Coupling C-GRASP with Direct Search methods

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1. Context

Unconstrained Global Optimization

Unconstrained Global Optimization is the problem of minimizing non-linear functions $f : S \rightarrow \mathbb{R},\ S \subset \mathbb{R}^n$ where the variables are only subject to bound constraints :

$$\begin{array}{ll} \min & f(x) \\ \text{s.t} & l_i \leq x_i \leq u_i \quad \forall i \in \{1, \cdots, n\} \end{array}$$

We can assume that:

- f is probably non convex and/or multi-modal and/or non smooth.
- a call to the evaluation of f is computationally expensive.
- the gradient can be unusable: maybe it does not exist, is not known or is too expensive.

We will focus on global methods with a preference on stochastic and gradient-free ones.

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1. Context

Overview of the literature

Direct Searches are gradient-free methods investigated in the 50's - 60's:

- Nelder-Mead (or Simplex Search) [NM65].
- Hooke and Jeeves (or Pattern Search) [HJ61].

Metaheuristics are now most commonly studied:

- Neighborhood-based (SA [HF02, HF04], TS [CS00b, CS05, HF03b], GRASP [HRP10]).
- Population-based (GA [Ped96, CS00a, CS03, HF03a], ACO [SD08], PSO [VV07], SS [LM05]).

Recently, there is a growing interest in hybridizing metaheuristics with Direct Search methods:

- SA [HF02, HF04]
- TS [CS05, HF03b]
- GA [CS03, HF03a]
- PSO [VV07]

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1. Context

Motivation

One of our needs is to find a good metaheuristic to use as a bound in an interval Branch & Bound method to solve global optimization problems. This metaheuristic shall be:

- efficient. It can give good approximations in a reasonable number of function evaluations.
- easy to tune in order not to increase the tuning difficulty of the whole method.
- gradient-free but with the possibility to easily include efficient procedures using the gradient.

We have selected a recent metaheuristic presenting these characteristics : C-GRASP from Hirsch and al [HMPR06, HRP10].

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2. C-GRASP

Presentation

Profile of the method:

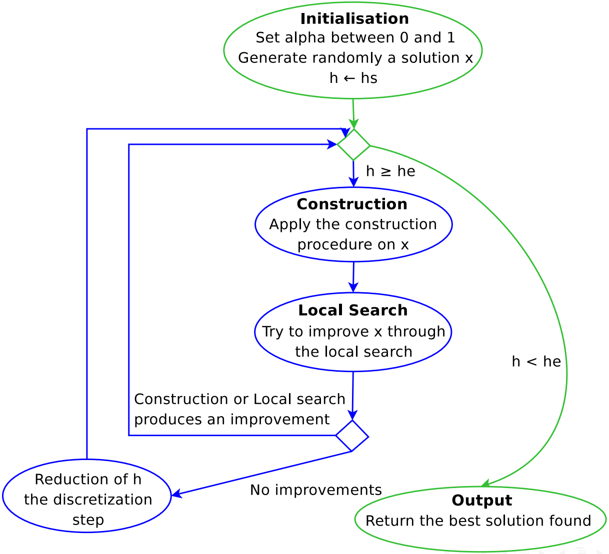
- Stochastic.
- Multi-start.
- Neighborhood-based.

C-GRASP is the extension of GRASP from Feo and Resende [FR95] to continuous non-linear problems.
The main points of the method are:

- to construct a solution through a greedy-randomized procedure. A parameter $\alpha \in [0, 1]$ controls the degree of randomness.
- to improve the solution with a local search method.
- to control the neighborhood density and distance of both procedures by a discretization step $h \in [h_e, h_s]$.

2. C-GRASP

The algorithm



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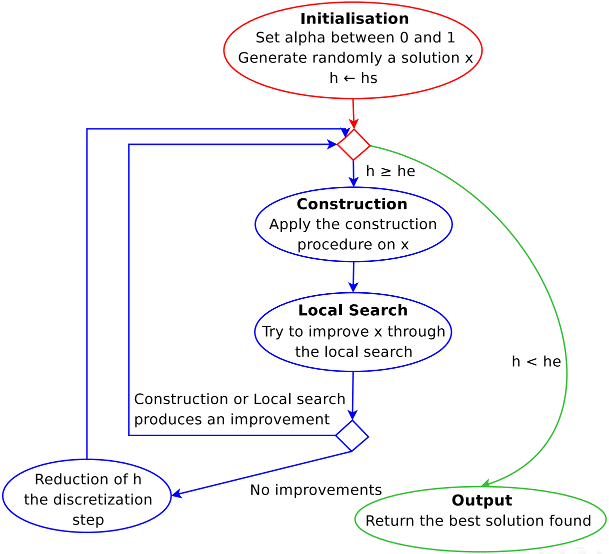

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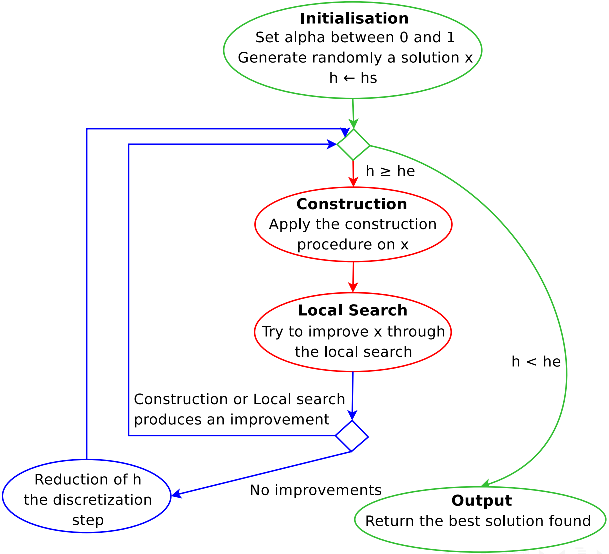

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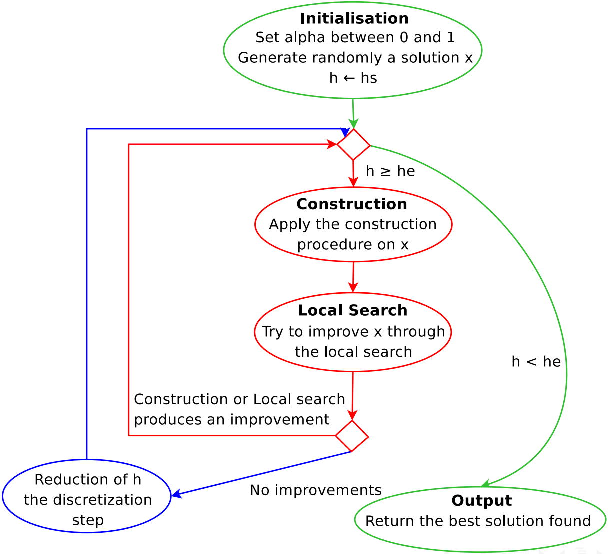

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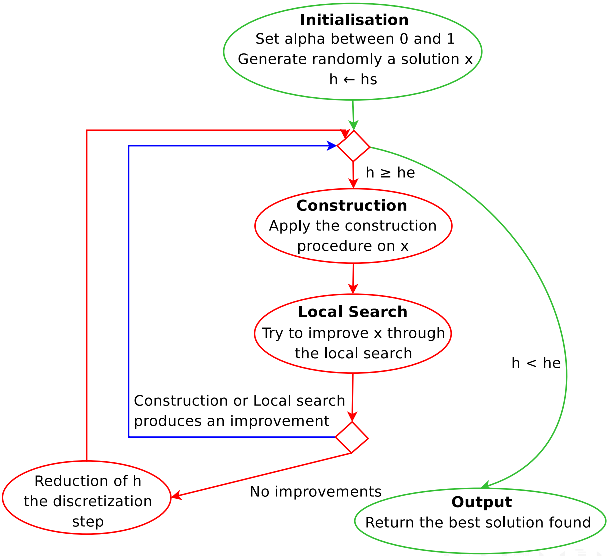

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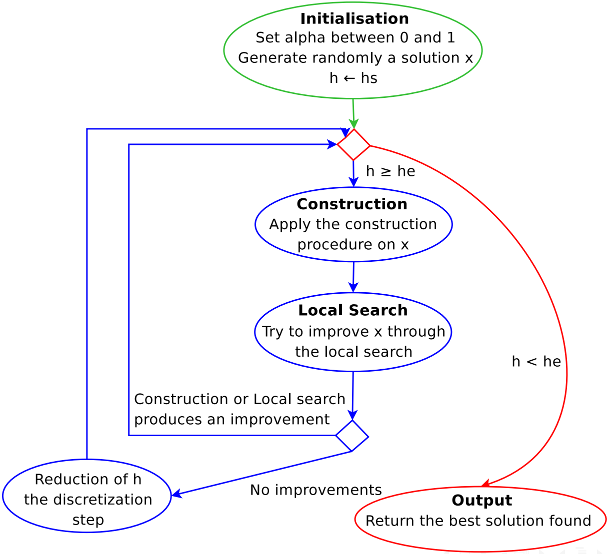

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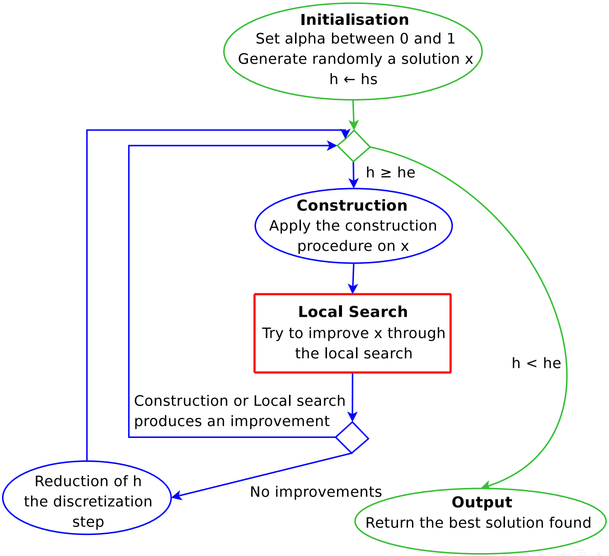

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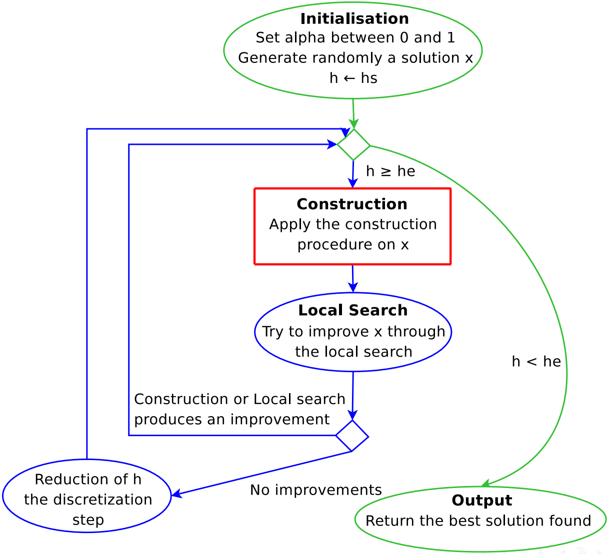
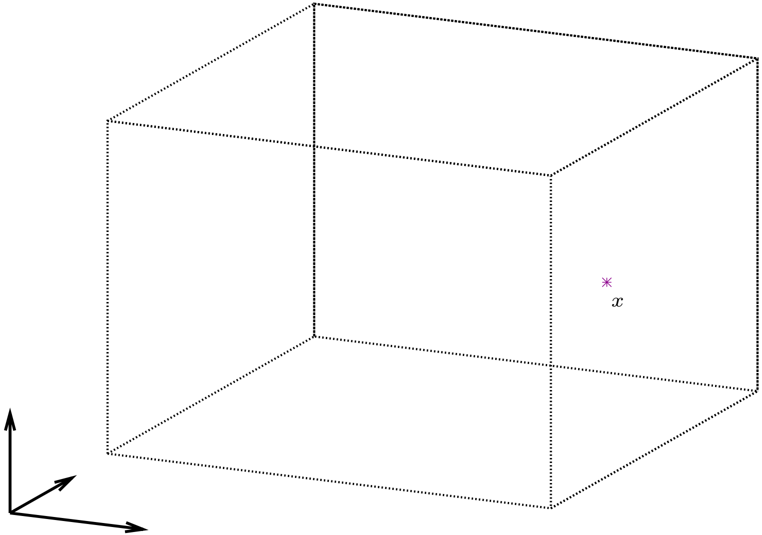


2. C-GRASP

Construction procedure



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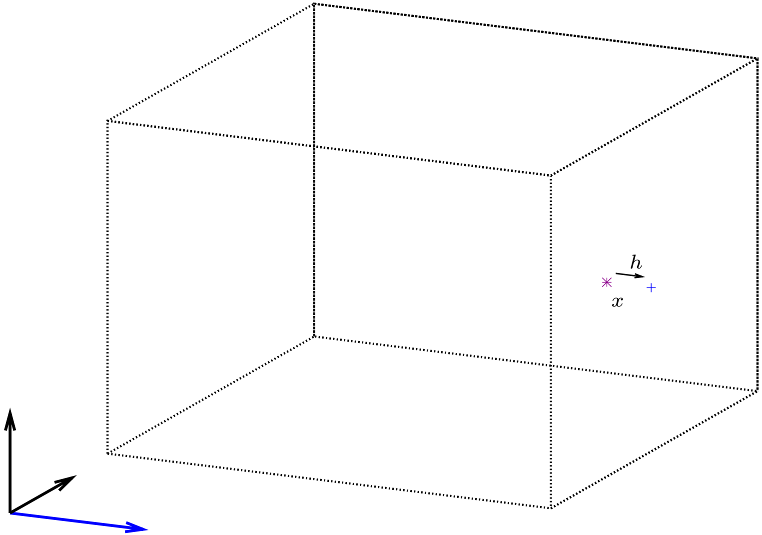

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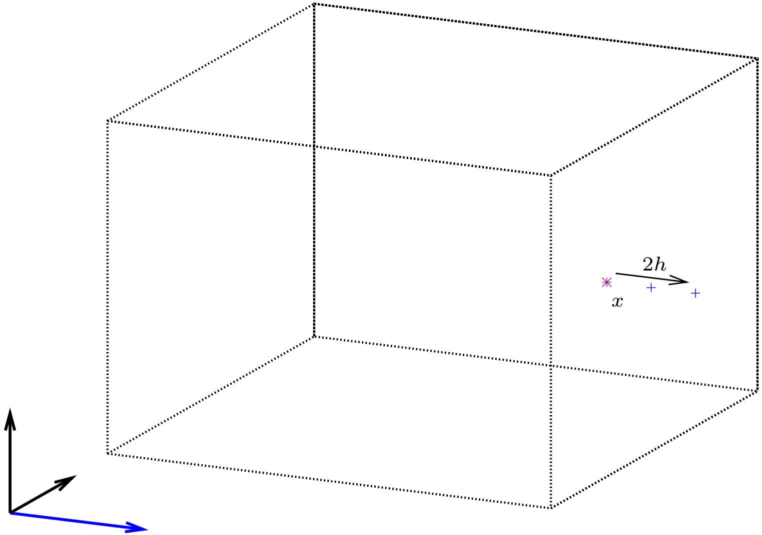

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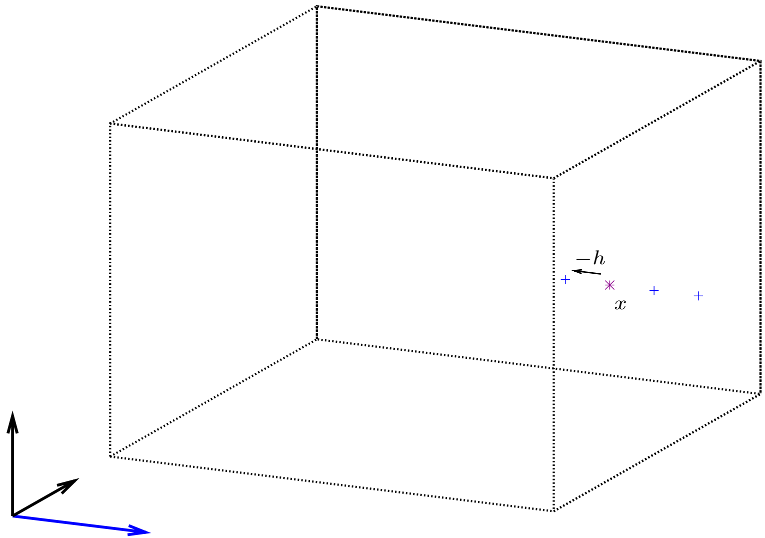

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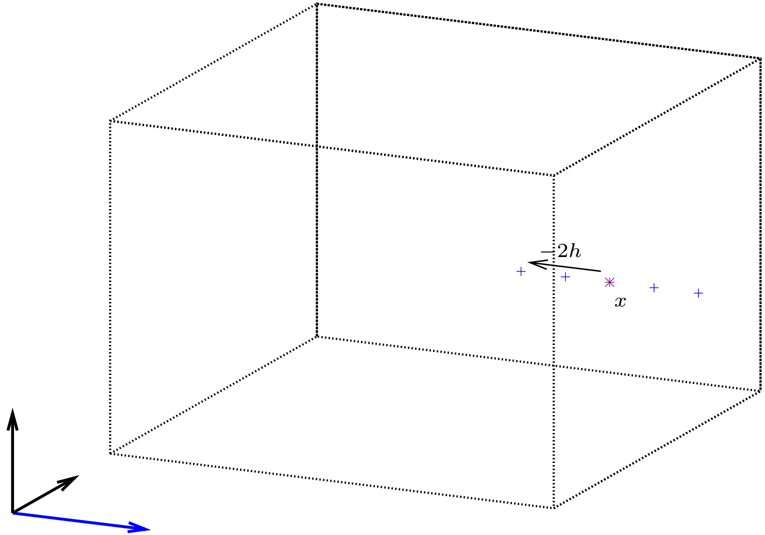

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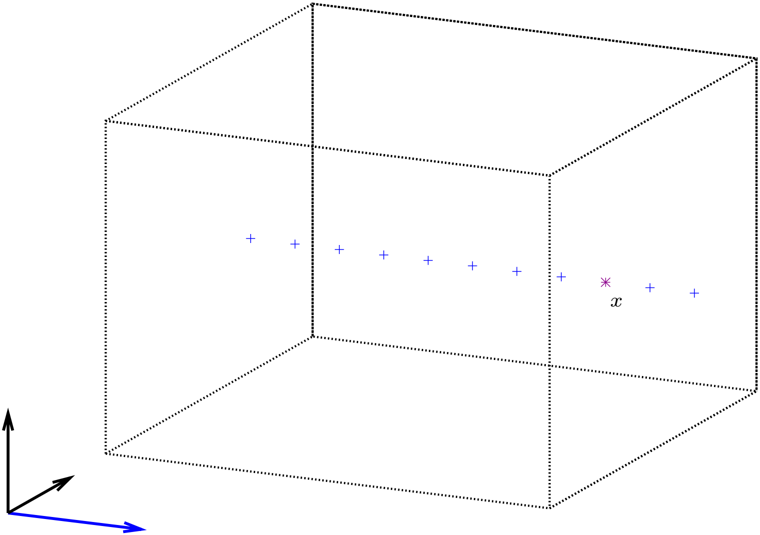

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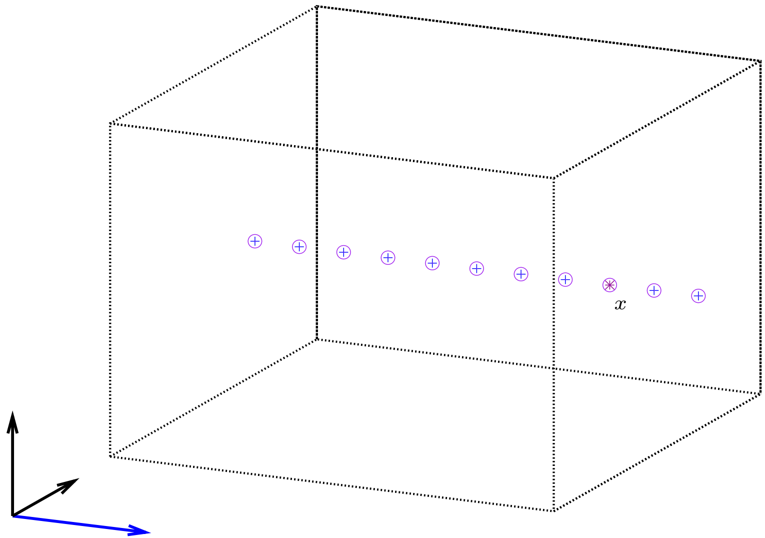

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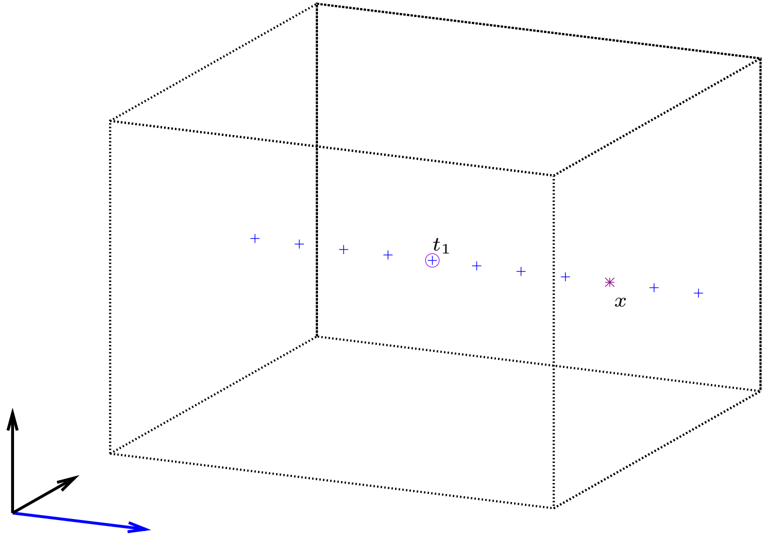

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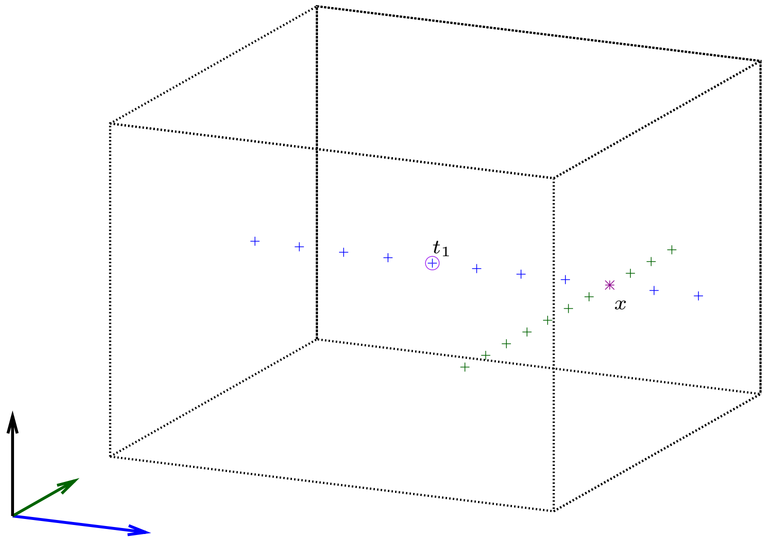

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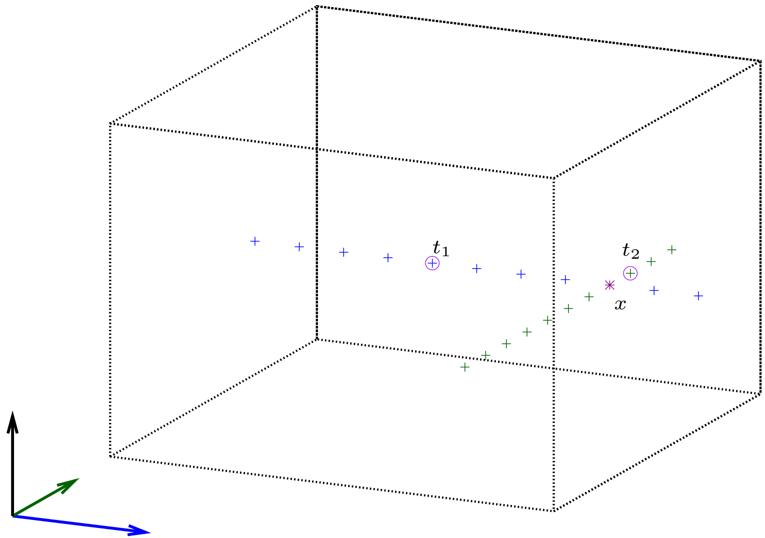

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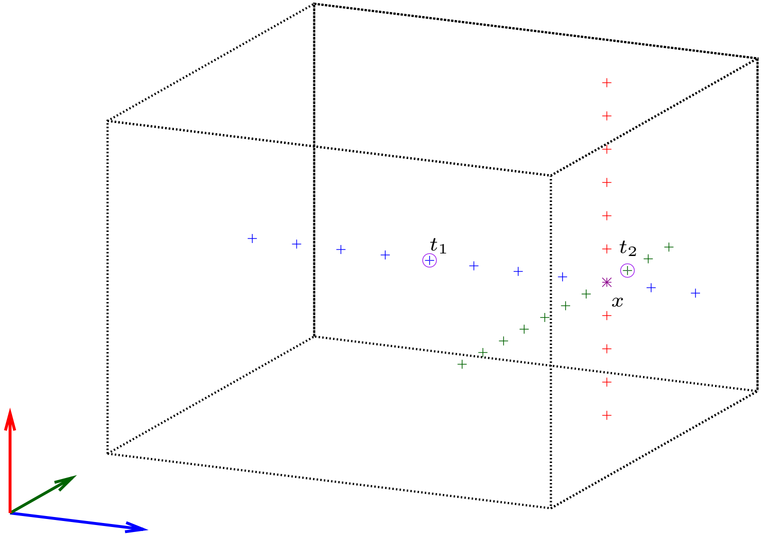

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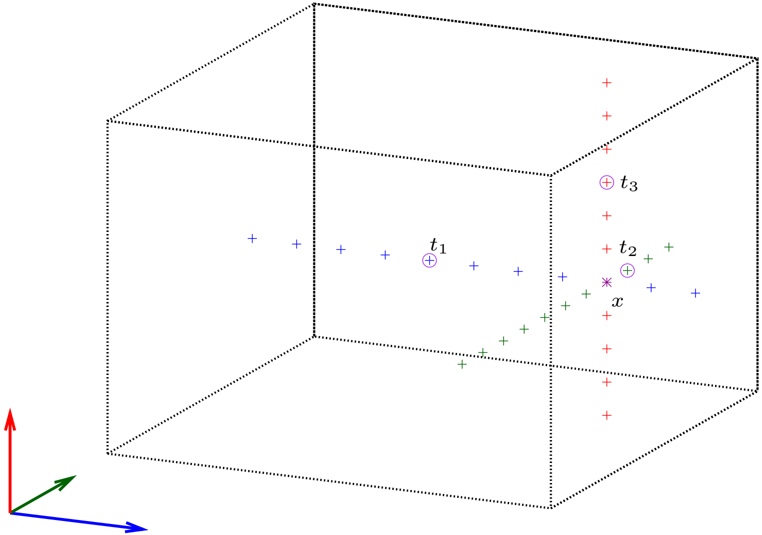
Construction procedure



2. C-GRASP

Construction procedure

Assuming we have $min = f(t_1) < f(t_2) < f(t_3) = max$, we define the set RCL like:

$$RCL = \{i | f(t_i) \leq min + \alpha * (max - min)\}$$

Suppose that $f(t_1) = min = -1$, $f(t_2) = -0.5$, $f(t_3) = max = 0$ and α is set to 0.5.
Thus, $RCL = \{i | f(t_i) \leq -0.5\} = \{1, 2\}$.
Select randomly an element of the RCL, for example 2. Then for the next iteration of the construction procedure:

- $x \leftarrow t_2$
- the second direction (green one) will not be checked.

Stopping criterion:

- no more directions to check.

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2. C-GRASP

Proposition

C-GRASP is a quite efficient method able to deal with a wide variety of problems.

But compared to other efficient metaheuristics, C-GRASP:

- need first a little more computation efforts before reaching good approximations (not very efficient in a short term vision).
- have some difficulty to converge fast to very precise solutions.

Thus, our purpose is to improve C-GRASP:

- by the use of new strategies (exploration / intensification, seeding of the search space).
- by hybridizing it with Direct Search methods.

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3. Proposed Approach

Proposition

Pre-optimization:

(1) Seeding of the search space. Similar to the initialisation method of the Scatter Search [LM05].

Construction procedure:

(2) Stopping mechanism of the construction procedure to avoid potentially non-improving call to it.

(3) New line search for the construction procedure, reducing its cost while *h* decreases.

Local improvement procedure:

(4) Use of the Direct Search Nelder-Mead as local improvement procedure: it has shown good results when used inside a multi-start method [Ped07].

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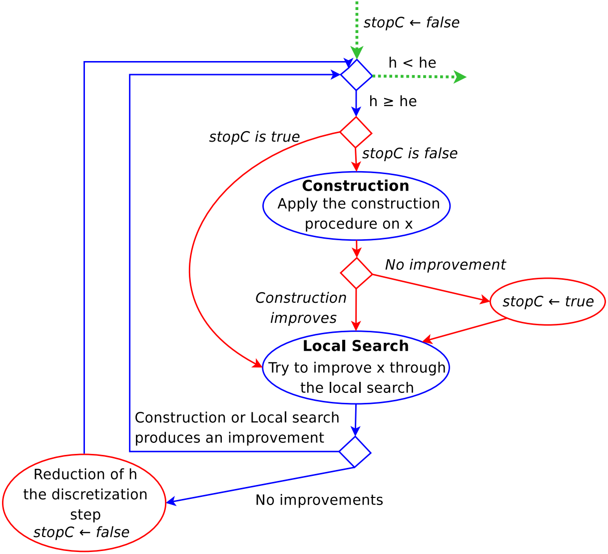
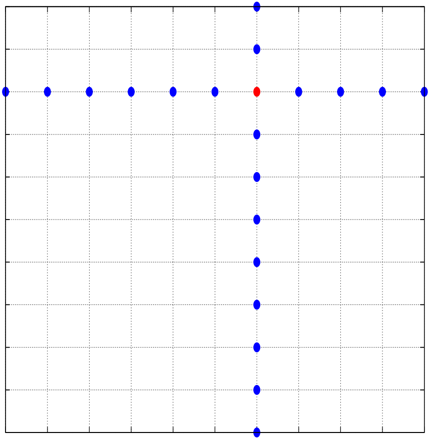
3. Proposed Approach

Construction's stopping mechanism (2)



3. Proposed Approach

New construction (3)



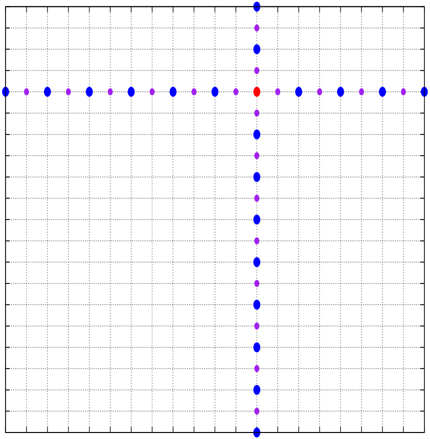
Considering the classic construction procedure at a given *h*.
20 points to evaluate (10 per directions).

3. Proposed Approach

New construction (3)

Decreases the value $h \leftarrow \frac{h}{2}$:

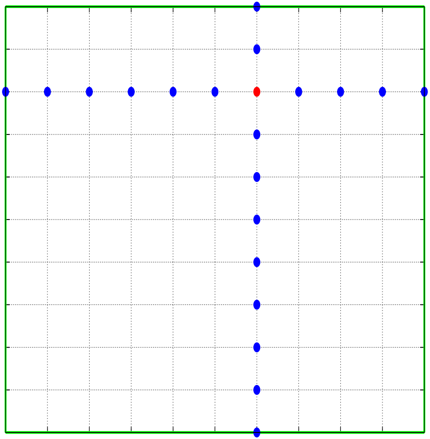
The construction method needs more evaluations (40 evaluations).



3. Proposed Approach

New construction (3)

Considering the **new** construction procedure at a given *h*.
A window correspond to the whole search space.
20 points to evaluate (10 per directions).



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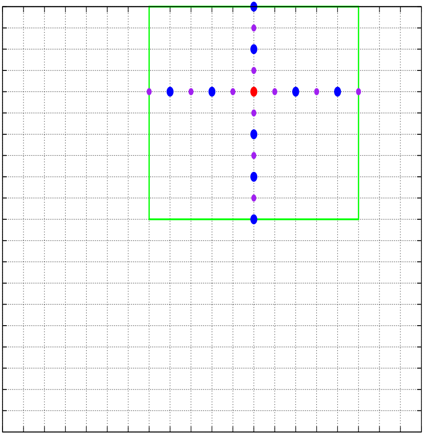
3. Proposed Approach

New construction (3)

Decreases the value $h \leftarrow \frac{h}{2}$
Decreases the window the same way as h:

> the new construction needs a constant number of evaluations (20 evaluations).



4. Experiments

Protocols

Two different experiments:

(1) Consumption of function evaluations for a given precision.
(2) Overall precision within a given number of function evaluations.

We compare the Hybrid C-GRASP with other metaheuristics:

- C-GRASP [HRP10].
- DTS_{APS} [HF03b].
- Scatter Search [LM05].

Results for these methods are taken from their respective papers.

Benchmark Functions ▶▶|

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4. Experiments

First experiment

Experiments over 14 simple functions : dimensions between 2 and 10.
100 runs performs on each function.
The algorithm is stopped when:

$$|f(x^*) - f(\hat{x})| < 10^{-4} * |f(x^*)| + 10^{-6}$$

If this condition is satisfied, the problem is said to be solved.
The results report:

- the % of successful runs.
- the average number of function evaluations over the successful runs.

4. Experiments

First experiment

		C-GRASP	DTS_{APS}	Hybrid C-GRASP
BR	Success	**100**	**100**	**100**
	f. Eval	10,090	212	**139**
EA	Success	**100**	82	**100**
	f. Eval	5,093	**223**	973
SH	Success	**100**	92	**100**
	f. Eval	18,608	274	**172**
GP	Success	**100**	**100**	**100**
	f. Eval	**53**	230	312
$H_{3,4}$	Success	**100**	**100**	**100**
	f. Eval	1,719	438	**217**
$H_{6,4}$	Success	**100**	83	**100**
	f. Eval	29,894	**1,787**	2,200

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First experiment

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$S_{4,5}$	Success	**100**	75	**100**
	f. Eval	9,274	**819**	4,157
$S_{4,7}$	Success	**100**	65	99
	f. Eval	11,766	**812**	5,963
$S_{4,10}$	Success	**100**	52	99
	f. Eval	17,612	**828**	6,857
R_2	Success	**100**	**100**	**100**
	f. Eval	23,544	**254**	400
R_5	Success	**100**	85	**100**
	f. Eval	182,520	**1,684**	1,773
R_{10}	Success	**100**	85	**100**
	f. Eval	725,281	**9,037**	17,703
Z_5	Success	**100**	**100**	**100**
	f. Eval	12,467	1,003	**549**
Z_{10}	Success	**100**	**100**	**100**
	f. Eval	2,297,937	**4,032**	4,776

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4. Experiments

Second experiment

Experiments over 40 standard benchmark functions: from 2 to 30 dimensions.
100 performs on each function.
Tune of h_s and h_e relative to the data (search spaces).

A *GAP* measure is defined as follows:

$$GAP = |f(x^*) - f(\hat{x})|$$

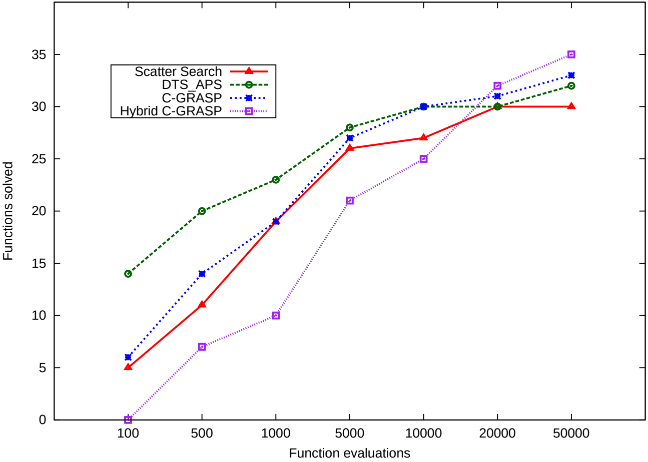
We consider a problem solved if:

$$GAP \leq \begin{cases} 0.001 * |f(x^*)| & \text{if } f(x^*) \neq 0 \\ 0.001 & \text{if } f(x^*) = 0 \end{cases}$$

The maximum number of funtions evaluations is set to $50,000$.
Numerical results are average sum of GAP values of all the 40 functions over 100 runs.

4. Experiments

Second experiment



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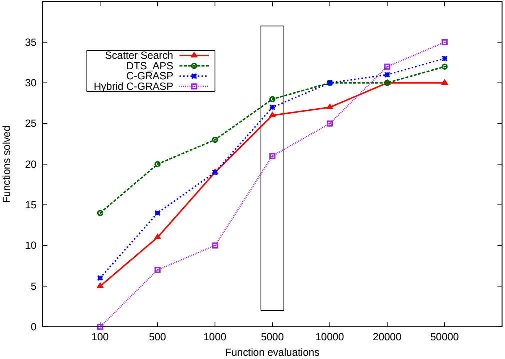
4. Experiments

Second experiment



Method	Function Evaluations 5,000
Scatter Search	4.96
DTS_{APS}	**4.22**
C-GRASP	6.20
Hybrid C-GRASP	4.722

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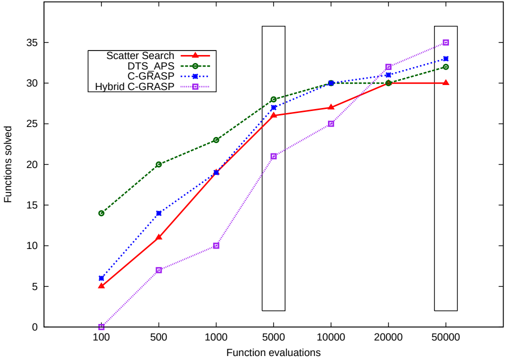
4. Experiments

Second experiment



Method	Function Evaluations 5,000	50,000
Scatter Search	4.96	3.46
DTS_{APS}	**4.22**	1.29
C-GRASP	6.20	3.02
Hybrid C-GRASP	4.722	**0.028**

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5. Conclusion

Discussion

The Hybrid C-GRASP:

- has a small cost in order to get very precise solutions with good guarentee of success on easy functions (First experiments).
- is robust: no particular difficulty or ease to solve a wide variety of functions (Second experiments).

But some drawbacks remain:

- need more computational effort before getting interesting solutions (Second experiments).
- have some difficulty to deal with high dimensional problems (as it is known for Direct Search methods).

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5. Conclusion

Perspectives

Future work:

- study of new strategies. The construction procedure still needs to be improved (Hirsch [Hir06] proposed some ideas).
- incorporation of stopping rules in order to get a true multi-start procedure.
- a more complete benchmark of the different methods, in order to know if some are better suited in some situations or not.
- integration of the method inside a rigorous B & B algorithm.

Further possible study:
Hybridization of the Scatter Search [LM05] with the Hybrid C-GRASP. It seems to be a promising idea to combine the respective behaviors of the two methods.

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Appendices

Nelder-Mead

We have studied different Direct Searches to use with C-GRASP, we have selected Nelder & Mead [NM65].

We use this method instead of the classical local improvement procedure. The method consist of:

- generate n new points around x at distance h.
- the set of $n+1$ points (x + n new points) is called *simplex*.
- we try to improve the *simplex* by performing geometric modifications, modifying the worst point.

Stopping criterion:

- number of call to the evaluation of the function.
- the difference between the evaluation of the best and worst points of the *simplex*.

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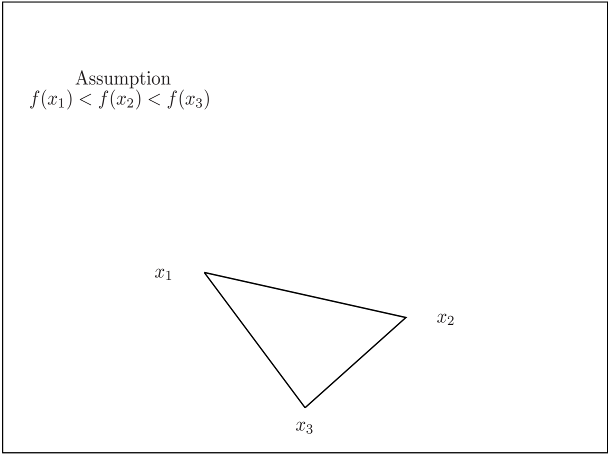
Appendices

Nelder-Mead



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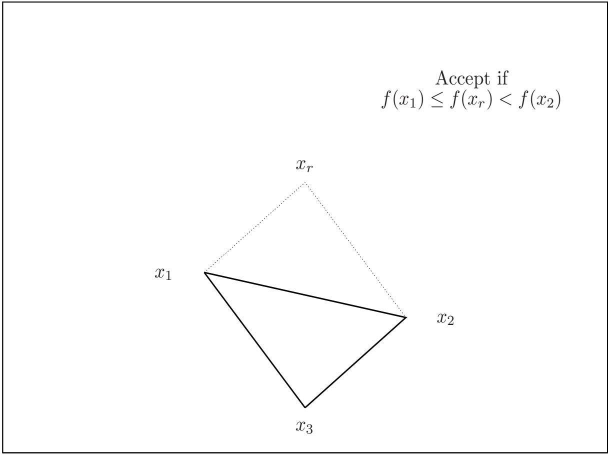
Nelder-Mead



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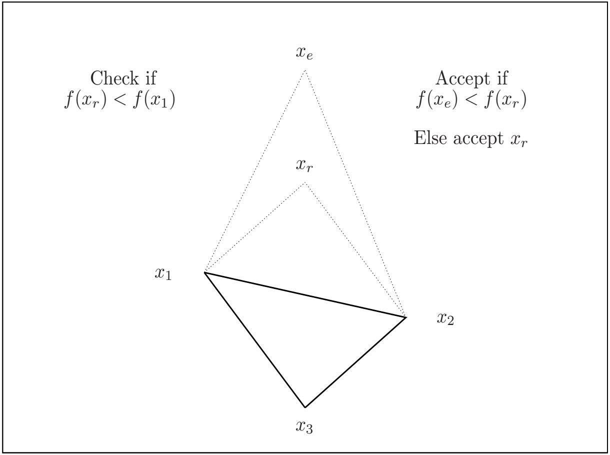
Nelder-Mead



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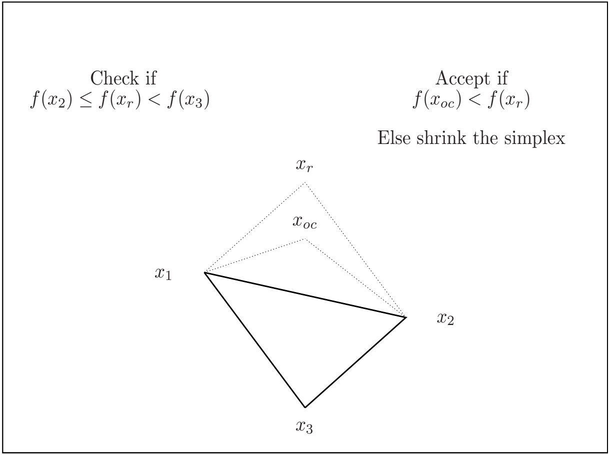
Nelder-Mead



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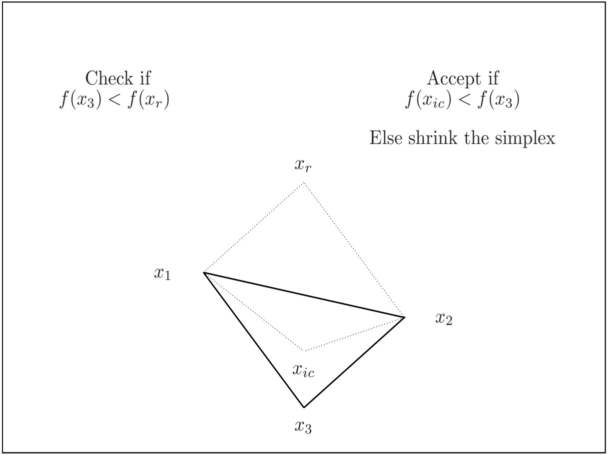
Nelder-Mead



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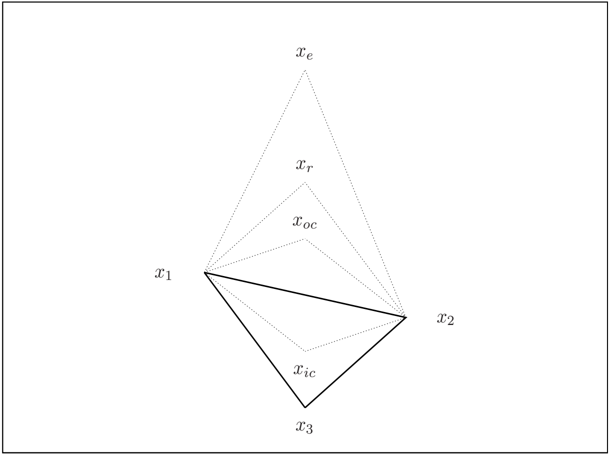
Nelder-Mead



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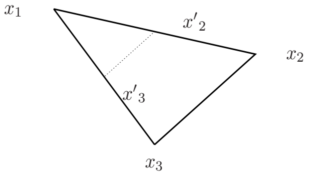
Nelder-Mead

No points accepted → shrinkage



Appendices

Benchmark Functions

Function	Dimension	Function	Dimension
Six-Hump Camelback (CA)	2	Beale (BE)	2
Bohachevsky (B_2)	2	Boole (BO)	2
Branin (BR)	2	**Easom** (EA)	2
Goldstein and Price (GP)	2	Matyas (M)	2
Rosenbrock (R_2)	2	Schwefel (SC_2)	2
Shubert (SH)	2	**Zakharov** (Z_2)	2
De Joung (SP_3)	3	**Hartmann** ($H_{3,4}$)	3
Colville (CV)	4	Perm$_0$ $P^0_{4,10}$	4
Perm ($P_{4,\frac{1}{2}}$)	4	Power Sum ($PS_{4,\{8,18,44,114\}}$)	4
Shekel ($S_{4,5}$)	4	**Shekel** ($S_{4,7}$)	4
Shekel ($S_{4,10}$)	4	**Rosenbrock** (R_5)	5
Zakharov (Z_5)	5	**Hartmann** ($H_{6,4}$)	6
Schwefel (SC_6)	6	Trid (T_6)	6
Griewank GR_{10}	10	Rastrigin (RA_{10})	10
Rosenbrock (R_{10})	10	Sum Squares (SS_{10})	10
Trid (T_{10})	10	**Zakharov** (Z_{10})	10
Griewank GR_{20}	20	Rastrigin (RA_{20})	20
Rosenbrock (R_{20})	20	Sum Squares (SS_{20})	20
Zakharov (Z_{20})	20	Powell (PW_{24})	24
Dixon and Price (DP_{25})	25	Ackley (A_{30})	30
Levy (L_{30})	30	Sphere (SP_{30})	30

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Appendices

First experiment

Parameters are:

- $\alpha = 0.4$.
- Maximum number of starts: 20.
- Number of generated solutions with the seeding strategy: $min(10 * n, 100)$.
- Nelder-Mead stopping criterion:
  - $100 * n$ function evaluations.
  - $|f(x_1) - f(x_{n+1})| < 10^{-6}$.

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Appendices

First experiment

h_s and h_e:

Function	h_s	h_e	Function	h_s	h_e
SH	1	0.01	EA	10	0.02
GP	0.4	0.004	BR	1	0.005
$H_{3,4}$	0.1	0.001	$H_{6,4}$	0.1	0.001
$S_{4,5}$	1	0.002	$S_{4,7}$	1	0.002
$S_{4,10}$	1	0.002	R_2	1	0.01
R_5	1	0.01	R_{10}	1	0.01
Z_5	1.5	0.015	Z_{10}	1.5	0.015

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Appendices

Second experiment

Parameters:

- $\alpha = 0.4$.
- h_s is a percentage of the input box range, value set to 10%.
- h_e is a percentage of the input box range, value set to 1%.
- Number of generated solutions with the seeding strategy: $min(10 * n, 100)$.
- Nelder-Mead stopping criterion:
  - $100 * n$ function evaluations.
  - $|f(x_1) - f(x_{n+1})| < 10^{-6}$.

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