Benchmarking DFO algorithms

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(v2)

Plan

Introduction and problems

Tables and convergence graph

Performance and data profiles

References

Introduction

- How to measure the performance of an algorithm?
- How to compare algorithms amongst themselves?
- How to identify groups of problems?
- Are we interested in the final solution only, or in the progression of the algorithms?

How to benchmark DFO algorithms

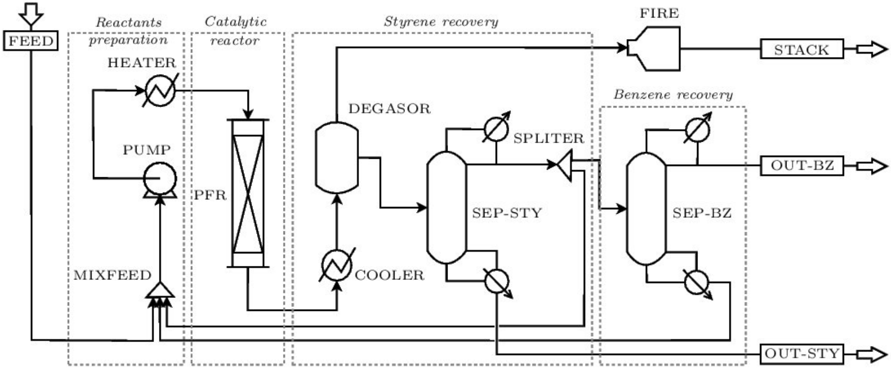
- Performance indicators:
  - Typically: Value of f and number of blackbox evaluations
  - Special measures for robustness, multiobjective optimization, etc.
- In the DFO context, CPU time is rarely relevant since the number of evaluations is a perfect machine-independent criterion
- However, CPU time is useful for:
  - Blackboxes with variable complexity
  - Parallelism
  - ...

How to find problems

- We want to achieve reproducibility. However most blackbox applications are proprietary and/or cannot be shared easily. There is not yet a universal and accepted collection of such problems.
- Typically, algorithms are tested on a mixture of analytic problems and real-life applications.
- When testing on real applications, it is necessary to use many instances, for example by changing the parameters of the applications, or by using several starting solutions.

A realistic blackbox for benchmarking

STYRENE problem [Audet et al., 2008]



8 variables, 11 constraints, one evaluation $\simeq$ 1s, $\simeq$20% of failures

Collections of analytic problems

The usual analytic collections are:

- The Hock and Schittkowski set [Hock and Schittkowski, 1981]
- The Lukšan and Vlček set [Lukšan and Vlček, 2000]
- Problems used in [Moré and Wild, 2009]. Core of 22 unconstrained CUTEst problems reformulated as 212 instances (smooth, nonsmooth, and noisy)
- CUTEst, the latest evolution of the CUTE and CUTEr collections [Gould et al., 2015]
- The COCO platform
- Isolated problems such as ROSENBROCK or GRIEWANK

Tables of numerical results

- Useful to summarize instance characteristics
- Give the exact values for each execution of Solver s on Problem p
- Problem: becomes difficult to read (*too much information*)

Table example

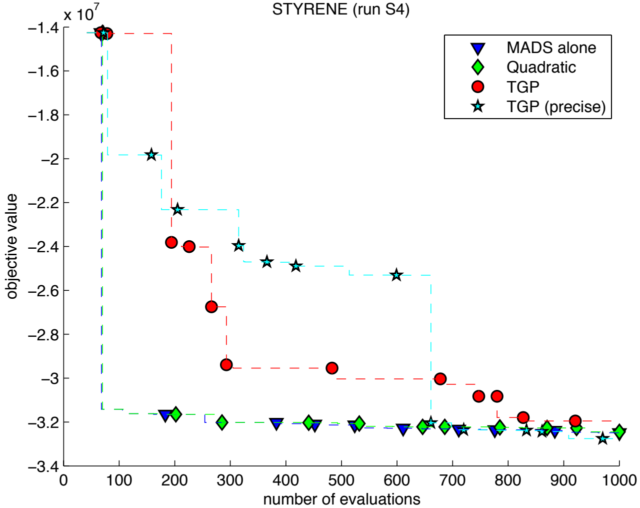
Table 6 Pooling Test Problems from the Literature

	Parameters			Solution				CPU time (sec)			Error (%)		
Example	*nsp*	k_{max}	*nt*	Exact	MSLP	MALT	VNS	MSLP	MALT	VNS	MSLP	MALT	VNS
Flow model													
AST1	1,000	10	1	549.803	276.661	532.901	545.27	2.20	2.45	2.81	49.68	3.07	0.82
AST2	1,500	10	1	549.803	284.186	535.617	543.909	9.18	5.21	5.68	48.31	2.58	1.07
AST3	1,000	10	1	561.048	255.846	397.441	412.145	18.71	4.96	5.34	54.35	29.09	26.47
AST4	230	0	0	877.649	—	876.206	876.206	0.82	0.77	1.01	—	0.16	0.16
BT4	5	0	0	45	39.6970	45	45	0.01	0.01	0.01	11.78	0	0
BT5	10	15	2	350	327.016	324.077	350	0.03	0.09	1.11	6.57	7.41	0
F2	120	10	1	110	100	107.869	110	0.07	0.44	0.57	9.09	1.94	0
H1	5	0	0	40	40	40	40	0.02	0.01	0.01	0	0	0
H2	5	0	0	60	60	60	60	0.02	0.01	0.01	0	0	0
H3	5	3	1	75	60.7332	70	75	0.02	0.01	0.03	19.02	6.67	0
RT1	5	0	0	4,136.22	126.913	4,136.22	4,136.22	1.34	0.04	0.04	96.93	0	0
RT2	5	5	1	4,391.83	—	4,330.78	4,391.83	0.04	0.47	0.60	—	1.39	0
GP1	50	5	1	60.5	28.732	35	46	0.01	0.04	0.08	52.51	42.15	23.97
Proportion model													
AST1	1,000	10	1	549.803	544.307	532.901	533.783	1.14	2.38	2.61	1	3.07	2.91
AST2	1,500	10	1	549.803	548.407	535.617	542.54	3.04	4.97	5.37	0.25	2.58	1.32
AST3	1,000	10	1	561.048	551.081	397.441	558.835	4.98	4.98	5.93	1.68	29.09	0.3
AST4	230	0	0	877.649	—	876.206	876.206	1.19	1.21	1.55	—	0.16	0.16
BT4	5	0	0	45	39.7019	45	45	0.01	0.02	0.02	11.77	0	0
BT5	10	15	2	350	292.532	323.12	350	0.12	0.16	1.53	16.42	7.68	0
F2	120	0	0	110	110	110	110	0.15	0.49	0.49	0	0	0
H1	5	0	0	40	40	40	40	0.02	0.01	0.01	0	0	0
H2	5	0	0	60	60	60	60	0.02	0.01	0.01	0	0	0
H3	5	3	1	75	69.9934	70	75	0.02	0.01	0.02	6.68	6.67	0
RT1	5	0	0	4,136.22	3,061.03	4,136.22	4,136.22	0.07	0.03	0.03	25.99	0	0
RT2	5	5	1	4,391.83	4,391.02	4,330.77	4,391.82	0.04	0.58	0.72	0.02	1.39	0

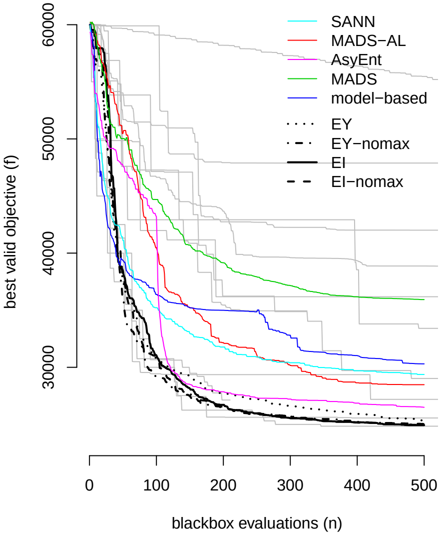
Convergence graph

- Provides a picture of the convergence of one or several methods for one given instance of a problem
- Represents only the successes or all evaluations
- Horizontal steps between two f values
- Problem: Only for one instance. Does not allow to draw any general conclusion

Convergence graph example (1)

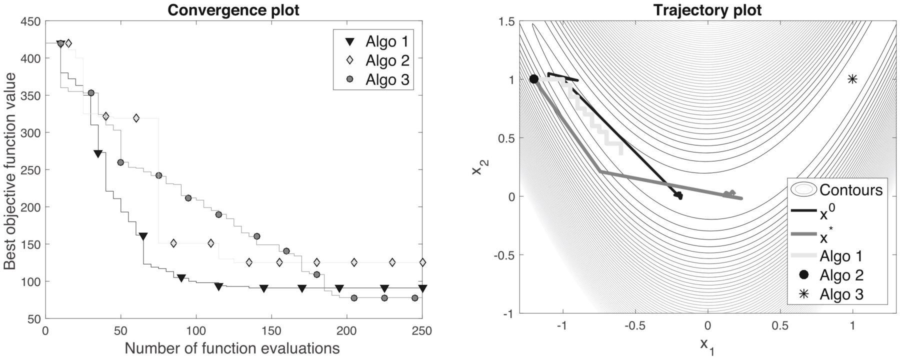


Convergence graph example (2)



From [Gramacy et al., 2015]

Convergence + trajectory plots for 2D examples



From [Audet and Hare, 2017]

Introduction and problems

Tables and convergence graph

Performance and data profiles

References

Performance and data profiles

- Introduced by [Dolan and Moré, 2002, Moré and Wild, 2009]
- Graphical and straightforward way of comparing methods on sets of problems
- **Relative** comparison of the methods
- Moré and Wild give the MATLAB tools to draw profiles at `http://www.mcs.anl.gov/~more/dfo/`
- We consider:
  - Unconstrained problems
  - Single-objective problems
  - Deterministic instances and algorithms
  - No parallelism

Profiles: Original version from the M&W paper

- $\mathcal{P}$: set of problems or instances
- $\mathcal{S}$: set of solvers, or algorithms, or methods
- Performance measure $t_{p,s} > 0$ available for each $p \in \mathcal{P}$ and $s \in \mathcal{S}$. Typically the number of evaluations required to satisfy a convergence test
- Small values of the performance measure are preferable
- Performance ratio for problem $p \in \mathcal{P}$ and solver $s \in \mathcal{S}$:

$$r_{p,s} = \frac{t_{p,s}}{\min\{t_{p,a} : a \in \mathcal{S}\}}$$

Convergence test (1/2)

- One possible convergence test is, for the candidate solution x:

$$f(x_0) - f(x) \geq (1 - \tau)(f(x_0) - f_L)$$

- Where:
  - $\tau > 0$: tolerance
  - x_0: **unique** and **feasible** starting point
  - f_L: smallest value of f obtained by any solver within a given budget of evaluations, for each $p \in \mathcal{P}$
- It requires that the reduction $f(x_0) - f(x)$ achieved by x be at least $1 - \tau$ times the best possible reduction $f(x_0) - f_L$
- τ represents the percentage decrease from $f(x_0)$. As it decreases, the accuracy of $f(x)$ as an approximation to f_L increases

Convergence test (2/2)

- **Example 1**: Values of $f(x_0)$ and of f after 100 evaluations, for 3 algorithms on 2 problems:

	Pb 1	Pb 2
$f(x_0)$	10	-703.57
f Algo. 1	0.01	-1,907.47
f Algo. 2	1.2	-3,964.20
f Algo. 3	0	-3,682.12

For $\tau = 0.1$, when does the convergence test pass?

- Other convergence tests include the relative error between $f(x)$ and f_L. For example $\frac{f(x)-f_L}{|f_L|} \leq \tau$ if $f_L \neq 0$

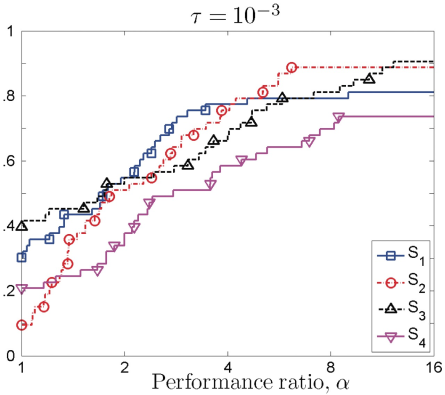
Performance profiles

- The best solver $s^* \in \mathcal{S}$ for a particular problem $p \in \mathcal{P}$ attains the lower bound $r_{p,s^*} = 1$
- $t_{p,s} = r_{p,s} = \infty$ when s fails to satisfy the convergence test on p
- The performance profile of s is the fraction of problems where the performance ratio is at most α:

$$\rho_s(\alpha) = \frac{1}{|\mathcal{P}|}\text{size}\{p \in \mathcal{P} : r_{p,s} \leq \alpha\}$$

- It is the probability distribution for the ratio $r_{p,s}$
- $\rho_s(1)$ is the fraction of problems for which s performs the best
- For α sufficiently large, $\rho_s(\alpha)$ is the fraction of problems solved by s
- Solvers with high values for ρ_s are preferable

Performance profiles: Example



Accurate view of the performance for $\tau = 10^{-3}$. Taken from [Moré and Wild, 2009]

Example 2

Draw the performance profiles for the following table:

$t_{p,s}$	Pb 1	Pb 2
Algo. 1	35	∞
Algo. 2	∞	1,200
Algo. 3	112	500

$t_{p,s}$ represents the number of evaluations for which the convergence test succeeded, for a given value of τ

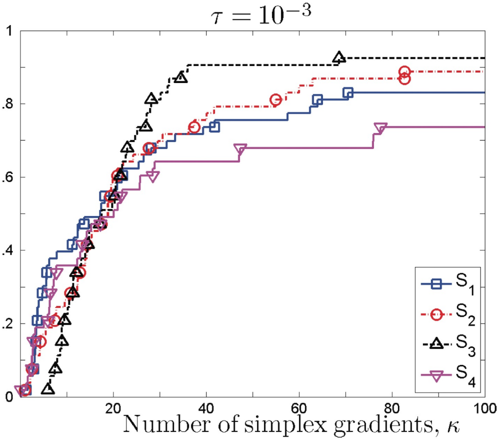
Data profiles

- We are interested in the percentage of problems that can be solved, for a given tolerance τ with a variable budget of evaluations
- The data profile of Solver s is

$$d_s(\kappa) = \frac{1}{|\mathcal{P}|}\text{size}\left\{p \in \mathcal{P} : \frac{t_{p,s}}{n_p + 1} \leq \kappa\right\},$$

  where n_p is the number of variables in Problem p
- It represents the percentage of problems that can be solved with κ groups of $n_p + 1$ function evaluations, or simplex gradient estimates
- $n_p + 1$ is the number of evaluations needed to compute a one-sided finite-difference estimate of the gradient

Data profiles: Example



Taken from [Moré and Wild, 2009]

Example 3

Draw the data profiles for the following table.

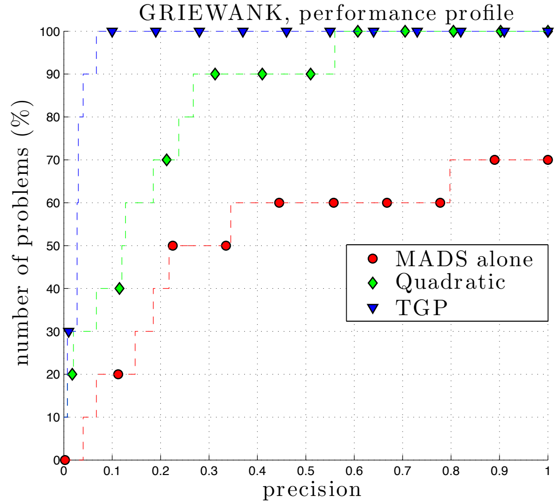
$t_{p,s}$	Pb 1	Pb 2
Algo. 1	35	∞
Algo. 2	∞	1,200
Algo. 3	112	500

$t_{p,s}$ represents the number of evaluations for which the convergence test succeeded, for a given value of τ. Problem 1 has 2 variables and Problem 2 has 9 variables

Simplified performance profiles

- Consider only the final solutions. The stopping criteria must be the same for all the algorithms (i.e. same budget of evaluations)
- x-axis: tolerance τ
- y-axis: percentage of problems *solved* given the τ tolerance
- "solved" must be defined
- At $\tau = 0$:
  - We see the methods that gave the best solutions
  - The performance values may sum up to a value $< 100\%$

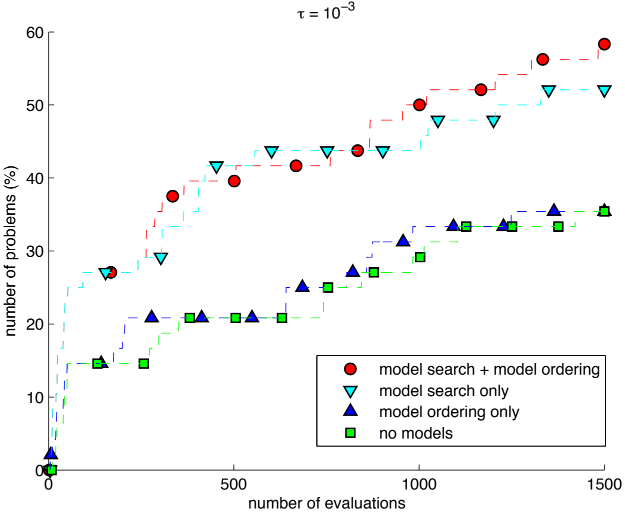
Simplified performance profiles: Example



Simplified data profiles

- We consider the entire history of all executions: We focus on the convergence
- The tolerance τ is fixed
- x-axis: Convergence measure: Number of evaluations or number of simplex gradients when the problems have different dimensions
- y-axis: Percentage of problems *solved* given the τ tolerance
- For $x = 0$, we should have $y = 0$
- For $x = x_{max}$, we should observe the same values on the performance profiles, at τ
- Equivalent to the original version. Only the presentation differs

Simplified data profiles: Example



Extensions

- How to extend performance and data profiles
  - To the constrained case?
  - With parallelism?
  - With stochastic algorithms?
- Several choices have to be taken. This is the subject of Homework #1 for the constrained case
- Accuracy profiles [Audet and Hare, 2017] for the robustness and quality of the final solution

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- Performance and data profiles [Dolan and Moré, 2002, Moré and Wild, 2009]
- Test problems [Hock and Schittkowski, 1981, Lukšan and Vlček, 2000, Moré and Wild, 2009, Gould et al., 2015]
- Some benchmark papers [Whitley et al., 2006, Fowler et al., 2008, Moré and Wild, 2009, Rios and Sahinidis, 2013, Martelli and Amaldi, 2014]

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