Combining Interval Methods with Evolutionary Algorithms for Global Optimization

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1. Global optimization methods
   - Interval methods
   - Evolutionary algorithms

2. Charibde: a cooperative hybrid solver
   - Hybrid metaheuristics
   - Architecture of Charibde

3. Experimental results
   - Benchmark of difficult constrained problems
   - New optimality results for multimodal functions
   - Molecular dynamics: an open problem
   - Aeronautical application: conflict resolution

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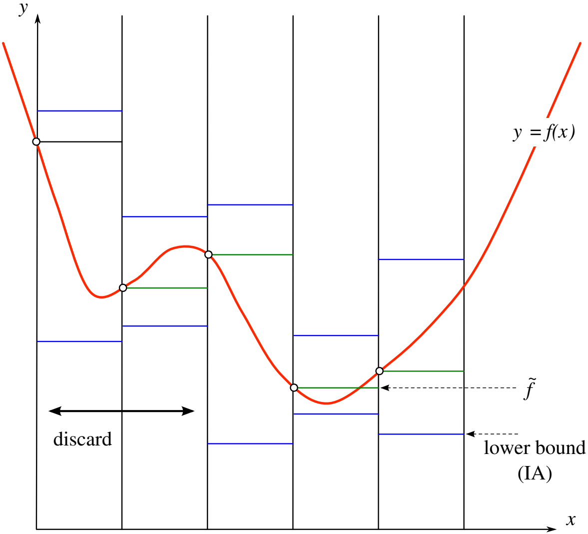
Interval branch and bound framework (IB&B)

Computation of **guaranteed lower bounds** in B&B



Interval branch and bound framework (IB&B)

Non-uniform search

- best upper bound $\tilde{f} = \overline{F(\tilde{x})}$ of global minimum x^*
- If $\tilde{f} \leq \underline{F(X)}$, discard X
- otherwise store in priority queue $\mathcal{L}$
  - exploration strategy: breadth first, best first, depth first

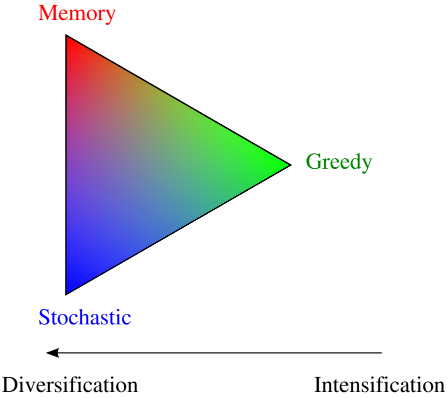
In n dimensions

- dichotomy variable after variable
- iterate until required precision ϵ on image
- **exponential** complexity $\Rightarrow$ n small

Metaheuristics

Metaheuristics combine memory, greedy search and/or stochastic search

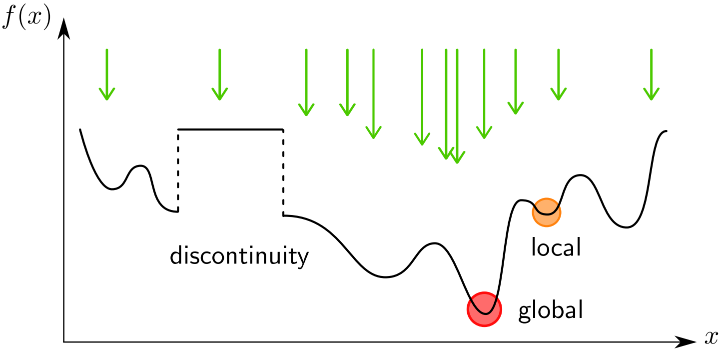
- do not require specific properties on f (black box)
- single (pattern search, simulated annealing) or multiple solutions (EA)
- costly methods, **no guarantee of optimality**



Evolutionary algorithms

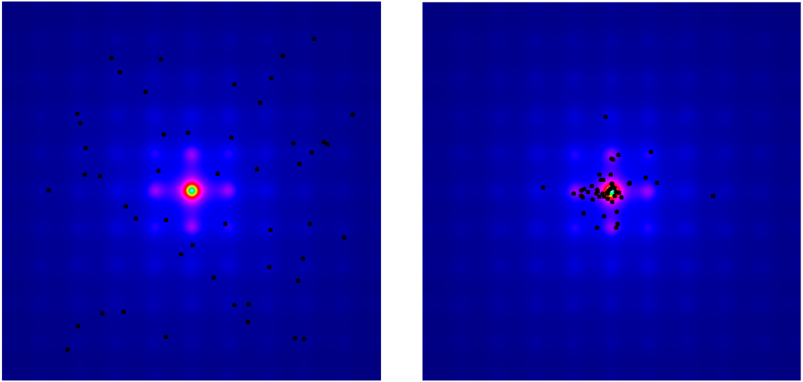
Evolutionary algorithms are random walks guided by heuristics

- stochastic sampling of the search-space
- based on the theory of evolution (selection, crossover, mutation operators)
- iterative improvement of a population of individuals x_i
- adaptation criterion (fitness) $f(x_i)$



Evolutionary algorithms

Genetic algorithm [Holland, 1975], differential evolution [Storn and Price, 1997]



Initial population

After 50 iterations

Figure: DE on Griewank function ($n = 2$), 50 individuals

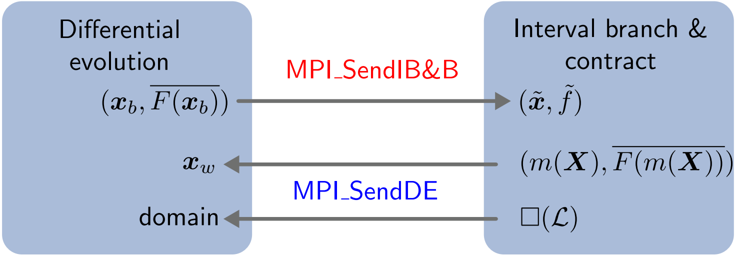
Hybrid metaheuristics

Hierarchical classification of hybrid methods (metaheuristic + exact method)

- integrative (low-level) approaches
  - metaheuristic is master
    memetic algorithms
  - metaheuristic is slave
    GA in IB&B [Zhang and Liu, 2007]
- cooperative (high-level) approaches
  - sequential execution (preprocessing)
    IB&B + GA [Sotiropoulos et al., 1997]
  - parallel execution
    BB // memetic algorithm [Gallardo et al., 2007]

Charibde: a new cooperative solver [Vanaret et al., 2013]

- cooperative ($\neq$ integrative) parallel hybridization, inspired by [Alliot et al., 2012]
- **fully reliable** $>$ complete (BARON, Couenne)



- differential evolution: efficient on continuous problems, few hyperparameters
- interval branch and contract: interleaves branching and filtering (constraint propagation)
- independent processes exchange bounds and solutions (MPI)

An advanced cooperation

IB&C exploration strategy

- extract from $\mathcal{L}$ the *farthest* box from $\tilde{\boldsymbol{x}}$ ($\sum$ of componentwise distances)
  - either $\tilde{\boldsymbol{x}}$ close to $\boldsymbol{x}^*$: fast local exploration by DE
  - or $\tilde{\boldsymbol{x}}$ far from $\boldsymbol{x}^*$: might as well search in area not reachable by DE
- postpone tedious interval search around $\boldsymbol{x}^*$, waiting for the best possible $\tilde{f}$
- adaptive heuristic: recompute priorities when $\tilde{\boldsymbol{x}}$ updated

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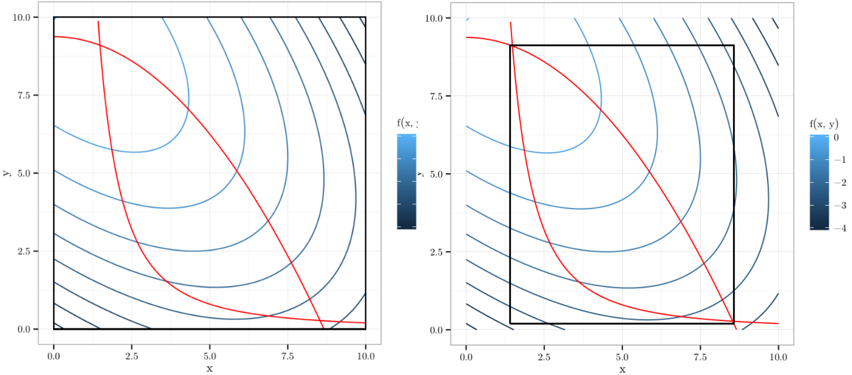
DE domain reduction operator

- restart of DE in smaller search-space
- IB&C maintains remaining boxes $\rightarrow$ take the hull!

$$
(\mathcal{P}) \quad \min_{(x,y)\in[0,10]^2} -\frac{(x+y-10)^2}{30} - \frac{(x-y+10)^2}{120}
$$

$$
\text{s.c.} \quad \frac{20}{x^2} - y \le 0
$$

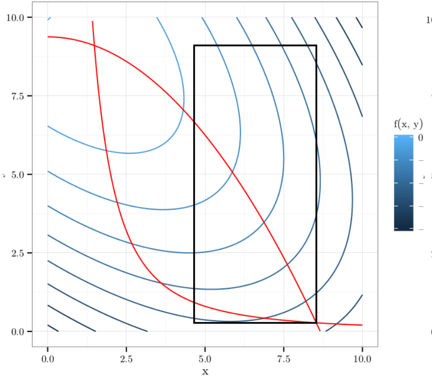
$$
x^2 + 8y - 75 \le 0
$$



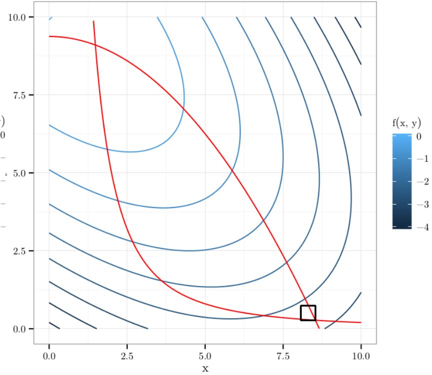
Initial domain

Initial domain (contracted)

Sporadically trigger MPI communication to send $\mathcal{L}$ to DE



After 10 generations



After 20 generations

Why does it work? The exploration strategy

- "peels off" domain from outside $\rightarrow$ boosts hull reduction
- maintains a low (≤ 200) number of boxes in $\mathcal{L}$
  - cheap MPI communication and hull operation ($O(|\mathcal{L}|)$)

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Benchmark of difficult constrained problems

Comparison of interval solvers

- difficult COCONUT problems selected by [Araya et al., 2012]
  - ex2_1_7, ex2_1_9, ex6_2_6, ex6_2_8, ex6_2_9, ex6_2_11, ex6_2_12, ex7_2_3, ex7_3_5, ex14_1_7, ex14_2_7
- GlobSol [Kearfott, 1996], IBBA [Ninin et al., 2010] and Ibex [Chabert and Jaulin, 2009]

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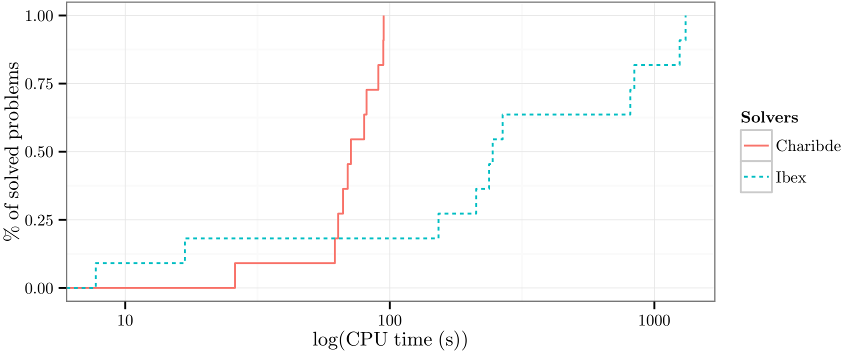
Cumulative CPU time

- GlobSol and IBBA time out ($>$ 3600s on several problems)
- Ibex: 1312.32s
- Charibde: **94.85s**

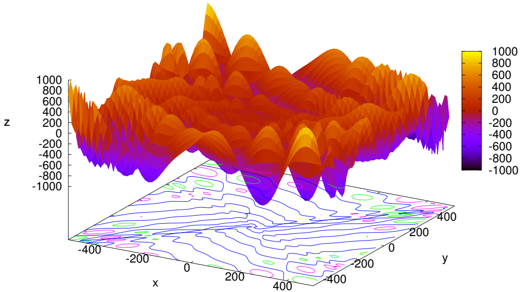
Benchmark of difficult constrained problems



New optimality results for multimodal functions

Multimodal functions, few *approximate* solutions known

Function	Type	Domain	Best known	Charibde
Michalewicz	unconst	$[0, \pi]^n$	up to 50	70
Sine Envelope	unconst	$[-100, 100]^n$	2	5
Egg Holder	unconst	$[-512, 512]^n$	2	10
Keane	inequality const	$[0, 10]^n$	up to 100	5
Rana	unconst	$[-512, 512]^n$	2	7



Lennard-Jones clusters [Jones, 1924]

Find the most stable configuration of a cluster of n atoms

- potential describes pairwise interactions between atoms

$$f(x) = \sum_{i<j}^{n} v(r_{ij}) = 4 \sum_{i<j}^{n} \left(\frac{1}{r_{ij}^{12}} - \frac{1}{r_{ij}^{6}} \right) = 4 \sum_{i<j}^{n} \left[\left(\frac{1}{r_{ij}^{6}} - \frac{1}{2} \right)^2 - 1 \right]$$

  where $r_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$
- non-convex and highly combinatorial ($O(e^n)$ local minima)
- *open problem* for $n \geq 5$
- putative minimum for $n = 5$: -9.103852415708 (triangular bipyramid)

Lennard-Jones clusters [Jones, 1924]

Find the most stable configuration of a cluster of n atoms

- potential describes pairwise interactions between atoms

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	BARON	Couenne	Charibde
Minimum	$-9.10385\underline{346444055}$	$-9.10387\underline{0325603582}$	-9.103852415707552
Search time (s)	0.23	41.94	0.11
Overall total (s)	0.23	61.7	1436
Given status	locally optimal	optimal	certified ($\varepsilon = 10^{-9}$)

Conflict resolution between aircraft

En-route traffic

- guarantee separation ($S = 5NM$) between aircraft at any moment
- if separation lost on trajectory forecast, maneuver the aircraft

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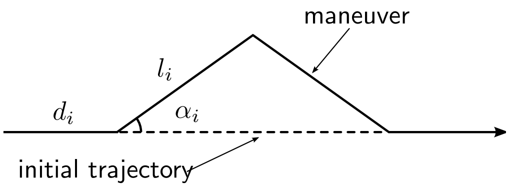
Conflict resolution using *lateral* maneuvers

- modeled as constrained optimization problem with separation constraints
- smallest possible maneuvers
- existing approaches: MINLP [Pallottino et al., 2002] and EA [Durand et al., 1996]



Conflict resolution between aircraft

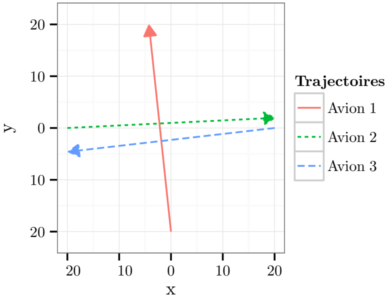
Vector of variables $\boldsymbol{x} = (d_1, \alpha_1, l_1, \ldots, d_n, \alpha_n, l_n)$

$$
\begin{aligned}
(\mathcal{P}) \quad & \min_{\boldsymbol{x}} \sum_{i=1}^{N} \left((1 - \frac{d_i}{\overline{d_i}})^2 + (\frac{\alpha_i}{\overline{\alpha_i}})^2 + (\frac{l_i}{\overline{l_i}})^2 \right) \\
\text{s.c.} \quad & d_i \in [\underline{d_i}, \overline{d_i}] \\
& \alpha_i \in [\underline{\alpha_i}, \overline{\alpha_i}] \\
& l_i \in [\underline{l_i}, \overline{l_i}] \\
& \forall i < j, \quad \forall t \in [0, t_f], \quad S^2 \leq \|\vec{p_i}(t) - \vec{p_j}(t)\|^2
\end{aligned}
$$

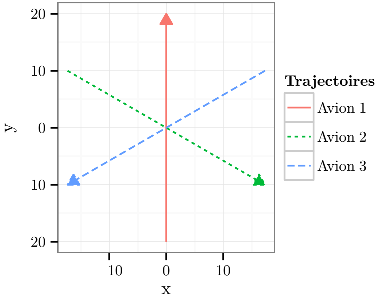
Universally quantified constraints

- violated if $\exists t \in [0, t_f], \quad S^2 > \|\vec{p_i}(t) - \vec{p_j}(t)\|^2$
- handled by specific interval contractors [Goldsztejn et al., 2009]

Conflict resolution between aircraft

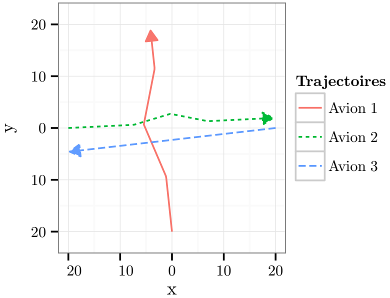


Noisy configuration

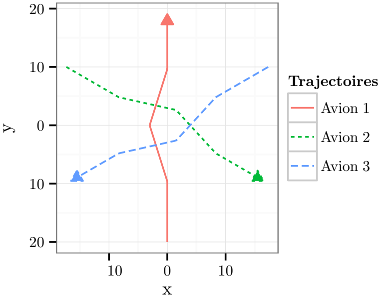


Roundabout configuration

Conflict resolution between aircraft



Noisy configuration (4min)



Roundabout configuration (11.5h)

Conclusion

Our hybrid solver Charibde

- combines an EA and interval-based methods in a cooperative way
- exploits EA's feasible points to update $\tilde{f}$
- prevents premature convergence toward local minima by injecting solutions into EA population
- **proves the optimality** of the solution

Perspectives

- affine arithmetic (alternative enclosure method)
- parallel IB&C

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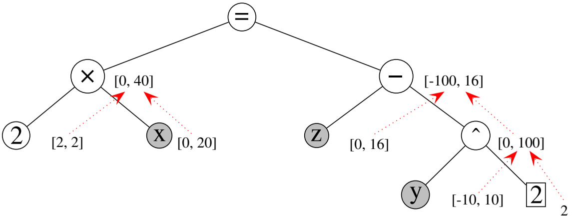
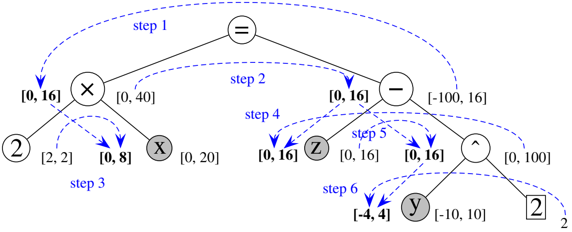
HC4Revise algorithm (w.r.t. $2x = z - y^2$)

- bottom-up: evaluate each node using IA



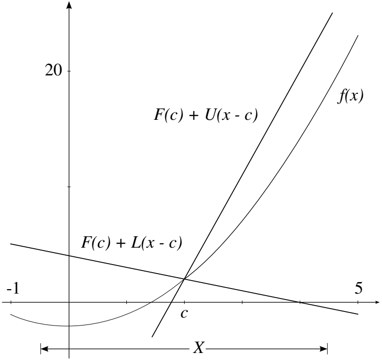
- top-down: constraint propagation using inverse functions



Interval Newton algorithm

Equality constraint $f = 0$

- Newton operator: $N(X,c) = c - \frac{F(c)}{F'(X)}$
- **Any zero** of f in X lies in $X \cap N(X,c)$
- If $N(X,c) \subset int(X)$, then **existence of a unique zero** in X



$$f(x) = x^2 - 2, x \in X = [-\tfrac{1}{2}, \tfrac{9}{2}], c = 2$$

$$N(X,c) = 2 - \frac{2^2 - 2}{2[-\frac{1}{2}, \frac{9}{2}]}$$
$$= [-\infty, \frac{16}{9}] \cup [4, +\infty]$$

(separation of possible zeros)

$$X \cap N(X,x) = [-\frac{1}{2}, \frac{16}{9}] \cup [4, \frac{9}{2}]$$