A new hybrid algorithm for linear constrained global optimization
and an application in Astrophysics

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University of Southampton - Southampton, November 10, 2008

Outline

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Problem formulation

The problem we are addressing is:

Problem definition

$$\min_{z \in \mathbb{R}^n} \; f(z)$$
$$\text{s.t.} \quad \ell \leq z \leq u,$$

where $\ell \leq z \leq u$ are understood componentwise.

Smoothness

To apply particle swarm or coordinate search, smoothness of the objective function $f(z)$ is not required.

Assumption

For the convergence analysis of coordinate search, and therefore of the hybrid algorithm, some smoothness of the objective function $f(z)$ is imposed.

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Particle Swarm paradigm (PS)

- Population based algorithms that try to mimic the social behavior of a population (swarm) of individuals (particles).
- An individual behavior is a combination of its past experience (cognitive influence) and of the society experience (social influence).
- In the optimization context, one particle p, at time instance t, is represented by its current position ($x^p(t)$), its best ever position ($y^p(t)$) and a *traveling* velocity ($v^p(t)$).
- Let $\hat{y}(t)$ represent the best particle position of the population.

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New position and velocity

The new particle position is updated by

Update particle

$$x^p(t+1) = x^p(t) + v^p(t+1),$$

where $v^p(t+1)$ is the new velocity given by

Update velocity

$$v_j^p(t+1) = \iota(t)v_j^p(t) + \mu\omega_{1j}(t)\left(y_j^p(t) - x_j^p(t)\right) + \nu\omega_{2j}(t)\left(\hat{y}_j(t) - x_j^p(t)\right),$$

for $j = 1, \ldots, n$.

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Handling bound constraints

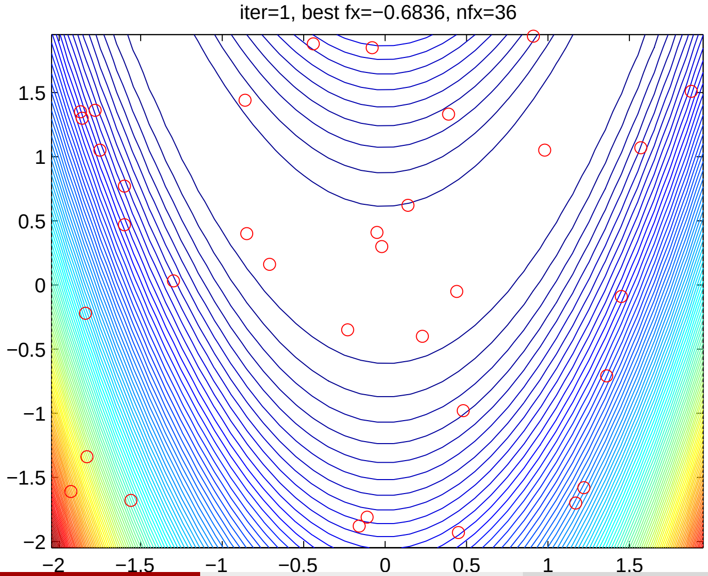
In particle swarm, simple bound constraints are handled by a projection onto $\Omega = \{x \in \mathbb{R}^n : \ \ell \leq x \leq u\}$, for all particles $i = 1, \ldots, s$.

Projection

$$proj_{\Omega}(x_j^i(t)) = \begin{cases} \ell_j & \text{if } \ x_j^i(t) < \ell_j, \\ u_j & \text{if } \ x_j^i(t) > u_j, \\ x_j^i(t) & \text{otherwise,} \end{cases}$$

for $j = 1, \ldots, n$.

Example



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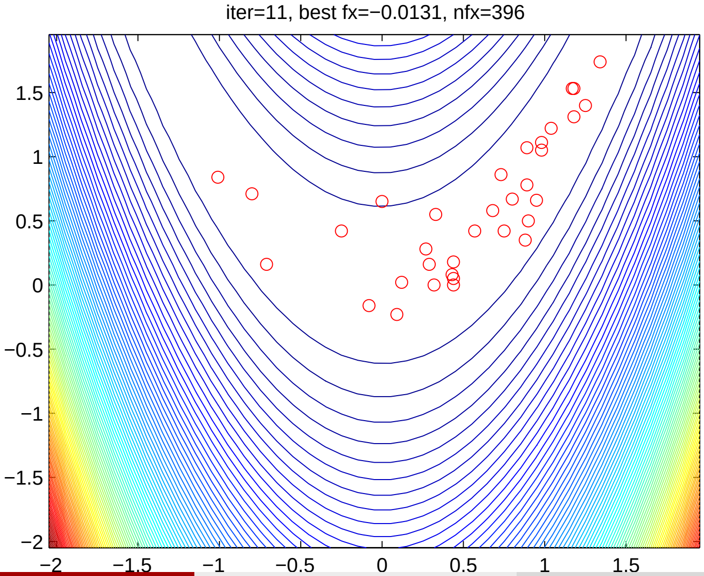

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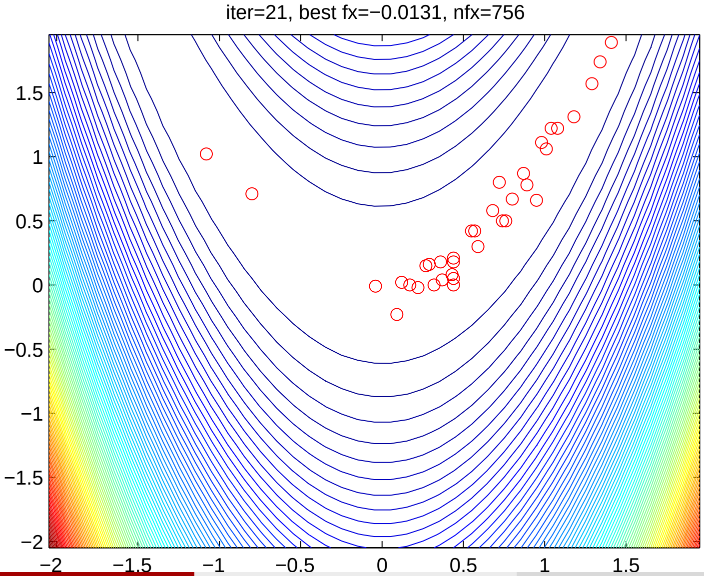

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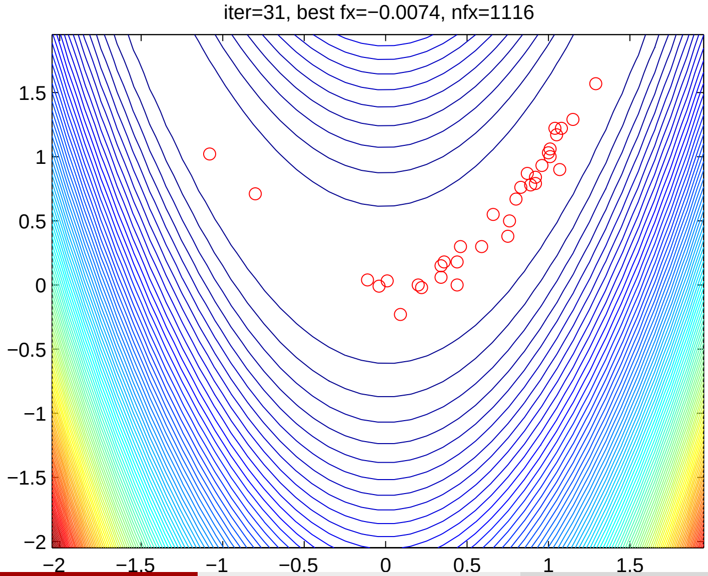

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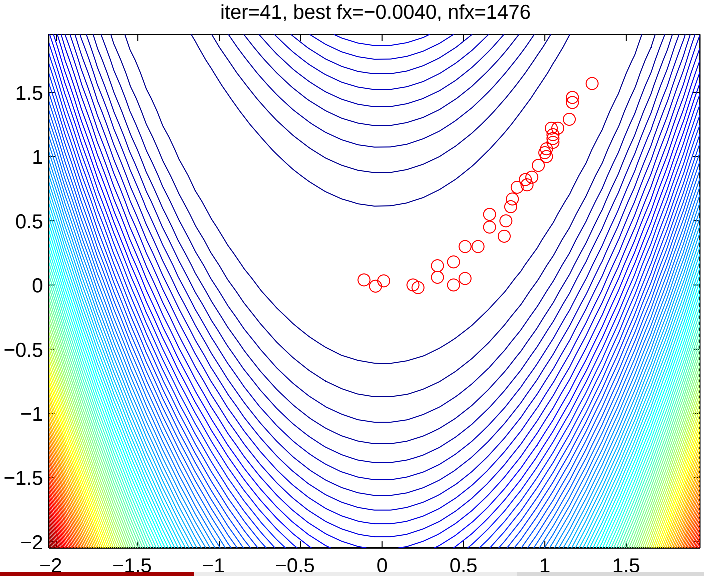

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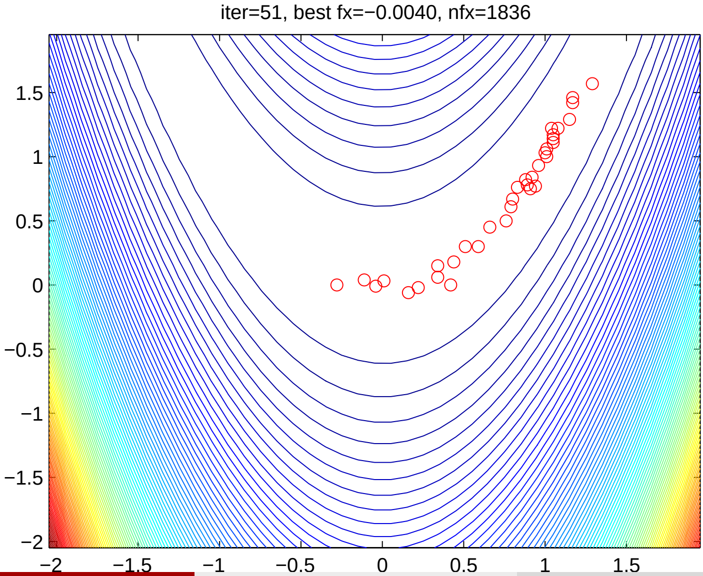

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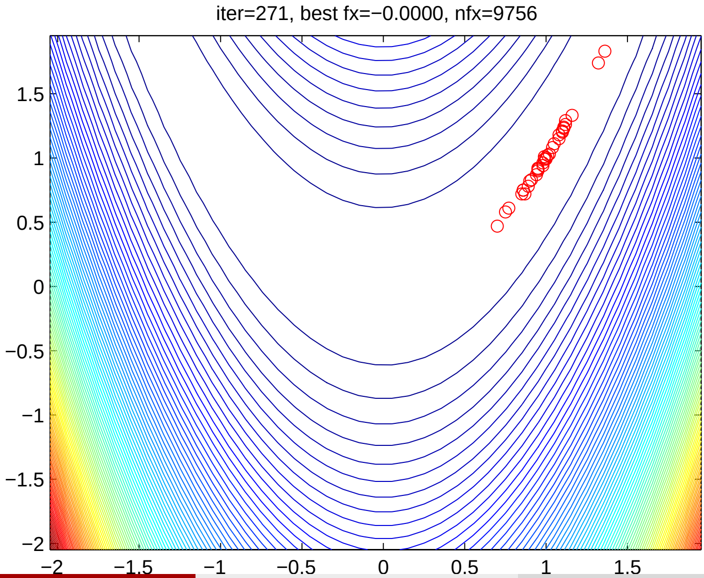

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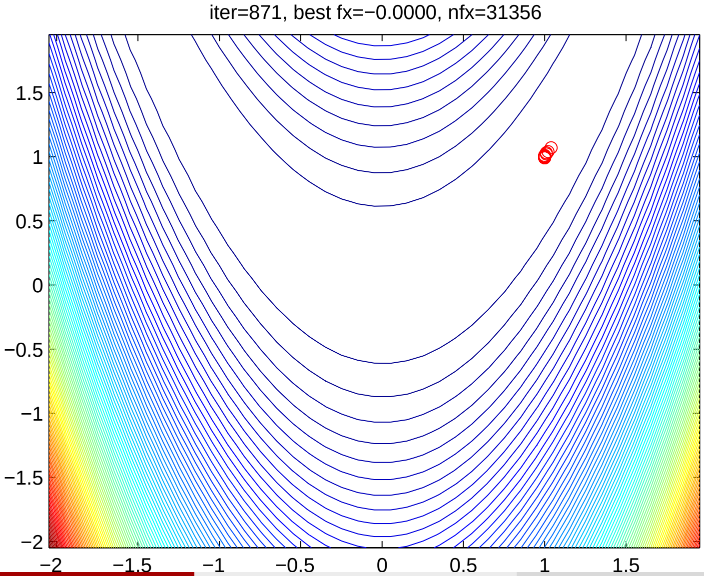
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1.5
1
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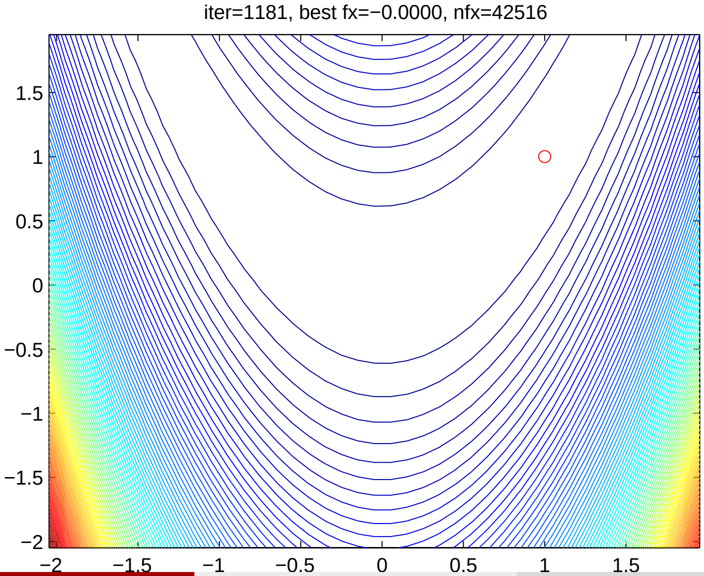
iter=1181, best fx=−0.0000, nfx=42516
1.5
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−0.5
−1
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−2
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Some properties

- Easy to implement.
- Easy to deal with discrete variables.
- Easy to parallelize.
- For a correct choice of parameters the algorithm terminates ($\lim_{t \to +\infty} v(t) = 0$).
- Uses only objective function values.
- Convergence for a global optimum under strong assumptions (unpractical).
- High number of function evaluations.

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Introduction to direct search methods

- Direct search methods are an important class of optimization methods that try to minimize a function by comparing objective function values at a finite number of points.
- Direct search methods do not use derivative information of the objective function nor try to approximate it.
- Coordinate search is a simple direct search method.

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Some definitions

Positive maximal basis

Formed by the coordinate vectors and their negative counterparts:

$$D_\oplus = \{e_1, \ldots, e_n, -e_1, \ldots, -e_n\}.$$

$D_\oplus$ spans $\mathbb{R}^n$ with nonnegative coefficients.

Coordinate search

The direct search method based on $D_\oplus$ is known as coordinate or compass search.

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Sets

Given $D_\oplus$ and the current point $y(t)$, two sets of points are defined: a grid M_t and the poll set P_t.

The grid M_t is given by

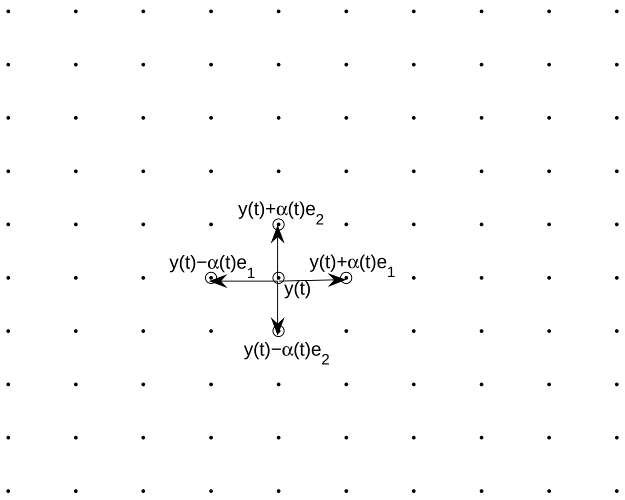
$$M_t = \left\{ y(t) + \alpha(t) D_\oplus z,\ z \in \mathbb{N}_0^{|D_\oplus|} \right\},$$

where $\alpha(t) > 0$ is the grid size parameter.

The poll set is given by

$$P_t = \{ y(t) + \alpha(t) d,\ d \in D_\oplus \}.$$

Example of M_t and P_t



The grid M_t and the set P_t when $D_\oplus = \{e_1, e_2, -e_1, -e_2\}$

Coordinate search

- The search step conducts a finite search on the grid M_t.
- If no success is obtained in the search step then a poll step follows.
- The poll step evaluates the objective function at the elements of P_t, searching for points which have a lower objective function value.
- If success is attained, the value of $\alpha(t)$ may be increased, otherwise it is reduced.

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Handling bound constraints

For the coordinate search method it is sufficient to initialize the algorithm with a feasible initial guess ($y(0) \in \Omega$) and to use $\hat{f}$ as the objective function.

Penalty/Barrier function

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

Motivation for PSwarm

Hybrid algorithm

The hybrid algorithm tries to combine the best of both algorithms.

From particle swarm

The particle swarm ability of searching for the global optimum.

From coordinate search

The guarantee to obtain at least a stationary point. Some robustness.

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Motivation for PSwarm

Central idea

A particle swarm iteration is performed in the search step and if no progress is attained a poll step is taken.

Key points

- In the first iterations the algorithm takes advantage of the particle swarm ability to find a global optimum (exploiting the search space), while in the last iterations the algorithm takes advantage of the pattern search robustness to find a stationary point.
- The number of particles in the swarm search can be decreased along the iterations (no need to have a large number of particles around a local optimum).

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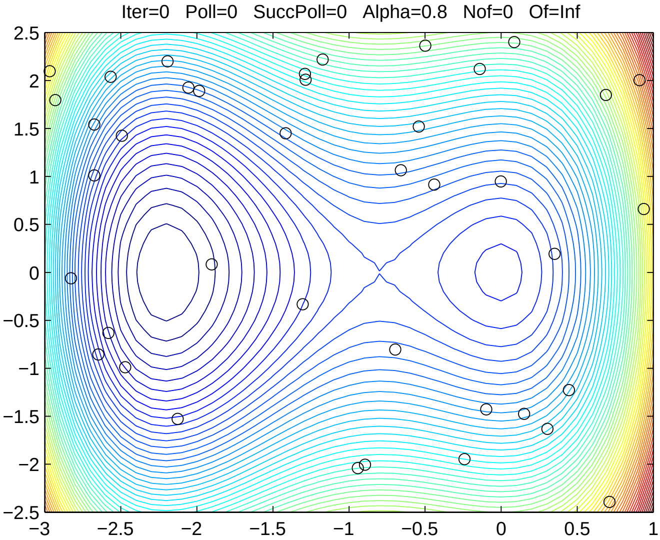

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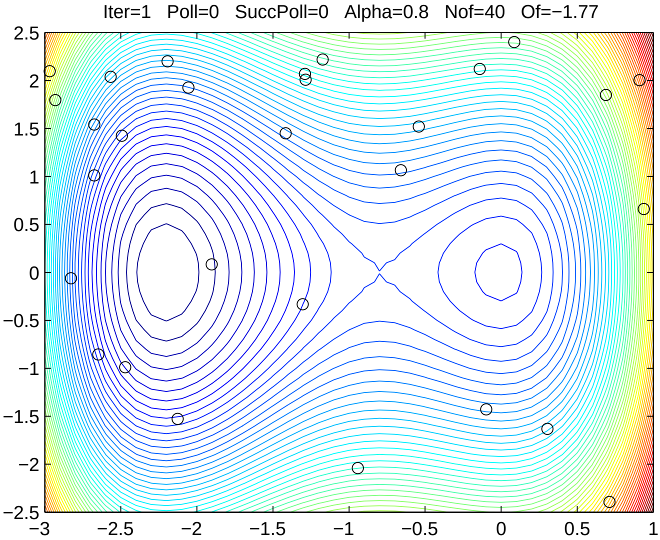

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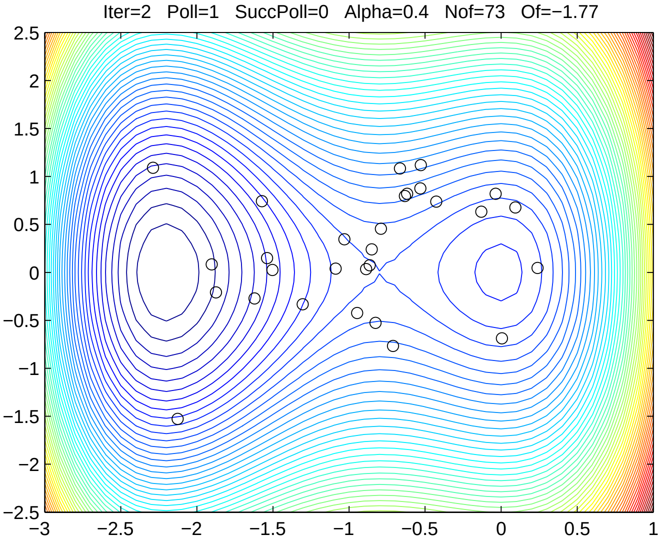

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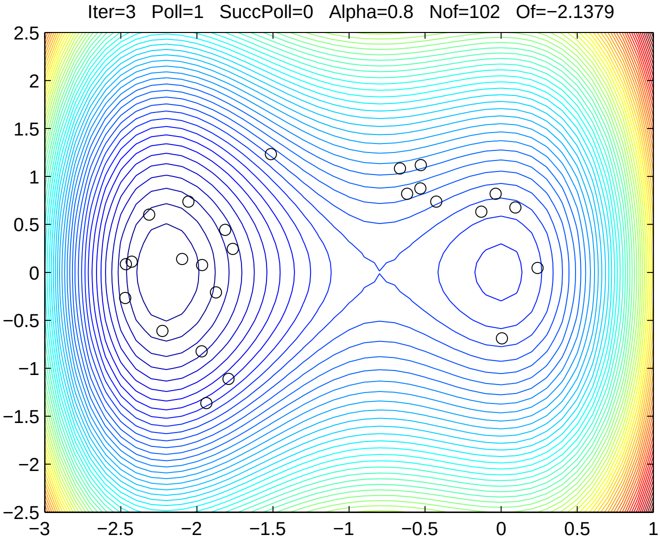

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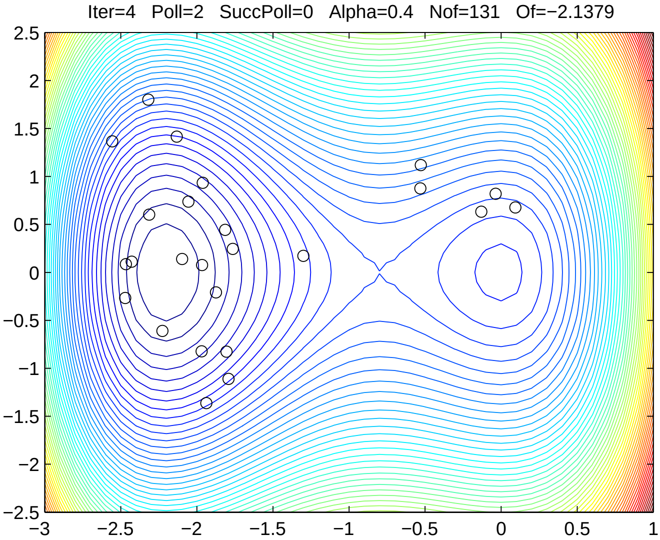

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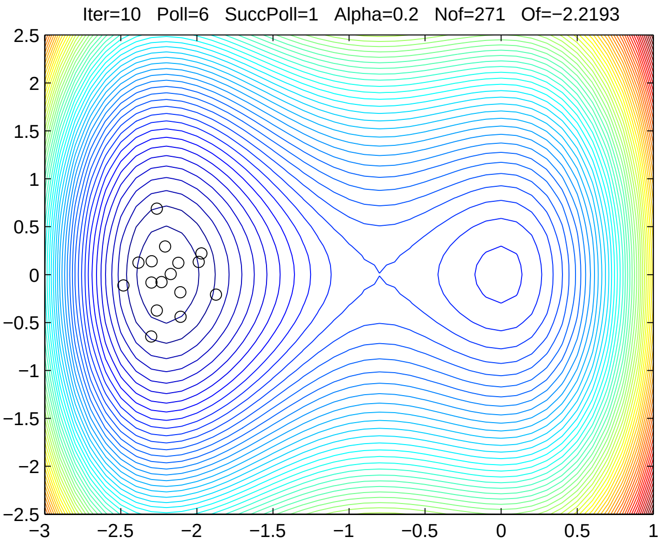

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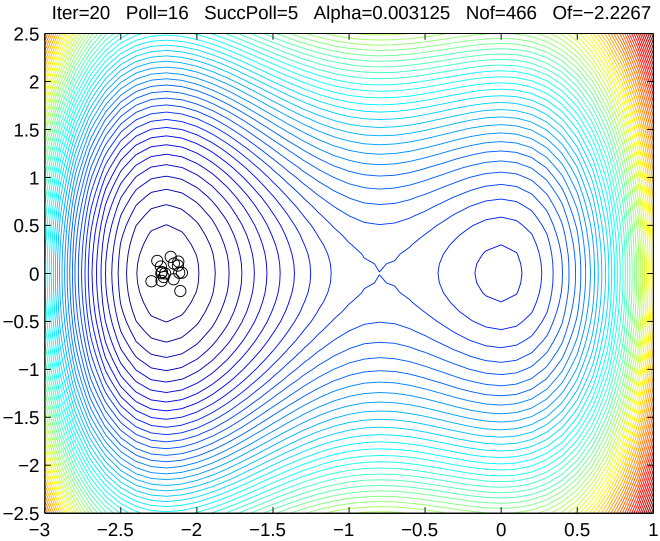

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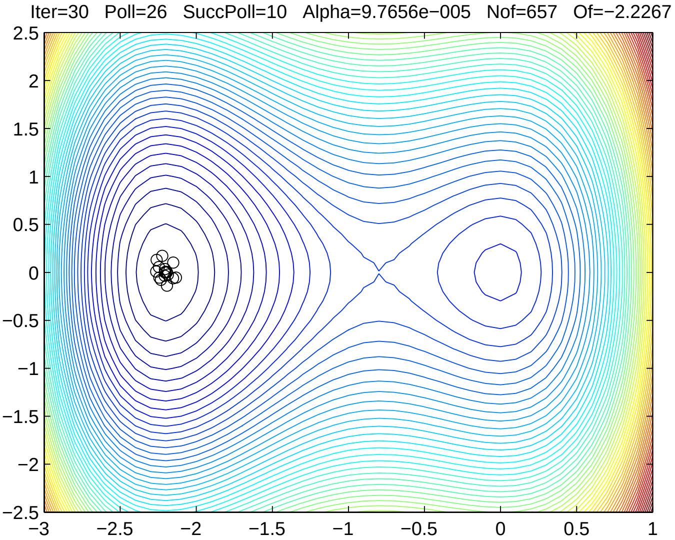

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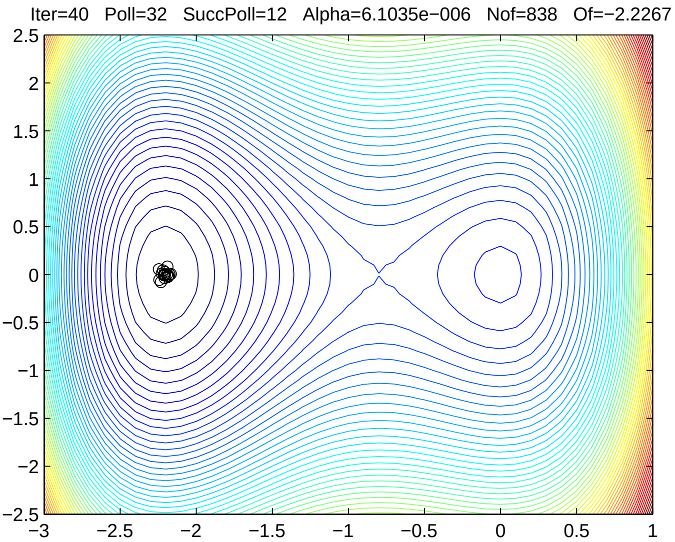

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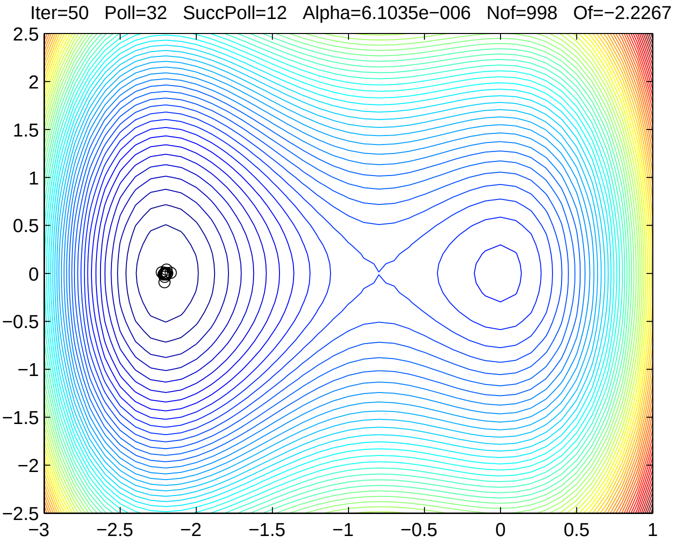

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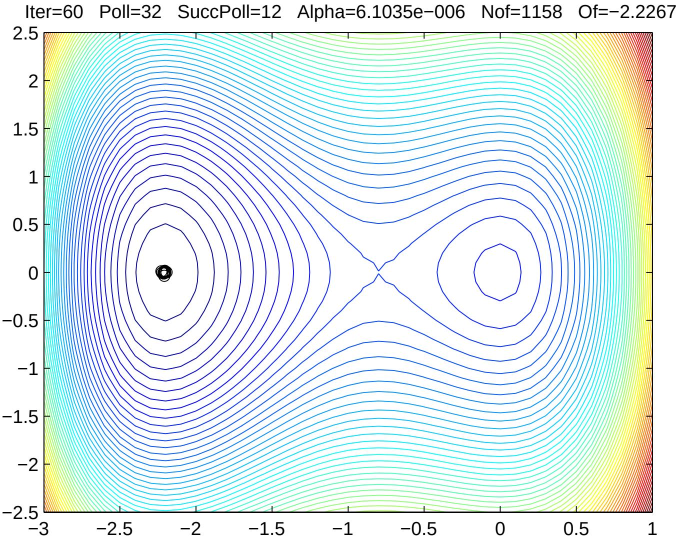

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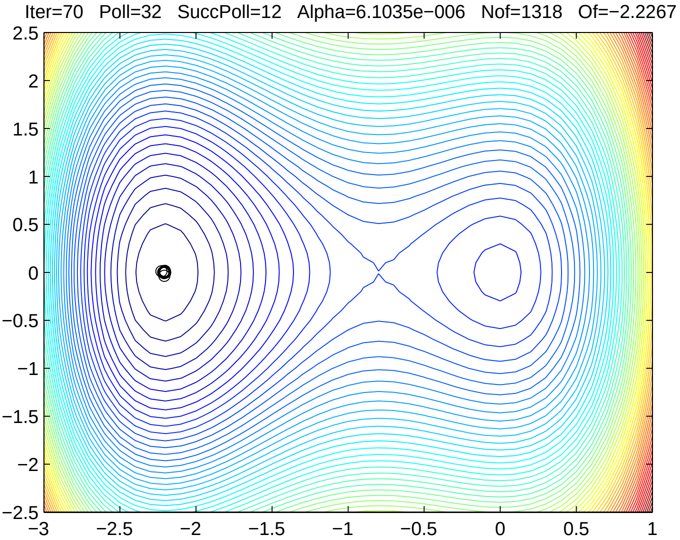

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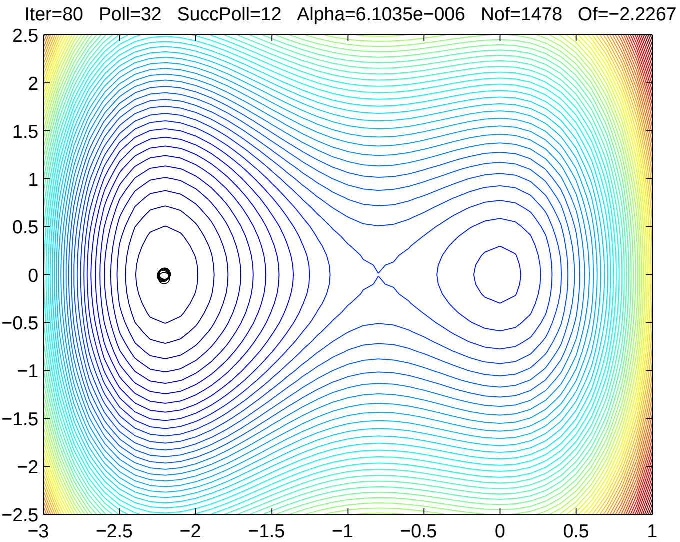

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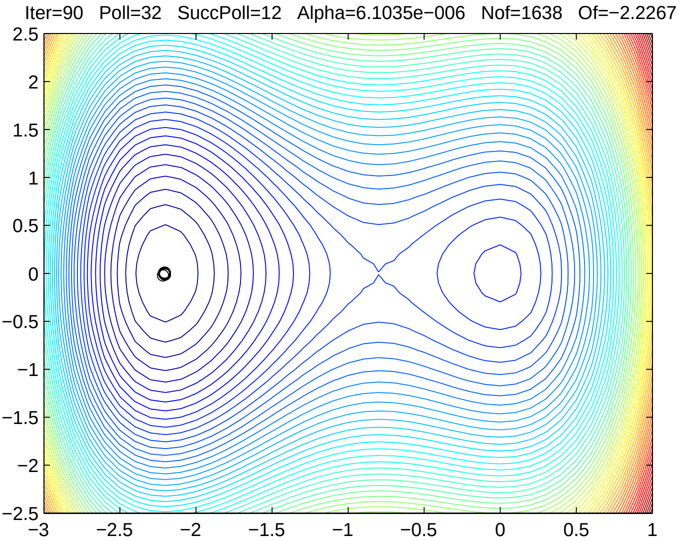

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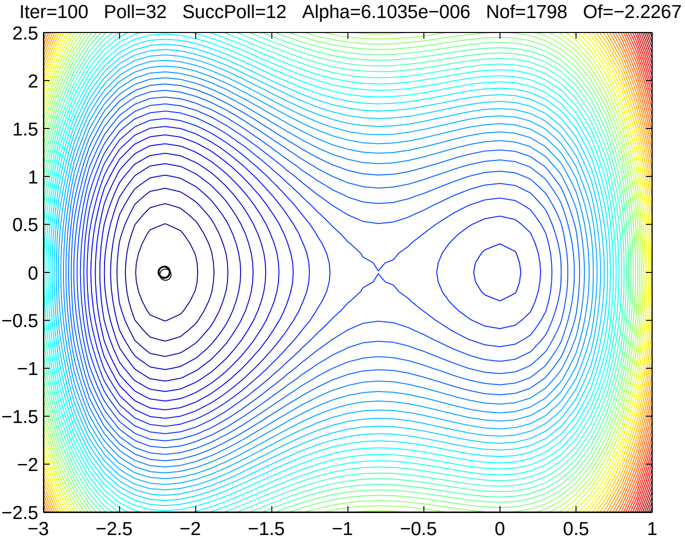

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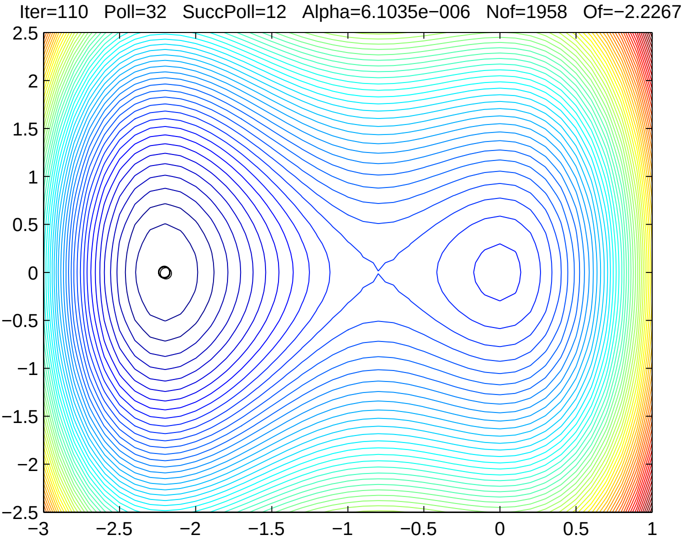

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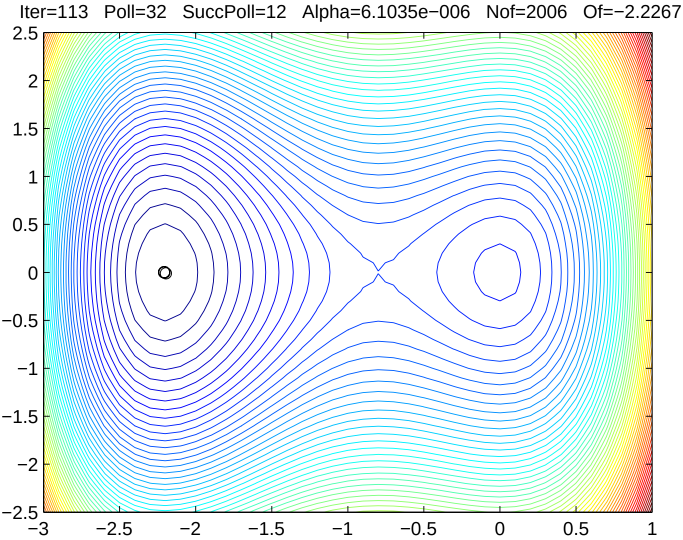

Test problems

- 122 problems were collected from the global optimization literature.
- 12 problems of large dimension (between 100 and 300 variables). The others are small (< 10) and medium size (< 30).
- Majority of objective functions are differentiable, but non-convex.
- All problems have simple bounds on the variables (needed for the search step — particle swarm).
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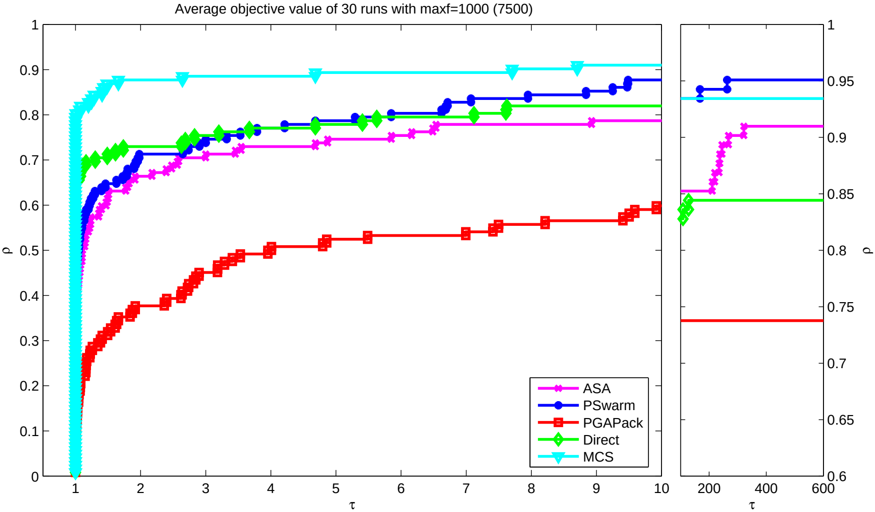
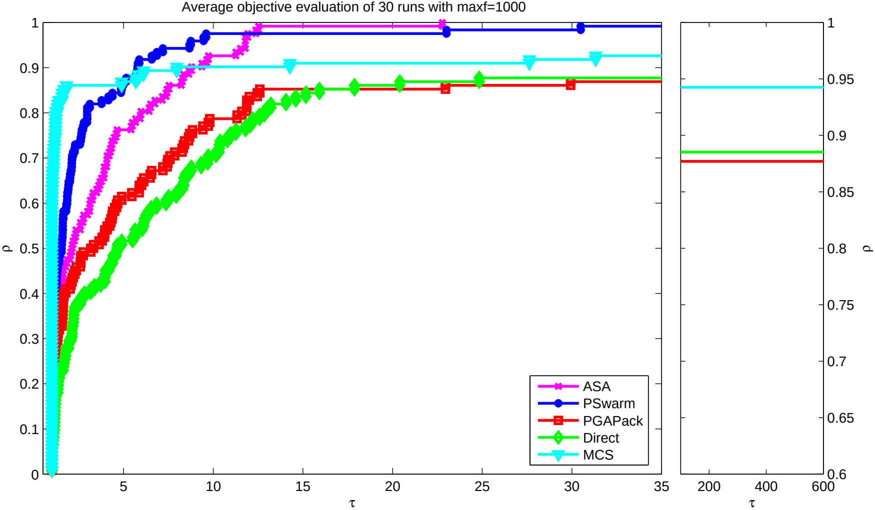
Average objective value



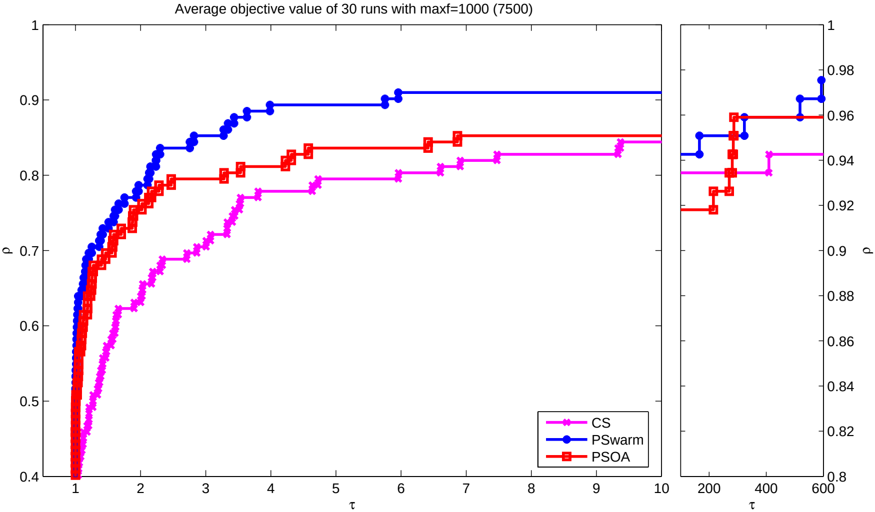
Average of objective function evaluations



Average number of objective function evaluations

$maxf$	ASA	PGAPack	PSwarm	Direct	MCS
1000	857	1009*	686	1107*	1837*
10000	5047	10009*	3603	11517*	4469

Coordinate search *vs* Particle swarm *vs* PSwarm



For further details see Vaz and Vicente, JOGO, 2007

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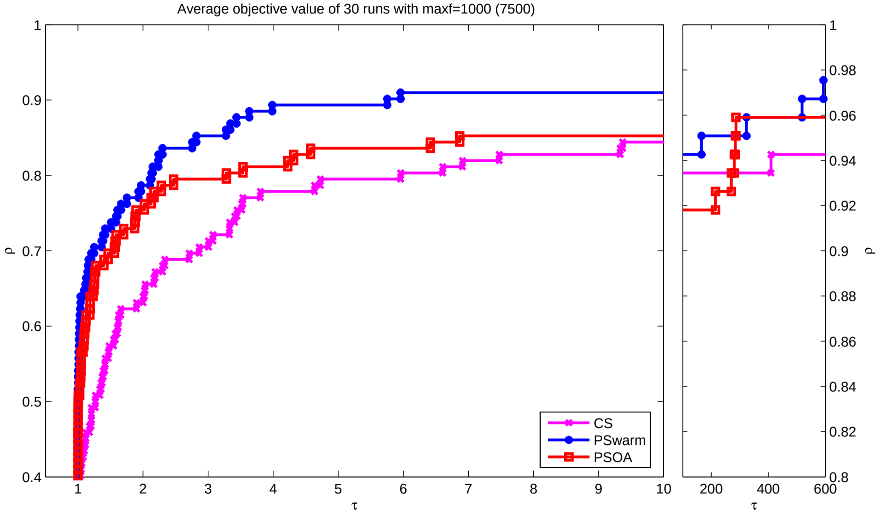

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Outline

Problem formulation

The problem we are now addressing is:

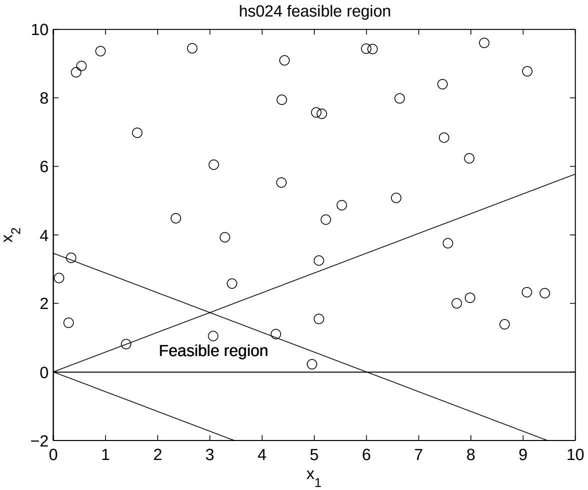
Problem definition - bound and linear constraints

$$\begin{aligned} \min_{z \in \mathbb{R}^n} \quad & f(z) \\ \text{s.t.} \quad & Az \leq b, \\ & \ell \leq z \leq u, \end{aligned}$$

where A is a $m \times n$ matrix, b is a m column vector and $\ell \leq z \leq u$ are understood componentwise.

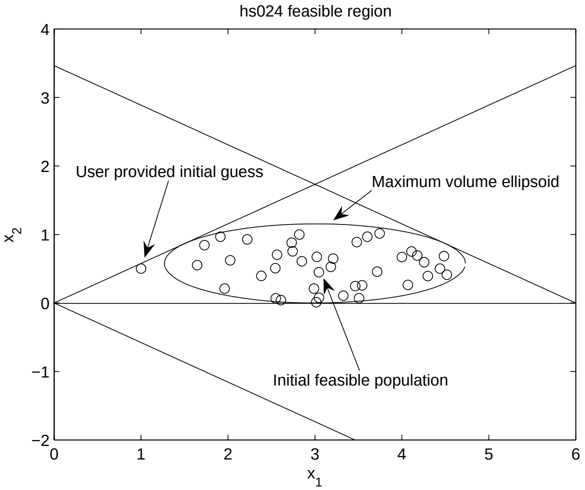
Feasible initial population

Obtaining an initial feasible population and controlling feasibility in the linear constrained case is critical.



Feasible initial population

Getting an initial feasible population allows a more efficient search for the global optimum.



Zhang and Gao interior-point code is being used to compute the maximum volume ellipsoid.

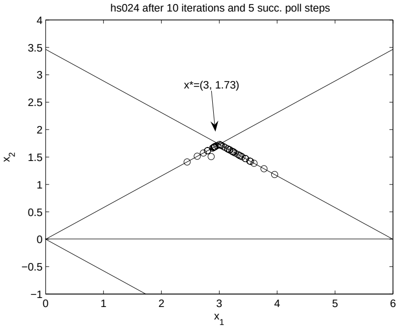
Search step (Particle Swarm)

Feasibility is kept during the optimization process for all particles. This is achieved by introducing a maximum allowed step in the "search" direction.

Maximum allowed step

$$x^p(t+1) = x^p(t) + \alpha_{max} v^p(t+1),$$

where α_{max} is the maximum step allowed to keep $x^p(t+1)$ inside the feasible region.



Poll step

For the coordinate search method applied to bound constrained problems it is sufficient to initialize the algorithm with a feasible initial guess $(y(0) \in \Omega)$ and to use $\hat{f}$ as the objective function.

Penalty/Barrier function

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

Linear constraints

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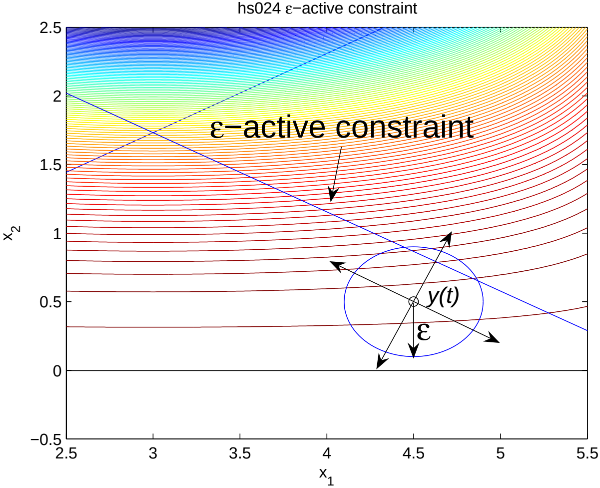
Positive generators for the tangent cone

The set of polling directions needs to conform with the geometry of the feasible set.



Positive generators for the tangent cone

No ϵ-active constraints

The positive spanning set is the maximal positive basis $D_{\oplus}$.

For ϵ-active constraint(s)

The polling directions are the positive generators for the tangent cone of the ϵ-active constraints (obtained by QR factorization)

Degeneracy

The ϵ parameter is dynamically adapted when degeneracy in the ϵ-active constraints is detected. If no success is attained the maximal positive basis is used.

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- 23 linear, 55 quadratic and 32 general nonlinear.
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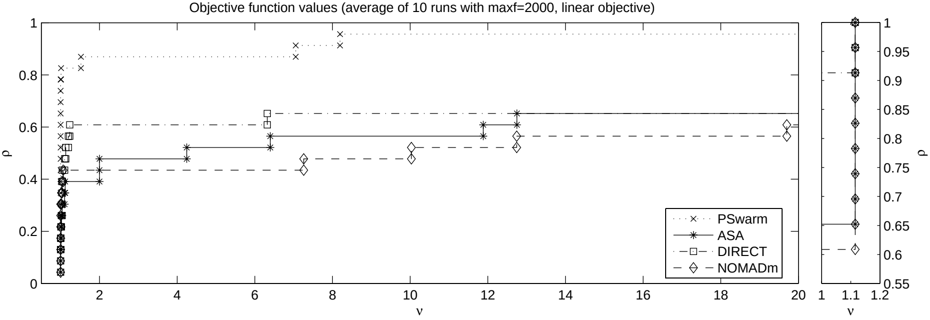
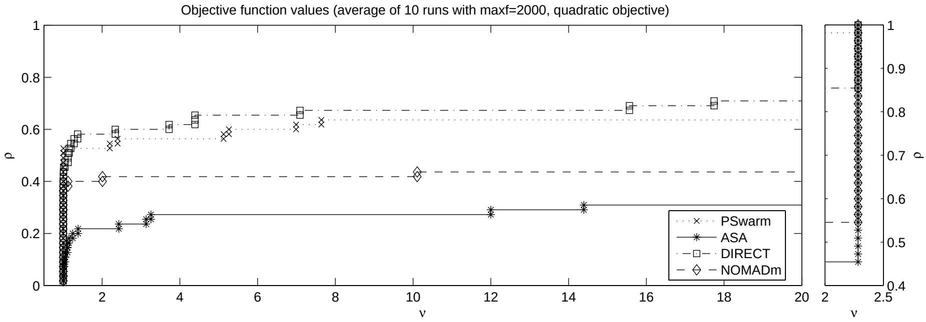
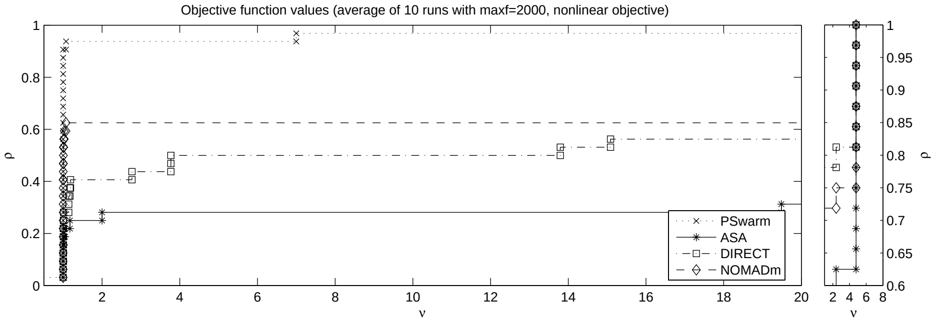


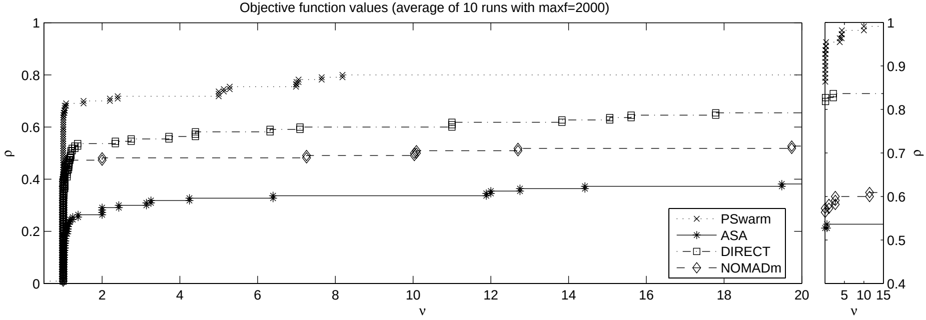
Quadratic objective functions



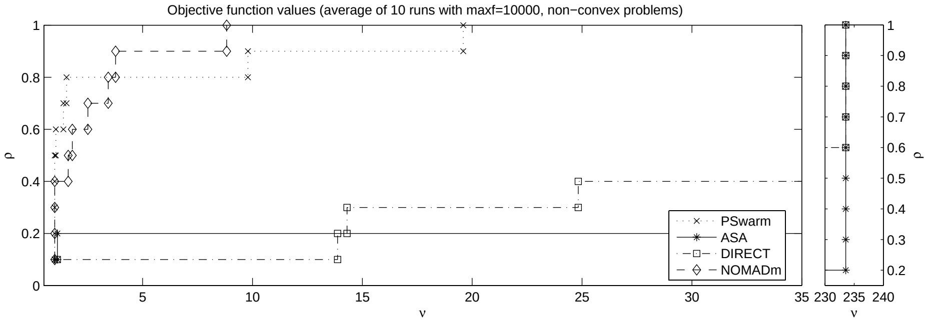
General nonlinear objective functions



All objective functions



Highly non-convex objective functions



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- PSwarm shown to be a robust and competitive solver.

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The problem

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To determine a set of stellar parameters (that define the star internal structure and evolution) from observable information.

Set of parameters to be determined

- M — stellar mass (relative to Sun mass $M_{\odot}$).
- X — abundance of hydrogen ($\%$).
- Y — abundance of helium ($\%$).
- Z — abundance of other elements ($Z = 100\% - X - Y$).
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Observable data from spectrum analysis

- t_{eff} — stellar surface temperature.
- lum — total stellar luminosity.
- $\left(\frac{Z}{X}\right)$ — relation between the abundance of other elements and hydrogen.
- g — surface gravity (less accurate).

Parameters and observable data for Sun

$M = 1$ and $t = 4.6$Gyr, with $t_{eff} = 5777$, $lum = 1$ and $Z/X = 0.0245$.

This information is only available for Sun.

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$$\min_{M,t,X,Y} \quad \left(\frac{t_{eff} - t_{eff,obs}}{\delta t_{eff,obs}}\right)^2 + \left(\frac{lum - lum_{obs}}{\delta lum_{obs}}\right)^2 + \left(\frac{\frac{1-X-Y}{X} - \left(\frac{Z}{X}\right)_{obs}}{\delta\left(\frac{Z}{X}\right)_{obs}}\right)^2 + \left(\frac{g - g_{obs}}{\delta g_{obs}}\right)^2$$

Given M, t and fixing X, Y (α and ov) the parameters t_{eff}, lum and g are computed by simulating (CESAM code) a system of differentiable equations.

The equations of internal structure are five: conservation of mass and energy, hydrostatic equilibrium, energy transport, production and destruction of chemical elements by thermonuclear reactions.

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Numerical results

Getting t_{eff}, lum and g – CESAM

t_{eff}, lum and g are computed by CESAM (Fortran 77 code), which is viewed as a black box function for the optimization process.

Optimization solver – PSwarm

PSwarm (C code).
Solver used with default options.

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Preliminary numerical results

Parallel approach

- Each objective function evaluation takes around 1 minute to compute (on a desktop computer). One day for a full algorithm run (serial).
- We tested 5 fake stars (in order to validate the approach) and 10 real stars.
- For each star we performed 28 runs. (28*15=420 days!).
- A parallel version was implemented using MPI-2. The Centopeia (University of Coimbra) and SeARCH (University of Minho) parallel platforms were used to obtain the numerical results.
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- About one day for 10 runs (parallel in 8 processors) — 42 particles with a maximum of 2000 o.f. evaluations.

Numerical results

Average obtained results (in Red) *vs* the real data.

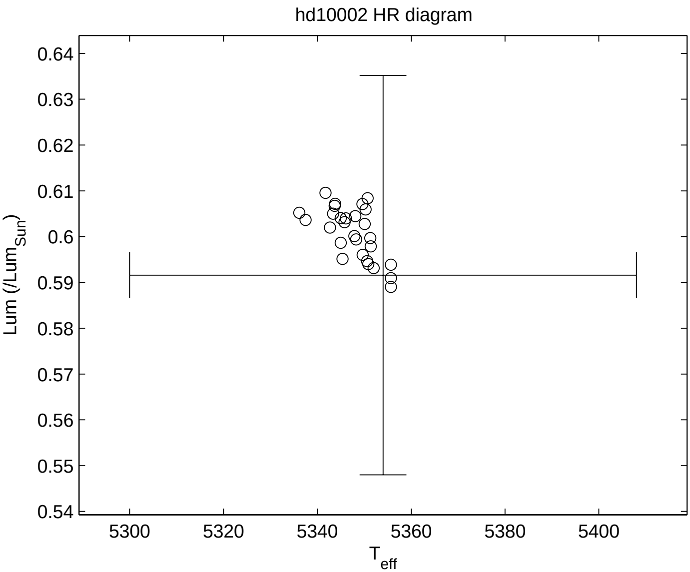
Star	M	t (Myr)	X	Y	α	ov	o.f. (average)
Sun	1.00	4600	0.715	0.268	1.63	0.00	
Sun	0.96	4691	0.68	0.31	1.55	0.265	0.272511931
fake1	0.85	1600	0.70	0.29	1.9	0.0	
fake1	0.84	2989	0.69	0.30	2.0	0.36	0.846046483
fake2	1.30	850	0.72	0.25	1.0	0.25	
fake2	1.20	4403	0.70	0.27	1.27	0.33	0.250562107
fake3	1.00	5000	0.68	0.30	0.7	0.15	
fake3	1.00	5499	0.68	0.30	0.72	0.28	0.209947500
fake4	0.70	5000	0.66	0.33	2.0	0.0	
fake4	0.71	3786	0.66	0.33	2.0	0.26	0.040181857
fake5	1.10	2500	0.62	0.36	1.4	0.3	
fake5	1.10	2956	0.62	0.36	1.57	0.22	0.232024714

Numerical results

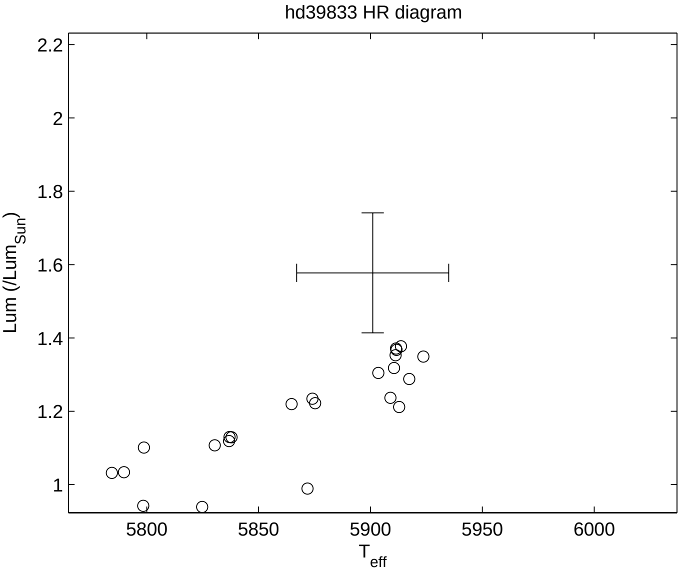
Average obtained results for real stars.

Star	M	t (Myr)	X	Y	α	ov	o.f. (average)
hd10002	0.87	5455	0.62	0.35	1.39	0.22	0.454073286
hd11226	1.12	3524	0.67	0.30	1.63	0.29	1.449135786
hd19994	1.28	2539	0.63	0.34	1.37	0.22	1.242964393
hd30177	1.02	5381	0.62	0.34	1.48	0.23	0.215747107
hd39833	1.24	1787	0.74	0.23	2.18	0.36	4.535001821
hd40979	1.08	3286	0.63	0.35	1.76	0.26	0.083869821
hd72659	1.18	4064	0.71	0.27	1.47	0.28	0.905840517
hd74868	1.26	2081	0.64	0.33	1.74	0.28	0.310089143
hd76700	1.15	4964	0.64	0.32	1.64	0.28	0.303584679
hd117618	1.09	4248	0.69	0.29	1.72	0.30	0.581501536

HR diagram with hd10002



HR diagram with hd39833



Further numerical results

Parallel approach

- A set of 193 stars was used (Stars belonging to spectral types F, G, or K).
- 25 runs were made for each star ($193 \times 2000 \times 25 = 18.40$ years computational time in parallel).
- The runs with objective function value greater than 1 were considered unsuccessful.
- Stars with less than 5 successful runs were removed from the analysis.
- The Milipeia (University of Coimbra) parallel platform was used to obtain the numerical results.

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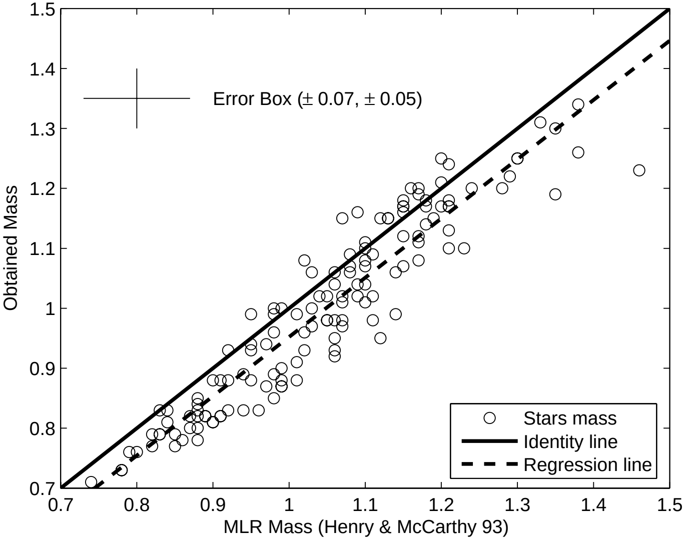
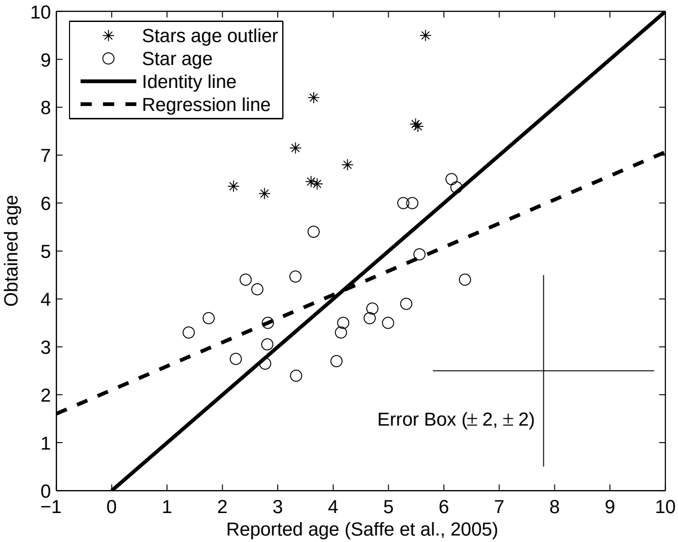
Further numerical results

MLR - Mass-luminosity relation.



Further numerical results



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The end

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