Stochastic (Randomized) Optimization via Natural Gradient Descent

Nikolaus Hansen
INRIA, Research Centre Saclay
Machine Learning and Optimization Group TAO
LRI, Univ. Paris-Sud

...don't hesitate with asking questions, expressing disbelief, giving comments...

Natural Evolution Strategies

...a natural (canonical) view point based on

- Wierstra et al, *Natural Evolution Strategies*, IEEE WCCI 2008.
- Glasmachers et al, *Exponential Natural Evolution Strategies*, GECCO 2009.
- Akimoto et al, *Bidirectional Relation between CMA Evolution Strategies and Natural Evolution Strategies*, PPSN 2010.

$\Longleftrightarrow$ $\Longleftrightarrow$

{randomized, stochastic} {optimization, search}

The Problem

Black-Box Optimization (Search)

Minimize (or maximize) a continuous domain objective (cost, loss, error, fitness) function

$$f : \mathbb{R}^n \to \mathbb{R}, \quad x \mapsto f(x)$$

where f is considered as a black-box

$x \longrightarrow$  $\longrightarrow f(x)$

and in particular

- gradients are not available or useful
- problem specific knowledge is used *within* the black box, e.g. with an appropriate encoding

Objective: find $x \in \mathbb{R}^n$ with small $f(x)$, where the search costs are the number of back-box calls (function evaluations)

On-line registration of spline images

Intraoperative ultrasound image CT image

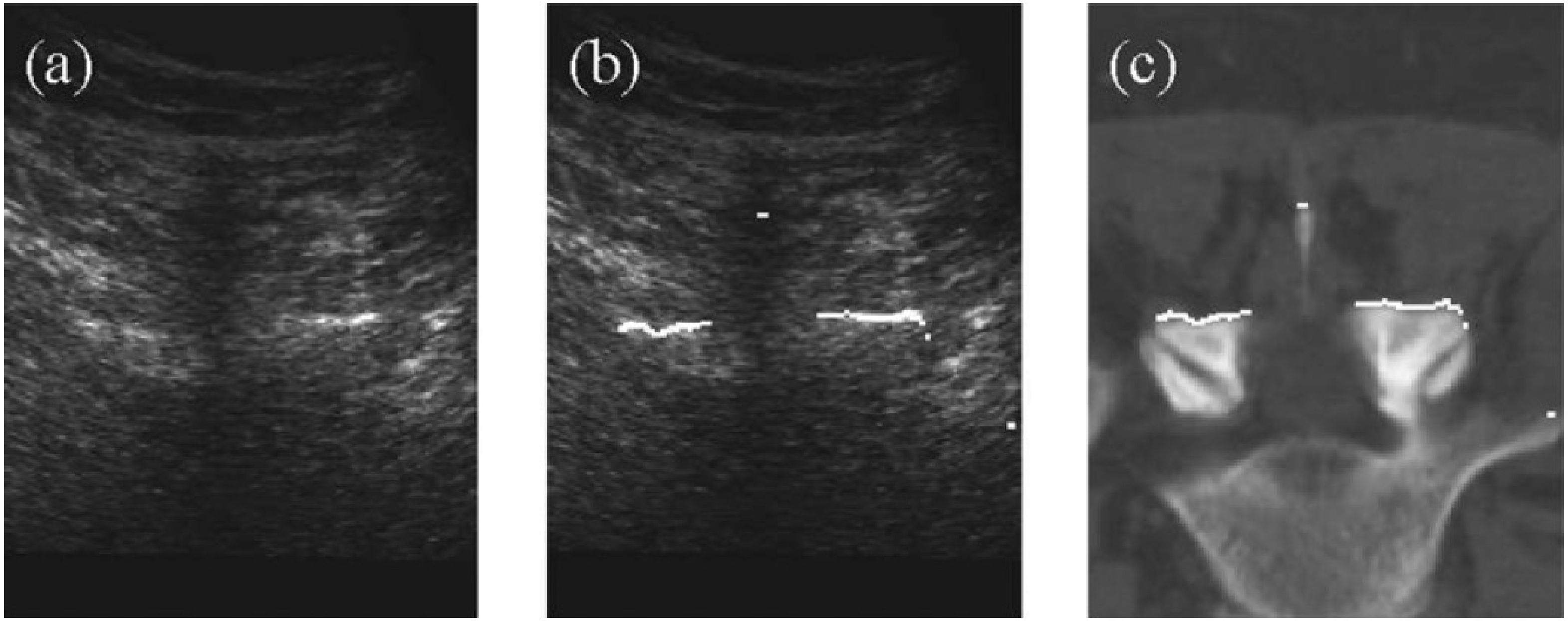


Fig. 6. (a) Intraoperative axial ultrasound image of a vertebra. (b) Bone surface at the registered position. (c) Corresponding CT image.

from [Winter et al 2008]

Distribution of final misalignment

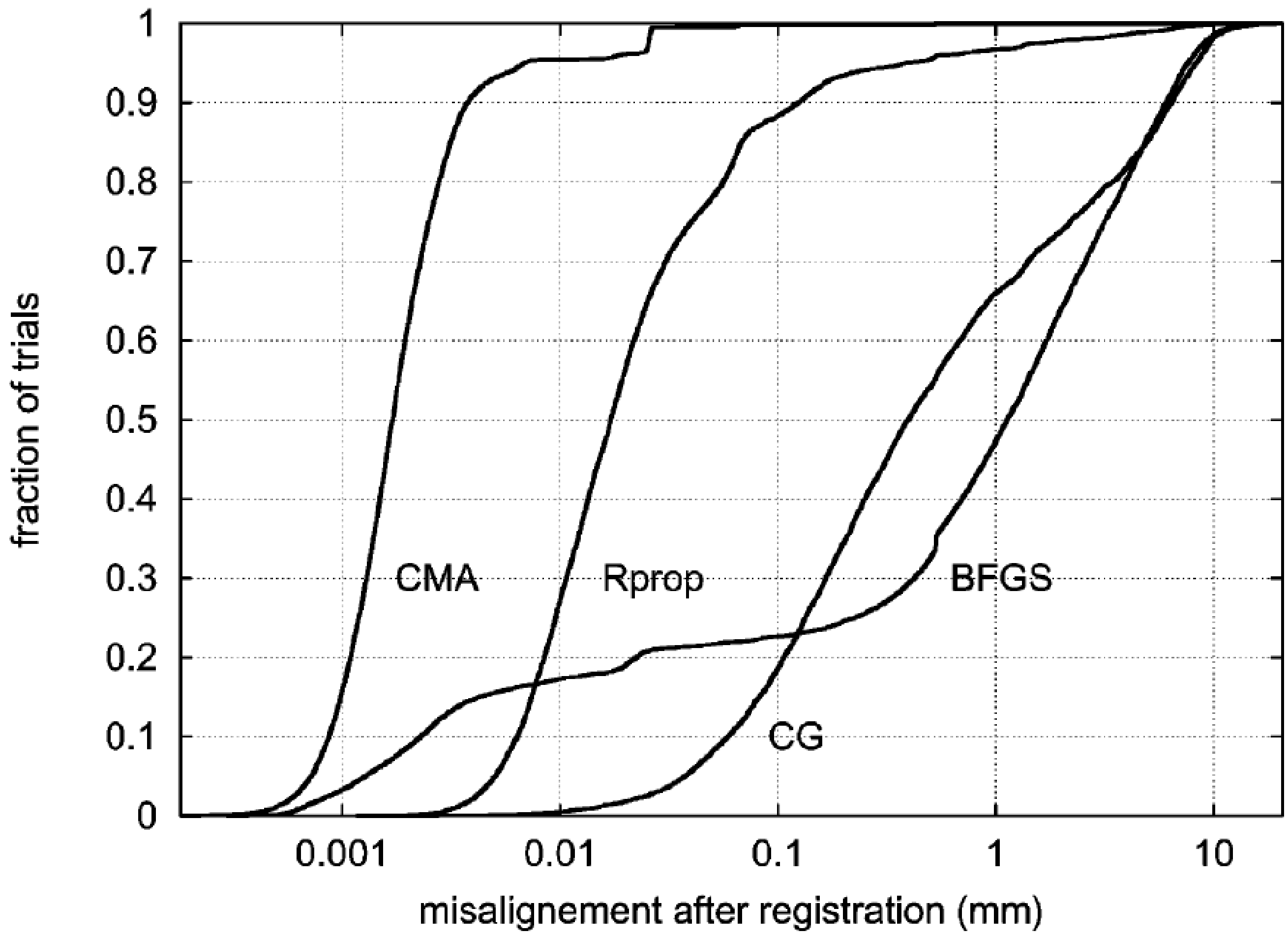
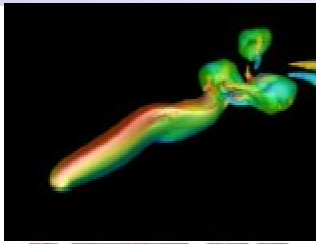


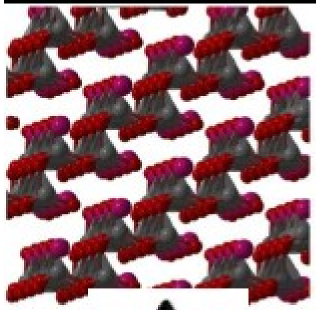
Fig. 9. Misalignment of all registration trials in the multistart optimization scenario; registration of 12 vertebrae, each with 1000 different starting positions and the different optimization methods BFGS, CG, iRprop, CMA.

from [Winter et al 2008]

More selected applications

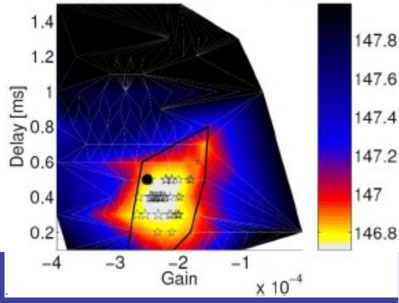


- Swimming fish simulation [Kern et al 2007]
  computational flow simulation, motion control



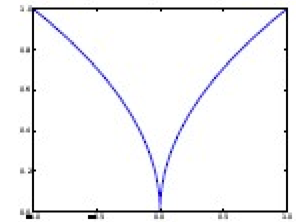
- Crystal structure prediction [Glass et al 2006]
  specialized algorithm: encoding, operators etc.
  new structure of $CaCO_3$ above 137GPa predicted and subsequently confirmed in experiment

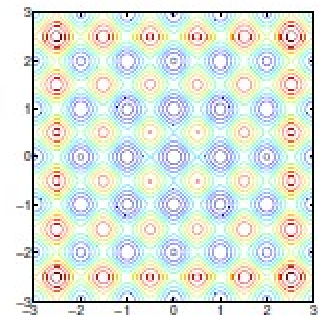
- Modelling of volcanic magma [Halter et al 2006]
  bilevel energy optimization
- Space launcher design to maximize the payload per EUR [Collange et al 2010]
  for Ariane in collaboration with EADS Astrium
- Combustion control [Hansen et al 2009]
  real-time laboratory experiment in collaboration with Alstom

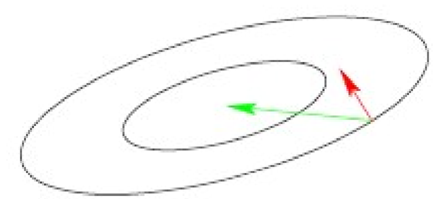


Difficulties in black-box optimization

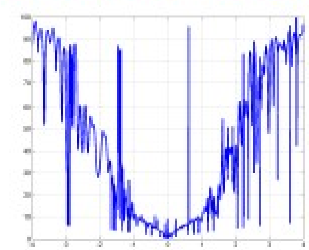
- non-linear, non-quadratic, non-convex
  on linear/quadratic functions better search policies are available
- dimensionality
  (considerably) larger than three
- non-separability
  dependencies between the objective variables
- ill-conditioning
  widely varying sensitivity
- ruggedness
  non-smooth, discontinuous, multimodal, and/or noisy function







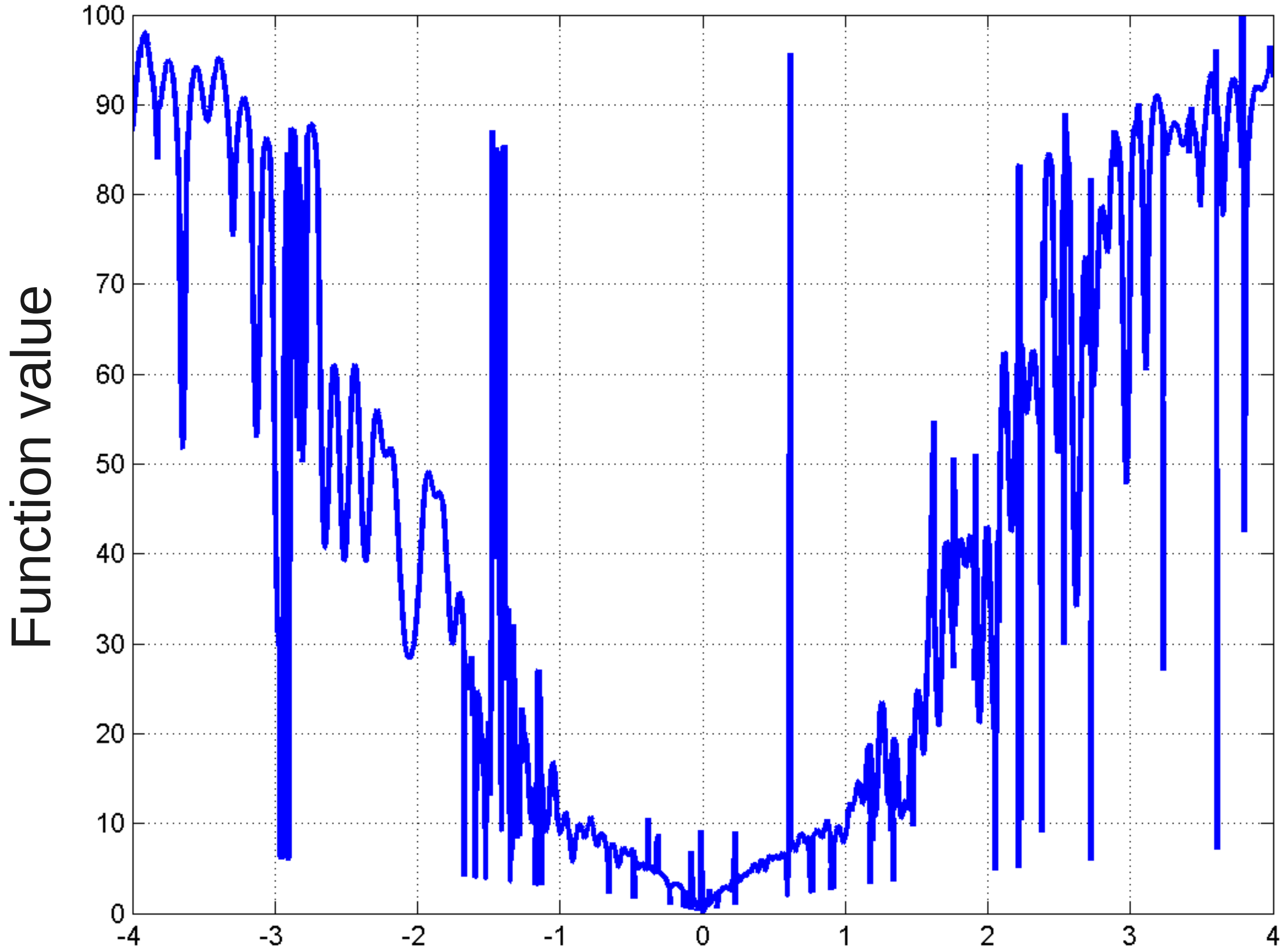
gradient direction Newton direction



in any case the objective function must be highly regular

Rugged landscape

Section through 5-D ($n = 5$) landscape



The Methods

Incomplete taxonomy of search methods

Gradient-based methods (Taylor, smooth)

local search

- Conjugate gradient methods [Fletcher & Reeves 1964]
- Quasi-Newton methods (BFGS) [Broyden et al 1970]

Derivative-free optimization (DFO)

- Trust-region methods (NEWUOA) [Powell 2006]
- Simplex downhill [Nelder & Mead 1965]
- Pattern search [Hooke & Jeeves 1961] [Audet & Dennis 2006]

Stochastic search methods

- Evolution strategies [Rechenberg 1965]
- Simulated annealing (SA) [Kirkpatrick et al 1983]
- Simultaneous perturbation stochastic approximation (SPSA) [Spall 2000]

A Reminder: the Classical Approach

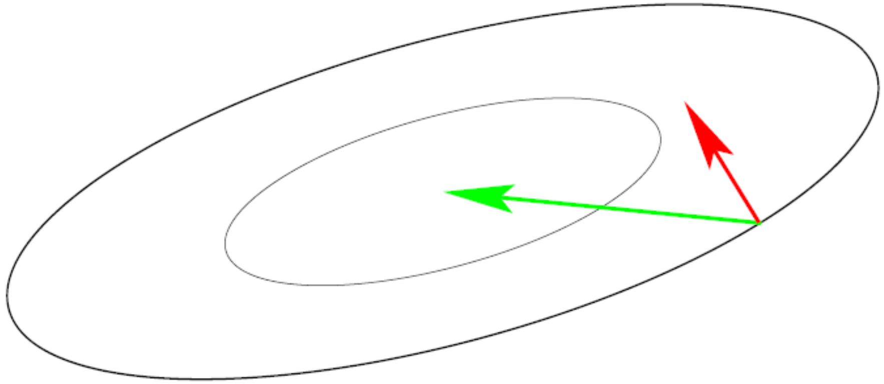
Let $x_k \in \mathbb{R}^n, \eta > 0$
In order to improve (reduce) $f(x_k)$, descend in gradient direction (first order):

$$x_{k+1} = x_k - \eta \vec{\nabla} f(x_k)$$ with η small

or even better in Newton direction (second order):

$$x_{k+1} = x_k - \eta H^{-1}(x_k) \vec{\nabla} f(x_k)$$

incorporating the Hessian matrix H of f (f'', curvature)
Remark: H depends on f and might also depend on x



gradient direction $-f'(\boldsymbol{x})^{\mathrm{T}}$

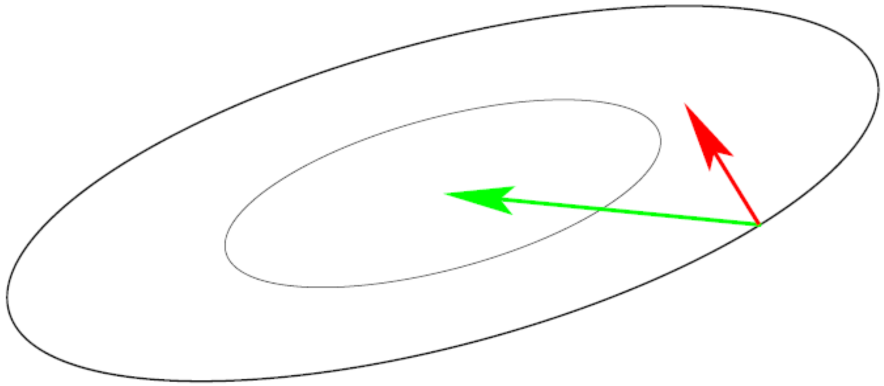
Newton direction $-\boldsymbol{H}^{-1} f'(\boldsymbol{x})^{\mathrm{T}}$

View points of the second order approach

- higher order Taylor approximation
- (proper) choice of a variable metric or inner product $\langle x, y \rangle_H = x^T H y$

in order to define the gradient

- is invariant under *affine* coordinate transformations $x \mapsto Ax + b$



gradient direction $-f'(\boldsymbol{x})^{\mathrm{T}}$

Newton direction $-\boldsymbol{H}^{-1} f'(\boldsymbol{x})^{\mathrm{T}}$

...a randomized view point of search...

Rank-based stochastic optimization template

Given: a parametrized distribution $P(.|\theta)$
Initialize θ and set population size $\lambda \in \mathbb{N}$
While not happy

1. Sample $P(x|\theta) \to x_1, \dots, x_\lambda \in \mathbb{R}^n$
2. Evaluate $x_1, \dots, x_\lambda$ on $f : \mathbb{R}^n \to \mathbb{R}$
$$f(x_{1:\lambda}) \le \dots \le f(x_{\mu:\lambda}) \le \dots \le f(x_{\lambda:\lambda})$$
3. Update parameters $\theta \leftarrow Update(\theta, x_{1:\lambda}, \dots, x_{\mu:\lambda})$

Return, for example, the expected value of P, $m \in \theta$

Algorithm 1 Controlled Markov chain Monte Carlo

- Sample initial values $\theta_0, X_0 \in \Theta \times$ X.
- Iteration $i + 1$ $(i \ge 0)$, given $\theta_i = \theta_i(\theta_0, X_0, \dots, X_i)$ from iteration i
  1. Sample $X_{i+1}|(\theta_0, X_0, \dots, X_i) \sim P_{\theta_i}(X_i, \cdot)$.
  2. Compute $\theta_{i+1} = \theta_{i+1}(\theta_0, X_0, \dots, X_{i+1})$.

Andrieu & Thoms 2008

A new search problem

Original problem: find (approach)

$$x^* = \arg\min_{x\in\mathbb{R}^n} f(x)$$

New problem: considering a parameterized distribution $P(.|\theta)$ for $x \in \mathbb{R}^n$ and find (approach)

$$\arg\min_\theta E(f(x)|\theta) \quad \text{or}$$

$$\arg\min_\theta E(f(x)\,\mathbf{1}_{f(x)<f_\theta}|\theta) \quad \text{(disregarding bad samples) or} \dots$$

Remark 1 (same solution): $x^* \sim P(x|\theta^*)$

with $\theta^* = \arg\min_\theta E(g(f(x))|\theta)$ and any g monotonically increasing

Remark 2: $P(.|\theta)$ can be interpreted as *construction method* for (good) solutions

Objective: evolve $P(.|\theta)$ (updating θ) to achieve a small $E(f(x)|\theta)$ with a small number of f-evaluations

Now let $\theta \in \mathbb{R}^m \dots$

...let's start from zero...

Steepest Descent

Let the likelihood $p(x|\theta)$ define a parameterized family of distributions for $x \in X$, such that $\min_\theta E(f(x)|\theta) = \min_{x\in X} f(x)$. We want to approach

$$\arg\min_{\theta\in\mathbb{R}^m} E(f(x)|\theta)$$

We consider the steepest descent

$$\theta_{k+1} = \theta_k - \eta\nabla_\theta E(f(x)|\theta_k)$$

Q1: does that make sense? Q2: can we implement this?

a gradient ∇_θ is defined via a ”small” change of θ, that is, a small change of the probability distribution

what is the appropriate metric (what is ”small”)?

Curvature

the *Fisher information metric* implies an *informational difference* between probability distributions (and is the curvature of the relative entropy) $F_{ij}(\theta) = -E\frac{\partial^2 \log p(x|\theta)}{\partial\theta_i\partial\theta_j}$

only the *natural gradient* $\tilde{\nabla}$ complies with the Fisher information metric and is invariant under reparameterization

the $\tilde{\nabla}$-steepest descent reads

$$\begin{aligned}\theta_{k+1} &= \theta_k - \eta\tilde{\nabla}E(f(x)|\theta_k)\\ &= \theta_k - \eta F_\theta^{-1}\nabla_\theta E(f(x)|\theta_k)\end{aligned}$$

where F_θ is the Fisher information matrix

Remark: F_θ^{-1} does not depend on the underlying problem f!

A Rephrasing

the $\tilde{\nabla}$-steepest descend reads

$$\begin{aligned}\theta_{k+1} &= \theta_k - \eta \tilde{\nabla} E(f(x)|\theta_k) \\ &= \theta_k - \eta F_\theta^{-1} \underbrace{\nabla_\theta E(f(x)|\theta_k)}_{\text{how compute this?}}\end{aligned}$$

where F_θ is the Fisher information matrix

we find (under mild regularity assumptions on P)

$$\begin{aligned}\nabla_\theta E(f(x)|\theta) &= \int_x f(x) \frac{p(x|\theta)}{p(x|\theta)} \nabla_\theta p(x|\theta) dx \\ &= E(f(x) \nabla_\theta \log p(x|\theta))\end{aligned}$$

and therefore ...

MC-Approximation

we have

$$\theta_{k+1} = \theta_k - \eta\,\tilde{\nabla} E(f(x)|\theta_k)$$
$$= \theta_k - \eta E(f(x) F_\theta^{-1} \nabla_\theta \log p(x|\theta_k))$$

with a Monte-Carlo approximation of E (i.e. taking an average) we implement

the expensive part, a weight value for each x_i

$$\theta_{k+1} = \theta_k - \frac{\eta}{\lambda} \sum_{i=1}^{\lambda} f(x_i) F_\theta{}^{-1} \nabla_\theta \ln p(x_i|\theta_k)$$

where $x_i \sim P(.|\theta)$ for $i = 1 \ldots \lambda$ and F_θ is the Fisher information matrix

a stochastic steepest natural descent on $E(f(x)|\theta)$

Finally: Some Practical Details

we have a stochastic steepest natural descend on $E(f(x)|\theta)$

the expensive part, a weight value for each x_i

$$\theta_{k+1} = \theta_k - \frac{\eta}{\lambda} \sum_{i=1}^{\lambda} f(x_i) \underbrace{{F_\theta}^{-1} \nabla_\theta \ln p(x_i|\theta_k)}$$

where $x_i \sim P(.|\theta_k)$ for $i = 1 \ldots \lambda$ and F_θ is the Fisher information matrix

using the maximum entropy (normal) distribution for p,
${F_\theta}^{-1} \nabla_\theta \ln p(x_i|\theta_k)$ can be explicitly computed

a first hint of how to choose the learning rate ("step-size"):

$$\frac{\eta}{\lambda} \approx \frac{1}{\sum |f(x_i)|} \times \left(1 \wedge \overbrace{\frac{\left(\sum |f(x_i)|\right)^2}{\sum f(x_i)^2}}^{\text{amount of input information}} \times \frac{2}{\underbrace{n^2 + 3n}_{\text{degrees of freedom in } \theta}}\right)$$

Natural Evolution Strategy = CMA-ES with $c_1 = c_\sigma = 0$

Input: $m \in \mathbb{R}^n$, $\lambda \in \{2, 3, 4, \dots\}$

Set $w_{i=1,\dots,\lambda}$ suitably, $c_\mu \approx \mu_w / n^2$ where $\mu_w = 1/\sum_{i=1}^{\lambda} w_i^2$
Initialize covariance matrix $\mathbf{C} = \mathbf{I}$

Note: θ = $(m, \mathbf{C})$

While not *happy*

$$\mathbf{x}_i \sim \mathcal{N}(m, \mathbf{C}), \quad \text{for } i = 1, \dots, \lambda$$ sampling

$$\mathbf{y}_i := \mathbf{x}_i - m \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$$

$$m \leftarrow m + \sum_{i=1}^{\lambda} w_{\rho(i)} \, \mathbf{y}_i, \quad \rho(i) = \operatorname{rank}(f(\mathbf{x}_i))$$ $\tilde{\nabla}$-update of the mean

$$\mathbf{C} \leftarrow \mathbf{C} + c_\mu \sum_{i=1}^{\lambda} w_{\rho(i)} (\mathbf{y}_i \mathbf{y}_i^{\mathrm{T}} - \mathbf{C})$$ $\tilde{\nabla}$-update of $\mathbf{C}$

using predetermined weights w_i instead of $w_i = -f(\mathbf{x}_{\rho^{-1}(i)})/\lambda$ and
using different learning rates (η, here 1 and c_μ) for m and $\mathbf{C}$
adding a few more tricks and design principles
leads to CMA-ES...

[Akimoto et al, PPSN 2010, Bidirectional Relation between CMA Evolution...]

Covariance Matrix Adaptation Evolution Strategy

CMA-ES = natural gradient descent + cumulation + step-size control

Input: $m \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\lambda \in \{2, 3, 4, \ldots\}$

Set $c_c \approx 4/n$, $c_\sigma \approx 4/n$, $c_1 \approx 2/n^2$, $c_\mu \approx \mu_w/n^2$, $c_1 + c_\mu \leq 1$, $d_\sigma \approx 1$,
set $w_{i=1,\ldots,\lambda}$ decreasing in i, $\sum_i |w_i| = 1$ and $\mu_w^{-1} := \sum_i {w_i}^2 \approx 3/\lambda$
Initialize $\mathbf{C} = \mathbf{I}$, and $\mathbf{p}_c = \mathbf{0}$, $\mathbf{p}_\sigma = \mathbf{0}$

While not *terminate*

$$\mathbf{x}_i = m + \sigma\, \mathbf{y}_i \sim \mathcal{N}\left(m, \sigma^2 \mathbf{C}\right), \quad \text{for } i = 1, \ldots, \lambda \qquad \text{sampling}$$

$$m \leftarrow m + \sigma \sum_i w_i\, \mathbf{y}_{i:\lambda} =: m + \sigma \mathbf{y}_w, \quad f(\mathbf{x}_{1:\lambda}) \leq f(\mathbf{x}_{2:\lambda}) \ldots \qquad \text{update mean}$$

$$\mathbf{p}_\sigma \leftarrow (1 - c_\sigma)\, \mathbf{p}_\sigma + \sqrt{1 - (1 - c_\sigma)^2} \sqrt{\mu_w}\, \mathbf{C}^{-\frac{1}{2}}\, \mathbf{y}_w \qquad \text{path for } \sigma$$

$$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\mathbf{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|} - 1\right)\right) \qquad \text{update of } \sigma$$

$$\mathbf{p}_c \leftarrow (1 - c_c)\, \mathbf{p}_c + \mathbb{1}_{[0,2n]}\left\{\|\mathbf{p}_\sigma\|^2\right\} \sqrt{1 - (1 - c_c)^2} \sqrt{\mu_w}\, \mathbf{y}_w \qquad \text{path for } \mathbf{C}$$

$$\mathbf{C} \leftarrow (1 - c_1 - c_\mu)\, \mathbf{C} + c_\mu \sum_{i=1}^{\lambda} w_i\, \mathbf{y}_{i:\lambda} \mathbf{y}_{i:\lambda}^{\mathrm{T}} + c_1\, \mathbf{p}_c\, \mathbf{p}_c^{\mathrm{T}} \qquad \text{update } \mathbf{C}$$

Evolution Strategies on the Sphere Function

$$f(x) = \|x\|^2 = \sum_{i=1}^{n} x_i^2$$

- Evolution Window for the step-size

  [Rechenberg 1973]

- One-fifth success rule (single parent, $\mu = 1$)

  $\mu = |\{w_i \neq 0 \mid w_i \in \{0, \frac{1}{\mu}\}\}|$

  [Schumer&Steiglitz TAC 1968, Rechenberg 1973]

- Optimal truncation ratio for (μ, λ)-ES $\frac{\mu}{\lambda} \approx 0.27$

  [Beyer 2001]

- Known optimal recombination weights

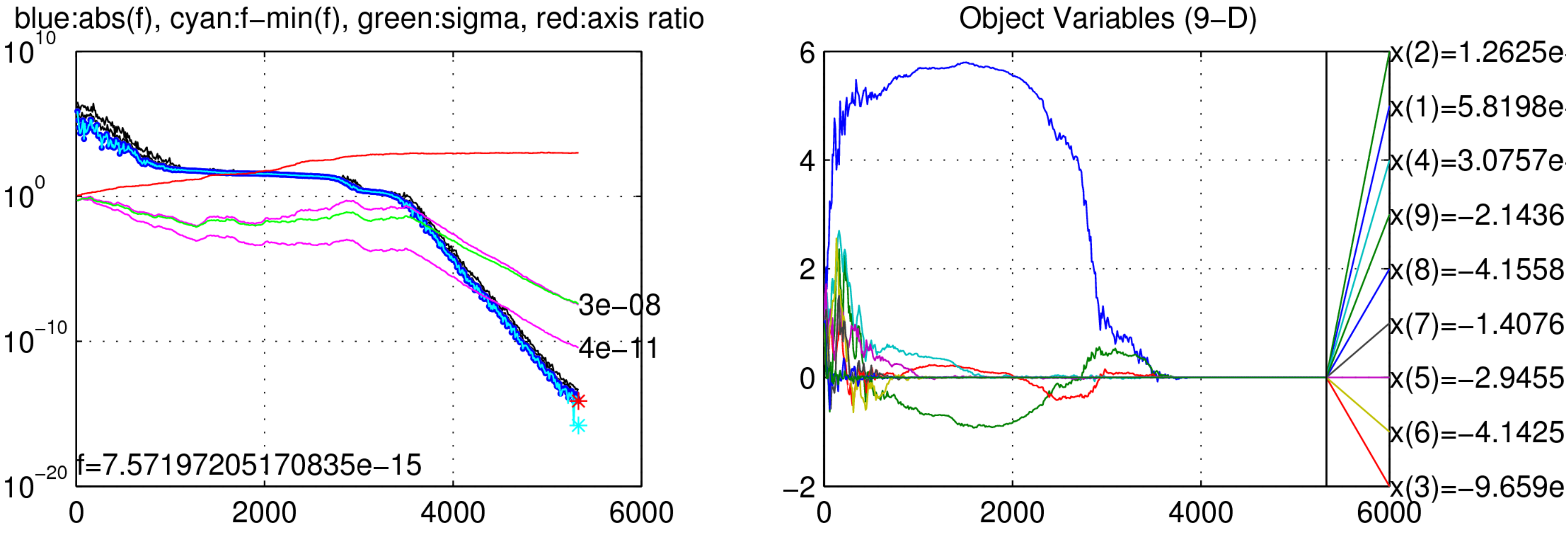
  [Arnold TEC 2006]

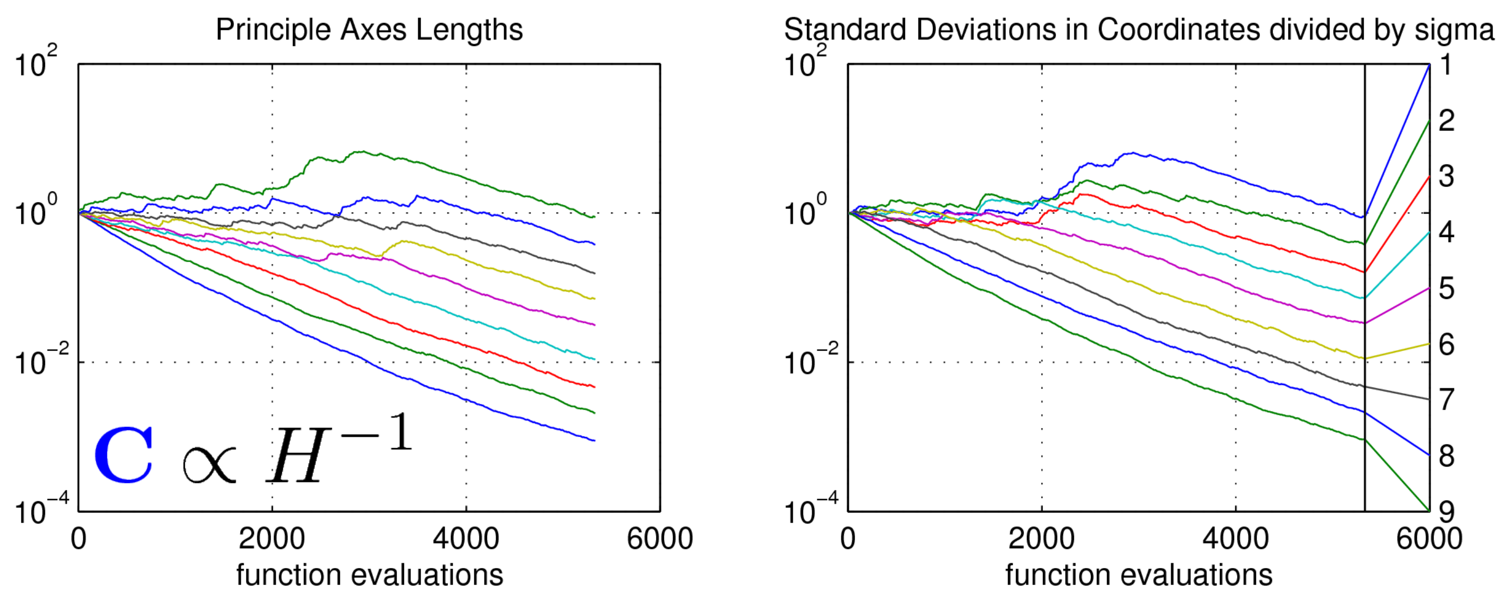
- Convergence proofs (linear convergence)

  [Auger TCS 2005, Jägersküpper TCS 2006] $\frac{m_k - \mathbf{x}^*}{\sigma_k}$ is stationary

- Optimal progress rates $\|m_k - x^*\| \approx \|m_0 - x^*\| \exp\left(-0.2k\frac{\mu}{n}\right)$

Experimentum crucis

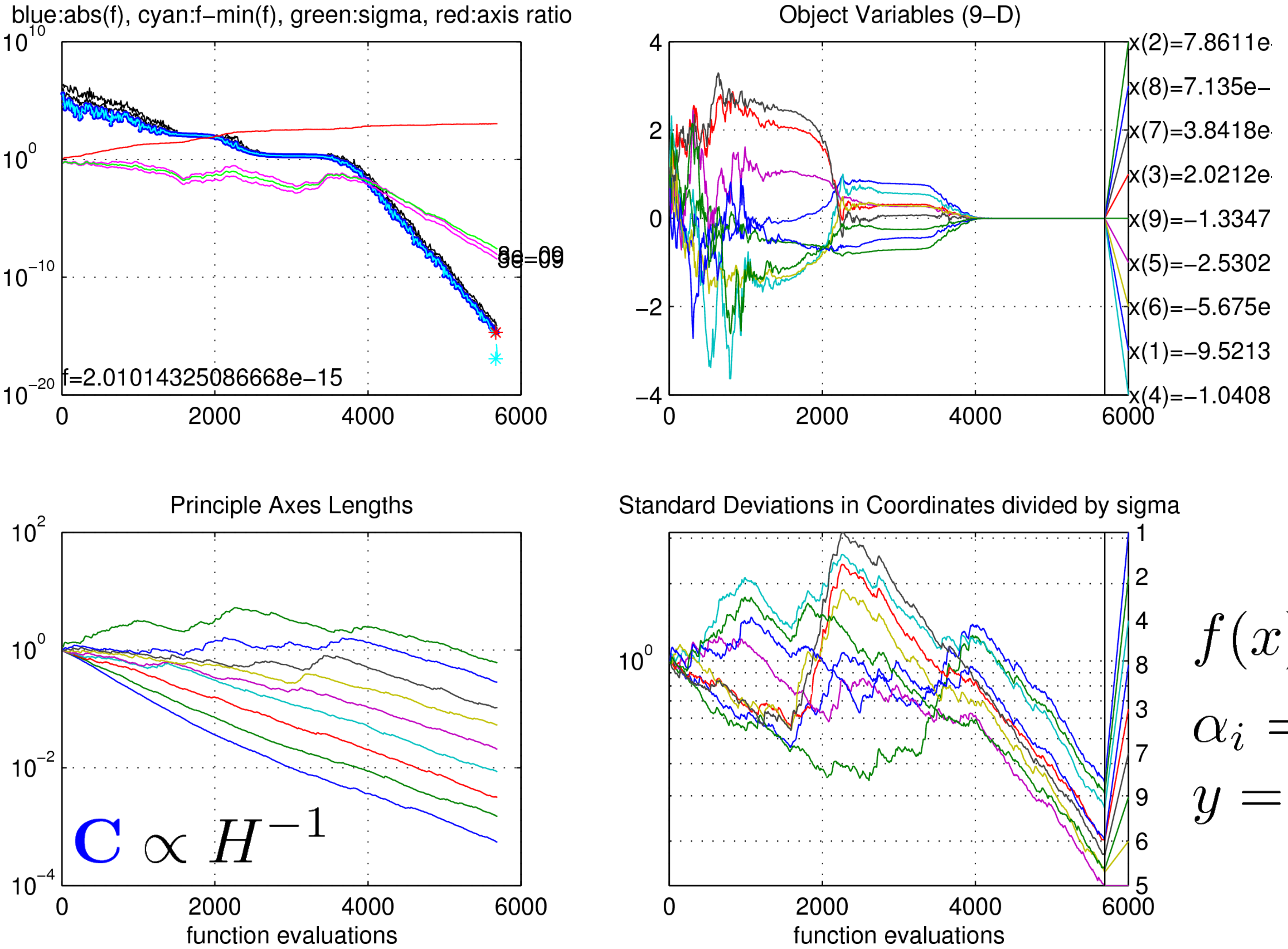




$$f(x) = \sum_{i=1}^{n} \alpha_i x_i^2$$

$$\alpha_i = 10^{6\frac{i-1}{n-1}}$$

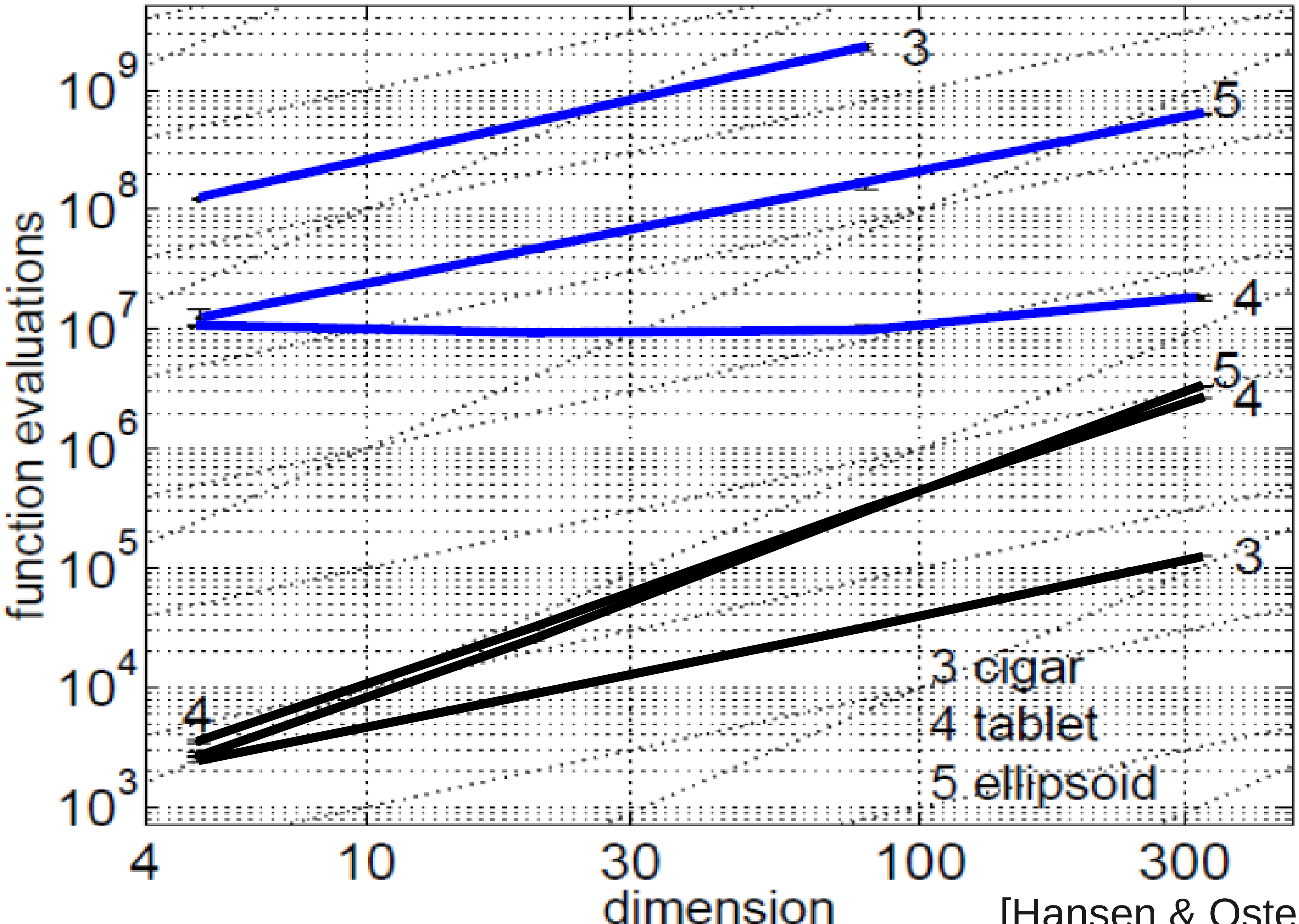
Experimentum crucis



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

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i^2$$
$$\alpha_i = 10^{6\frac{i-1}{n-1}}$$
$$y = \mathrm{rotation}(x)$$

Quantifying the enhancement



[Hansen & Ostermeier 2001]

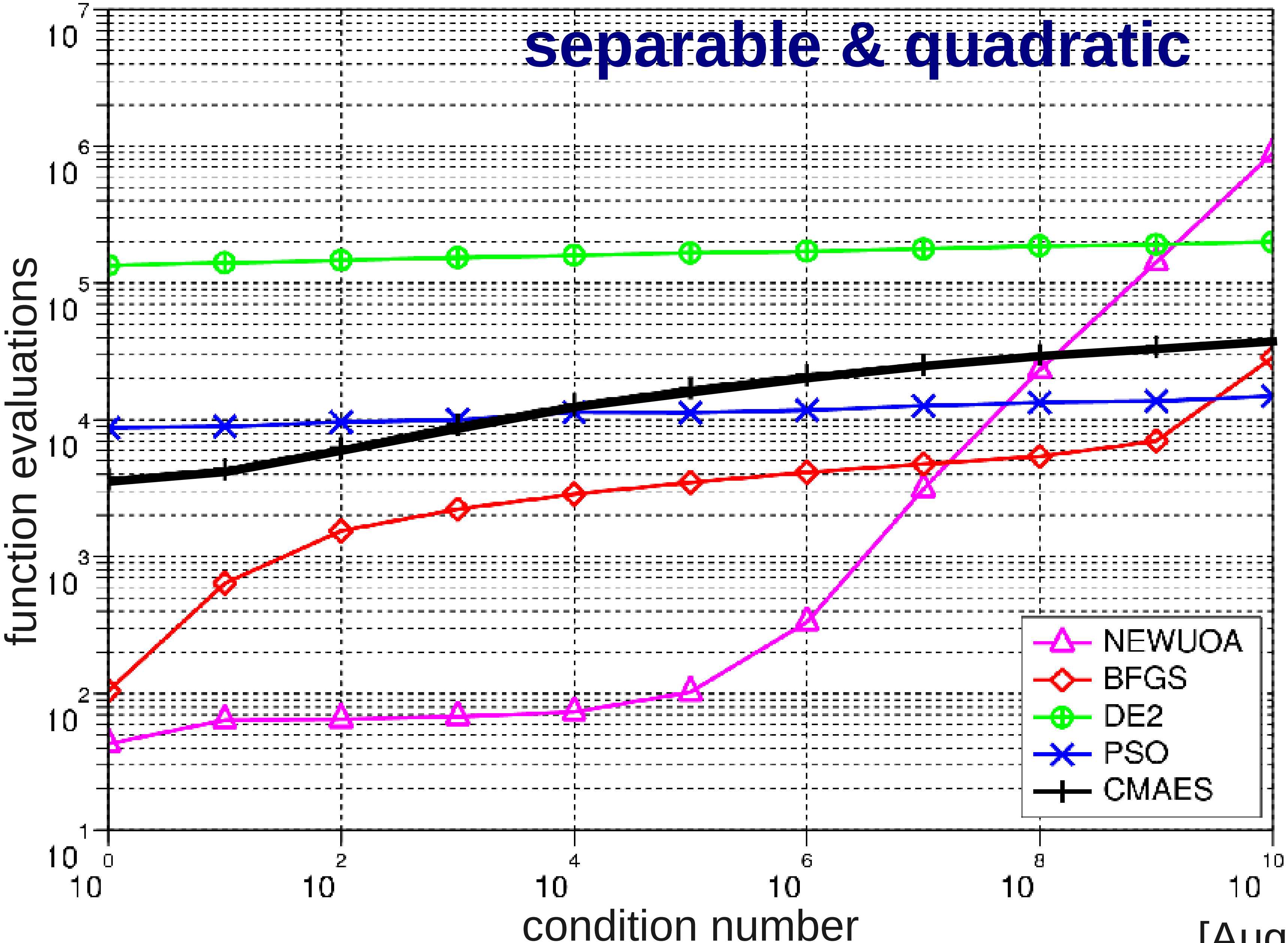
black: CMA-ES ($c_1 \approx 2/n^2$), blue: CSA-ES ($c_1 = 0$)

Unimodal test functions

$$f(x) = g\left(\frac{1}{2}x^T H x\right)$$

for different order-preserving $g : \mathbb{R} \rightarrow \mathbb{R}$
with uniform eigenspectrum of the Hessian H
in dimension 20

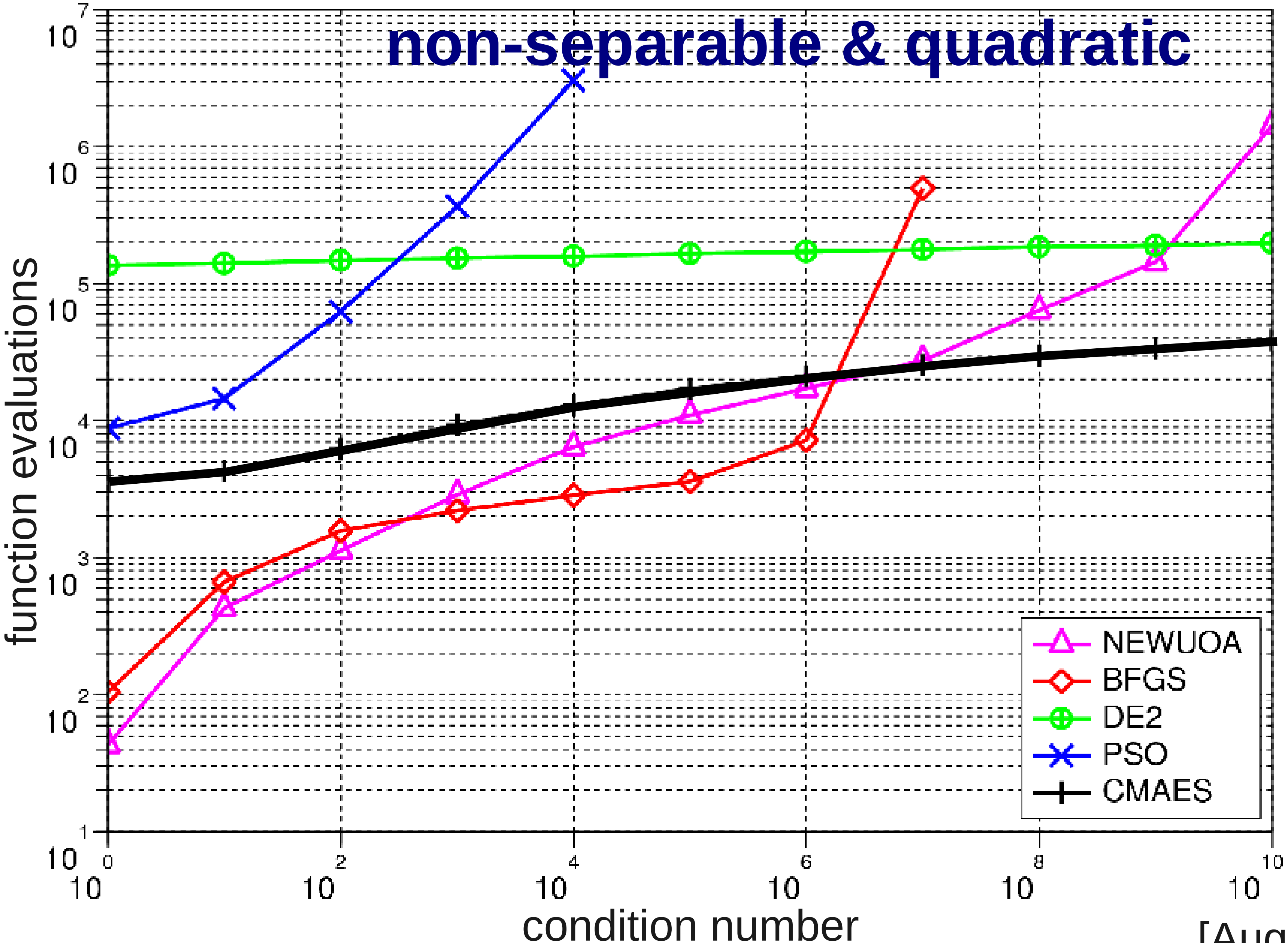
Runtime versus condition number



1

[Auger et al 2009]

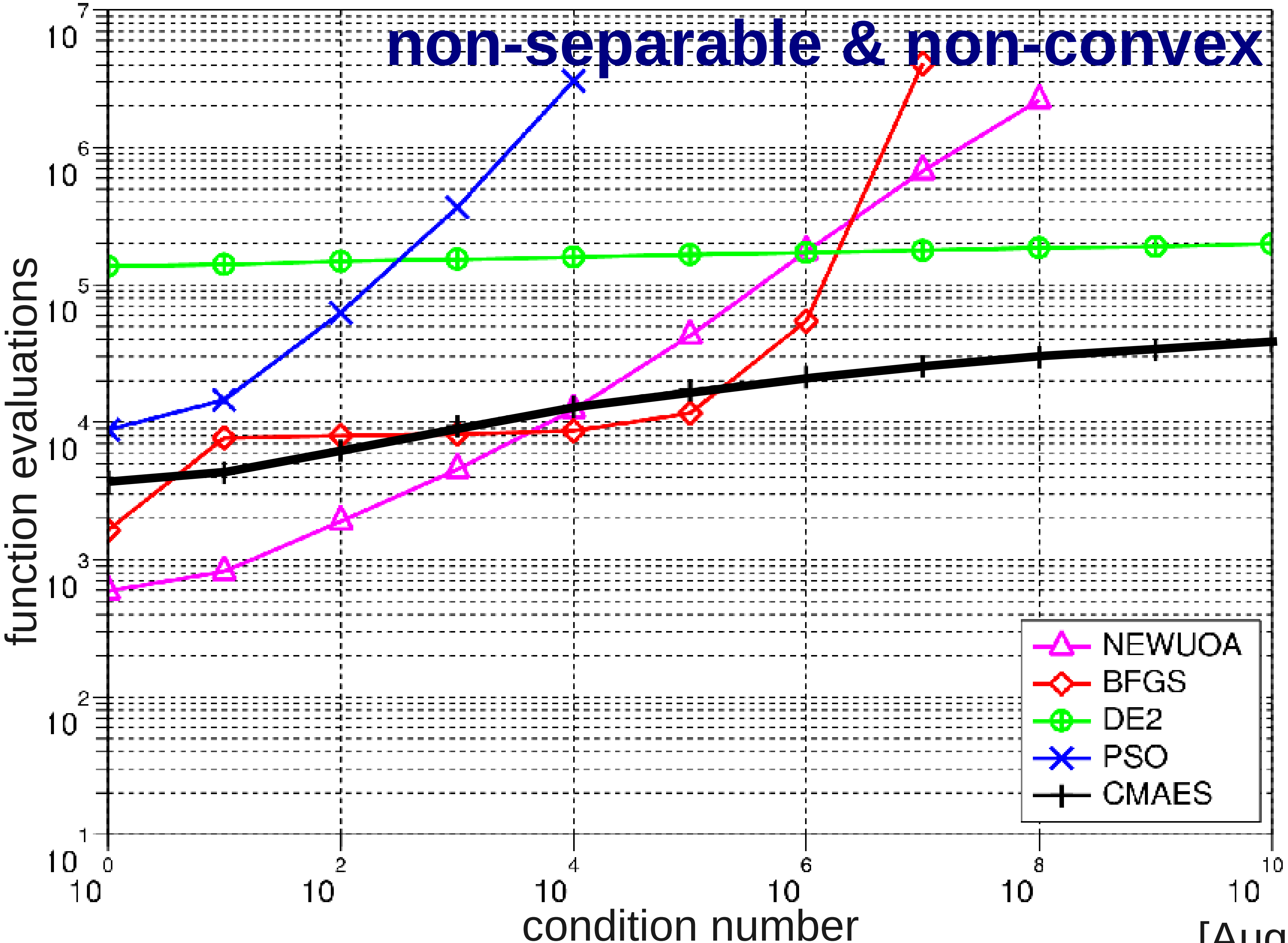
Runtime versus condition number



2

[Auger et al 2009]

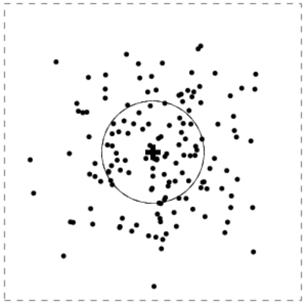
Runtime versus condition number



3

[Auger et al 2009]

CMA-ES in a nutshell



1) Sample maximum entropy distribution

$\mathbf{x}_i = m + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C})$ multivariate normal distribution

2) Ranking solutions according to their fitness

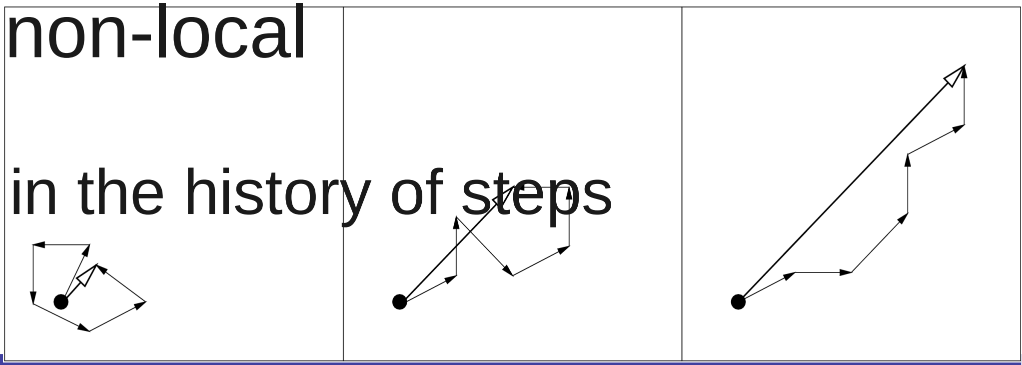
invariance to order-preserving transformations

3) Update mean and covariance matrix by natural gradient descend, increasing the expected fitness and likelihood of good steps

natural gradient descend,
PCA → variable metric, new problem representation,
invariant under changes of the coordinate system

4) Update step-size based on non-local information

exploit correlations in the history of steps



CMA-ES is widely recognized

- ≈ 1000 citations to the two seminal papers
- $\gg 100$ published applications
- implemented in libraries for
  - evolutionary computation [EO, Beagle,. . .]
  - pattern search [NOMADm]
  - machine learning [Shark]
  - robotics [PACLib]
  - chart analysis [AmiBroker]
  - water model calibration [PEST]
- ≈ 20 daily hits to the source code download page

Questions?

COCO/BBOB

- Is an environment for COmparing Continuous Optimizers
- under development with contributions from
  - Raymond Ros
  - Steffen Finck
  - Anne Auger
  - Marc Schoenauer
  - Petr Pošík
  - Mike Preuss
  - Dimo Brockhoff
  - …

http://coco.gforge.inria.fr

COCO: objectives

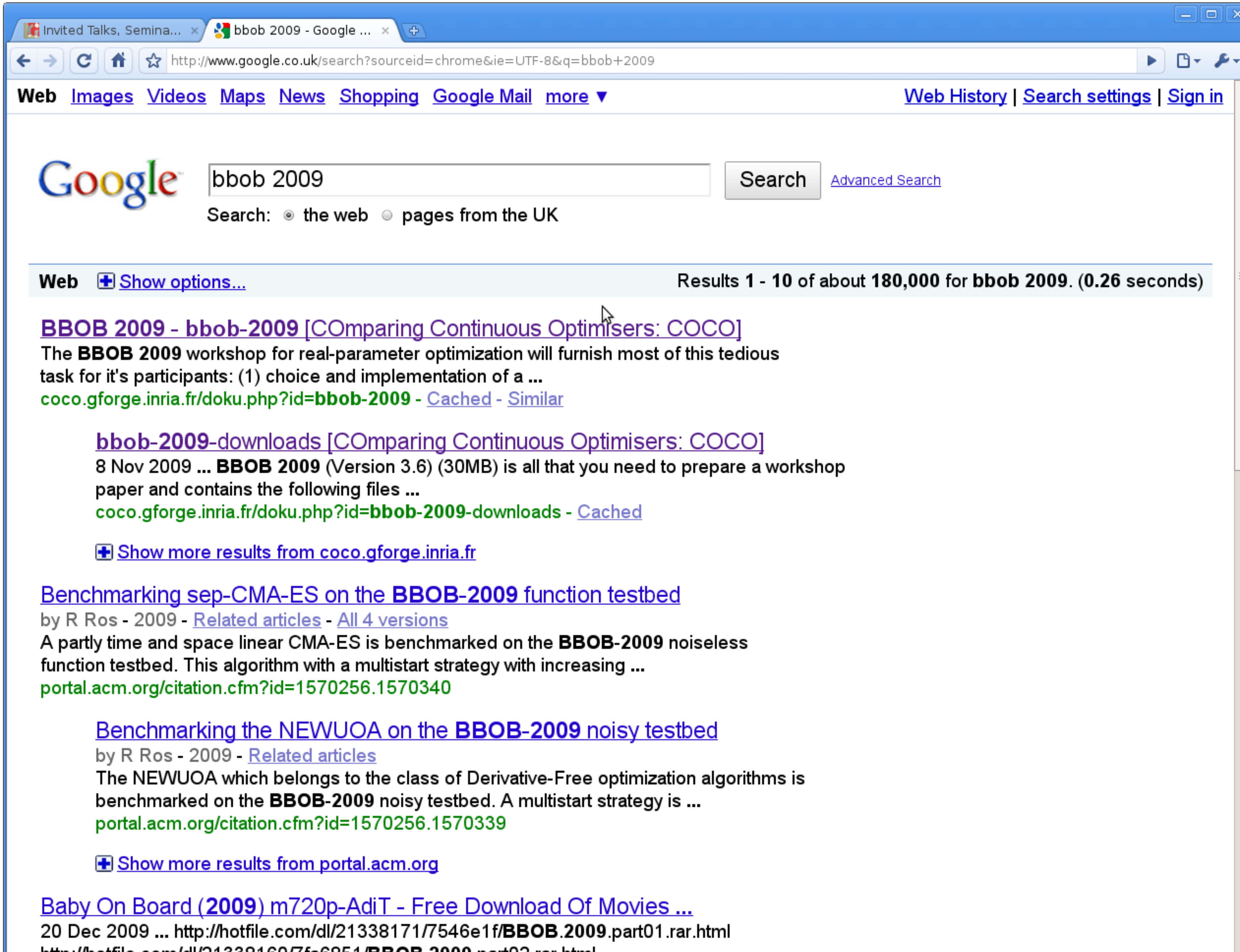
- function testbed:
  - should "reflect reality"
  - mainly non-convex and non-separable
  - scalable with the search space dimension
  - not too easy to solve, but yet comprehensible

- provide data acquisition at the interface of solver and objective function

  lean but sufficient data for quantitative analyses

- data presentation yields quantitative assessment, stratified by function properties...

BBOB in practice



BBOB in practice

Invited Talks, Semina... | bbob-2009-downloa...

http://coco.gforge.inria.fr/doku.php?id=bbob-2009-downloads

[[bbob-2009-downloads]] COMPARING CONTINUOUS OPTIMISERS: COCO

Show pagesource Old revisions Recent changes Index Login

This is the BBOB 2009 download page.

BBOB 2009 (Version 3.6) (30MB) is all that you need to prepare a workshop paper and contains the following files

- CODE:
  - tar code in Matlab/Octave
  - tar code in C
  - tar post-processing Python package + workshop paper LaTeX templates
  - soon available: post-processing Python package including comparing analysis
- DOCS:
  - pdf description of experimental procedure
  - pdf (13MB) noiseless functions documentation with figures
  - pdf noiseless functions documentation, version without figures
  - pdf (20MB) noisy function documentation with figures
  - pdf noisy function documentation, version without figures
  - pdf software user documentation
- TECHNICAL DOCS:
  - html post-processing package documentation

Here are the results from the workshop in July 2009

Search

Index
- **playground**
- **wiki**
- bbob-2009-downloads
- bbob-2009-results
- bbob-2009
- start

BBOB in practice

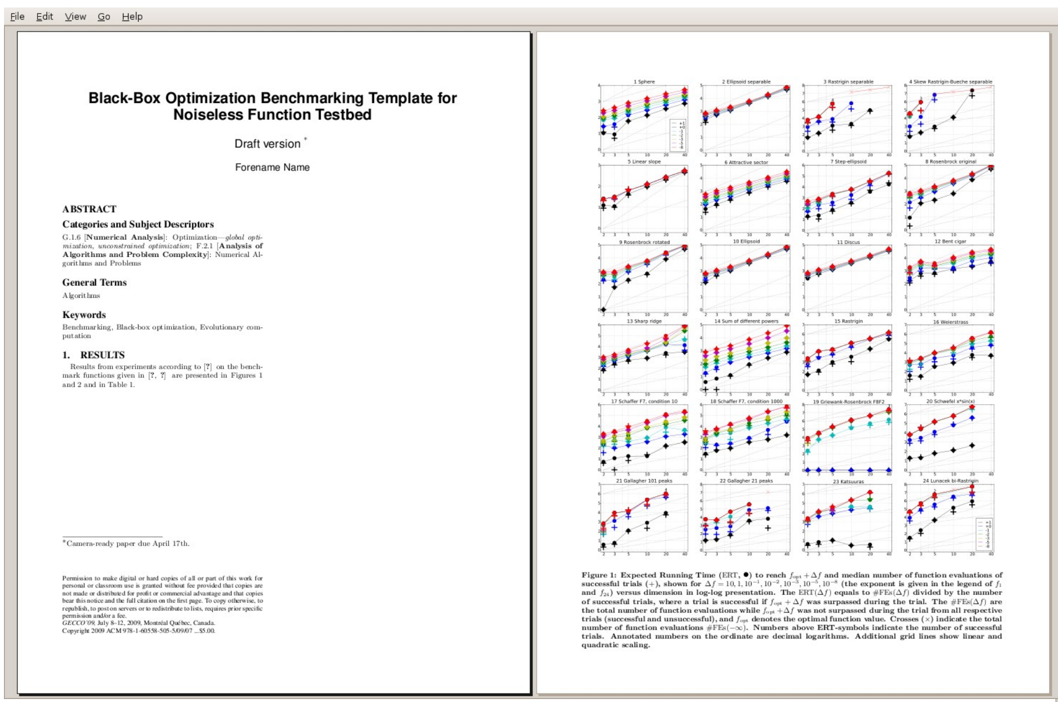
Matlab script:

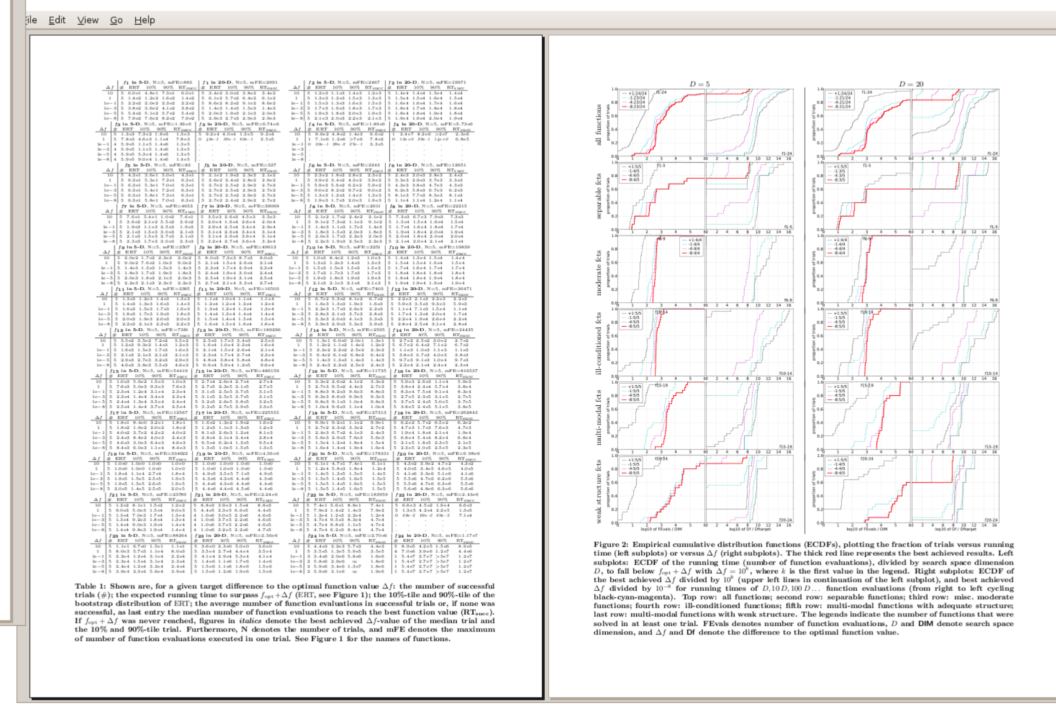
```
for dim = [2,3,5,10,20,40]  % small dimensions first, for CPU reasons
  for ifun = benchmarks('FunctionIndices')  % or benchmarksnoisy(...)
    for iinstance = [1:5, 1:5, 1:5]  % first 5 fct instances, three times
      fgeneric('initialize', ifun, iinstance, datapath);

      MY_OPTIMIZER('fgeneric', dim, ...   % necessary parameters
                   fgeneric('ftarget'));  % optional termination parameter

      fgeneric('finalize');
    end
    disp(['      date and time: ' num2str(clock, ' %.0f')]);
  end
  disp(sprintf('---- dimension %d-D done ----', dim));
end
```

BBOB in practice

Post-processing at the OS shell:

```
python codepath/bbob_pproc/run.py datapath
pdflatex templateACMarticle.tex
```



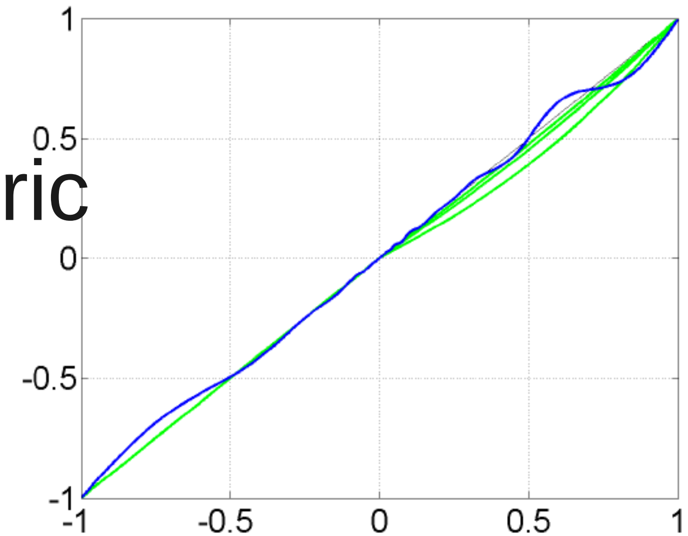


COCO: the noiseless functions

24 functions within five sub-groups

- Separable functions
- Essential unimodal functions
- Ill-conditioned unimodal functions
- Multimodal structured functions
- Multimodal functions with weak or without structure

functions are not perfectly symmetric and are locally deformed



COCO: the noisy functions

three noise-”models”, so-called:

- Gauss, Uniform (severe), Cauchy (outliers)
- Utility-free noise

$$E(f(x)) \leq E(f(y)) \Rightarrow U(f(x)) \leq U(f(y)) \; \forall x, y, U$$

30 functions with three sub-groups

- 2x3 functions with weak noise
- 5x3 unimodal functions
- 3x3 multimodal functions

How should we measure performance?

Evaluation of Search Algorithms

needs

- Meaningful quantitative measure on benchmark functions or real world problems
- Account for meta-parameter tuning

tuning to specific problems can be quite expensive

- Account for invariance properties

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

- Account for algorithm internal costs

often negligible, depending on the objective function cost

A performance measure

should be

- quantitative, with a ratio scale
- well-interpretable with a meaning
- relevant in the “real world”
- simple

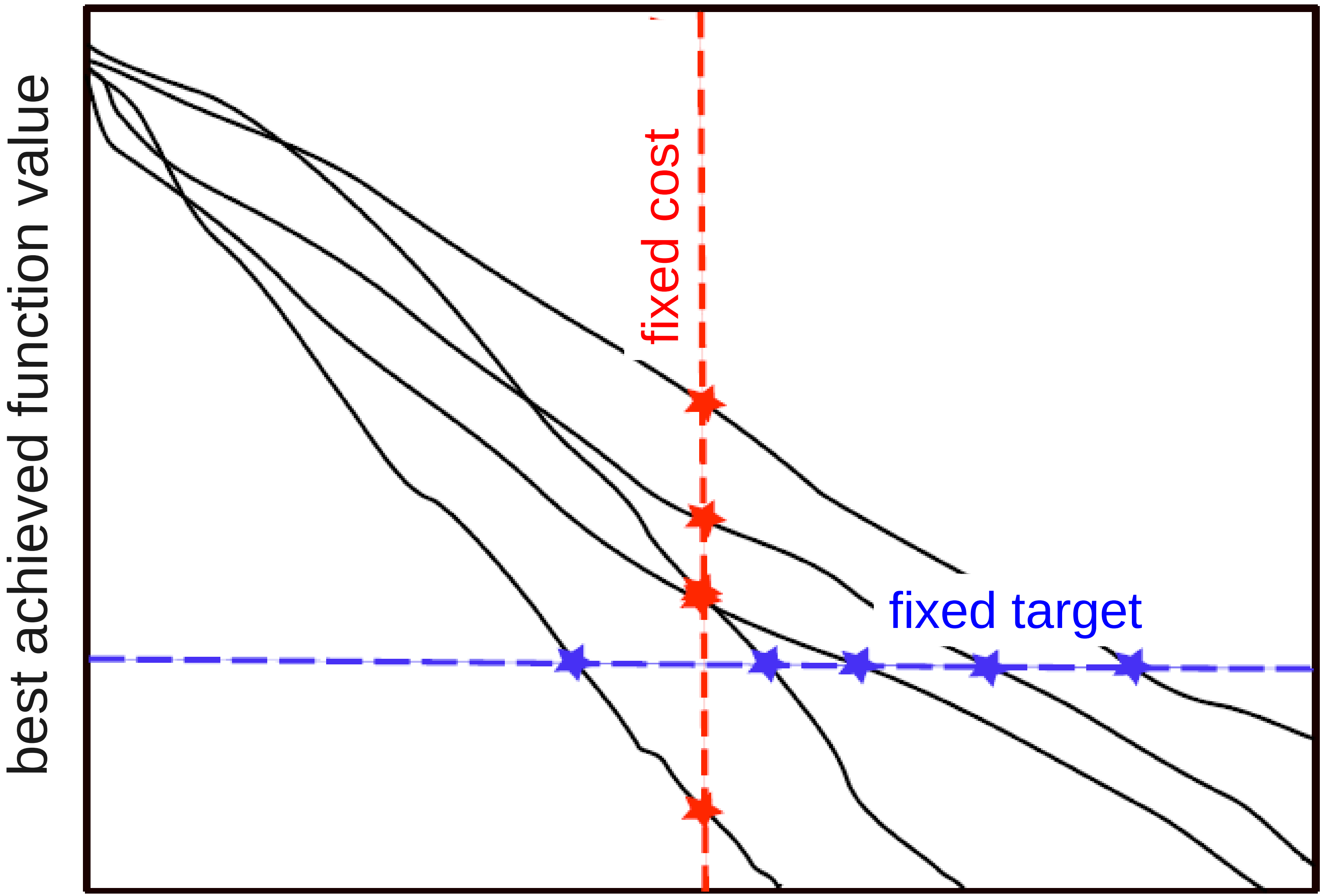
(recall) Black-Box Optimization

Two objectives:

- Find solution with a smallest possible function value
- With the least possible search costs (number of function evaluations)
- For measuring performance: fix one and measure the other

How should we measure performance?

fixed-cost versus fixed-target



A performance measure

should be

- quantitative, with a ratio scale
- well-interpretable with a meaning
- relevant in the "real world"
- simple

running time

- empirical distribution [Hoos & Stützle 1998]
- expectation, median, ...

Runtime

We measure runtime in number of function evaluations

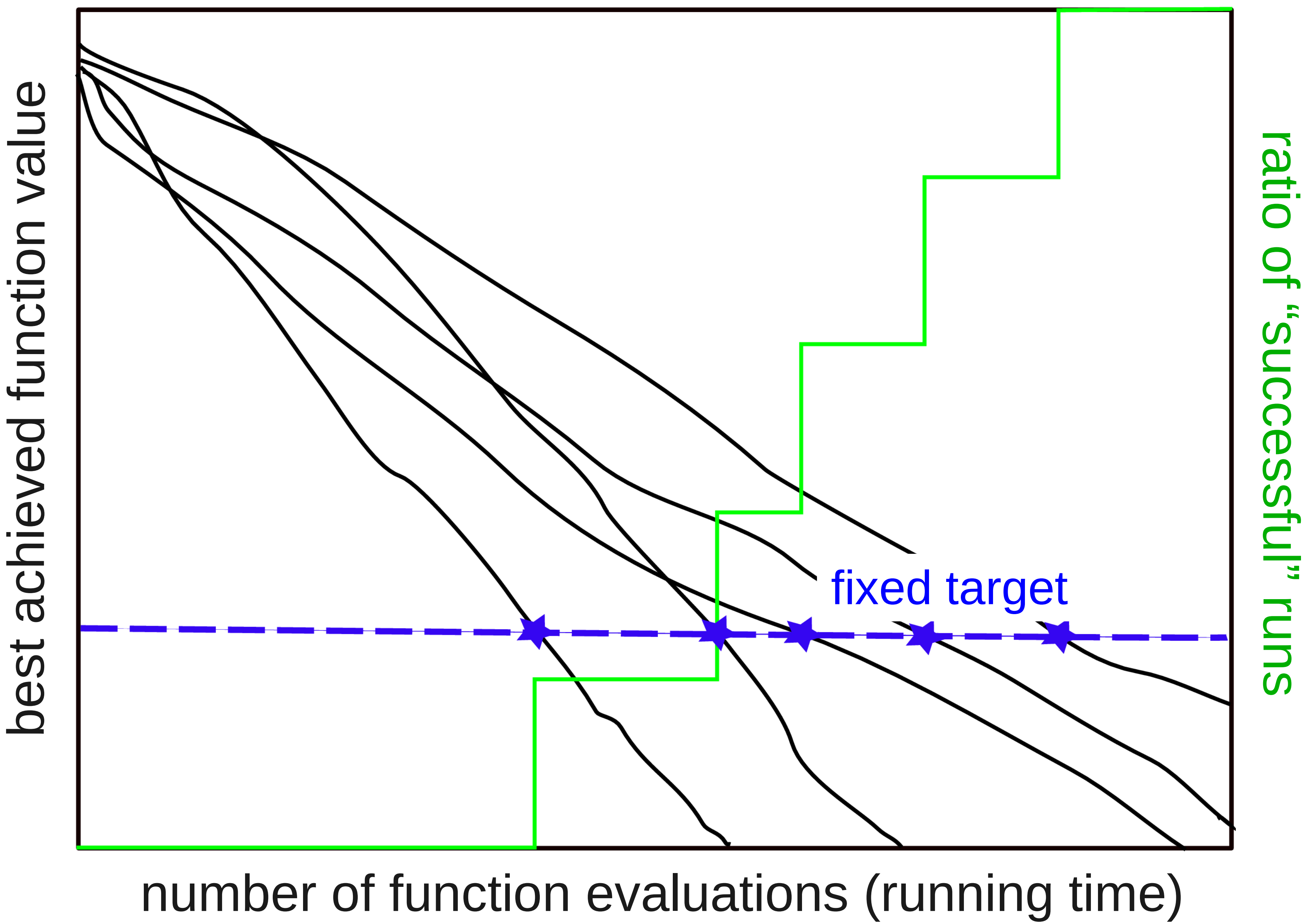
- As a distribution of runtimes
- As expected runtime ERT

For success probability $0 < p < 1$: (simulated) restarts until a successful run is observed.

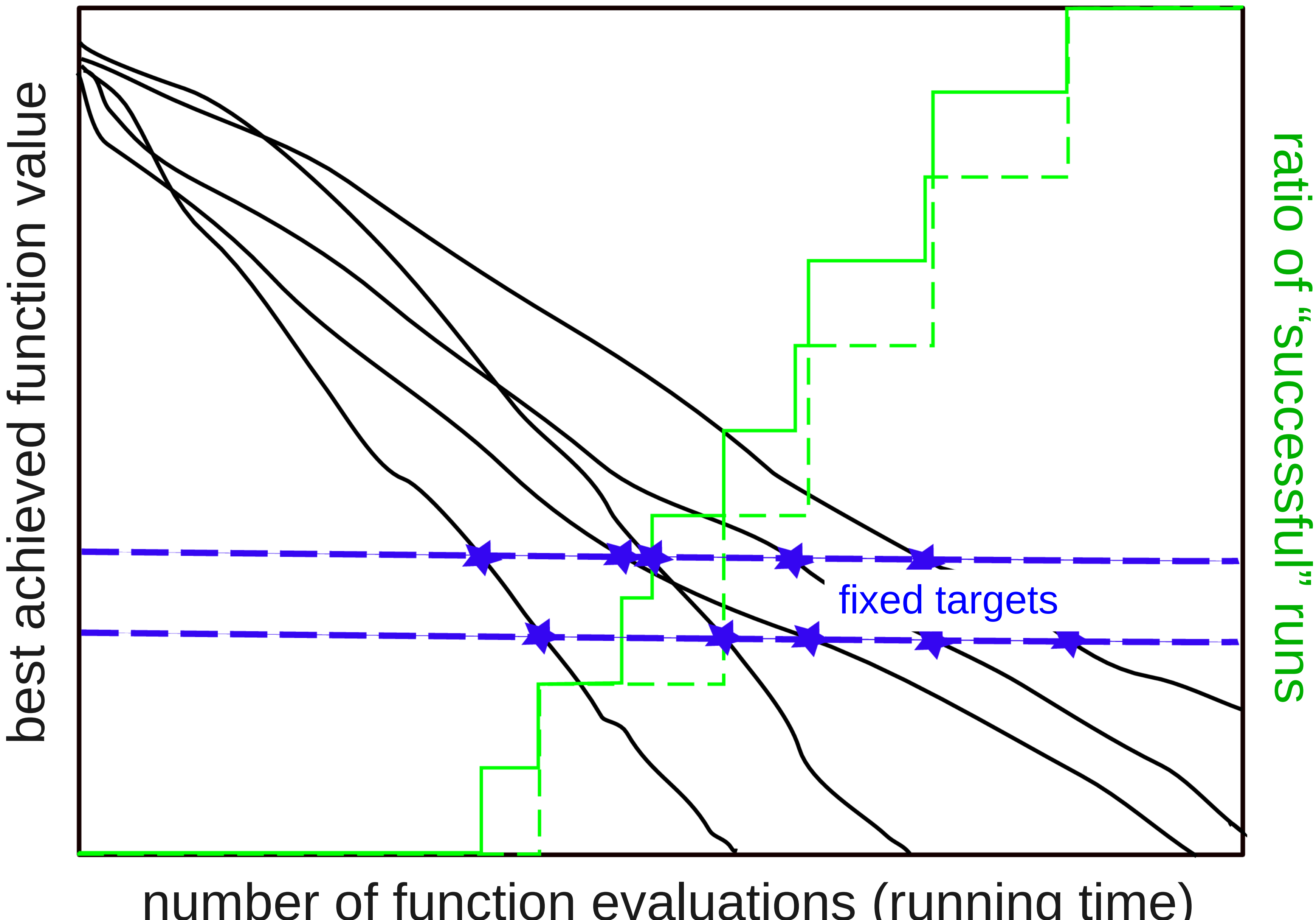
$$\begin{aligned}\mathsf{RT} &= \mathsf{RT}_{\mathrm{succ}} + \sum \mathsf{RT}_{\mathrm{unsucc}} \\ &\approx E(\mathsf{RT}_{\mathrm{succ}}) + \frac{1-p}{p} E(\mathsf{RT}_{\mathrm{unsucc}})\end{aligned}$$

Feature/drawback: termination method for unsuccessful trials can be critical

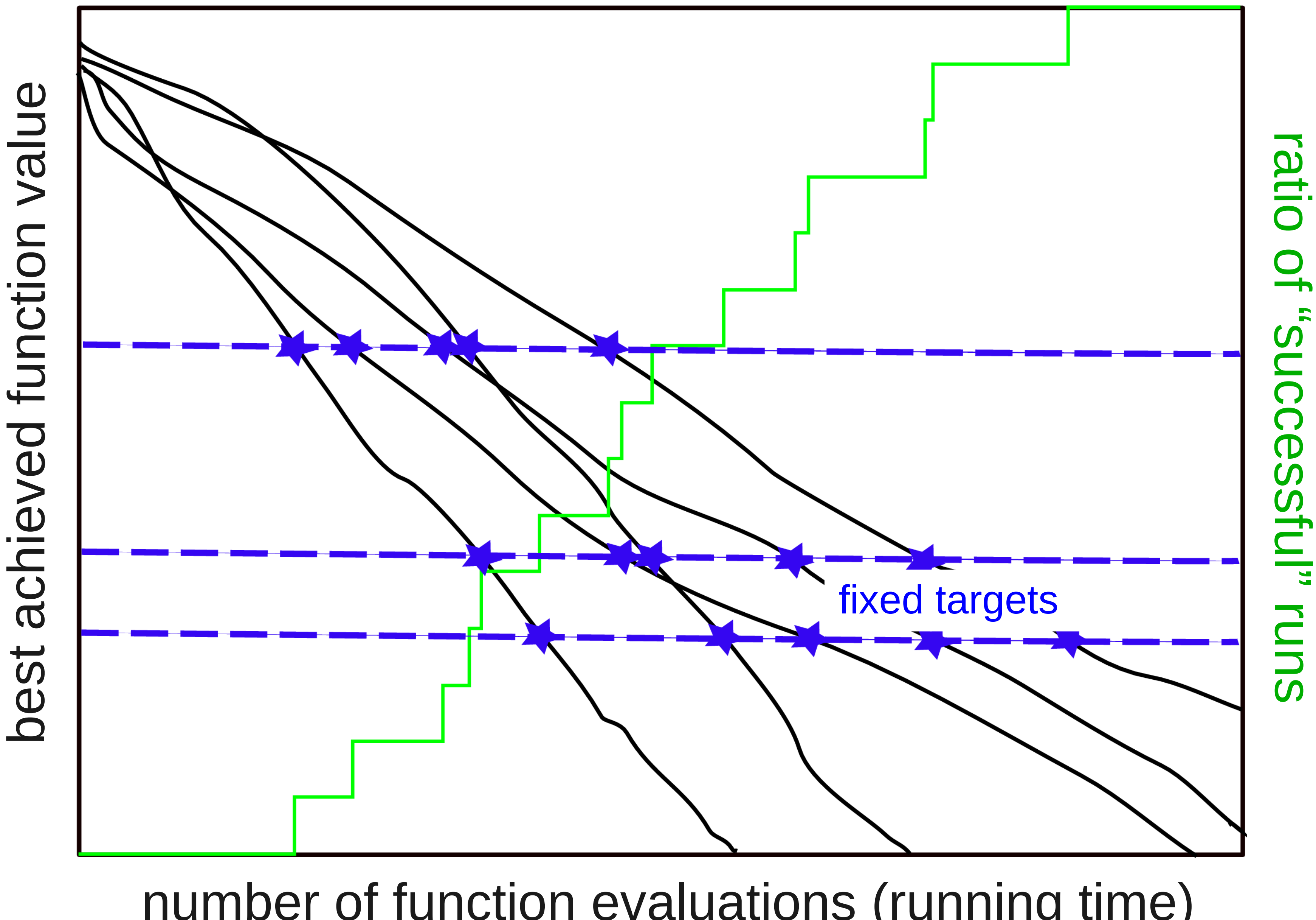
Measuring Performance with given target values



Measuring Performance with given target values



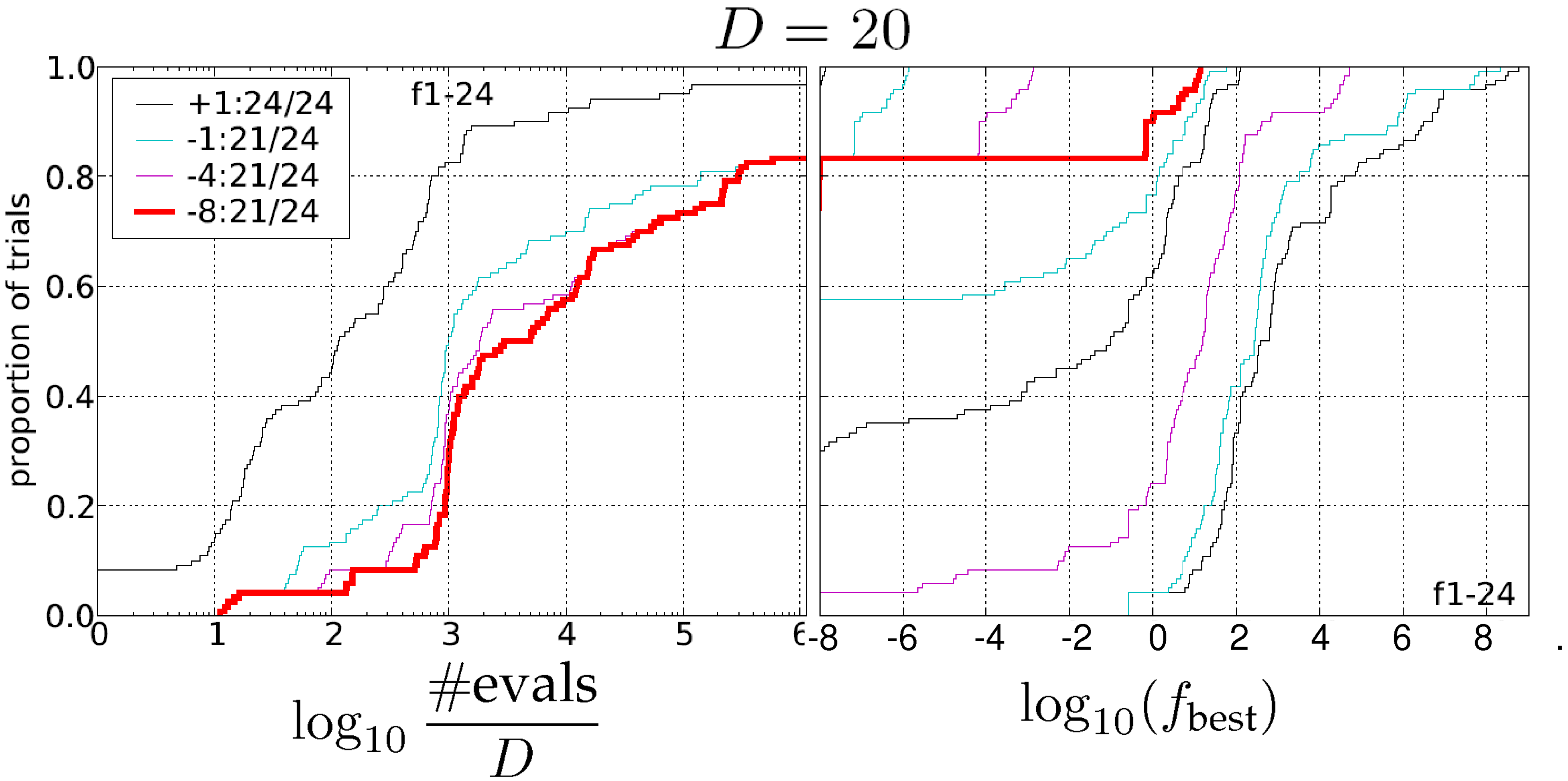
Measuring Performance with given target values



Cumulative Distribution of Runtimes

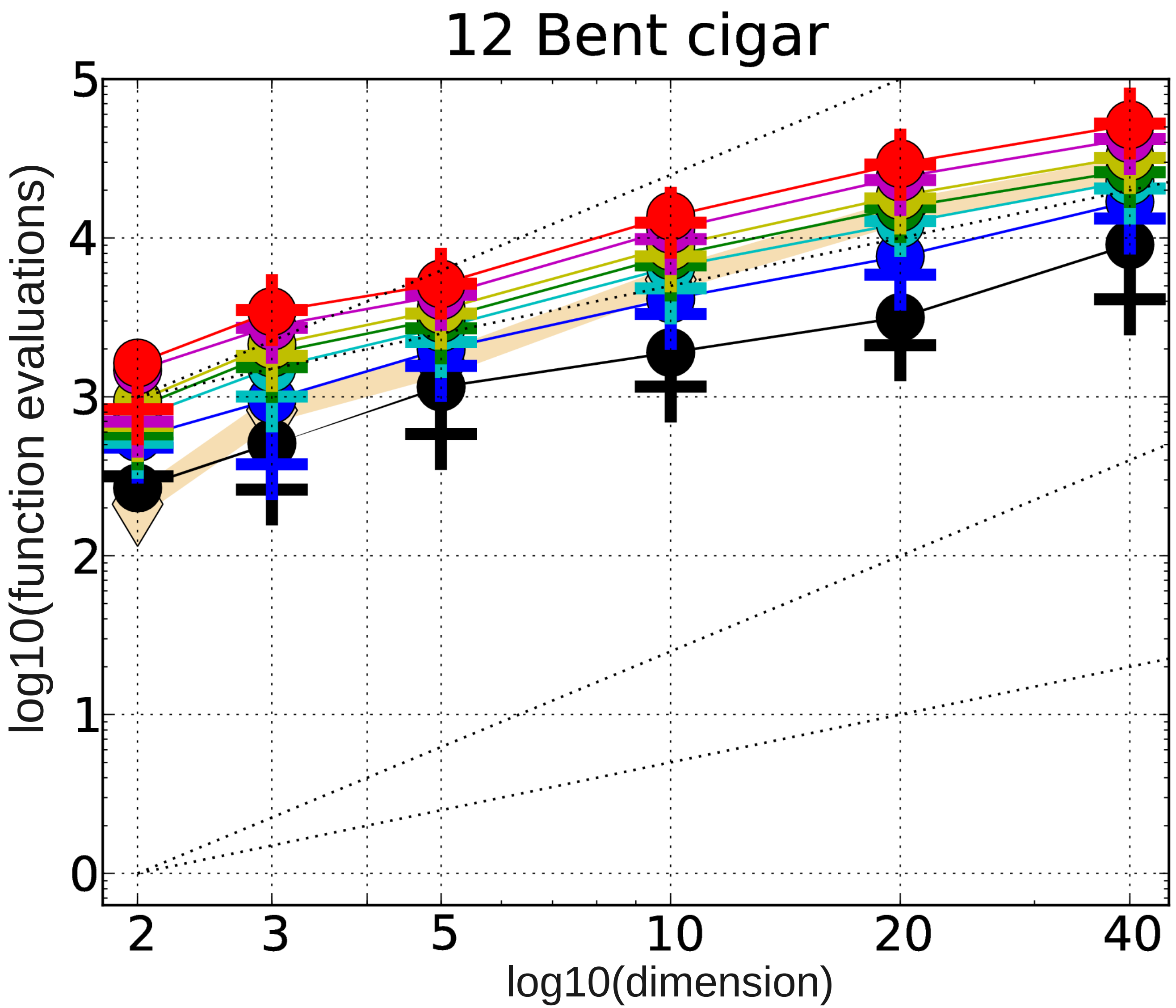
- Given a set of functions and for each function a (weighted) set of target values, the cumulative distribution of (simulated) RTs captures all(?) aspects of the performance in a single graph
- Remark: this performance measure can aggregate over any set of functions and target values
- Here: 50 target values, log-uniform in [1e-8,100] and 15 trials per function

Example for ECDFs



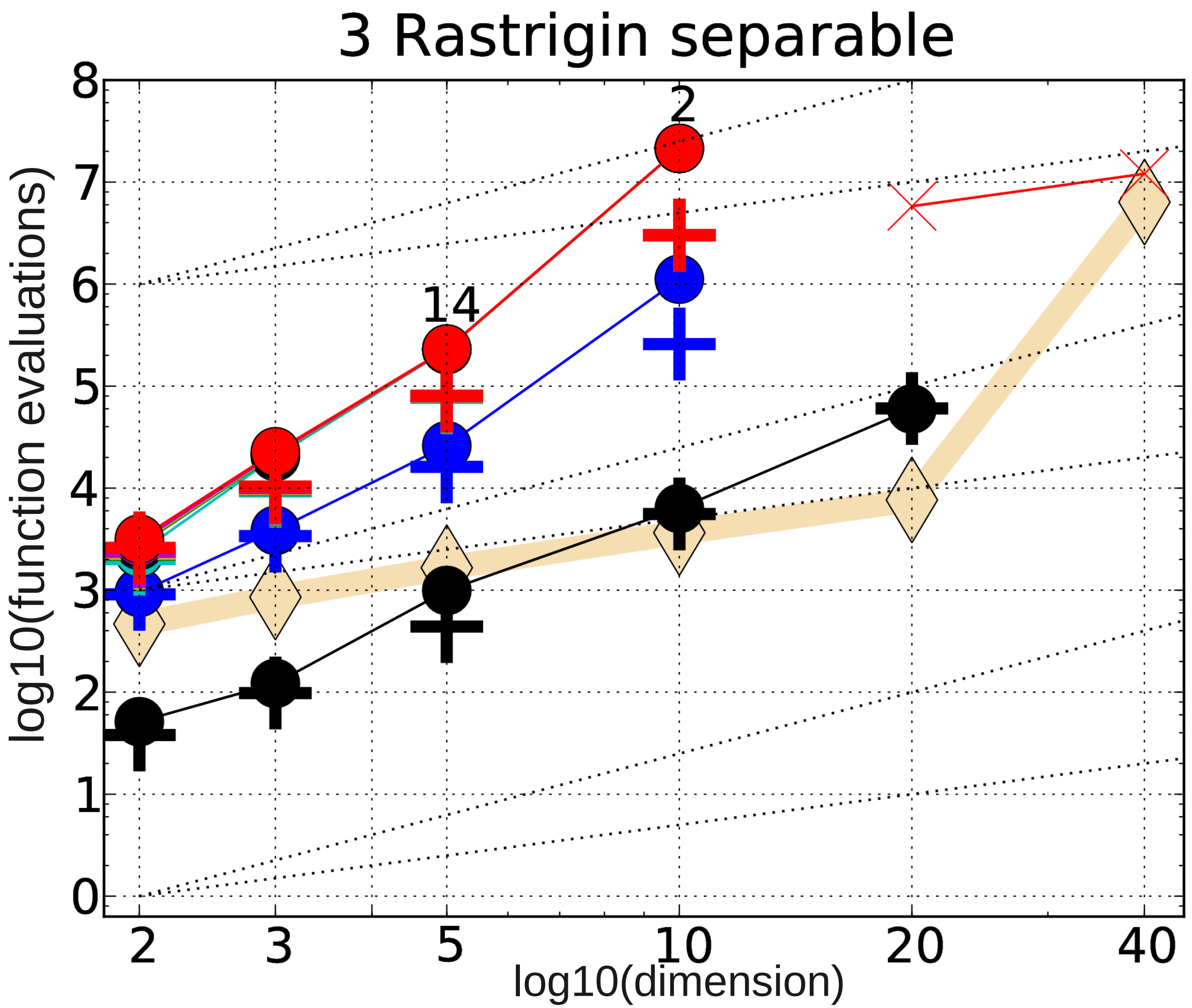
Empirical cumulative distribution functions (ECDFs) of running lengths (left) and function values (right)

Example: Scaling Behaviour



- ERT on f12: linear scaling of BIPOP-CMA-ES

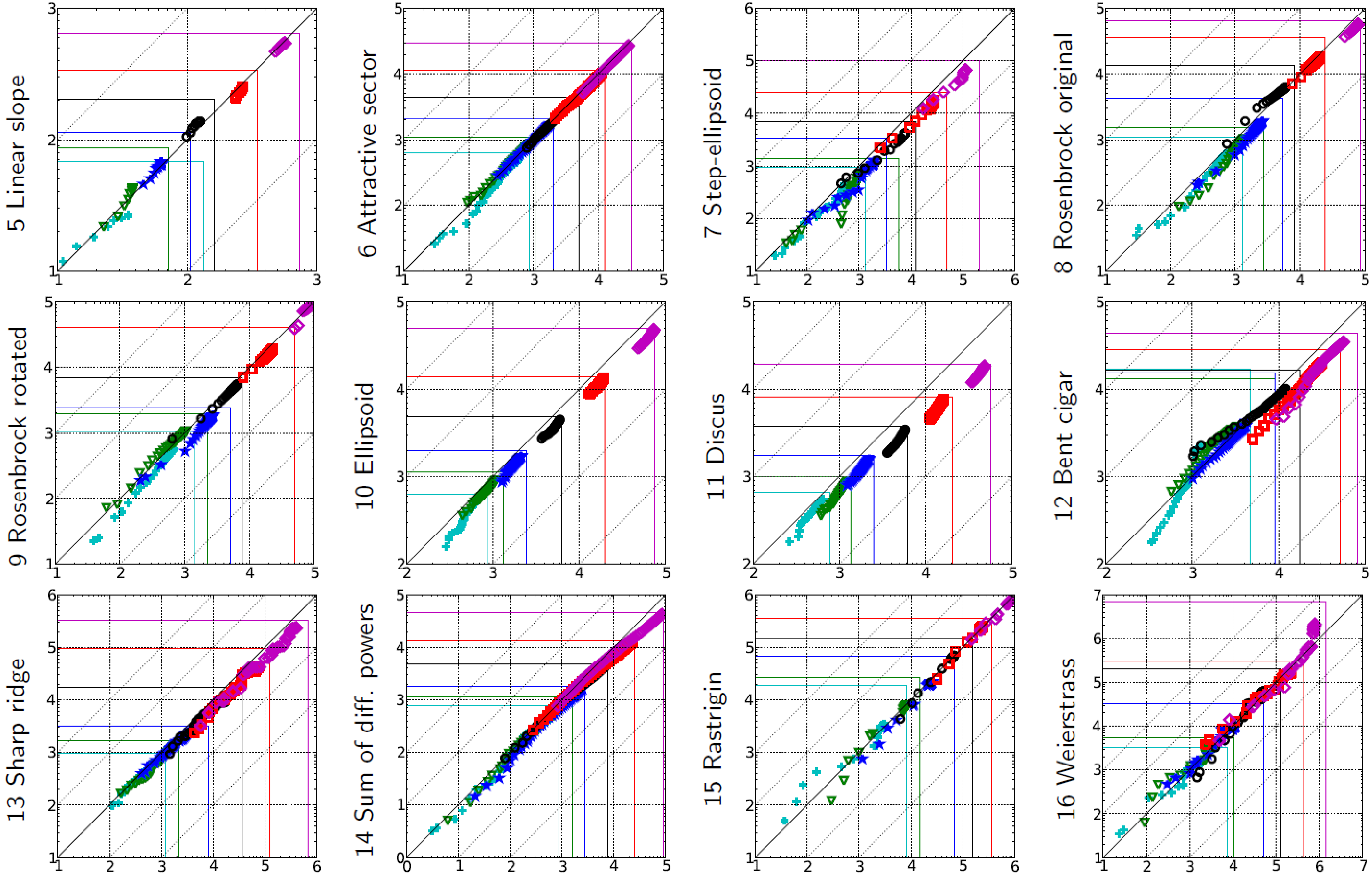
Example: Scaling Behaviour



- Experiments in >100-D are more often than not virtually superfluous

ERT scatter plots comparing two algorithms

all dimensions & targets



Overall Collected Data Sets

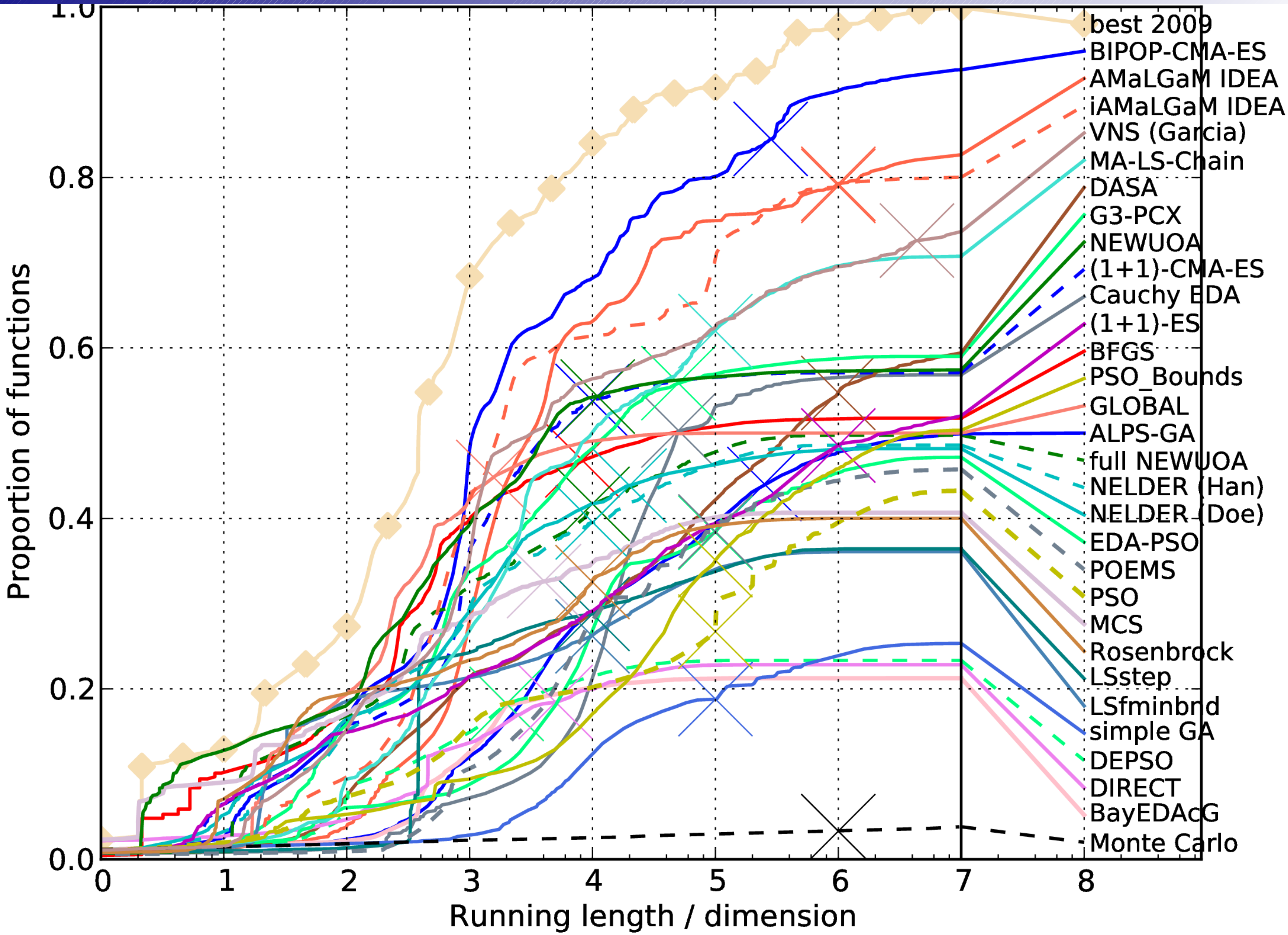
during the *Black-Box Optimization Benchmarking* (BBOB) workshops at the *Genetic and Evolutionary Computation Conference* GECCO

- 2009: 31 noiseless and 21 noisy “data sets”
- 2010: 24 noiseless and 16 noisy “data sets”

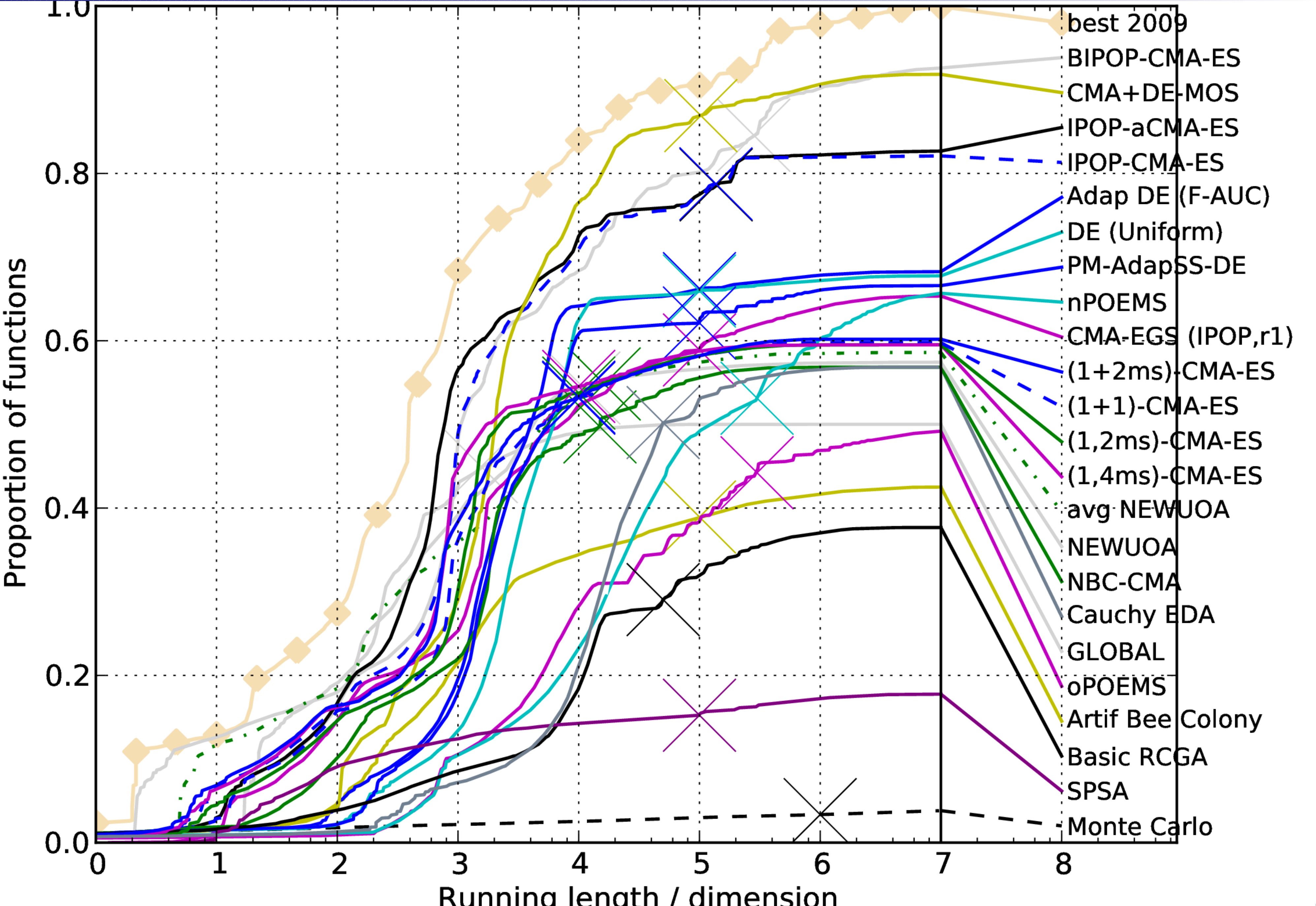
- Algorithms: RCGAs (eg plain, PCX), EDAs (eg IDEA), BFGS & (many) other “classical” methods, ESs (eg CMA), PSO, DE, Ant-Stigmergy Alg, Bee Colony, EGS, SPSA, Meta-Strategies...

Results

Results of 2009 (noisefree, 20-D)

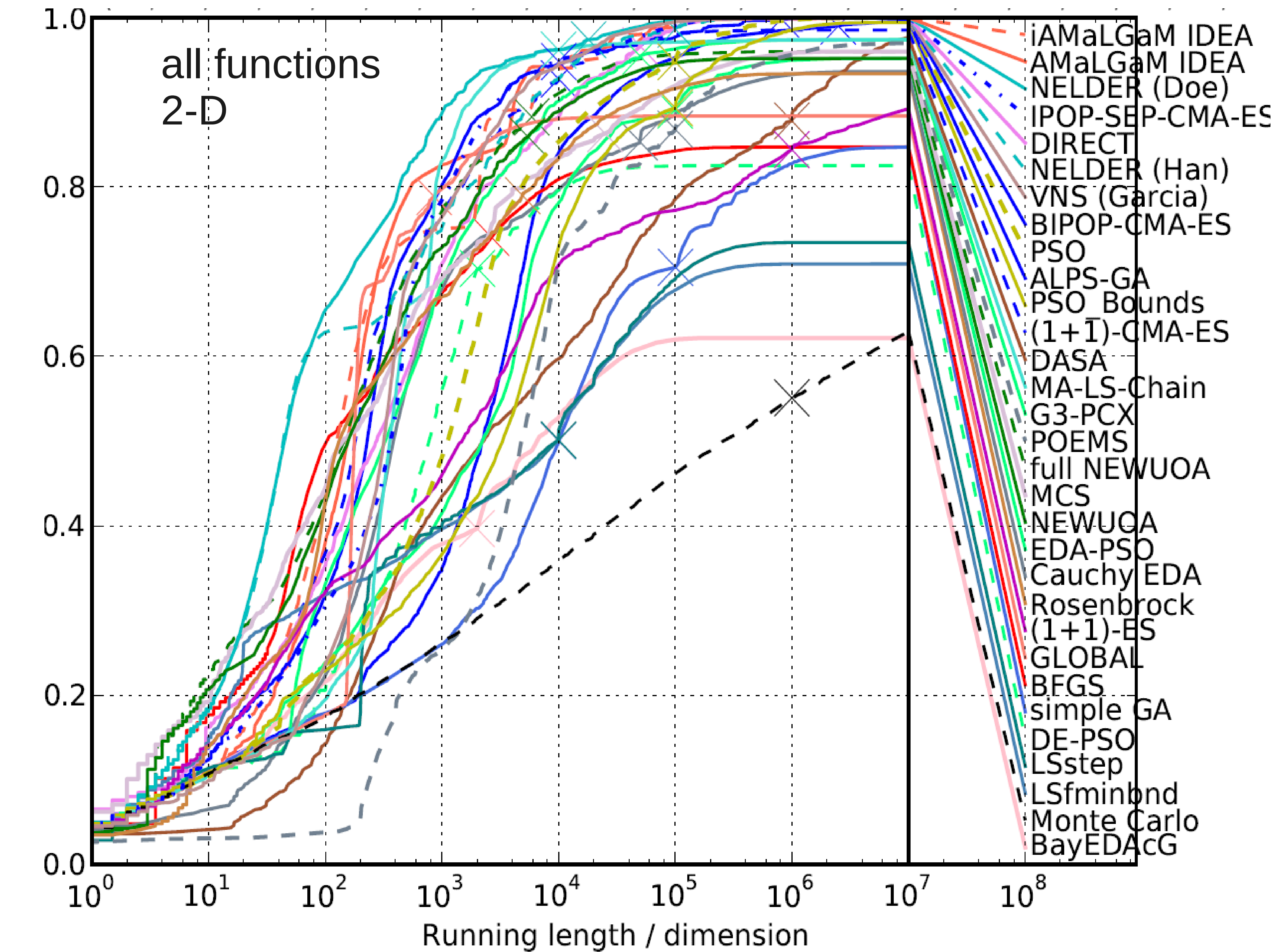


Results of 2010 (noisefree, 20-D)

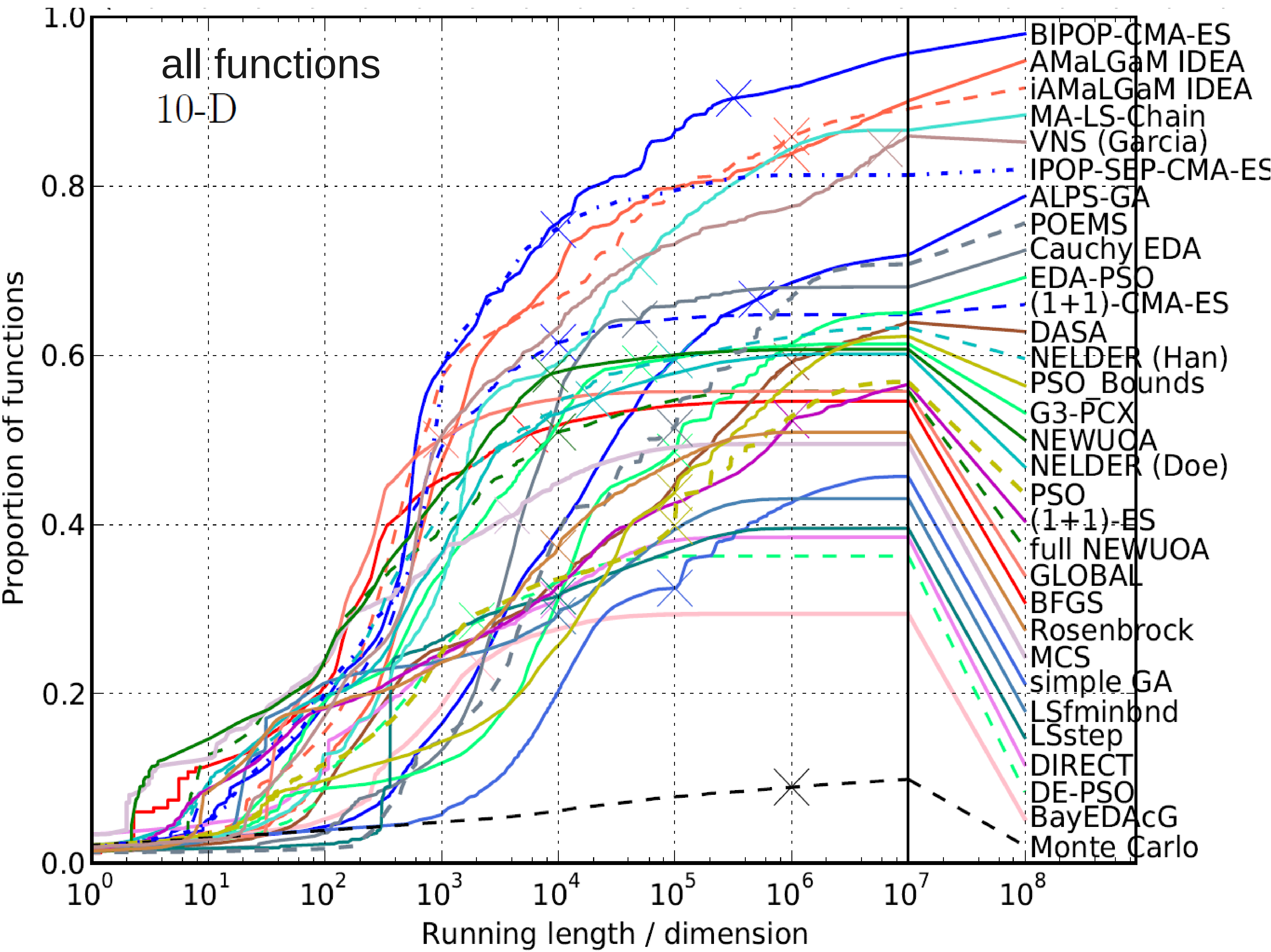


Results

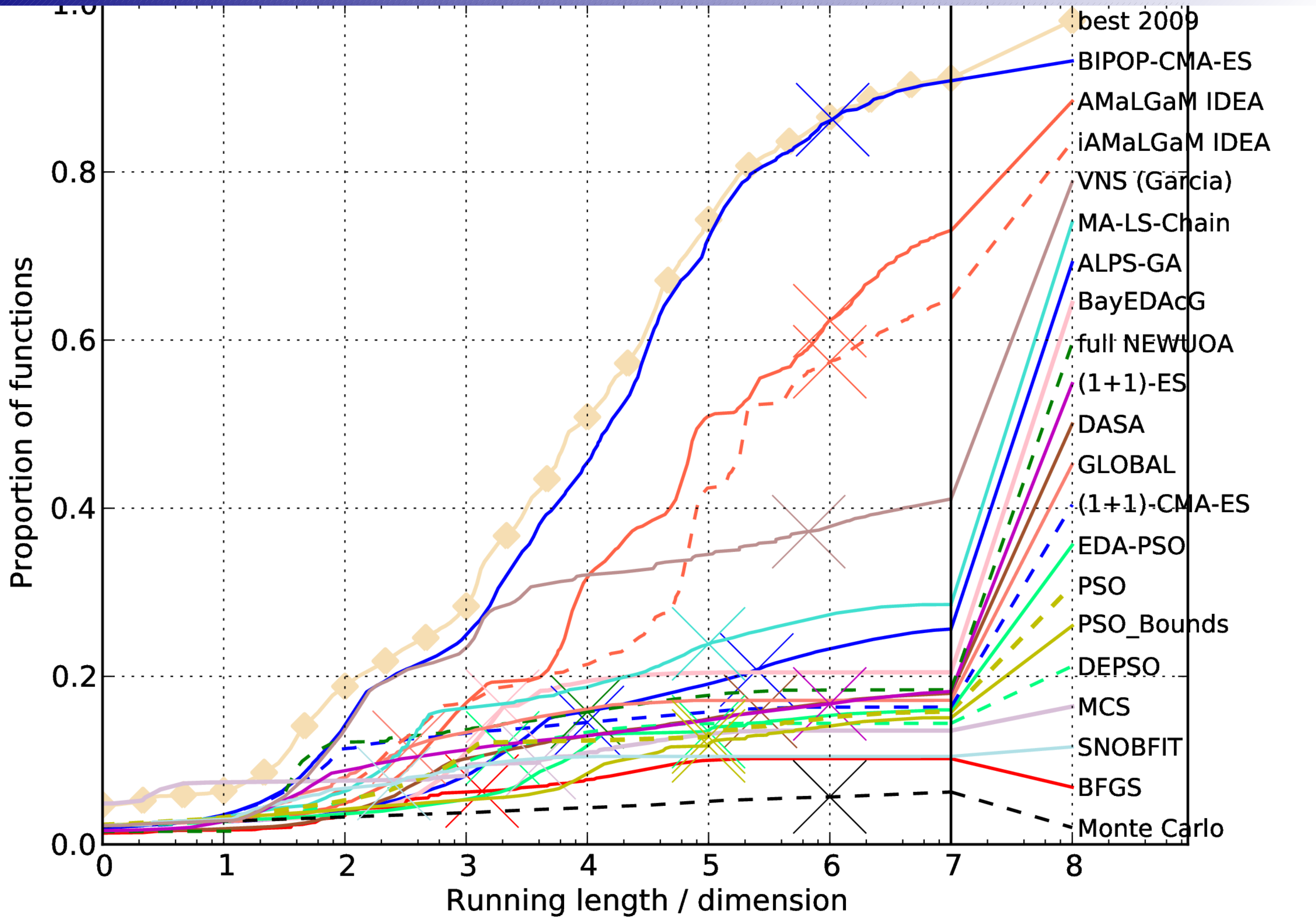
- Functions are not that easy to solve: the best algorithms need 10000 D function evaluations to solve 75% of the problems (function-target pairs)
- Given at most 500 D evaluations: MCS, NEWUOA and GLOBAL do well
- Given more evaluations: variants of CMA-ES and AMaLGaM-IDEA do well
- In very low dimension Nelder-Mead is superior



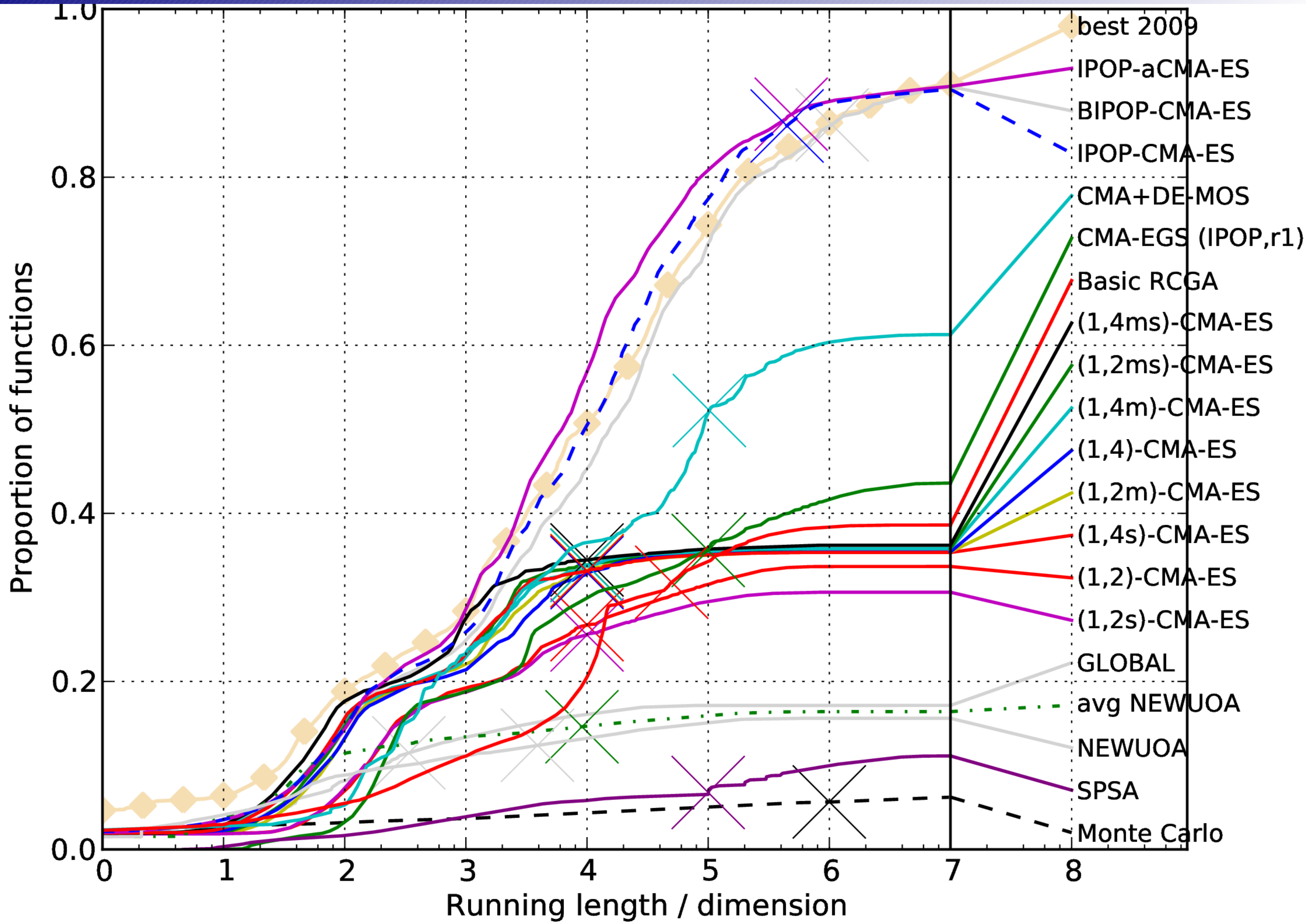
all functions
2-D
1.0
0.8
0.6
0.4
0.2
0.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
Running length / dimension
iAMaLGaM IDEA
AMaLGaM IDEA
NELDER (Doe)
IPOP-SEP-CMA-ES
DIRECT
NELDER (Han)
VNS (Garcia)
BIPOP-CMA-ES
PSO
ALPS-GA
PSO_Bounds
(1+1)-CMA-ES
DASA
MA-LS-Chain
G3-PCX
POEMS
full NEWUOA
MCS
NEWUOA
EDA-PSO
Cauchy EDA
Rosenbrock
(1+1)-ES
GLOBAL
BFGS
simple GA
DE-PSO
LSstep
LSfminbnd
Monte Carlo
BayEDAcG

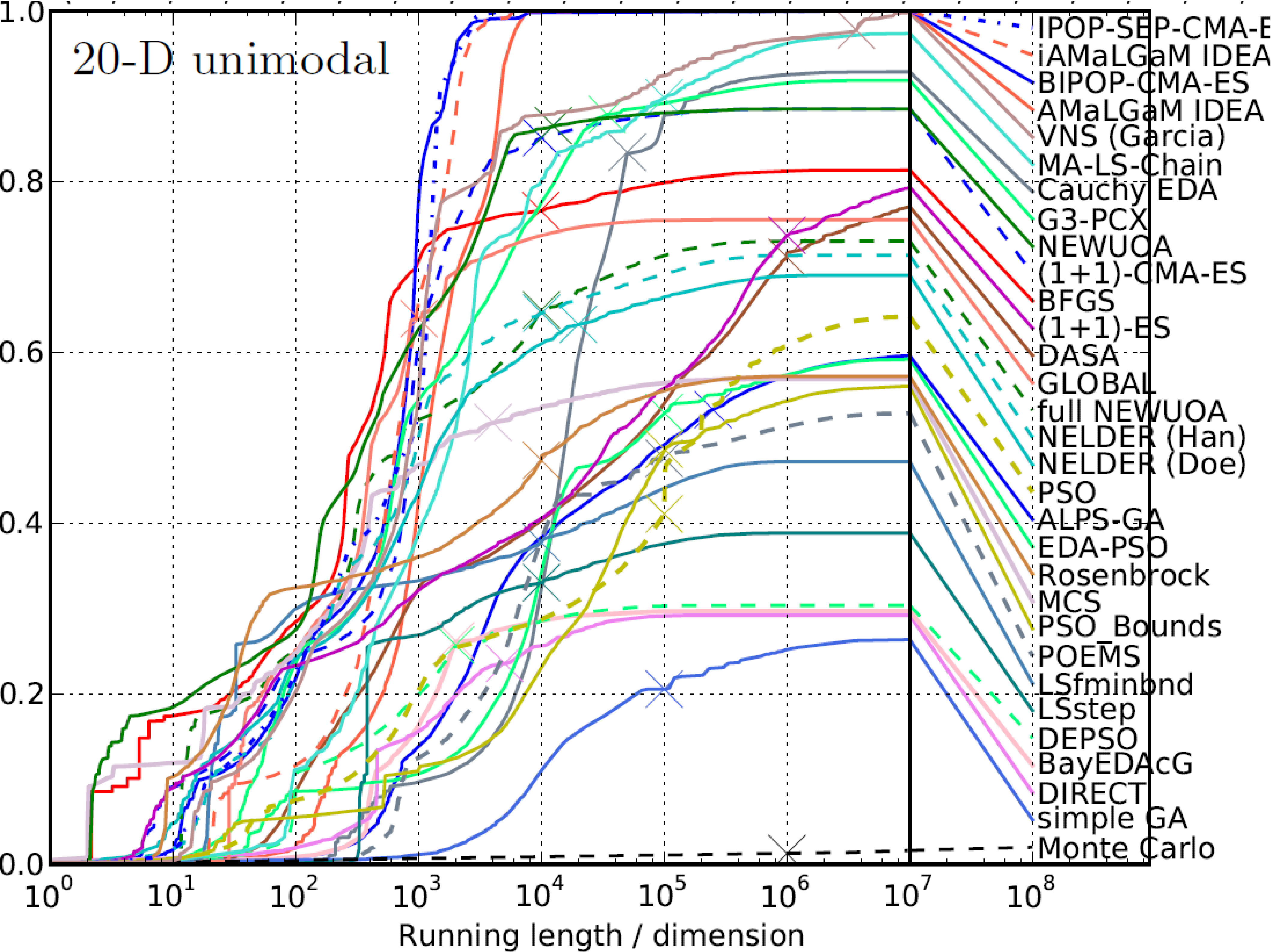

all functions
10-D
Proportion of functions
Running length / dimension
0.0
0.2
0.4
0.6
0.8
1.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
BIPOP-CMA-ES
AMaLGaM IDEA
iAMaLGaM IDEA
MA-LS-Chain
VNS (Garcia)
IPOP-SEP-CMA-ES
ALPS-GA
POEMS
Cauchy EDA
EDA-PSO
(1+1)-CMA-ES
DASA
NELDER (Han)
PSO_Bounds
G3-PCX
NEWUOA
NELDER (Doe)
PSO
(1+1)-ES
full NEWUOA
GLOBAL
BFGS
Rosenbrock
MCS
simple GA
LSfminbnd
LSstep
DIRECT
DE-PSO
BayEDAcG
Monte Carlo

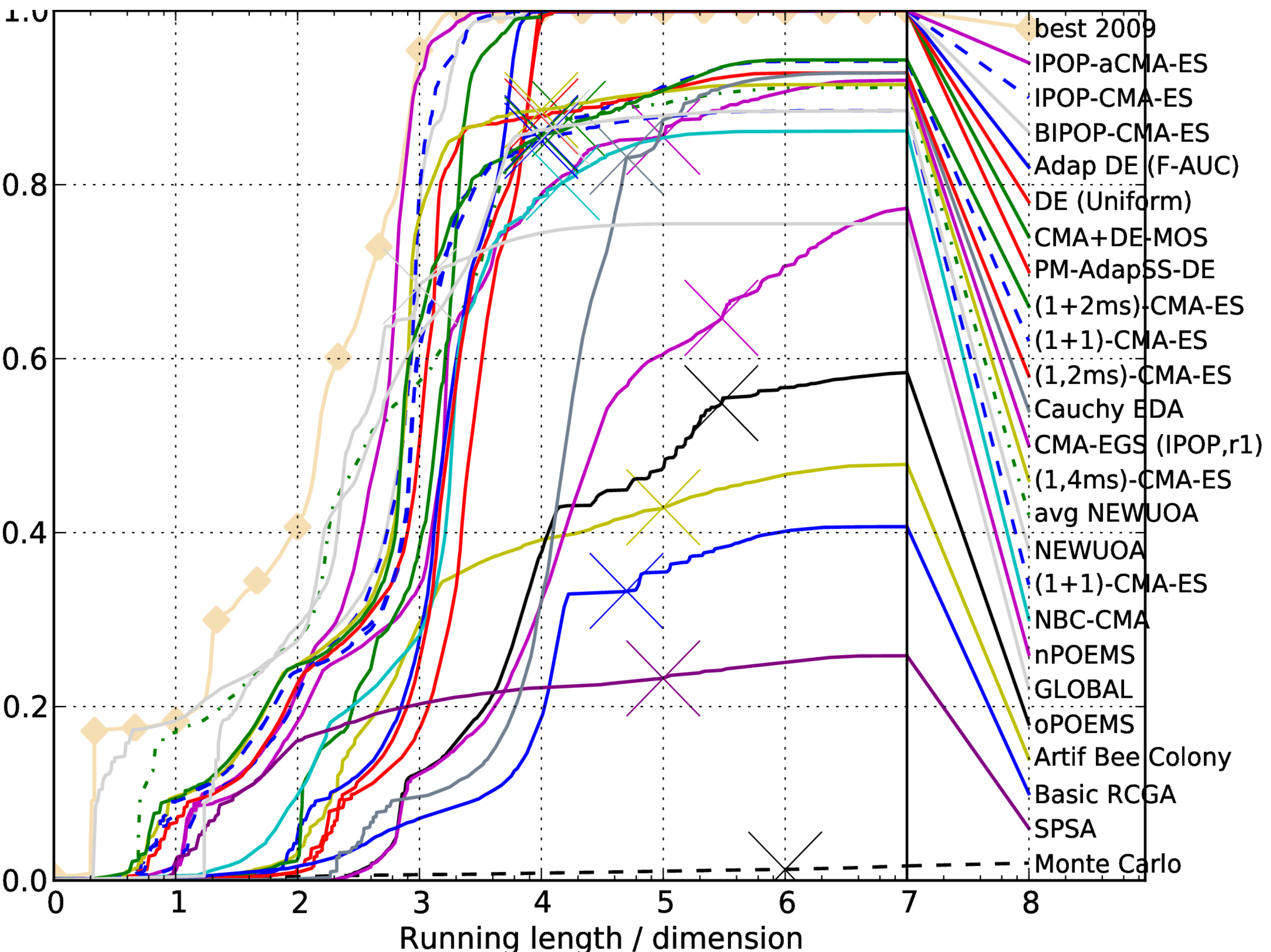
Results of 2009 (noisy, f_{101}-f_{130}, 20-D)



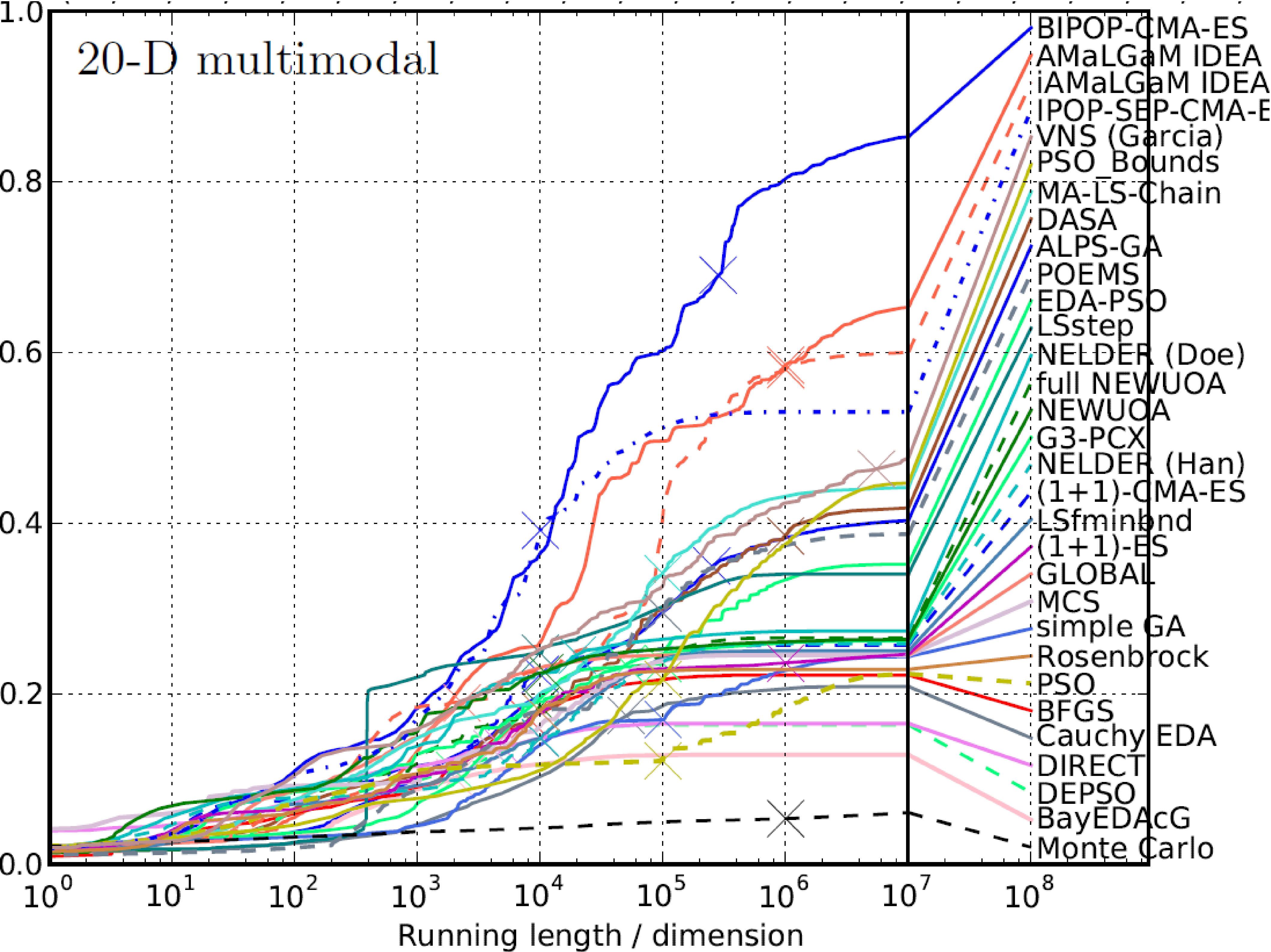
Results of 2010 (noisy, 20-D)



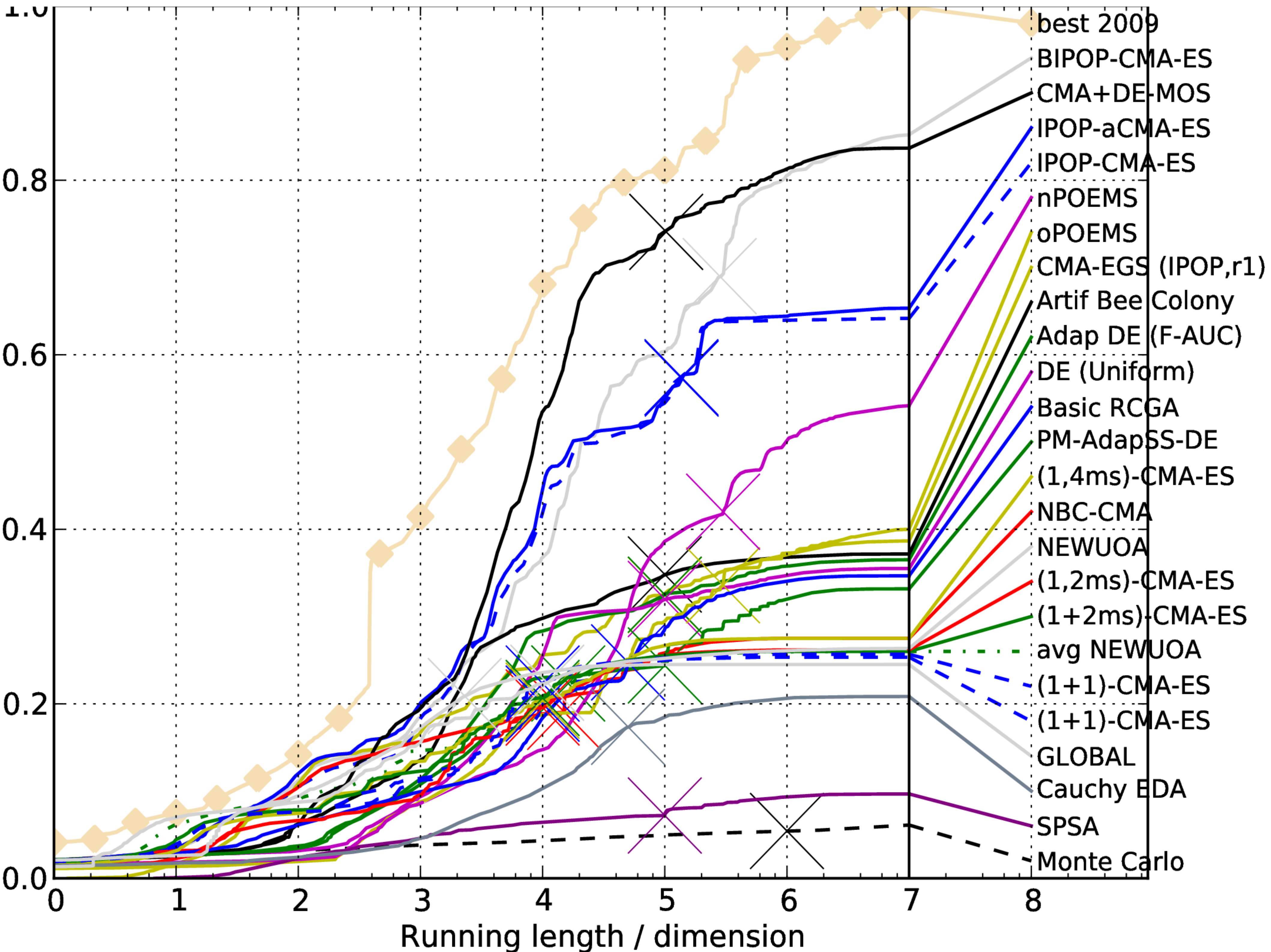

20-D unimodal
1.0
0.8
0.6
0.4
0.2
0.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
Running length / dimension
IPOP-SEP-CMA-E
iAMaLGaM IDEA
BIPOP-CMA-ES
AMaLGaM IDEA
VNS (Garcia)
MA-LS-Chain
Cauchy EDA
G3-PCX
NEWUOA
(1+1)-CMA-ES
BFGS
(1+1)-ES
DASA
GLOBAL
full NEWUOA
NELDER (Han)
NELDER (Doe)
PSO
ALPS-GA
EDA-PSO
Rosenbrock
MCS
PSO_Bounds
POEMS
LSfminbnd
LSstep
DEPSO
BayEDAcG
DIRECT
simple GA
Monte Carlo



1.0
0.8
0.6
0.4
0.2
0.0
0
1
2
3
4
5
6
7
8
Running length / dimension
best 2009
IPOP-aCMA-ES
IPOP-CMA-ES
BIPOP-CMA-ES
Adap DE (F-AUC)
DE (Uniform)
CMA+DE-MOS
PM-AdapSS-DE
(1+2ms)-CMA-ES
(1+1)-CMA-ES
(1,2ms)-CMA-ES
Cauchy EDA
CMA-EGS (IPOP,r1)
(1,4ms)-CMA-ES
avg NEWUOA
NEWUOA
(1+1)-CMA-ES
NBC-CMA
nPOEMS
GLOBAL
oPOEMS
Artif Bee Colony
Basic RCGA
SPSA
Monte Carlo



20-D multimodal
1.0
0.8
0.6
0.4
0.2
0.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
Running length / dimension
BIPOP-CMA-ES
AMaLGaM IDEA
iAMaLGaM IDEA
IPOP-SEP-CMA-E
VNS (Garcia)
PSO_Bounds
MA-LS-Chain
DASA
ALPS-GA
POEMS
EDA-PSO
LSstep
NELDER (Doe)
full NEWUOA
NEWUOA
G3-PCX
NELDER (Han)
(1+1)-CMA-ES
LSfminbnd
(1+1)-ES
GLOBAL
MCS
simple GA
Rosenbrock
PSO
BFGS
Cauchy EDA
DIRECT
DEPSO
BayEDAcG
Monte Carlo



best 2009
BIPOP-CMA-ES
CMA+DE-MOS
IPOP-aCMA-ES
IPOP-CMA-ES
nPOEMS
oPOEMS
CMA-EGS (IPOP,r1)
Artif Bee Colony
Adap DE (F-AUC)
DE (Uniform)
Basic RCGA
PM-AdapSS-DE
(1,4ms)-CMA-ES
NBC-CMA
NEWUOA
(1,2ms)-CMA-ES
(1+2ms)-CMA-ES
avg NEWUOA
(1+1)-CMA-ES
(1+1)-CMA-ES
GLOBAL
Cauchy EDA
SPSA
Monte Carlo
0.0
0.2
0.4
0.6
0.8
1.0
0
1
2
3
4
5
6
7
8
Running length / dimension

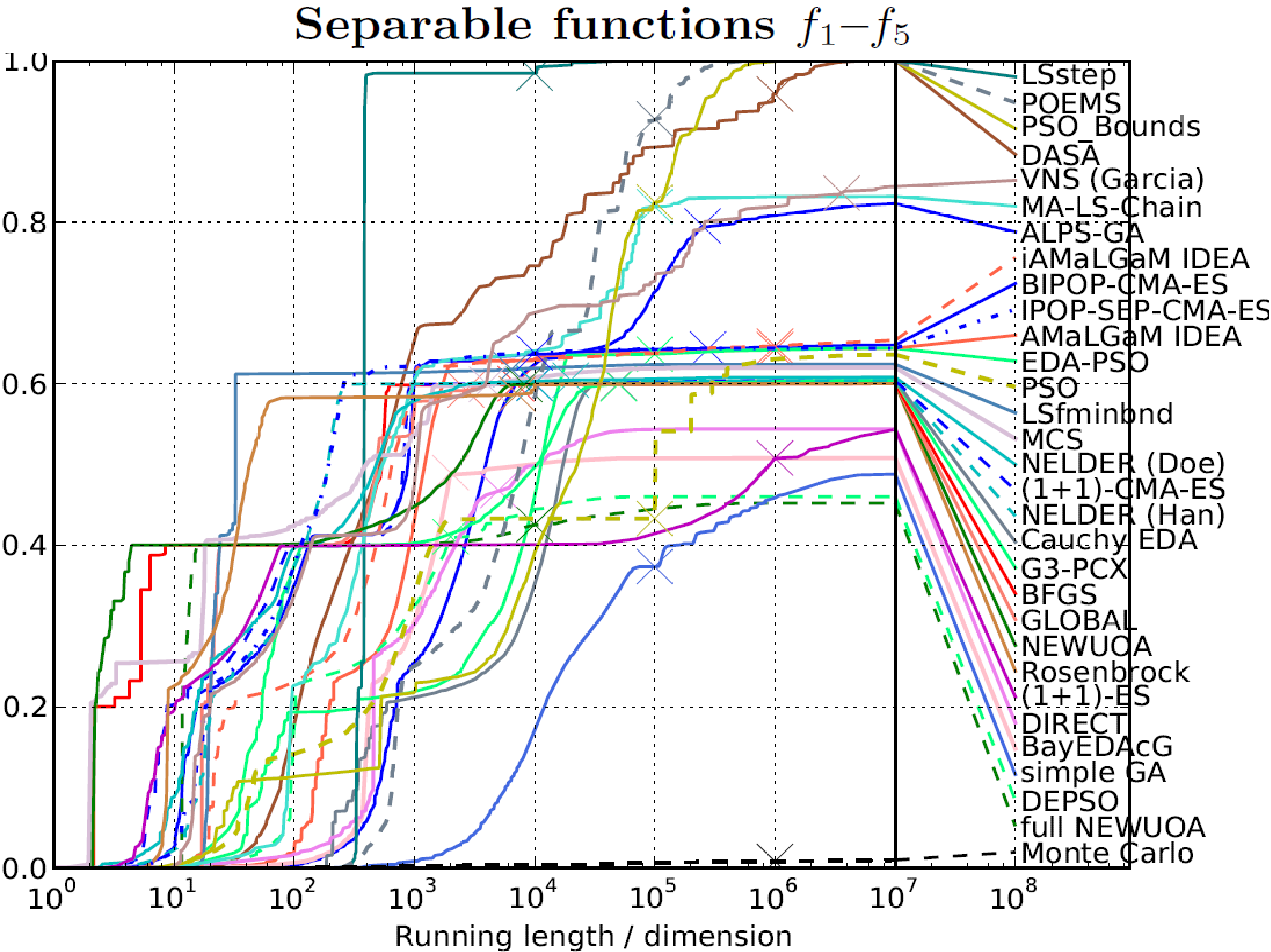
% SEPARABLE
1 Sphere
2 Ellipsoid separable with monotone x-transformation, condition 1e6
3 Rastrigin separable with both x-transformations "condition" 10
4 Skew Rastrigin-Bueche separable, "condition" 10, skew-"condition" 100
5 Linear slope, neutral extension outside the domain (not flat)

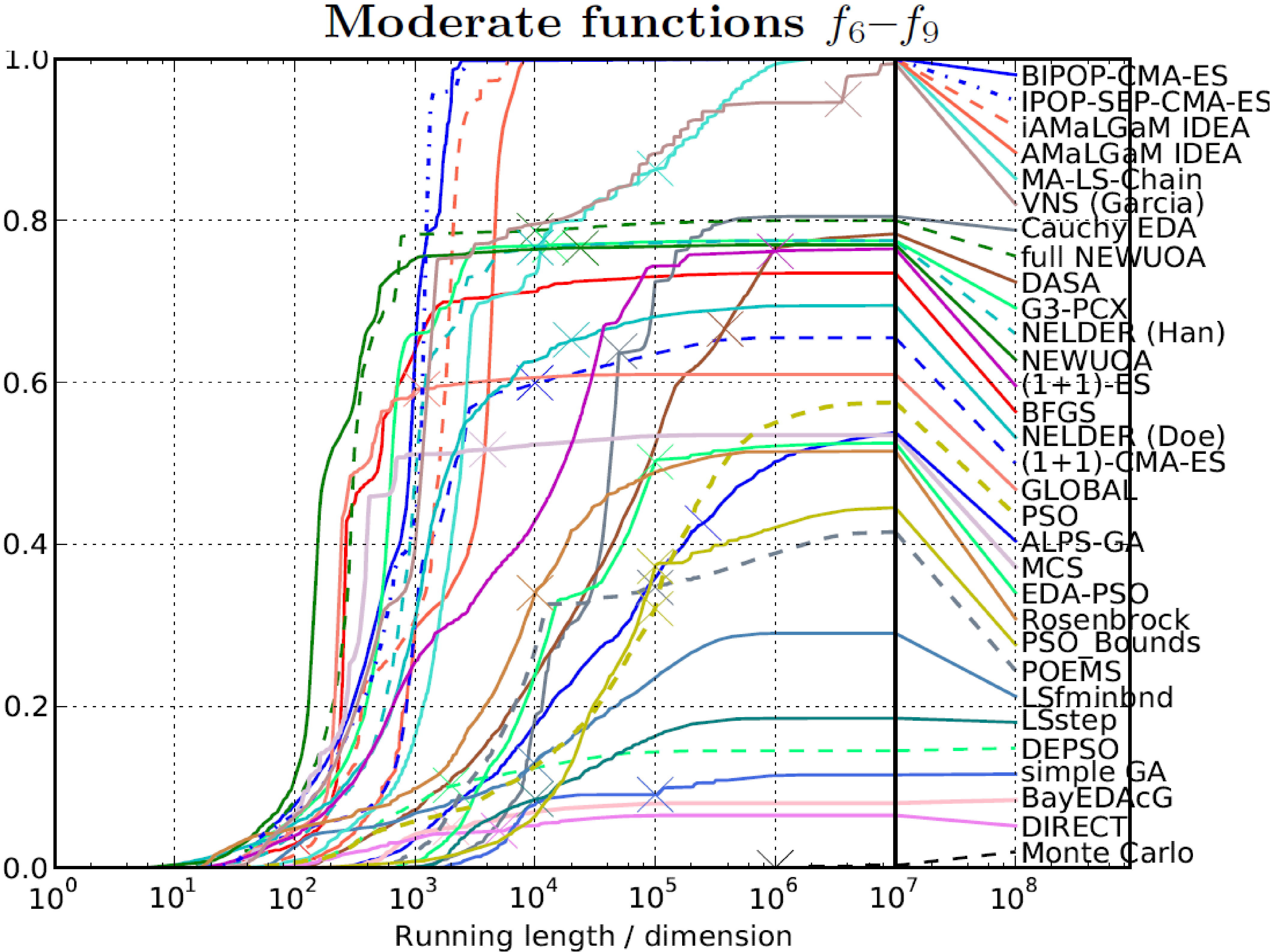
% LOW OR MODERATE CONDITION
6 Attractive sector function
7 Step-ellipsoid, condition 100
8 Rosenbrock, original
9 Rosenbrock, rotated

% HIGH CONDITION
10 Ellipsoid with monotone x-transformation, condition 1e6
11 Discus with monotone x-transformation, condition 1e6
12 Bent cigar with asymmetric x-transformation, condition 1e6
13 Sharp ridge, slope 1:100, condition 10
14 Sum of different powers

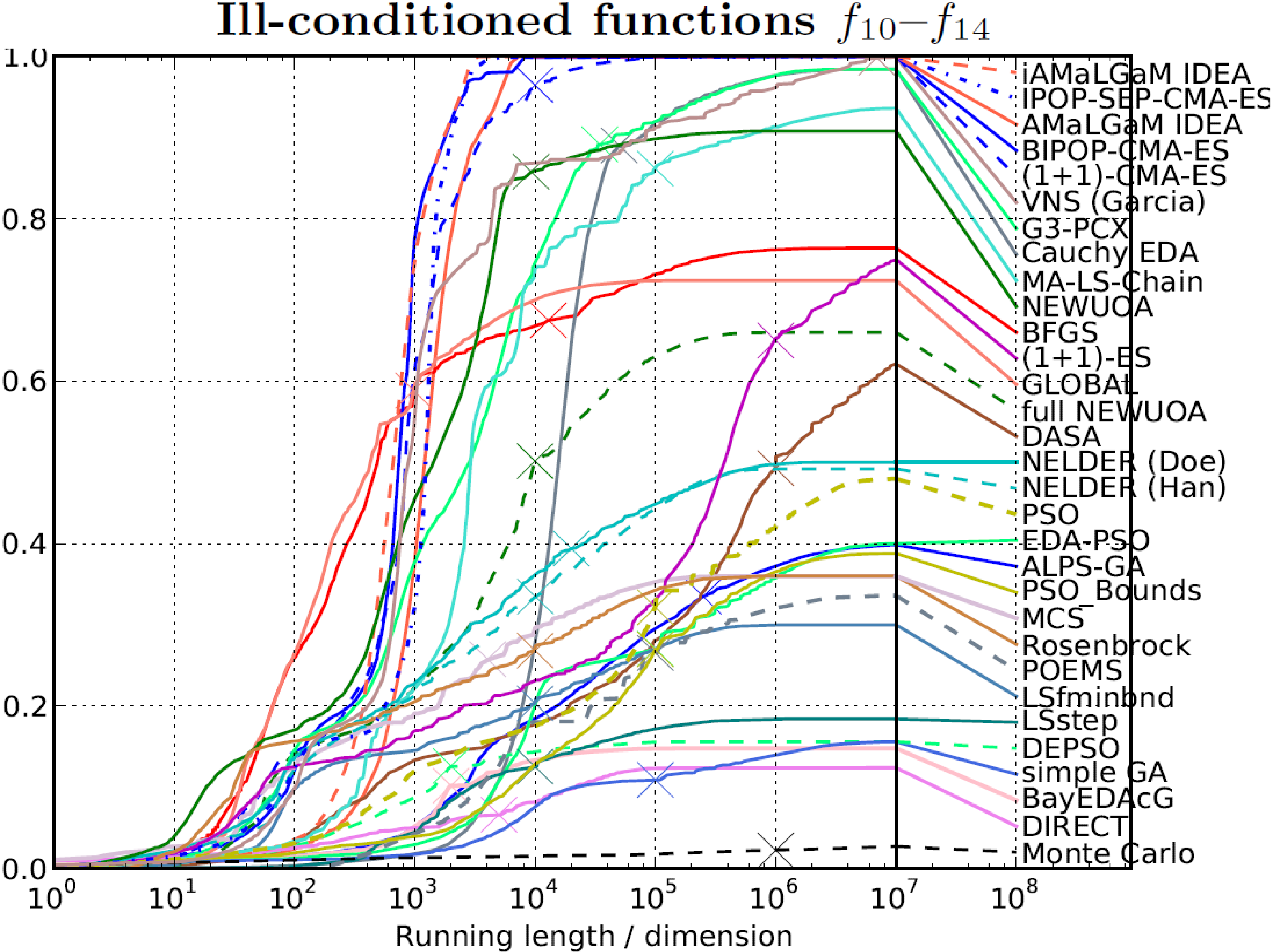
% MULTI-MODAL
15 Rastrigin with both x-transformations, condition 10
16 Weierstrass with monotone x-transformation, condition 100
17 Schaffer F7 with asymmetric x-transformation, condition 10
18 Schaffer F7 with asymmetric x-transformation, condition 1000
19 F8F2 composition of 2-D Griewank-Rosenbrock

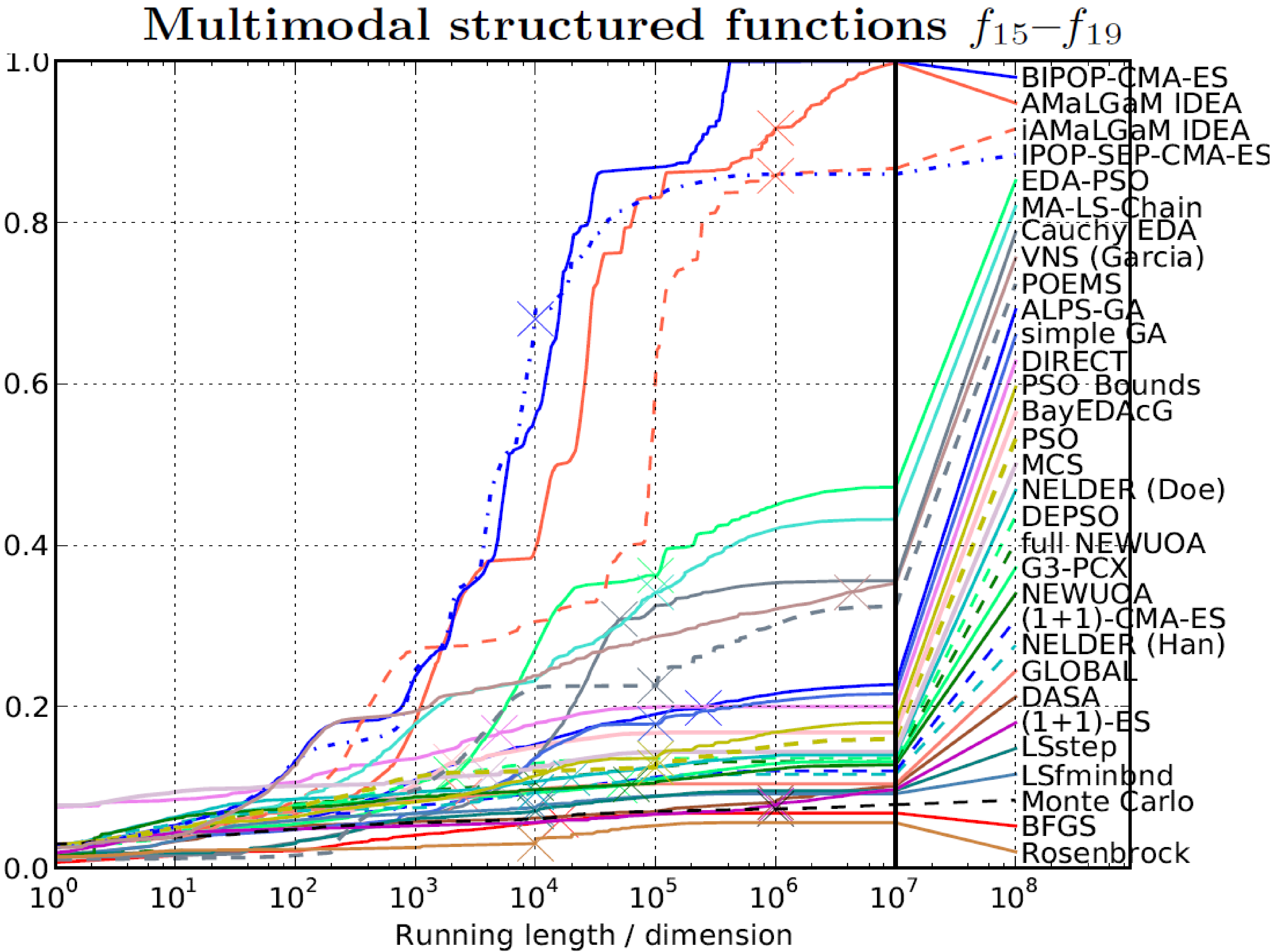
% MULTI-MODAL WITH WEAK GLOBAL STRUCTURE
20 Schwefel x*sin(x) with tridiagonal transformation, condition 10
21 Gallagher 101 Gaussian peaks, condition up to 1000
22 Gallagher 21 Gaussian peaks, condition up to 1000, 1000 for global opt
23 Katsuuras repetitive rugged function
24 Lunacek bi-Rastrigin, condition 100


Separable functions f_1–f_5
1.0
0.8
0.6
0.4
0.2
0.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
Running length / dimension
LSstep
POEMS
PSO_Bounds
DASA
VNS (Garcia)
MA-LS-Chain
ALPS-GA
iAMaLGaM IDEA
BIPOP-CMA-ES
IPOP-SEP-CMA-ES
AMaLGaM IDEA
EDA-PSO
PSO
LSfminbnd
MCS
NELDER (Doe)
(1+1)-CMA-ES
NELDER (Han)
Cauchy EDA
G3-PCX
BFGS
GLOBAL
NEWUOA
Rosenbrock
(1+1)-ES
DIRECT
BayEDAcG
simple GA
DEPSO
full NEWUOA
Monte Carlo



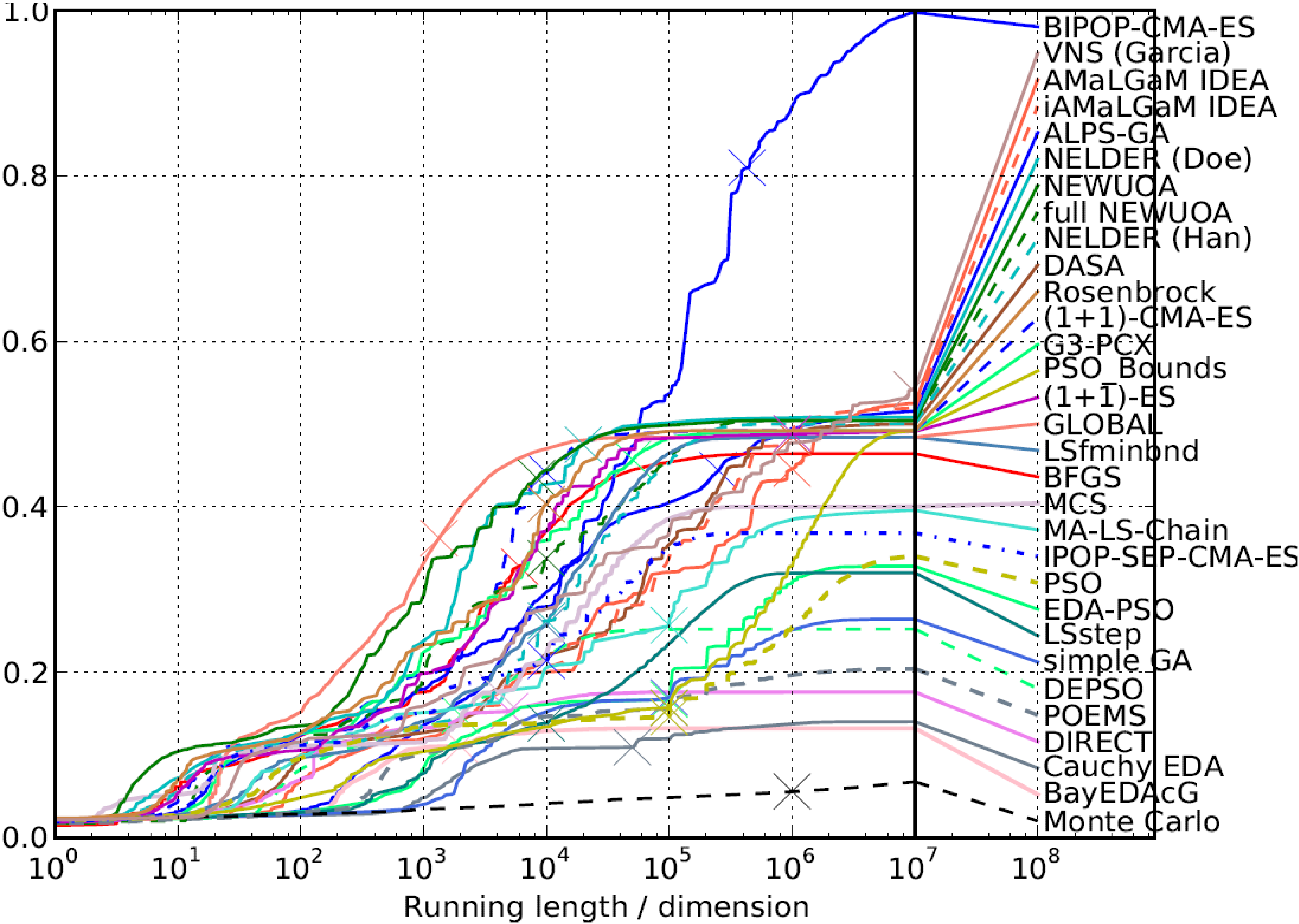
Moderate functions f_6–f_9
1.0
0.8
0.6
0.4
0.2
0.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
Running length / dimension
BIPOP-CMA-ES
IPOP-SEP-CMA-ES
iAMaLGaM IDEA
AMaLGaM IDEA
MA-LS-Chain
VNS (Garcia)
Cauchy EDA
full NEWUOA
DASA
G3-PCX
NELDER (Han)
NEWUOA
(1+1)-ES
BFGS
NELDER (Doe)
(1+1)-CMA-ES
GLOBAL
PSO
ALPS-GA
MCS
EDA-PSO
Rosenbrock
PSO_Bounds
POEMS
LSfminbnd
LSstep
DEPSO
simple GA
BayEDAcG
DIRECT
Monte Carlo

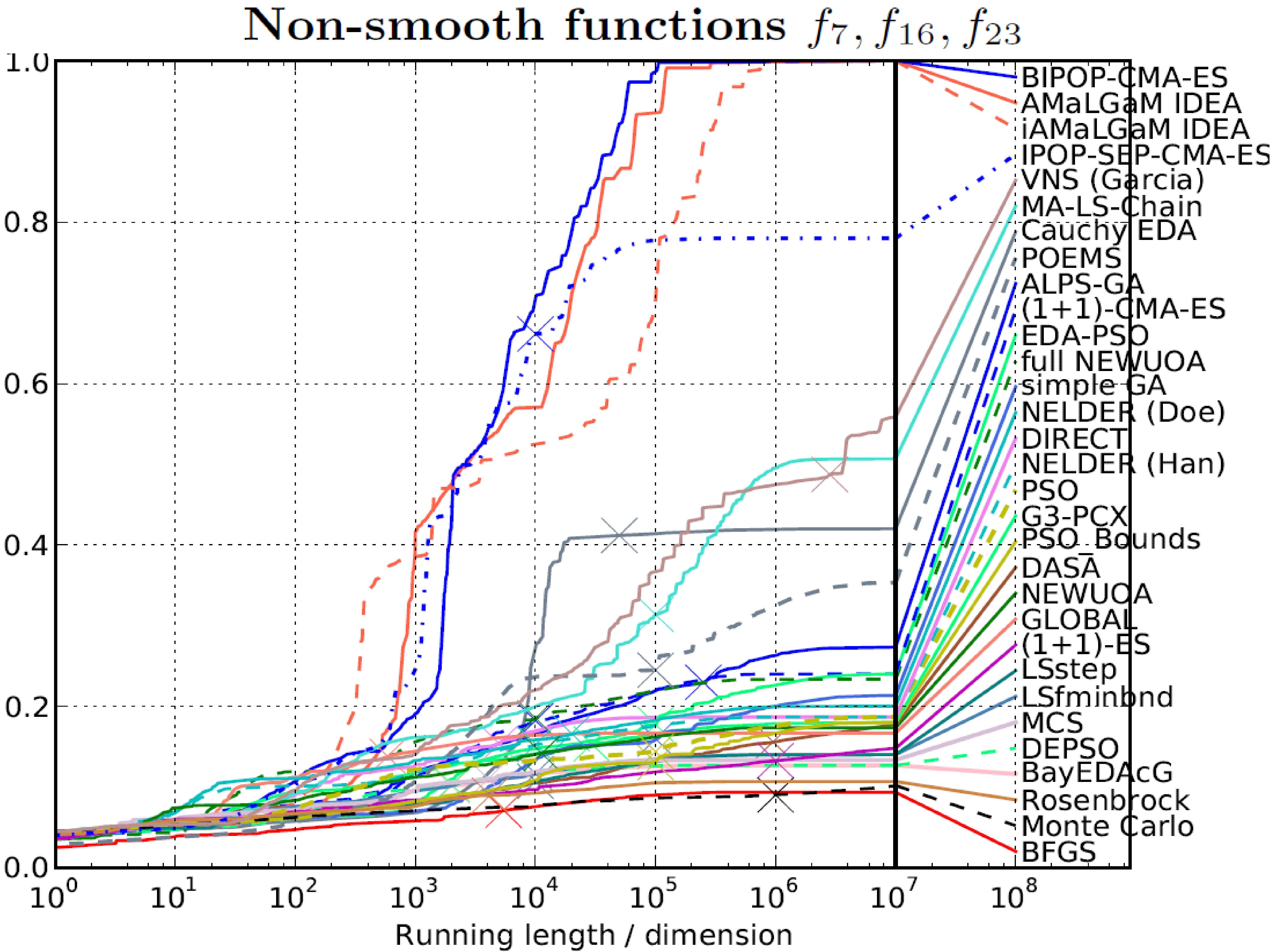

Ill-conditioned functions f_{10}–f_{14}
1.0
0.8
0.6
0.4
0.2
0.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
Running length / dimension
iAMaLGaM IDEA
IPOP-SEP-CMA-ES
AMaLGaM IDEA
BIPOP-CMA-ES
(1+1)-CMA-ES
VNS (Garcia)
G3-PCX
Cauchy EDA
MA-LS-Chain
NEWUOA
BFGS
(1+1)-ES
GLOBAL
full NEWUOA
DASA
NELDER (Doe)
NELDER (Han)
PSO
EDA-PSO
ALPS-GA
PSO_Bounds
MCS
Rosenbrock
POEMS
LSfminbnd
LSstep
DEPSO
simple GA
BayEDAcG
DIRECT
Monte Carlo



Multimodal structured functions f_{15}–f_{19}
1.0
0.8
0.6
0.4
0.2
0.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
Running length / dimension
BIPOP-CMA-ES
AMaLGaM IDEA
iAMaLGaM IDEA
IPOP-SEP-CMA-ES
EDA-PSO
MA-LS-Chain
Cauchy EDA
VNS (Garcia)
POEMS
ALPS-GA
simple GA
DIRECT
PSO_Bounds
BayEDAcG
PSO
MCS
NELDER (Doe)
DEPSO
full NEWUOA
G3-PCX
NEWUOA
(1+1)-CMA-ES
NELDER (Han)
GLOBAL
DASA
(1+1)-ES
LSstep
LSfminbnd
Monte Carlo
BFGS
Rosenbrock

Multimodal weakly structured functions f_{20}–f_{24}





Non-smooth functions f_7, f_{16}, f_{23}
1.0
0.8
0.6
0.4
0.2
0.0
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
10^8
Running length / dimension
BIPOP-CMA-ES
AMaLGaM IDEA
iAMaLGaM IDEA
IPOP-SEP-CMA-ES
VNS (Garcia)
MA-LS-Chain
Cauchy EDA
POEMS
ALPS-GA
(1+1)-CMA-ES
EDA-PSO
full NEWUOA
simple GA
NELDER (Doe)
DIRECT
NELDER (Han)
PSO
G3-PCX
PSO_Bounds
DASA
NEWUOA
GLOBAL
(1+1)-ES
LSstep
LSfminbnd
MCS
DEPSO
BayEDAcG
Rosenbrock
Monte Carlo
BFGS

Single Function Table

Table 6: 20-D, running time excess ERT/ERT_{best} on f_6, in italics is given the median final function value and the median number of function evaluations to reach this value divided by dimension

6 Attractive sector

Δftarget	1e+03	1e+02	1e+01	1e+00	1e-01	1e-02	1e-03	1e-04	1e-05	1e-07	Δftarget
ERT_{best}/D	4.03	26	64.7	87.2	123	152	184	219	248	309	ERT_{best}/D
ALPS	59	25	34	54	64	78	100	150	370	*14e-7/2e5*	ALPS [17]
AMaLGaM IDEA	26	22	19	22	21	22	22	21	22	22	AMaLGaM IDEA [4]
avg NEWUOA	**2.3**	**1.1**	1	**1**	1	**1**	1	**1**	**1**	1	avg NEWUOA [31]
BayEDAcG	46	41	*60e+0/2e3*	.	.	.	.	.	.	.	BayEDAcG [10]
BFGS	**2.2**	**2.7**	3.6	4.7	4.7	4.9	5	4.8	4.9	61	BFGS [30]
Cauchy EDA	6200	1500	1e3	1700	*17e-1/5e4*	.	.	.	.	.	Cauchy EDA [24]
BIPOP-CMA-ES	**2.9**	**2.2**	**1.5**	**1.7**	**1.6**	**1.6**	**1.6**	**1.5**	**1.6**	**1.6**	BIPOP-CMA-ES [15]
(1+1)-CMA-ES	**1.9**	4.5	13	180	1200	*13e-1/1e4*	.	.	.	.	(1+1)-CMA-ES [2]
DASA	12	6.8	9.9	19	25	33	49	58	63	74	DASA [19]
DEPSO	11	7.5	12	64	*13e-1/2e3*	.	.	.	.	.	DEPSO [12]
DIRECT	18	31	*40e+0/5e3*	.	.	.	.	.	.	.	DIRECT [25]
EDA-PSO	27	46	40	45	44	44	44	44	44	44	EDA-PSO [6]
full NEWUOA	5	**1.9**	**1.5**	**1.4**	**1.4**	**1.4**	**1.4**	**1.4**	**1.4**	**1.4**	full NEWUOA [31]
G3-PCX	4.1	**1.4**	**1.4**	**2**	**2.1**	**2.1**	**2.2**	**2.2**	**2.3**	**2.4**	G3-PCX [26]
simple GA	320	130	2e3	*11e+0/1e5*	.	.	.	.	.	.	simple GA [22]
GLOBAL	5	**2.9**	3.6	4.9	8.5	*42e-3/2e3*	.	.	.	.	GLOBAL [23]
iAMaLGaM IDEA	5.1	5.6	5.4	6.8	7.1	7.7	7.8	7.7	8	8.3	iAMaLGaM IDEA [4]
LSfminbnd	9	31	160	760	1100	960	*72e-1/1e4*	.	.	.	LSfminbnd [28]
LSstep	140	260	2300	*59e+0/1e4*	.	.	.	.	.	.	LSstep [28]
MA-LS-Chain	11	4.9	7.5	8.9	8	7.7	7.2	6.7	6.5	6	MA-LS-Chain [21]
MCS (Neum)	**1.8**	33	*42e+0/4e3*	.	.	.	.	.	.	.	MCS (Neum) [18]
NELDER (Han)	**2.2**	**2.4**	**2.7**	3.3	3.2	3.5	3.5	3.5	4	7.4	NELDER (Han) [16]
NELDER (Doe)	**1.5**	**2.3**	9.1	20	28	65	110	430	*46e-5/2e4*	.	NELDER (Doe) [5]
NEWUOA	**1**	**1**	1	**1.3**	**1.4**	**1.5**	**1.6**	**1.6**	**1.7**	**1.7**	NEWUOA [31]
(1+1)-ES	**2**	**2.2**	**2.1**	**2.8**	3.9	5.2	6.1	6.5	6.4	6.7	(1+1)-ES [1]
POEMS	89	26	31	37	36	36	36	35	36	37	POEMS [20]
PSO	6.4	280	1100	1400	980	820	710	620	570	790	PSO [7]
PSO_Bounds	9.5	45	120	150	140	140	140	130	160	220	PSO_Bounds [8]
Monte Carlo	2.4e5	*48e+1/1e6*	.	.	.	.	.	.	.	.	Monte Carlo [3]
Rosenbrock	**2.1**	3.9	31	76	210	230	810	*21e-2/1e4*	.	.	Rosenbrock [27]
IPOP-SEP-CMA-ES	3.2	**2.1**	**1.7**	**1.9**	**1.9**	**1.9**	**1.9**	**1.9**	**2**	**2**	IPOP-SEP-CMA-ES [29]
VNS (Garcia)	5	**2.8**	**1.9**	**1.9**	**1.7**	**1.7**	**1.7**	**1.6**	**1.6**	**1.6**	VNS (Garcia) [11]

Overview of best algorithms (20-D)

Functions	short runtime	long runtime
separable	NEWUOA (BFGS), LS-fminbnd	LS-step
moderate	NEWUOA (BFGS, GLOBAL)	IPOP-aCMA-ES
ill-conditioned	(NEWUOA) BFGS, GLOBAL	IPOP-aCMA-ES
non-smooth (2009)	IDEA (CMA-ES)	CMA-ES, IDEA
multimodal	(MCS, DIRECT, CMA-ES, IDEA)	IPOP-CMA-ES (ID
weak structure	(NEWUOA) GLOBAL	(BIPOP-CMA-ES)
noisy	(MCS, CMA-ES)	IPOP-aCMA-ES

(more) questions?

Any intelligent fool can make things bigger, more complex, and more violent. It takes a touch of genius, and a lot of courage, to move in the opposite direction.

Albert Einstein