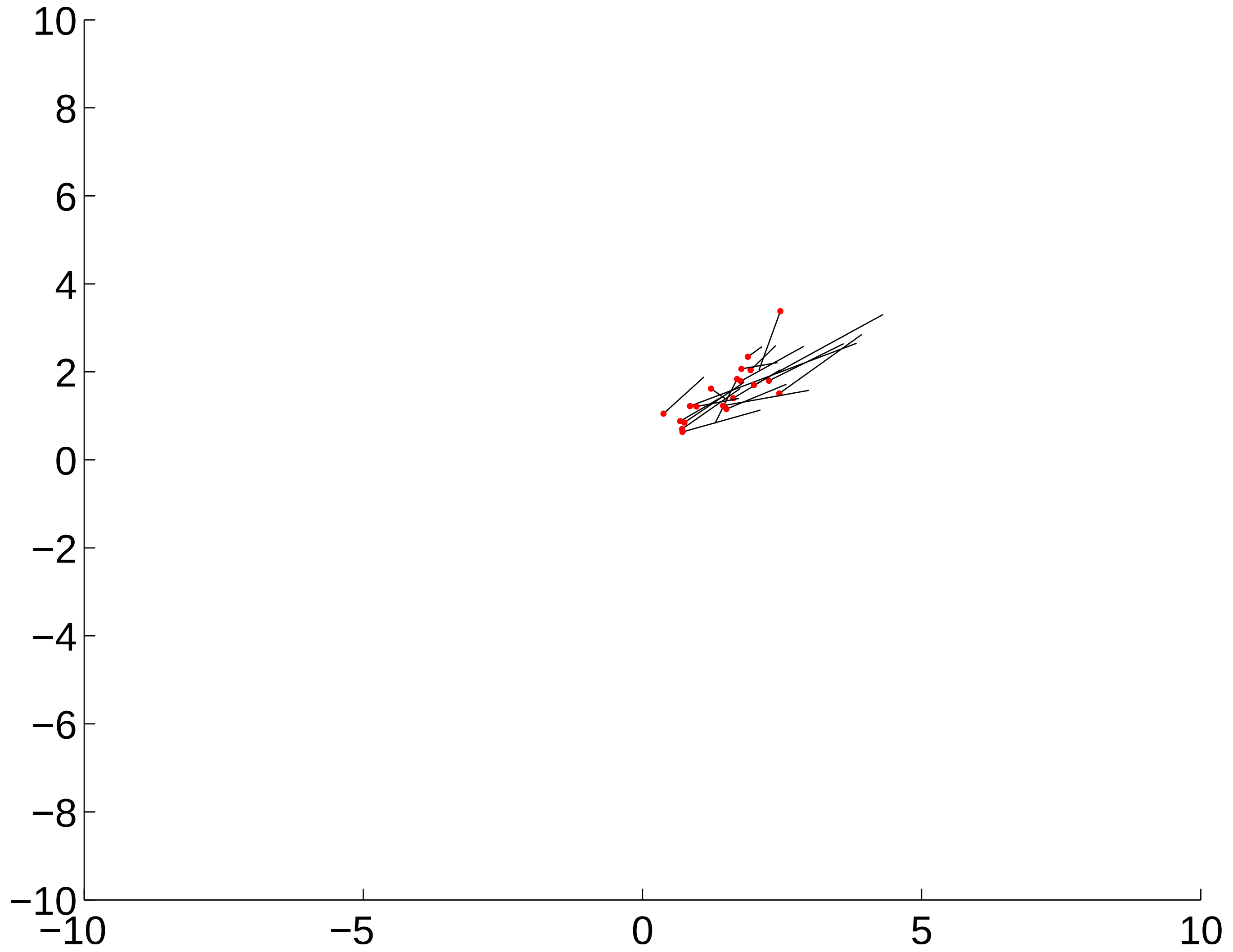

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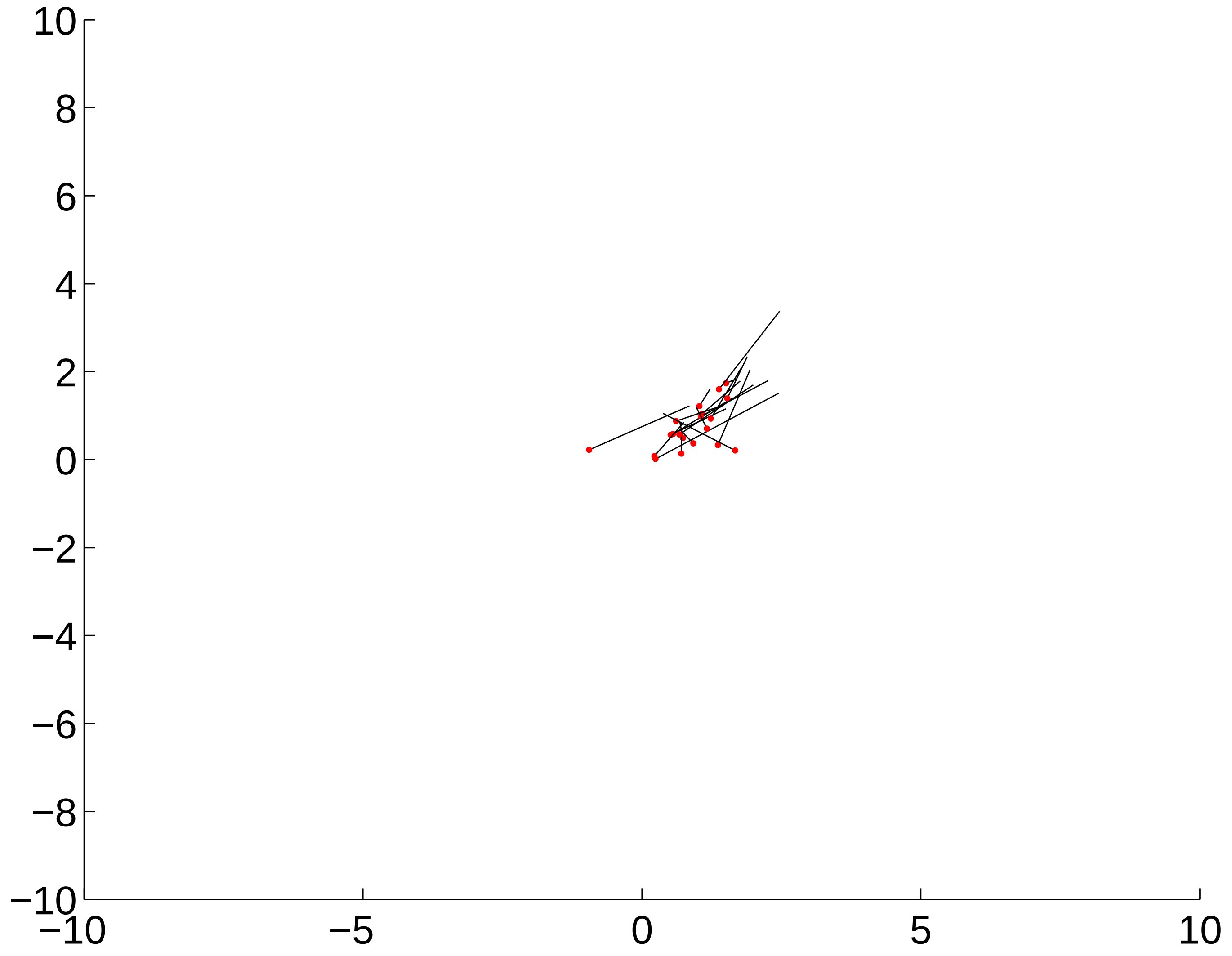

Evolution Strategy with Covariance Matrix Adaptation

Derandomized (m, λ)-ES [HO01]:

Initialize model:

- ✔ center μ, covariance matrix C and the global step size σ of the Gaussian

Select $\mathcal{P}$:

- ✔ select m best members of $\mathcal{B}$

Model update:

- ✔ Adapt μ and C using maximum likelihood estimation

$$\mu^{t+1} \leftarrow \bar{\mathbf{x}}^t_{\text{sel}}, \quad \mathbf{x}_{\text{sel}} \in \mathcal{P}$$

$$C^{t+1} \leftarrow \text{Cov}\left(\frac{\mathbf{x}^t_{\text{sel}} - \mu^t}{\sigma^t}\right)$$

- ✔ Adapt the global step size σ so that two consecutive steps, $\mu^t \rightarrow \mu^{t+1}$ and $\mu^{t+1} \rightarrow \mu^{t+2}$, are conjugated, i.e. conceptually

$$\left(\mu^{t+2} - \mu^{t+1}\right) \times C^{-1} \times \left(\frac{\mu^{t+1} - \mu^t}{(\sigma^{t+1})^2}\right) = 0$$

Generate $\mathcal{C}$ (λ candidates):

$$\mathbf{y}_i = \mu + \mathbf{z}_i, \quad \mathbf{z}_i \sim \mathcal{N}(0, \sigma \cdot C)$$

Population update:

- ✔ set $\mathcal{B}_{new}$ to $\mathcal{C}$

Summary in ODF:

- ✔ $|\mathcal{B}| = \lambda > 1$, $|\mathcal{P}| = m$, $|\mathcal{C}| = |\mathcal{B}|$
- ✔ Neighb. type: PDF
- ✔ Neighb. adaptativity: population, model

DEMO

[HO01] Nikolaus Hansen and Andreas Ostermeier. Completely derandomized self-adaptation in evolution strategies. *Evolutionary Computation*, 9(2):159–195, 2001.

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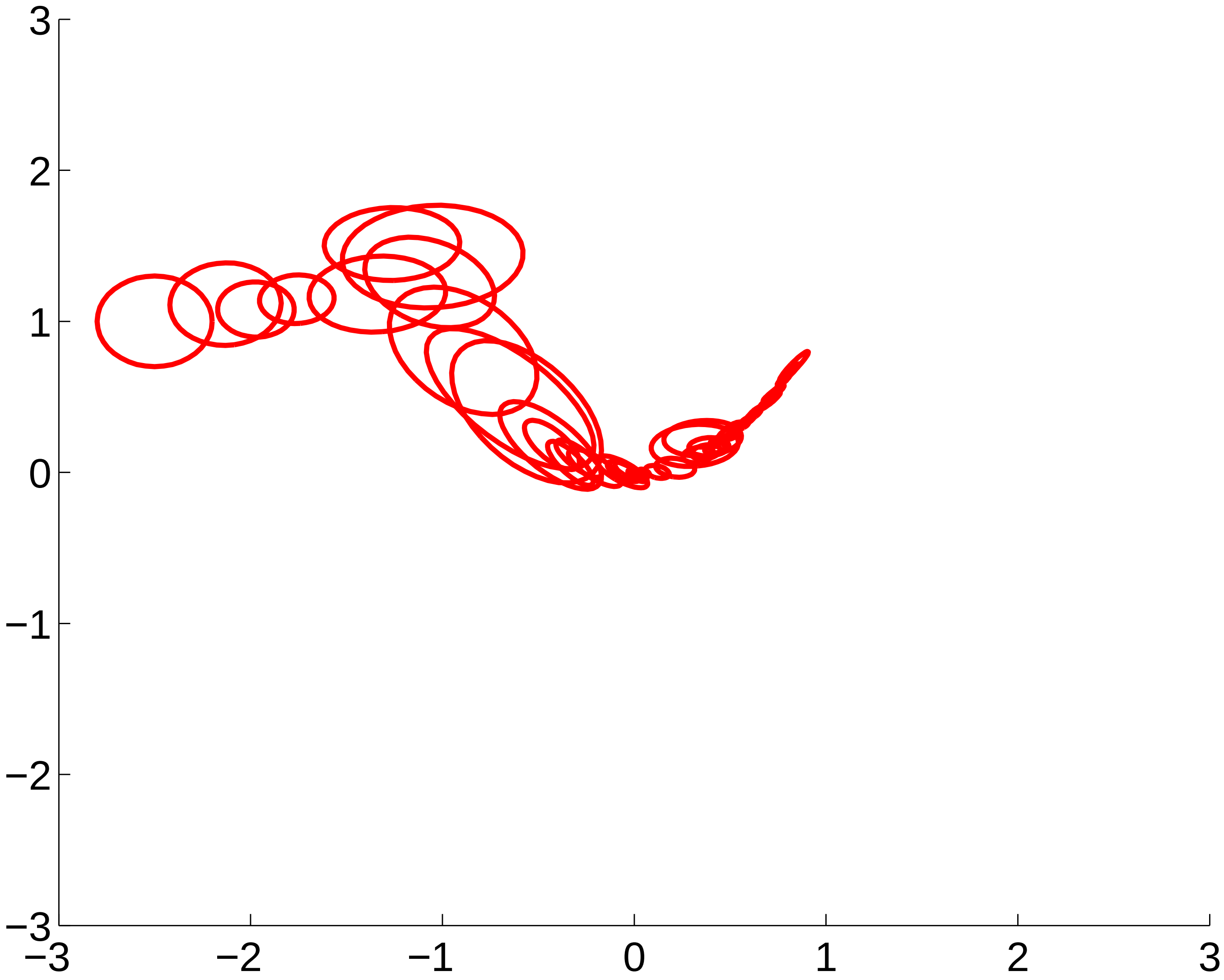
CMA-ES on the Rosenbrock function:



G3+mPCX

Generalized Generation Gap [DAJ02]:

Select $\mathcal{P}$:

- ✔ select the best member of $\mathcal{B}$ and $\mu - 1$ members randomly

Model update: none

Generate $\mathcal{C}$:

- ✔ Create λ candidates by mPCX operator

Population update:

- ✔ Choose r members of $\mathcal{B}$, create $\mathcal{R}$.
- ✔ Replace $\mathcal{R}$ with the r best sol. of $\mathcal{R} \cup \mathcal{C}$

Summary in ODF:

- ✔ $|\mathcal{B}| \approx 100$, $|\mathcal{P}| = \mu \approx 3$, $|\mathcal{C}| = \lambda \approx 2-6$
- ✔ Neighb. type: PDF
- ✔ Neighb. adaptativity: population

[DAJ02] Kalyanmoy Deb, Ashish Anand, and Dhiraj Joshi. A computationally efficient evolutionary algorithm for real-parameter optimization. *Evolutionary Computation*, 10(4):371–395, 2002.

Modified Parent Centric Xover (mPCX) [Deb05]:

Algorithm 5: Modified Parent Centric Crossover

Input: μ D-dimensional parents
Output: λ D-dimensional offspring

begin
- Mean of the parents: $\mathbf{g} \leftarrow \frac{1}{\mu}\sum_{i=1}^{\mu} \mathbf{x}_i$
- Direction vectors: $\mathbf{d}_i \leftarrow \mathbf{x}_i - \mathbf{g}$
- Base vectors: $\mathbf{e}_i \leftarrow \mathbf{d}_i / |\mathbf{d_i}|$
- **foreach** *offspring* $\mathbf{y}$ **do**
  - Choose 1 parent $\mathbf{x}_p$ randomly
  - Perpendicular distances D_i of the other $\mu - 1$ parents, $i \neq p$, to the line $\mathbf{g} -> \mathbf{x}_p$
  - Average distance: $\bar{D} = \frac{1}{\mu-1}\sum_{i=1, i\neq p}^{\mu} D_i$
  - Compute offspring as $\mathbf{y} \leftarrow \mathbf{x}_p + w_1 \mathbf{d}_p + \sum_{i=1, i\neq p}^{\mu} w_2 \bar{D} \mathbf{e}_i$ where $w_1 \sim \mathcal{N}(0, \sigma_1)$ and $w_1 \sim \mathcal{N}(0, \sigma_2)$

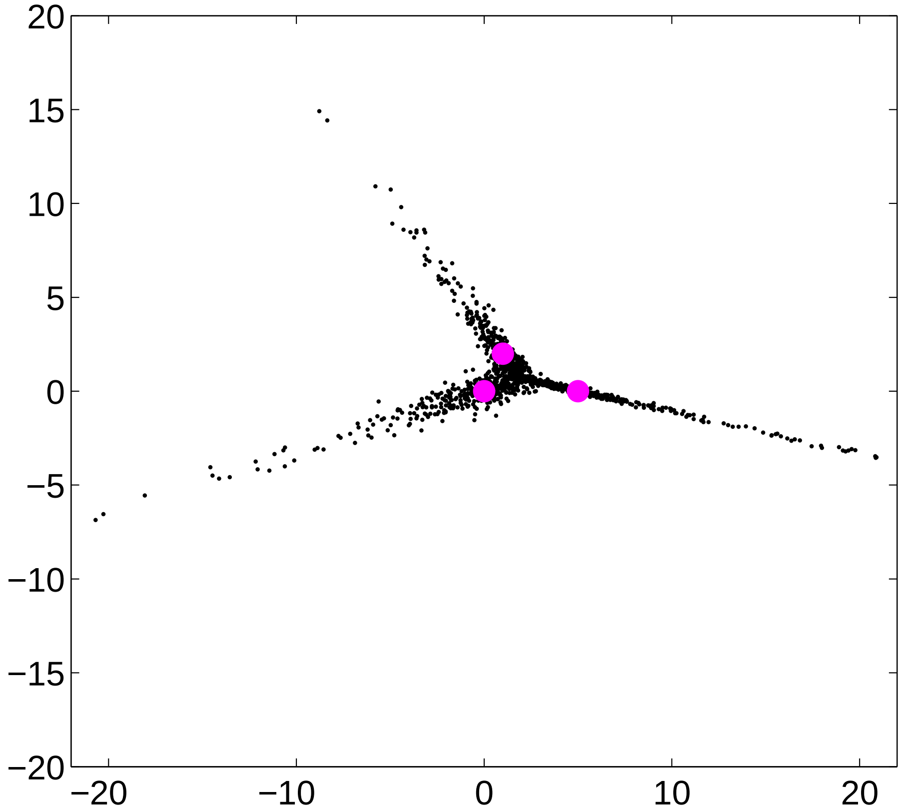
end

DEMO

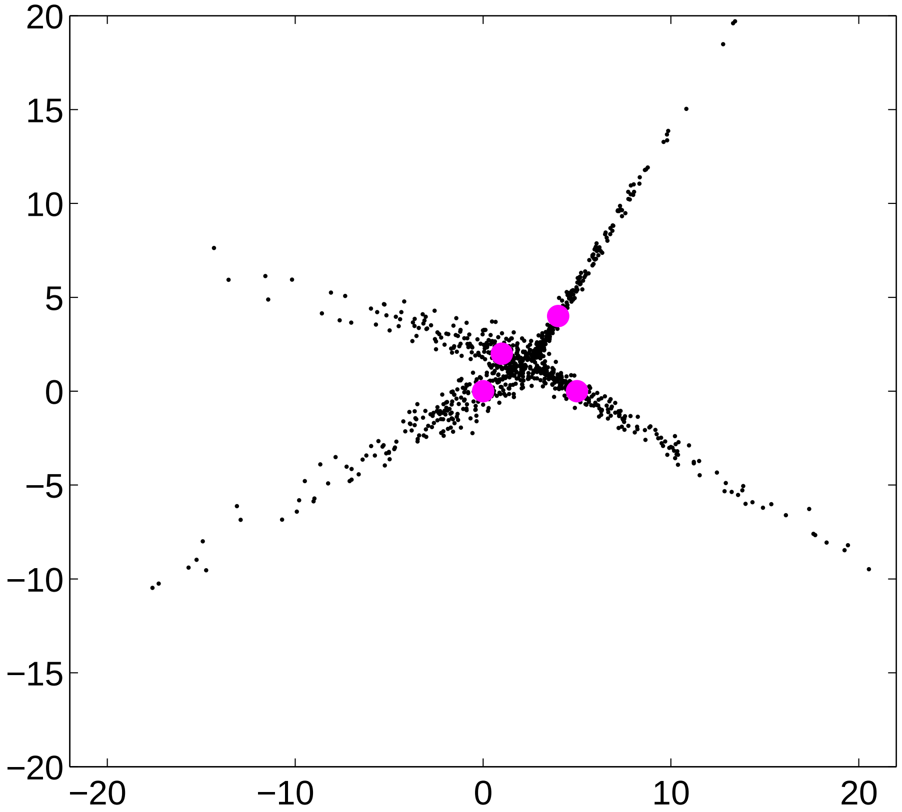
[Deb05] Kalyanmoy Deb. A population-based algorithm-generator for real-parameter optimization. *Soft Computing*, 9:236–253, 2005.

mPCX Operator Demo

Distribution of offspring when 3 2D points are used with mPCX over and over:



Distribution of offspring when 4 2D points are used with mPCX over and over:



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Special Session on Unconstrained Real-parameter Optimization:

Comparison of 11 particular representants of

- ✔ CMA-ES
- ✔ DE
- ✔ PSO
- ✔ EDA
- ✔ Co-evolution
- ✔ BLX-α operator

on 25 reference 10- and 30-dimensional optimization tasks [SHL+05].

Results comparison: thanks to Nikolaus Hansen! [Han05]

[Han05] Nikolaus Hansen. Compilation of results on the 2005 cec benchmark function set, 2005. http://www.bionik.tu-berlin.de/user/niko/cec2005compareresults.pdf.

[SHL+05] P. N. Suganthan, N. Hansen, J. J. Liang, K. Deb, Y.-P. Chen, A. Auger, and S. Tiwari. Problem definitions and evaluation criteria for the CEC 2005 Special Session on Real-Parameter Optimization. Technical report, Nanyang Technological University, Singapore, May 2005. http://www.ntu.edu.sg/home/epnsugan.

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So, what is the best algorithm?

"Hmmm, it depends. . . "

Important note: Initialization

- around the true optimum (favors mean-centric algos), or
- far away form the true optimum.

Another view of the candidate creation phase:

- parent-centric
  - (LS, Box, Rosenbrock)
  - Nelder-Mead, ES, DE, PSO, G3+mPCX
- mean-centric
  - CMA-ES
  - Not discussed here: EDA, e.g. SDR-AVS-IDEA [BGR07]

Observation: those promising techniques (in red color) *combine information from more than 2 parents* when creating offspring.

[BGR07] Peter A. N. Bosman, Jörn Grahl, and Franz Rothlauf. SDR: A better trigger for adaptive variance scaling in normal EDAs. In *GECCO '07: Proceedings of the 9th annual conference on Genetic and Evolutionary Computation*, pages 492–499, New York, NY, USA, 2007. ACM Press.

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Summary and Conclusions

Summary:

- ✔ Survey of several "historical" optimization strategies and their important features
- ✔ One of possible taxonomies of the optimization algorithms
- ✔ Survey of several "new" nature-inspired techniques
- ✔ Recent comparison results

Conclusions:

- ✔ There is NO BEST ALGORITHM FOR ALL PROBLEMS...
  - ✘ ... but a variant of CMA-ES should be the first try.
- ✔ In real spaces it seems better to select algorithm which combines more than 2 parents to create offspring.

Not covered here:

- ✔ constraints
- ✔ multiobjective optimization

Thank you for your attention

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Any questions?