Introduction to Optimization: Benchmarking

September 13, 2016 TC2 - Optimisation Université Paris-Saclay, Orsay, France

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India

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Course Overview

1	Fri, 16.9.2016	Introduction to Optimization					
	Wed, 21.9.2016	groups defined via wiki					
	Thu, 22.9.2016	everybody went (actively!) through the github.com/numbbo/coco	erybody went (actively!) through the Getting Started part of hub.com/numbbo/coco				
2	Fri, 23.9.2016	Today's lecture: Benchmarking; final a everybody can run and postprocess the questions/help during the lecture)	day's lecture: Benchmarking; final adjustments of groups erybody can run and postprocess the example experiment (~1h for final estions/help during the lecture)				
3	Fri, 30.9.2016	ecture					
4	Fri, 7.10.2016	Lecture	ecture				
	Mon, 10.10.2016	deadline for intermediate wiki report: what has been done and what remain	s to be done?				
5	Fri, 14.10.2016	Lecture					
6	Tue, 18.10.2016	Lecture	All deadlines:				
	Tue, 18.10.2016	deadline for submitting data sets	23:59pm Paris time				
	Fri, 21.10.2016	deadline for paper submission					
		vacation					
7	Fri, 4.11.2016	Final lecture					
	711.11.2016	oral presentations (individual time slot	s)				
	14 - 18.11.2016	Exam (exact date to be confirmed)					

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challenging optimization problems appear in many scientific, technological and industrial domains









Numerical Blackbox Optimization

Optimize $f: \Omega \subset \mathbb{R}^n \mapsto \mathbb{R}^k$



derivatives not available or not useful

Practical Blackbox Optimization



Not clear:

which of the many algorithms should I use on my problem?

Numerical Blackbox Optimizers

Deterministic algorithms

Quasi-Newton with estimation of gradient (BFGS) [Broyden et al. 1970] Simplex downhill [Nelder & Mead 1965] Pattern search [Hooke and Jeeves 1961] Trust-region methods (NEWUOA, BOBYQA) [Powell 2006, 2009]

Stochastic (randomized) search methods Evolutionary Algorithms (continuous domain) Differential Evolution [Storn & Price 1997] Particle Swarm Optimization [Kennedy & Eberhart 1995] Evolution Strategies, CMA-ES [Rechenberg 1965, Hansen&Ostermeier 2001] Estimation of Distribution Algorithms (EDAS) [Larrañaga, Lozano, 2002] Cross Entropy Method (same as EDA) [Rubinstein, Kroese, 2004]

• Genetic Algorithms [Holland 1975, Goldberg 1989] Simulated annealing [Kirkpatrick et al. 1983] Simultaneous perturbation stochastic approx. (SPSA) [Spall 2000]

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- choice typically not immediately clear
- although practitioners have knowledge about problem difficulties (e.g. multi-modality, non-separability, ...)

Need: Benchmarking

- understanding of algorithms
- algorithm selection
- putting algorithms to a standardized test
 - simplify judgement
 - simplify comparison
 - regression test under algorithm changes

Kind of everybody has to do it (and it is tedious):

- choosing (and implementing) problems, performance measures, visualization, stat. tests, ...
- running a set of algorithms

that's where COCO comes into play

Comparing Continuous Optimizers Platform https://github.com/numbbo/coco

automatized benchmarking

How to benchmark algorithms with COCO?

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	Numerical Black-Box Optimization Be	nchmarking Framework http://	coco.gforge.inria.fr/	88.13 contributors	
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- C/C++
- Java
- MATLAB/Octave

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For more information,

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For more information,

- read our benchmarking guidelines introduction
- read the COCO experimental setup description
- see the bbob-biobj COCO multi-objective functions testbed documentation and the specificities of the performance



can the links below to leave more about the ideas behind CoCO.



4. On the computer where experiment data shall be post-processed, run



- Java read me and example experiment
- Matlab/Octave read me and example experiment



YOURDATAFOLDER folder. We can also compare more than one algorithm by specifying several data result folders generated by different algorithms.

example_experiment.c

```
_ D _ X
/* Iterate over all problems in the suite */
while ((PROBLEM = coco_suite_get_next_problem(suite, observer)) != NULL)
{
    size t dimension = coco problem get dimension(PROBLEM);
    /* Run the algorithm at least once */
    for (run = 1; run <= 1 + INDEPENDENT_RESTARTS; run++) {</pre>
      size t evaluations done = coco problem get evaluations(PROBLEM);
      long evaluations remaining =
         (long)(dimension * BUDGET_MULTIPLIER) - (long)evaluations_done;
      if (... || (evaluations_remaining <= 0))</pre>
        break:
      my random search(evaluate function, dimension,
               coco problem get number of objectives(PROBLEM),
                coco problem get smallest values of interest(PROBLEM),
                coco problem get largest values of interest(PROBLEM),
                (size t) evaluations remaining,
               random generator);
```

generated by different algorithms.



Description by Folder



result folder

							x
🕞 🕞 🗸 📕 🕨 numbbo-git	thuł	o 🕨 bbob-biobj-data 🕨 data 🕨 ppdata 🕨	_	🗸 🍫 Search ppdat	ta		٩
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🔆 Favorites	^	Name	Date modified	Туре	Size		
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😌 Dropbox		bbob_pproc_commands.tex	01/08/2016 14:58	LaTeX Document	6 K	В	
Recent Places		🥫 index.html	01/08/2016 14:58	Firefox HTML Doc	1 K	В	
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index.html Firefox HTML Doct	ume	State: 33 Shared ent Date modified: 01/08/2016 14:58 Date	Size: 522 bytes created: 01/08/2016 14	Shared with	n: root		

automatically generated results



automatically generated results



automatically generated results



so far:

data for about 165 algorithm variants [in total on single- and multiobjective problems] 118 workshop papers by 79 authors from 25 countries

Measuring Performance

On

- real world problems
 - expensive
 - comparison typically limited to certain domains
 - experts have limited interest to publish
- "artificial" benchmark functions
 - cheap
 - controlled
 - data acquisition is comparatively easy
 - problem of representativeness

Test Functions

define the "scientific question"

the relevance can hardly be overestimated

- should represent "reality"
- are often too simple?

remind separability

- a number of testbeds are around
- account for invariance properties

prediction of performance is based on "similarity", ideally equivalence classes of functions

Available Test Suites in COCO

bbob bbob-noisy bbob-biobj 24 noiseless fcts30 noisy fcts55 bi-objective fcts

140+ algo data sets 40+ algo data sets new in 2016 15 algo data sets

How Do We Measure Performance?

Meaningful quantitative measure

- quantitative on the ratio scale (highest possible)
 "algo A is two *times* better than algo B" is a meaningful statement
- assume a wide range of values
- meaningful (interpretable) with regard to the real world possible to transfer from benchmarking to real world

runtime or first hitting time is the prime candidate (we don't have many choices anyway)

How Do We Measure Performance?

Two objectives:

- Find solution with small(est possible) function/indicator value
- With the least possible search costs (number of function evaluations)

For measuring performance: fix one and measure the other
Measuring Performance Empirically

convergence graphs is all we have to start with...



number of function evaluations

ECDF:

Empirical Cumulative Distribution Function of the Runtime [aka data profile]

A Convergence Graph



First Hitting Time is Monotonous



15 Runs



15 Runs ≤ 15 Runtime Data Points



Empirical Cumulative Distribution



the ECDF of run lengths to reach the target

- has for each data point a vertical step of constant size
- displays for each x-value (budget) the count of observations to the left (first hitting times)

Empirical Cumulative Distribution



- interpretations possible:
- 0.8. 80% of the runs reached the target
 0.6 target
 - e.g. 60% of the runs need between 2000 and 4000 evaluations





50 equally spaced targets







the empirical CDF makes a step for each star, is monotonous and displays for each budget the fraction of targets achieved within the budget







15 runs



15 runs50 targets



15 runs 50 targets



15 runs50 targetsECDF with 750 steps



50 targets from 15 runs

...integrated in a single graph

Interpretation



50 targets from 15 runs integrated in a single graph

area over the ECDF curve

average log runtime (or geometric avg. runtime) over all targets (difficult and easy) and all runs

Fixed-target: Measuring Runtime



Fixed-target: Measuring Runtime

• Algo Restart A:



RT_B^r $p_s(Algo Restart A) = 1$

Fixed-target: Measuring Runtime

• Expected running time of the restarted algorithm:

$$E[RT^{r}] = \frac{1 - p_{s}}{p_{s}} E[RT_{unsuccessful}] + E[RT_{successful}]$$

• Estimator average running time (aRT):

$$\widehat{p_s} = \frac{\# \text{successes}}{\# \text{runs}}$$

 $\widehat{RT_{unsucc}}$ = Average evals of unsuccessful runs

 $\widehat{RT_{succ}}$ = Average evals of successful runs

$$aRT = \frac{\text{total #evals}}{\text{#successes}}$$

ECDFs with Simulated Restarts

What we typically plot are ECDFs of the simulated restarted algorithms:



Worth to Note: ECDFs in COCO

In COCO, ECDF graphs

- never aggregate over dimension
 - but often over targets and functions
- can show data of more than 1 algorithm at a time



Another Interesting Plot...

...comparing aRT values over several algorithms



Another Interesting Plot...

...comparing aRT values over several algorithms



Another Interesting Plot...

...comparing aRT values over several algorithms



Interesting for 2 Algorithms...

dimensions:

...are scatter plots

 $2:+, 3: \triangledown, 5:*, 10:\circ, 20:\Box, 40:\diamond$.



There are more Plots...

...but they are probably less interesting for us here

The single-objective BBOB functions

bbob Testbed

• 24 functions in 5 groups:

1 Separable Functions		4 Multi-modal functions with adequate global structure	
f1	Sphere Function	f15	Rastrigin Function
f2	Sellipsoidal Function	f16	Weierstrass Function
f3	Rastrigin Function	f17	Schaffers F7 Function
f4	Büche-Rastrigin Function	f18	Schaffers F7 Functions, moderately ill-conditioned
f5	♥Linear Slope	f19	Composite Griewank-Rosenbrock Function F8F2
2 Functions with low or moderate conditioning		5 Multi-modal functions with weak global structure	
f6	Attractive Sector Function	f20	Schwefel Function
f7	Step Ellipsoidal Function	f21	Gallagher's Gaussian 101-me Peaks Function
f8	Rosenbrock Function, original	f22	Gallagher's Gaussian 21-hi Peaks Function
f9	Rosenbrock Function, rotated	f23	Katsuura Function
3 Functions with high conditioning and unimodal		f24	Lunacek bi-Rastrigin Function
f10	Ellipsoidal Function		
f11	ODiscus Function		
f12	Bent Cigar Function		
f13	Sharp Ridge Function		
f14	ODifferent Powers Function		

• 6 dimensions: 2, 3, 5, 10, 20, (40 optional)

Notion of Instances

- All COCO problems come in form of instances
 - e.g. as translated/rotated versions of the same function
- Prescribed instances typically change from year to year
 - avoid overfitting
 - 5 instances are always kept the same

Plus:

 the bbob functions are locally perturbed by nonlinear transformations

Notion of Instances



the recent extension to multi-objective optimization
Multiobjective Optimization (MOO)

Multiple objectives that have to be optimized simultaneously

performance



Observations:

there is no single optimal solution, but
some solutions (

are better than others (

are better than others (

are better than others (

bette



u weakly Pareto dominates v ($u \leq_{par} v$): $\forall 1 \leq i \leq k : f_i(u) \leq f_i(v)$ u Pareto dominates v ($u <_{par} v$): $u \leq_{par} v \land v \not\leq_{par} u$ performance



u weakly Pareto dominates v ($u \leq_{par} v$): $\forall 1 \leq i \leq k : f_i(u) \leq f_i(v)$ u Pareto dominates v ($u <_{par} v$): $u \leq_{par} v \land v \not\leq_{par} u$ performance



Pareto set: set of all non-dominated solutions (decision space) Pareto front: its image in the objective space



Pareto set: set of all non-dominated solutions (decision space) Pareto front: its image in the objective space





solution of Pareto-optimal set
 vector of Pareto-optimal front
 non-optimal decision vector
 non-optimal objective vector



ideal point: best values nadir point: worst values

· obtained for Pareto-optimal points

Quality Indicator Approach to MOO

Idea:

- transfer multiobjective problem into a set problem
- define an objective function ("quality indicator") on sets

Important:

⇒ Underlying dominance relation (on sets) should be reflected by the resulting set comparisons!



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Examples of Quality Indicators



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Examples of Quality Indicators II



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Examples of Quality Indicators II



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bbob-biobj Testbed

• 55 functions by combining 2 ъъоъ functions

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f12	Bent Cigar Function							
f13	Sharp Ridge Function ✓							
f14	♥Different Powers Function ✓							
-								

bbob-biobj Testbed

• 55 functions by combining 2 ььоь functions

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f2	♥Ellipsoidal Function ✓			f16 @Weierstrass Function								
f3	Rastrigin Function			f17 Schaffers F7 Function 🗸								
f4	Büche-Rastrigin Function		f_1	fo	f_6	f_8	f_{12}	f_{14}	f_{15}	f_{17}	f_{20}	f_{21}
f5	♥Linear Slope	f,	f1	f2	f3	f4	f5	f6	f7	f8	f9	f10
2 F	unctions with low or moderate conditionir	51		12	10	17	10	10	<u></u>	10	12	<u>110</u>
f6		f_2		<u>†11</u>	<u>f12</u>	<u>†13</u>	<u>f14</u>	<u>t15</u>	<u>f16</u>	<u>f17</u>	<u>118</u>	<u>f19</u>
f7	Step Ellipsoidal Function	f_6			<u>f20</u>	<u>f21</u>	<u>f22</u>	<u>f23</u>	<u>f24</u>	<u>f25</u>	<u>f26</u>	<u>f27</u>
f8		f_8				<u>f28</u>	<u>f29</u>	<u>f30</u>	<u>f31</u>	<u>f32</u>	<u>f33</u>	<u>f34</u>
f9	Rosenbrock Function, rotated	f_{13}					<u>f35</u>	<u>f36</u>	<u>f37</u>	<u>f38</u>	<u>f39</u>	<u>f40</u>
3 Functions with high conditioning and unimo		f_{14}						<u>f41</u>	<u>f42</u>	<u>f43</u>	<u>f44</u>	<u>f45</u>
f10	Sellipsoidal Function	f_{15}							<u>f46</u>	<u>f47</u>	<u>f48</u>	<u>f49</u>
f11	ODiscus Function	f_{17}								<u>f50</u>	<u>f51</u>	<u>f52</u>
f12	Bent Cigar Function	f_{20}									f53	f54
f13	Sharp Ridge Function 🗸	fai										f55
f14	♥Different Powers Function	J 21										133

bbob-biobj Testbed

- 55 functions by combining 2 ььоь functions
- 15 function groups with 3-4 functions each
 - separable separable, separable moderate, separable ill-conditioned, ...
- 6 dimensions: 2, 3, 5, 10, 20, (40 optional)
- instances derived from ььоь instances:
- no normalization (algo has to cope with different orders of magnitude)
- for performance assessment: ideal/nadir points known

bbob-biobj Testbed (cont'd)

- Pareto set and Pareto front unknown
 - but we have a good idea of where they are by running quite some algorithms and keeping track of all nondominated points found so far
- Various types of shapes

bbob-biobj Testbed (cont'd)



Bi-objective Performance Assessment

algorithm quality =

normalized* hypervolume (HV) of all non-dominated solutions *if a point dominates nadir*



closest normalized* negative distance to region of interest [0,1]² *if no point dominates nadir*

* such that ideal=[0,0] and nadir=[1,1]

Bi-objective Performance Assessment

We measure runtimes to reach (HV indicator) targets:

- relative to a reference set, given as the best Pareto front approximation known (since exact Pareto set not known)
- actual absolute hypervolume targets used are

HV(refset) – targetprecision

with 58 fixed targetprecisions between 1 and -10⁻⁴ (same for all functions, dimensions, and instances) in the displays

Course Overview

1	Fri, 16.9.2016	Introduction to Optimization					
	Wed, 21.9.2016	groups defined via wiki					
	Thu, 22.9.2016	everybody went (actively!) through the Getting Started part of github.com/numbbo/coco					
2	Fri, 23.9.2016	Today's lecture: ⁽²⁾ Benchmarking; ⁽¹⁾ final adjustments of groups everybody can run and postprocess the example experiment (~1h for final ⁽³⁾ questions/help during the lecture)					
3	Fri, 30.9.2016	Lecture					
4	Fri, 7.10.2016	Lecture					
	Mon, 10.10.2016	deadline for intermediate wiki report: what has been done and what remains to be done?					
5	Fri, 14.10.2016	Lecture					
6	Tue, 18.10.2016	Lecture	All deadlines:				
	Tue, 18.10.2016	deadline for submitting data sets	23:59pm Paris time				
	Fri, 21.10.2016	deadline for paper submission					
		vacation					
7	Fri, 4.11.2016	Final lecture					
	711.11.2016	oral presentations (individual time slots)					
	14 - 18.11.2016	Exam (exact date to be confirmed)					

I hope it became clear...

...what are the important issues in algorithm benchmarking ...which functionality is behind the COCO platform ...and how to measure performance in particular ...what are the basics of multiobjective optimization ...and what are the next important steps to do: read the assigned paper and implement the algorithm document everything on the wiki Monday in 2 weeks: intermediate report on wiki And now...

...time for your questions and problems around COCO