Preventing Premature Convergence and Proving the Optimality in Evolutionary Algorithms

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Journée de présentation des doctorants, Equipe APO
13 septembre 2013

Objectives

- solve **nonlinear multimodal problems**
- find and **bound** a **global minimum** $(x^*,\ f^*)$

Hard task to find global optimum of numerical (un)constrained problems

- deterministic methods do not converge within reasonable time
- stochastic methods do not guarantee optimality

Considered approach: combine

- a **stochastic** research (Evolutionary Algorithms)
- a **deterministic** research (Interval-based algorithms)

1. Combining Evolutionary Algorithms and Interval-based methods

2. Speeding up the convergence

3. Experimental results

Evolutionary Algorithms (EA)

Evolutionary algorithms $\subset$ metaheuristics: random walk guided by heuristics

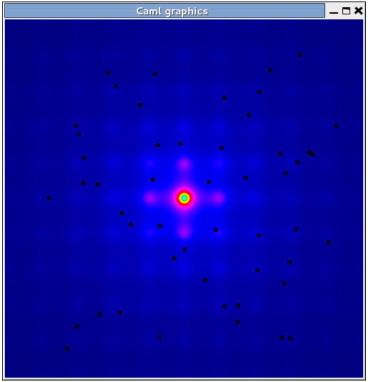
- do not require specific properties on f (black box)
- ideal for **difficult problems**: mixed variables, constraints
- costly methods, **no guarantee of optimality**

Stochastic global optimization algorithms

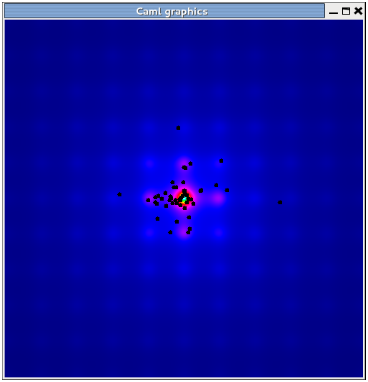
- based on the **theory of evolution**
- selection, crossover, mutation operators
- iterative improvement of a **population of individuals** x_i
- adaptation criterion (fitness) $f(x_i)$

Evolutionary Algorithms (EA)

- GA [Holland, 1975], DE [Storn and Price, 1997], PSO, ES, Genetic programming



Initial population



After 50 iterations

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

Interval Analysis (IA)

Numerical analysis method to bound round-off errors [Moore, 1966]

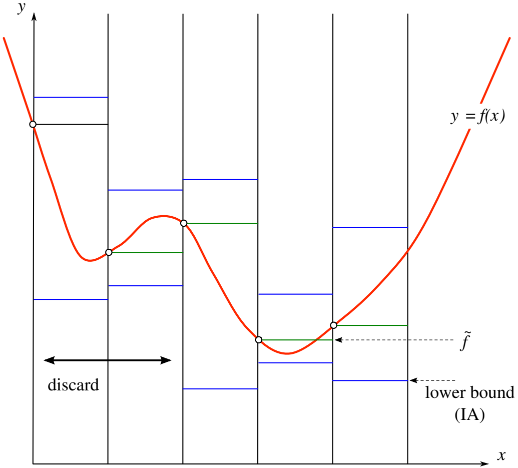
$$\text{Interval } X = [\underline{X}, \overline{X}] = \{x \in \mathbb{R} \mid \underline{X} \leq x \leq \overline{X}\}$$
$$\text{Box } \mathbf{X} = \text{interval vector}$$

Interval arithmetic

- computing with **sets** $\neq$ computing with points
- **rigorous enclosure** (outward rounding)
- **inclusion function** $F: f(X) = \{f(x) \mid x \in X\} \subset F(X)$ (natural, centered, mean value, etc.)

Branch and Bound framework (B&B)

Computation of **guaranteed lower bounds** in B&B [Hansen, 1992]



- If $\tilde{f} \leq \underline{F(X)}$, discard X
- otherwise store in priority queue $\mathcal{L}$

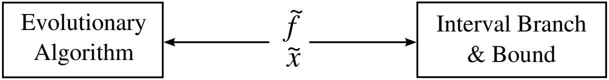
In n dimensions:

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

Cooperative hybrid algorithm

Hybridization between **efficiency** of EA and **reliability** of IA

- integrative approach [Sotiropoulos et al., 1997, Zhang and Liu, 2007]
- **cooperative** approach: [Alliot et al., 2012, Vanaret et al., 2013]
  - independent processes exchange bounds and solutions (MPI)
  - **fully reliable** $\neq$ complete (BARON, Couenne) or local (Minos, Ipopt)



- DE: Update $(\tilde{x}, \tilde{f})$ with $(x_{best}, \overline{F(x_{best})})$
- IB&B: Whenever the evaluation of $mid(\mathbf{X})$ improves $\tilde{f}$, add $mid(\mathbf{X})$ to DE population

Improvements

Preliminary results showed that

- on some problems, the EA quickly finds the global minimum
- it takes the IB&B ages to prove the optimality
- how to speed up convergence?

Issues to tackle

- problem inherent to Interval Analysis: large overestimation
- exploit the constraints: propagation of $g_i \leq 0$, $f \leq \tilde{f}$ and $\nabla f = 0$
- enhance the cooperation

The dependency problem

Quality of inclusion depends on syntactic form

- $f(x) = x^2 - 2x$, $F_N([1,4]) = [-7, 14]$
- $g(x) = x(x-2)$, $G_N([1,4]) = [-4, 8]$,
- $h(x) = (x-1)^2 - 1$, $H_N([1,4]) = [-1, 8] = f([1,4])$

Dependency problem = main source of **overestimation**

- multiple occurrences of a variable are decorrelated $(X - X = \{x - y \mid x \in X, y \in X\} \ni 0)$
- optimal range if single occurrence of each variable
- overerstimation error reduces
  - linearly for natural extension
  - quadratically for mean value form $F(X) = F(c) + (X - c)F'(X)$

How does dependency affect the convergence?

Rana's function, $x_i \in [-512, 512]$

- first syntax:

$$f(x) = \sum_{i=1}^{n-1} (x_i \cos u \sin v + (1 + x_{i+1}) \sin u \cos v)$$

where $u = \sqrt{|x_{i+1} + x_i + 1|}$ and $v = \sqrt{|x_{i+1} - x_i + 1|}$

- second syntax: rewriting using $\cos x \sin y = \frac{1}{2}(\sin(x+y) - \sin(x-y))$

Table: CPU times (s) of convergence ($\epsilon = 10^{-6}$, $NP = 70$, $W = 0.7$, $CR = 0.5$)

n	First syntax	Second syntax
2	0.25	0.009
3	6.5	0.12
4	254	1.45
5	∞	18.5
6	∞	244
7	∞	3300

Interval Constraint Programming (ICP)

Constraint propagation may

- **contract** (narrow bounds) a box without loss of solutions
- prove that a box **cannot contain** a global minimizer

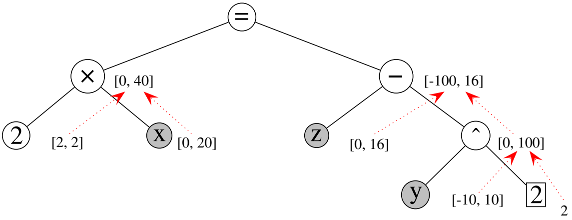
Filtering/Contraction algorithms [Chabert and Jaulin, 2009]

- `HC4` (`HC4Revise`) [Benhamou et al., 1999] for (in)equalities
- Interval Newton for equalities
- Mohc: monotonic `HC4Revise` + Newton [Araya et al., 2010]

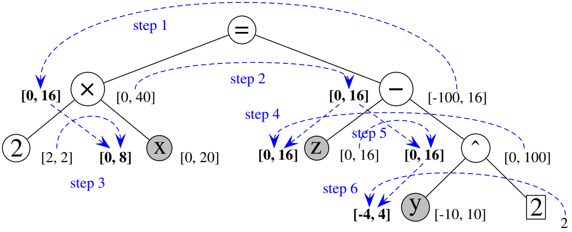
`Charibde` [Vanaret et al., 2013] = DE + Interval Branch and Contract (IB&C)
(IB&B + `HC4Revise` + Mohc + gradient info)

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

- bottom-up: evaluate each node using IA



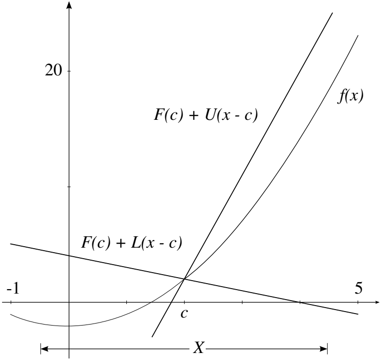
- top-down: constraint propagation using inverse functions



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)

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

Computing an upper bound

Computation of good upper bound $\tilde{f}$ crucial in B&B

- deterministic local solvers (MINOS, Ipopt) start from a feasible point
- if x is a feasible point, then $\overline{F(x)}$ is an upper bound of f^*

Identification of feasible solutions

- Evolutionary Algorithms
  - find feasible points from random starting points
  - exploration generally not limited to a neighborhood
- Interval-based methods
  - contraction w.r.t. to $g_i \leq 0$ discards inconsistent values
  - contraction w.r.t. to $g_i \geq 0$ discards **solutions**

New adaptive heuristic of box selection

Box selection from the priority queue determines the order of exploration

- depth first, breadth first, most promising box (smallest lower bound)

Approach that takes advantage of $\tilde{f}$ AND $\tilde{x}$

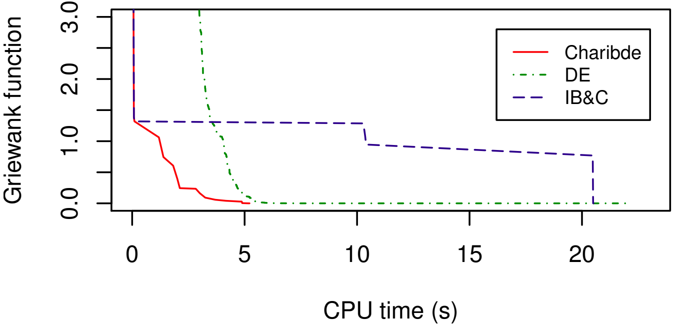
- idea: carry out research in the boxes that are **farthest** from $\tilde{x}$
  - either $\tilde{x}$ close to x^*: fast local exploration by EA
  - or $\tilde{x}$ far from x^*: might as well search elsewhere
- postpone tedious interval search around $\tilde{x}$, waiting for the best possible $\tilde{f}$
- **adaptive** heuristic: recompute priority when $\tilde{x}$ is updated

Experimental results

- generally more efficient than classical heuristics
- maintains a low size of the priority queue

Performance comparison

Griewank function $f(x) = 1 + \frac{1}{4000}\sum_{i=1}^{n} x_i^2 - \prod_{i=1}^{n} \cos\frac{x_i}{\sqrt{i}}$, $n = 200$



- DE: local optimum close to 0 (22s)
- IB&C: 20.5s
- `Charibde`: 5.2s

Certified optima for a benchmark of functions

Table: Test functions with best known and certified minima

	n	Type	Best known f^*	$\tilde{f}$ by `Charibde`	CPU time (s)
Bound-Constrained Problems					
Rastrigin	50	NL	0	0	0.3
Schwefel	10	NL	-4189.82887	-4189.82887	2.3
Rosenbrock	50	Q	0	0	3.3
Griewank	200	NL	0	0	12
Michalewicz	75	NL	-	**-74.6218112**	138
Egg Holder	10	NL	-8247	**-8291.2400675**	768
Rana	7	NL	-	**-3070.2475210**	3300
Inequality-Constrained Problems					
Himmelblau	5	Q	-31025.56024	-31025.56024	0.07
Beam	4	NL	1.7248523	1.7248523	2.2
Tension	3	P	0.01266523	0.01266523	3.8
Keane	5	NL	-0.63445	-0.63445	472

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)

	BARON [Sahinidis, 1996]	Charibde
Optimum	-9.1039	$\tilde{f} = -9.10385241570755$2
CPU (s)	0.002	0.12 + 1000
Status	"locally optimal"	certified ($\epsilon = 10^{-6}$)

Conclusion

`Charibde` algorithm

- prevents premature convergence toward local minima
- **proves the optimality** of the solution
- achieved new optimal results for difficult benchmark functions

Perspectives

- applications to aeronautics (conflict resolution), 3D computer graphics, geometry, optimization of neural networks
- parallelization of IB&B

Perspectives

Perform DE restarts

- add diversity in the search process
- possibly on a reduced search-space
  - IB&B contains list $\mathcal{L}$ of remaining boxes
  - our selection heuristic "peels" the search-space from outside
  - reduced search-space = convex hull (enclosing box) of $\mathcal{L}$
  - crude enclosure...

Table: Lennard-Jones clusters ($n = 5$)

DE iteration	Search-space retrieved from IB&B
0	$[0, 1.2] \times [0, 1.2]^5 \times [-1.2, 1.2] \times [-1.2, 1.2] \times [0, 1.2]$
50000	$[0.94, 1.2] \times [0, 1.2]^5 \times [-0.47, 1.2] \times [-1.2, 1.11] \times [0.24, 1.2]$
60000	$[0.94, 1.2] \times [0, 1.2]^5 \times [-0.47, 1.2] \times [-1.2, 1.11] \times [0.52, 1.2]$

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