Introduction to Optimization Derivative-Free Optimization II: Benchmarking

December 16, 2016 École Centrale Paris, Châtenay-Malabry, France



Dimo Brockhoff Inria Saclay – Ile-de-France

Course Overview

Date		Торіс	
Fri, 7.10.2016		Introduction	
Fri, 28.10.2016	D	Introduction to Discrete Opt	imization + Greedy algorithms I
Fri, 4.11.2016	D	Greedy algorithms II + Bran	ich and bound
Fri, 18.11.2016	D	Dynamic programming	
Mon, 21.11.2016	D	Approximation algorithms a	nd heuristics
Fri, 25.11.2016	С	Randomized Search Heuris	tics + Intro. to Continuous Opt. I
Mon, 28.11.2016	С	Introduction to Continuous (Optimization II
Mon, 5.12.2016	С	Introduction to Continuous (Optimization III
Fri, 9.12.2016	С	Constrained Optimization +	Descent Methods
Mon, 12.12.2016 in S103-S105	С	Derivative Free Optimization	n I: CMA-ES
Fri, 16.12.2016	С	Derivative Free Optimization with the COCO platform	n II: Benchmarking Optimizers
Wed, 4.1.2017		Exam	if not indicated otherwise, classes take place in S115-S117

Experimental Considerations around CMA-ES

Experimentum Crucis with CMA-ES

CMA-ES Summary

with CMA-ES

The Experimentum Crucis

Experimentum Crucis (0)

What did we want to achieve?

reduce any convex-quadratic function

$$f(\boldsymbol{x}) = \boldsymbol{x}^{\mathrm{T}} \boldsymbol{H} \boldsymbol{x}$$

e.g.
$$f(\mathbf{x}) = \sum_{i=1}^{n} 10^{6\frac{i-1}{n-1}} x_i^2$$

to the sphere model

$$f(\boldsymbol{x}) = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}$$

without use of derivatives

lines of equal density align with lines of equal fitness

 $\mathbf{C} \propto \mathbf{H}^{-1}$

in a stochastic sense

• • • • • • • from [Hansen; •p.• 91]

Experimentum Crucis with CMA-ES

CMA-ES Summary

The Experimentum Crucis

Experimentum Crucis (1)

f convex quadratic, separable



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• • • • • • • from [Hansen; p. 92]

Experimentum Crucis with CMA-ES

CMA-ES Summary

The Experimentum Crucis

Experimentum Crucis (2)

f convex quadratic, as before but non-separable (rotated)





• • • • • • • from [Hansen; p. 93]

Influence of Condition Number + Invariance

Comparing Experiments

Comparison to BFGS, NEWUOA, PSO and DE

f convex quadratic, separable with varying condition number α

Ellipsoid dimension 20, 21 trials, tolerance 1e-09, eval max 1e+07



BFGS (Broyden et al 1970) NEWUAO (Powell 2004) DE (Storn & Price 1996) PSO (Kennedy & Eberhart 1995) CMA-ES (Hansen & Ostermeier

 $f(\mathbf{x}) = g(\mathbf{x}^{\mathrm{T}}\mathbf{H}\mathbf{x})$ with

g identity (for BFGS and

g any order-preserving = strictly increasing function (for all other)

SP1 = average number of objective function evaluations¹⁴ to reach the target function value of $g^{-1}(10^{-9})$

¹⁴Auger et.al. (2009): Experimental comparisons of derivative free optimization algorithms, SEA < = > < = > 900

Influence of Condition Number + Invariance

Comparing Experiments

Comparison to BFGS, NEWUOA, PSO and DE

f convex quadratic, non-separable (rotated) with varying condition number α

Rotated Ellipsoid dimension 20, 21 trials, tolerance 1e-09, eval max 1e+07



BFGS (Broyden et al 1970) NEWUAO (Powell 2004) DE (Storn & Price 1996) PSO (Kennedy & Eberhart 1995) CMA-ES (Hansen & Ostermeier 2001) $f(\mathbf{x}) = g(\mathbf{x}^{T}\mathbf{H}\mathbf{x})$ with \mathbf{H} full

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Influence of Condition Number + Invariance

Comparing Experiments

Comparison to BFGS, NEWUOA, PSO and DE

f non-convex, non-separable (rotated) with varying condition number α

Sqrt of sqrt of rotated ellipsoid dimension 20, 21 trials, tolerance 1e-09, eval max 1e+07



SP1 = average number of objective function evaluations¹⁶ to reach the target function value of $g^{-1}(10^{-9})$

Performance on BBOB Testbed: Data Profile

Comparing Experiments

Comparison during BBOB at GECCO 2009



200

Summary CMA-ES I

Summary and Final Remarks

Main Characteristics of (CMA) Evolution Strategies

- Multivariate normal distribution to generate new search points follows the maximum entropy principle
- 2 Rank-based selection implies invariance, same performance on g(f(x)) for any increasing gmore invariance properties are featured
- Step-size control facilitates fast (log-linear) convergence and possibly linear scaling with the dimension in CMA-ES based on an evolution path (a non-local trajectory)
- Covariance matrix adaptation (CMA) increases the likelihood of previously successful steps and can improve performance by orders of magnitude

the update follows the natural gradient $\mathbf{C} \propto \mathbf{H}^{-1} \iff$ adapts a variable metric \iff new (rotated) problem representation $\implies f: \mathbf{x} \mapsto g(\mathbf{x}^{\mathrm{T}}\mathbf{H}\mathbf{x})$ reduces to $\mathbf{x} \mapsto \mathbf{x}^{\mathrm{T}}\mathbf{x}$

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Summary CMA-ES II

Summary and Final Remarks

Limitations of CMA Evolution Strategies

- internal CPU-time: 10⁻⁸n² seconds per function evaluation on a 2GHz PC, tweaks are available 1 000 000 *f*-evaluations in 100-D take 100 seconds *internal* CPU-time
- better methods are presumably available in case of
 - partly separable problems
 - specific problems, for example with cheap gradients

specific methods

• small dimension ($n \ll 10$)

for example Nelder-Mead

small running times (number of *f*-evaluations < 100*n*) model-based methods

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Introduction to Optimization @ ECP, Dec. 16, 2016

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I hope it became clear...

...that CMA-ES samples according to multivariate normal distributions ...how CMA-ES updates its mean, stepsize, and covariance matrix ...what are the invariance properties of CMA-ES ...and how to read the output of CMA-ES

Numerical Benchmarking of Blackbox Optimization Algorithms







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]

Numerical Blackbox Optimizers

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 Simultaneous perturbation stochastic approx. (SPSA) [Spall 2000]

- 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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numbbo/coco: Comparing Continuous Optimizers

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- C/C++
- Java
- MATLAB/Octave

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Contributions to link further languages (including a better example in C++) are more than welcome.

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

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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

Exercise (Part 1): Comparing Numerical Optimization Algorithms with COCO

https://github.com/numbbo/coco

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https://github.com/numbbo/coco



Matlab/Octave read me and example experiment

http://coco.gforge.inria.fr/doku.php?id=algorithms

Step 3: downloading data

[[algorithms]] **COMPARING CONTINUOUS OPTIMISERS: COCO** Show pagesource 🔜 Old revisions 📧 Recent changes 🔍 Sitemap 👰 Login Search The following table lists all algorithms related to the BBOB workshops and special sessions in the years 2009 till 2015 together with links to Navigation their data. In order to sort the table according to some columns, please click on the corresponding table header. If available, the source Home codes of the algorithms can be downloaded by clicking on the link with the corresponding algorithm name in the second column. Documentation download latest old code Data Noiseless Data Noisy related PDFs and Remarks No Algorithm Year Author(s) • Onew code homepage (Raw) (Raw) download new code directly noiselessData noisvData O PDF 1 ALPS 2009 Hornby BBOB 2016 noiselessData PDFnoiseless PDFnoisy noisyData 2 AMALGAM 2009 Bosman et al. BBOB 2015 @ GECCO Algorithms PDFnoiseless PDFnoi 3 BAYEDA Gallagher noiselessData noisyData 2009 noiselessData noisyData PDFnoiseless PDF BFGS 2009 Ros 4 for the moment: noisyData PDFnoiseless PDF 5 BIPOP-CMA-ES 2009 Hansen noiselessData noiselessData PDF 6 Cauchy-EDA 2009 Pošík n/a **IPOP-CMA-ES** Auger and noiselessData 7 CMA-ESPLUSSEL 2009 noisyData PDFnoiseless PDF Hansen Korošec and BBOB 2013 O PDFnoiseless O PDFnoisy 2009 noiselessData noisyData 8 DASA Šilc Algorithms Results García-Nieto noiselessData noisyData 😡 PDFnoiseless PDFnoisy 9 DE-PSO 2009 Schedule et al. Downloads O PDF BBOB 2012 noiselessData 10 DIRECT 2009 Pošík n/a algorithm is deterministic and thus, only run on each Algorithms instance once Results Downloads El-Abd and noiselessData noisyData O PDF 11 EDA-PSO 2009 Kamel BBOB 2010

https://github.com/numbbo/coco



Description by Folder

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:



• Algo Restart B:

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

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



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...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

Exercise (Part 2): Comparing Numerical Optimization Algorithms with COCO

Exercise (Part 2)

Objectives:

- investigate the performance of algorithms
 - CMA-ES ("IPOP-CMA-ES" version)
 - Nelder-Mead simplex (use "NelderDoerr" version here)
 - BFGS quasi-Newton
 - Genetic Algorithm: discretization of cont. variables ("GA")
 - plus 1-2 algos of your choice from <u>http://coco.gforge.inria.fr</u>
- postprocess (now) and investigate the data (after a few more slides)

tip: use --omit-single option to save time

The single-objective BBOB functions

The 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	Sellipsoidal 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



Exercise (Part 3): Comparing Numerical Optimization Algorithms with COCO

Exercise (Part 3)

Objective:

investigate the data:

- a) which algorithms are the best ones?
- b) does this depend on the dimension?
- c) look at single graphs: can we say something about the algorithms' invariances, e.g. wrt. rotations of the search space?
- d) what do you think: are the displayed algorithms well-suited for problems with larger dimension?
- e) what can you say about the algorithm, you chose yourself?

reminder: open thesis projects

one is related to this exercise but automatized & for 150+ data sets ("data science")

I hope it became clear...

...that the fixed-target approach is superior over the budget-based approach (and why)
...that COCO is easy to use and provides a lot of data to explore
...and which algorithms to use/investigate when you have to solve a numerical unconstrained blackbox problem yourself at some point