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Formulations for Surrogate-Based Constrained Blackbox Optimization

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Presentation outline

Blackbox optimization and the MADS algorithm

Surrogates

Surrogate problem formulations

Results and discussion

Blackbox optimization and the MADS algorithm

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Blackbox optimization problems

We consider the optimization problem:

$$\min_{x\in\Omega} \quad f(x)$$

with $\Omega = \left\{ x \in \mathcal{X} : c_j(x) \leq 0, j \in \{1, 2, \ldots, m\} \right\} \subset \mathbb{R}^n$.

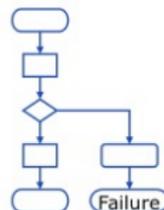The evaluations of f and of the c_j functions are usually the result of a computer code (a blackbox).

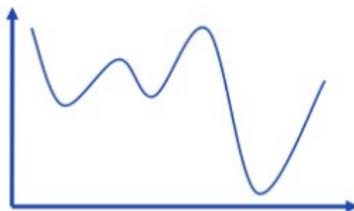# Blackboxes as illustrated by J. Simonis [ISMP 2009]
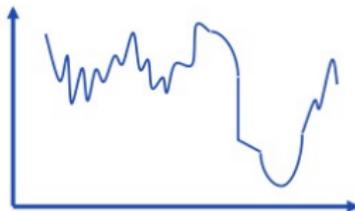

Long runtime

>2 GByte

Large memory
requirement

Software
might fail

$\nabla f(x)$

No derivatives
available

Local
optima

Non-smooth,
noisy

Example: Snow Water Equivalent (SWE) estimation

▶ Accurate estimate of water stored in snow is crucial to optimize hydroelectric plants management.

▶ Exact snow measurement is impossible.

▶ SWE is measured at specific sites and next interpolated over the territory.

▶ Territory is huge: Hydro-Québec (HQ) operates 565 dams, 75 reservoirs, and 56 hydroelectric power plants, located over 90 watersheds and covering more than 550,000 km^2.

SWE estimation

- ▶ Previously done manually by weighing snow cores at specific sites.
- ▶ Each measurement campaign requires 2 weeks.
- ▶ Missing measurements due to adverse meteorological conditions.

GMON device

- ▶ A new measuring instrument that provides daily automatic SWE.
- ▶ GMON for Gamma-MONitoring device: it measures the natural Gamma radiation emitted from the soil.
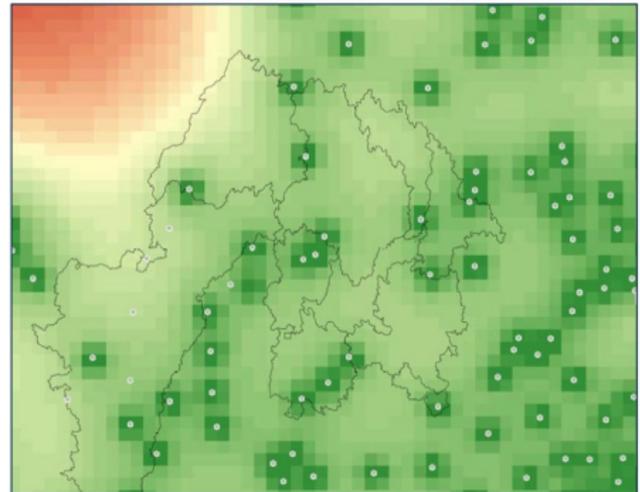- ▶ Communicates via satellites.

SWE estimation from GMON measures

- ▶ Kriging interpolation is used to obtain SWE estimation together with an error map.
- ▶ How to find the device locations that minimize the kriging interpolation error of the SWE?
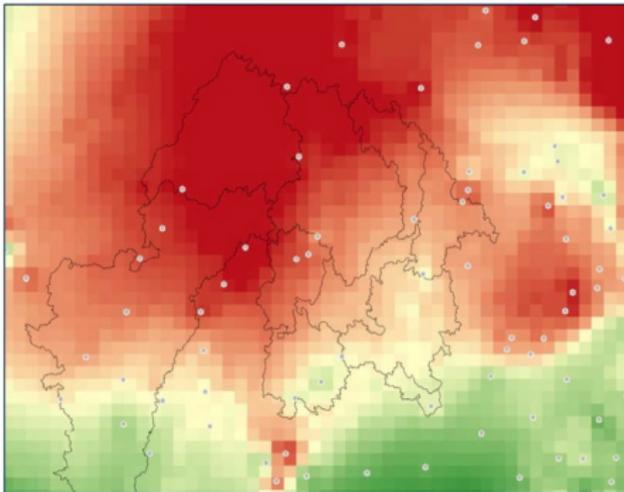
SWE estimation   standard deviation of estimation

Mesh Adaptive Direct Search (MADS)

▶ Audet and Dennis [SIOPT, 2006]

▶ Iterative algorithm that evaluates the blackbox at some trial points on a spatial discretization called the mesh.

▶ One iteration = search and poll.

▶ Algorithm is backed by a convergence analysis based on the Clarke Calculus for nonsmooth functions.

▶ MADS is available via the `NOMAD` free software package at `www.gerad.ca/nomad`.

BBO and MADS
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Surrogates
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Surrogate problem formulations
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Results and discussion
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[0] Initializations (x_0, Δ_0^m)
[1] Iteration k
    [1.1] Search
        select a finite number of mesh points
        evaluate candidates opportunistically
    [1.2] Poll (if the Search failed)
        construct poll set $P_k = \{x_k + \Delta_k^m d : d \in D_k\}$
        sort(P_k)
        evaluate candidates opportunistically
[2] Updates
    if success
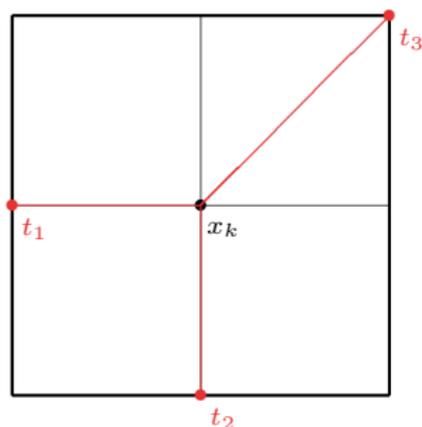 $x_{k+1} \leftarrow$ success point
        increase Δ_k^m
    else
        $x_{k+1} \leftarrow x_k$
        decrease Δ_k^m
    $k \leftarrow k+1$, stop or go to **[1]**

Poll illustration (successive fails and mesh shrink)
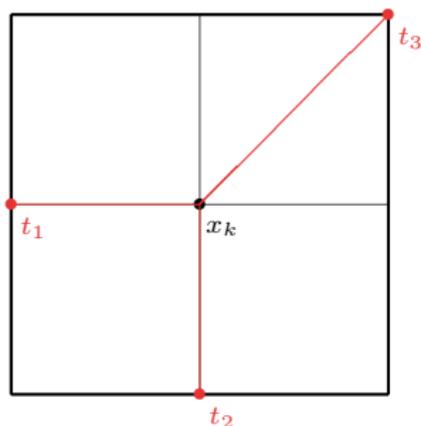
$$\Delta_k^m = \Delta_k^p = 1$$

poll trial points$=\{t_1, t_2, t_3\}$

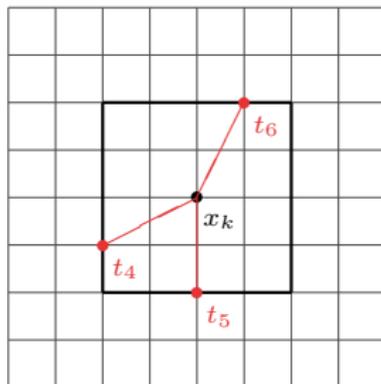## Poll illustration (successive fails and mesh shrink)

$$\Delta_k^m = \Delta_k^p = 1 \qquad \Delta_{k+1}^m = 1/4$$
$$\Delta_{k+1}^p = 1/2$$

poll trial points $= \{t_1, t_2, t_3\}$ $= \{t_4, t_5, t_6\}$

Poll illustration (successive fails and mesh shrink)

$$\Delta_k^m = \Delta_k^p = 1$$
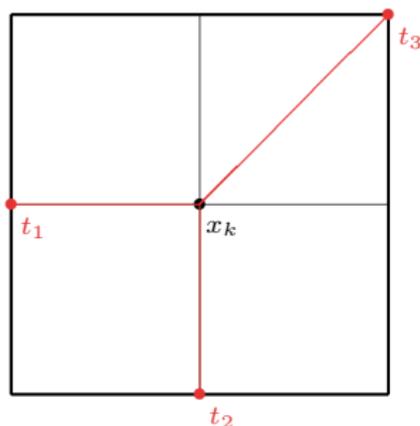
$$\Delta_{k+1}^m = 1/4$$
$$\Delta_{k+1}^p = 1/2$$

$$\Delta_{k+2}^m = 1/16$$
$$\Delta_{k+2}^p = 1/4$$
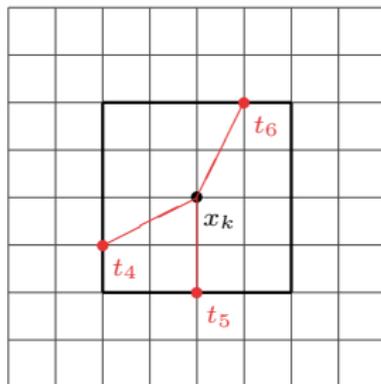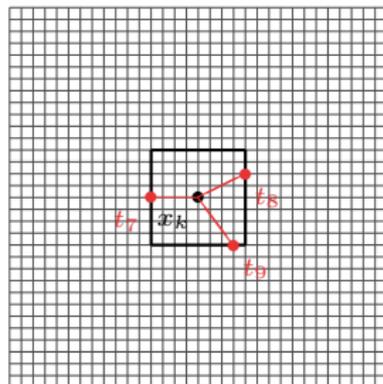
poll trial points=$\{t_1, t_2, t_3\}$ $= \{t_4, t_5, t_6\}$ $= \{t_7, t_8, t_9\}$

Blackbox optimization and the MADS algorithm

Surrogates

Surrogate problem formulations

Results and discussion

Static versus dynamic surrogates

▶ Static surrogate: A cheaper model defined a priori by the user. It is used as a blackbox too. Typically a simplified physics model. Variable precision is not yet considered.

▶ Dynamic surrogate: Model managed by the algorithm, based on past evaluations. It can be periodically updated.

In the remaining of this presentation, we focus on dynamic surrogates based on the `dynaTree` library.

General framework of MADS + surrogates

Only the additions to the MADS algorithm are reported.

[0] Initializations
[1] Iteration k

    [1.1] Model Search

        select data points from cache
        construct one model for each output (obj + cstrs)
        optimize model to determine oracle points
        ($\rightarrow$ the subproblem, or surrogate problem)
        project candidates to the mesh
        evaluate candidates opportunistically

    [1.2] Poll (if the Search failed)

        Model Ordering: use models to sort trial points

[2] Updates

The `dynaTree` **library**

▶ Developed for parameter-free regression by Taddy, Gramacy, and Polson [J. of the Am. Stat. Association, 2011].

▶ Based on Bayesian inference.

▶ `R` package available on CRAN.

dynaTree **outputs**

- The predictive mean $\hat{f}(x)$.
- The predictive standard deviation $\hat{\sigma}_f(x)$.
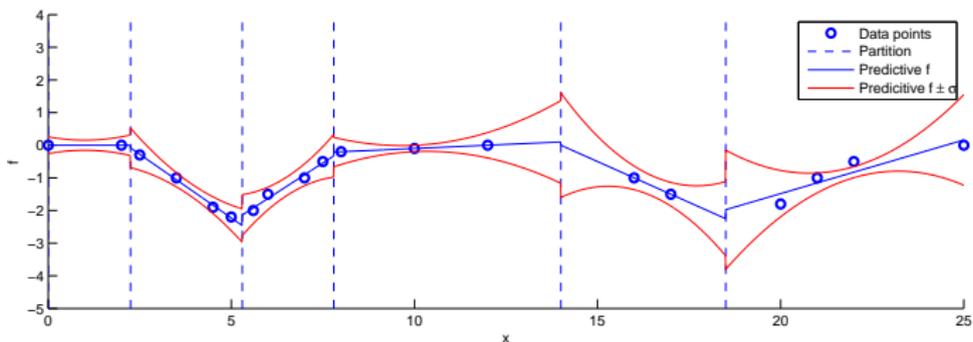
- The predictive cumulative distribution $\mathbb{P}[f(x) \leq f_0]$.
- Likewise for the constraints: $\hat{c}_j(x)$, $\hat{\sigma}_j(x)$, $\mathbb{P}[c_j(x) \leq c_0]$.

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▶ At each iteration, find the most promising candidates by solving the surrogate problem.

▶ The most basic formulation is:

$$\begin{cases} \min_{x \in \mathcal{X}} & \hat{f}(x) \\ \text{s.t.} & \hat{c}_j(x) \leq 0 \ \ \forall j \in J \ . \end{cases}$$

▶ We tested other formulations in the following submitted manuscript: B. Talgorn, S. Le Digabel, and M. Kokkolaras: *Problem Formulations for Simulation-based Design Optimization using Statistical Surrogates and Direct Search* [Optimization Online].

Diversification term

The standard deviation is added to the blackbox outputs:

$$(F\sigma) \quad \begin{cases} \min_{x \in \mathcal{X}} & \hat{f}(x) - \lambda.\hat{\sigma}_f(x) \\ \text{s.t.} & \hat{c}_j(x) - \lambda.\hat{\sigma}_j(x) \leq 0 \ \ \forall j \in J \ . \end{cases}$$

$\lambda > 0 \Rightarrow$ diversification: focus more on exploration than on a particular region. The feasible domain is extended and poor values of $\hat{f}$ may be considered if $\hat{\sigma}_f$ is large.

Probability of feasibility of a point

One continuous `dynaTree` model is built for each constraint.

$$\mathbb{P}[x] = \mathbb{P}[x \text{ is feasible}] = \prod_{j \in J} \mathbb{P}[c_j(x) \leq 0] \ .$$

$\Rightarrow$ one scalar statistical measure to handle the constraints.

BBO and MADS
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Chance constraint

$$(F\sigma P) \quad \begin{cases} \min_{x \in \mathcal{X}} & \hat{f}(x) - \lambda.\hat{\sigma}_f(x) \\ \text{s.t.} & \mathbb{P}[x \text{ is feasible}] \geq p_c \ . \end{cases}$$

Diversification is possible (with parameter λ), but only candidates which are likely to be feasible are evaluated.

Generally, $p_c = \frac{1}{2}$, but it can be tailored according to the number of constraints.

Improvement

Improvement: $I(x) = \max\{f_{min} - f(x), 0\}$:

- ▶ M. Schonlau, D.R. Jones, and W.J. Welch [JOGO, 1998].
- ▶ f_{min}: current best known solution value.
- ▶ $I(x) > 0$ if x is better than the incumbent solution.
- ▶ $I(x) = 0$ otherwise.

Two statistical measurements:

- ▶ Probability of improvement: $PI(x) = \mathbb{P}\left[I(x) > 0\right]$.
- ▶ Expected improvement: $EI(x) = \mathbb{E}\left[I(x)\right]$.

What to do with constraints?

Probability of feasible improvement

Probabilities on:

- ► The objective: $PI(x)$
- ► The feasibility: $\mathbb{P}[x]$

$\Rightarrow$ Probability of Feasible Improvement:

$$PFI(x) = \mathbb{P}[x \text{ is feasible}] \times PI(x)$$

$$(PFI) \quad \left\{ \begin{array}{l} \min_{x \in \mathcal{X}} \; -PFI(x) \end{array} \right.$$

Expected improvement subject to constraints

Maximization of the expected improvement under constraints:

$$(EI\sigma) \quad \begin{cases} \min\limits_{x \in \mathcal{X}} & -EI(x) - \lambda.\hat{\sigma}_f(x) \\ \text{s.t.} & \hat{c}_j(x) - \lambda.\hat{\sigma}_j(x) \leq 0 \ \ \forall j \in J \end{cases}$$

Expected feasible improvement (EFI)

Statistical measurement of

- ▶ The objective: $EI(x)$
- ▶ The feasibility: $\mathbb{P}[x]$

⇒ Expected Feasible Improvement:

$$EFI(x) = \mathbb{P}[x \text{ is feasible}] \times \mathbb{E}\left[I(x)\right]$$

The EFI represents what a candidate will statistically yield, in regard to the optimization problem.

Expected feasible improvement (EFI)

Maximization of the expected feasible improvement:

$$(EFI) \quad \left\{ \quad \min_{x \in \mathcal{X}} \ -EFI(x) \right.$$

EFI with a diversification term:

$$(EFI\sigma) \quad \left\{ \quad \min_{x \in \mathcal{X}} \ -EFI(x) - \lambda.\hat{\sigma}_f(x) \right.$$

List of (most of) surrogate problem formulations

$(F\sigma)\begin{cases} \min\limits_{x \in \mathcal{X}} & \hat{f}(x) - \lambda.\hat{\sigma}_f(x) \\ st: & \hat{c}_j(x) - \lambda.\hat{\sigma}_j(x) \leq 0 \end{cases}$		
$(F\sigma P)\begin{cases} \min\limits_{x \in \mathcal{X}} & \hat{f}(x) - \lambda.\hat{\sigma}_f(x) \\ st: & \mathbb{P}[x \text{ is feasible}] \geq p_c \end{cases}$	$\lambda \in$	
$(EI\sigma)\begin{cases} \min\limits_{x \in \mathcal{X}} & EI(x) - \lambda.\hat{\sigma}_f(x) \\ st: & \hat{c}_j(x) - \lambda.\hat{\sigma}_j(x) \leq 0 \end{cases}$	$\left\{0, \frac{1}{100}, \frac{1}{10}, 1\right\}$	
$(EFI\sigma) \quad \min\limits_{x \in \mathcal{X}} -EFI(x) - \lambda.\hat{\sigma}_f(x)$		
$(PFI) \quad \min\limits_{x \in \mathcal{X}} -PFI(x)$		

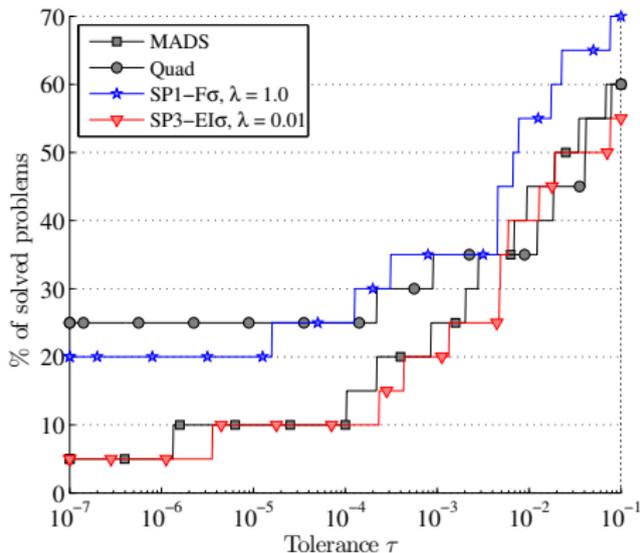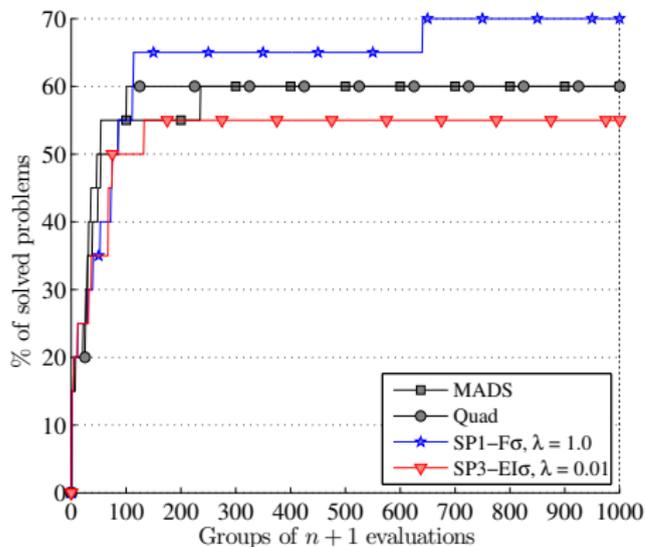Blackbox optimization and the MADS algorithm

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Set of analytic problems

Name	n	m	Bounds	Smooth	f^*
G2	10	3	yes	no	-0.740466
MAD6	5	8	no	no	0.101831
PENTAGON	6	16	no	no	-1.85962
SNAKE	2	3	no	yes	0
HS24	2	4	no	yes	-1
HS34	3	3	yes	yes	-0.833795
HS36	3	2	yes	yes	-3300
HS37	3	3	yes	yes	-3455.51
HS64	3	2	no	yes	6299.94
HS66	3	3	yes	yes	0.532397
HS72	4	3	yes	yes	727.701
HS73	3	4	no	no	29.8944
HS86	5	11	no	yes	-32.2879
HS93	6	3	no	yes	135.075961
HS101	7	7	yes	yes	1809.76
HS102	7	7	yes	yes	911.88
HS103	7	7	yes	yes	543.67
HS104	8	7	yes	yes	4.02305
HS105	8	4	yes	yes	1136.36
HS114	9	7	yes	no	-1192.28

Profiles for the analytic problems (20 instances)

Left: *Data profile* with $\tau = 10^{-1}$.   Right: *Performance profile* after $1000(n+1)$ evaluations.
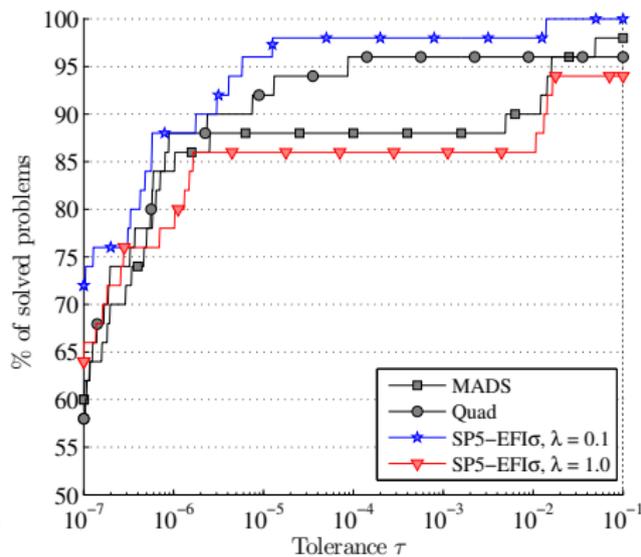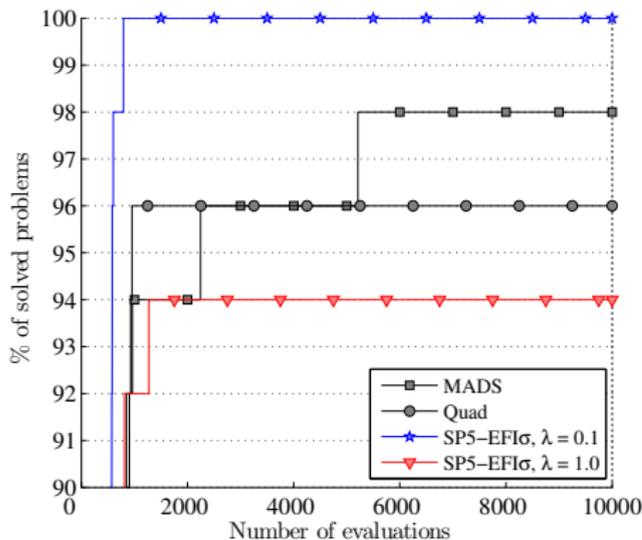
Realistic MDO application

- ▶ NASA Aircraft Range problem with $n = m = 10$.
- ▶ Supersonic business jet with 3 disciplines: aerodynamics, structure, and propulsion.
- ▶ The problem can be summarized as

$$
\begin{aligned}
\max \quad & \text{aircraft range} \\
\text{subject to} \quad & \text{normalized stress} \leq 1.09 \text{ (5 constraints)} \\
& \text{pressure gradient} \leq 1.04 \text{ Pa.m}^{-1} \\
& 0.5 \leq \text{eng. scale factor} \leq 1.5 \\
& \text{normalized engine temperature} \leq 1.02 \\
& \text{throttle setting} \leq \text{max throttle}
\end{aligned}
$$

Realistic MDO application: variables

Variables	Bounds		x^*
	Lower	Upper	
Taper ratio	0.1	0.4	0.4
Wingbox cross-section	0.75	1.25	0.75
Skin friction coeff.	0.75	1.25	0.75
Throttle	0.1	1.0	0.156
Thickness/chord	0.01	0.09	0.06
Altitude	30000	60000	60000
Mach number	1.4	1.8	1.4
Aspect ratio	2.5	8.5	2.5
Wing sweep	40	70	70
Wing surface area	50	1500	1500

Profiles for the MDO problem (50 instances)

Left: *Data profile* with $\tau = 10^{-1}$. Right: *Performance profile* after 10,000 evaluations.

Current conclusions

- ▶ Set of 20 analytic problems: $(F\sigma)$ with $\lambda = 1$ performs better.

- ▶ For two realistic MDO applications, $(EI\sigma)$ with $\lambda = 1/100$ and 1, and $(EFI\sigma)$ with $\lambda = 1/10$, gave the best results.

- ▶ `NOMAD` with `dynaTree` should be available in a future `NOMAD` release.

▶ S. Alarie, C. Audet, V. Garnier, S. Le Digabel, and L.A. Leclaire: *Snow water equivalent estimation using blackbox optimization.* Pacific Journal of Optimization, 2013.

▶ C. Audet and J. E. Dennis, Jr.: *Mesh adaptive direct search algorithms for constrained optimization.* SIAM Journal on Optimization, 2006.

▶ A.R. Conn and S. Le Digabel: *Use of quadratic models with mesh-adaptive direct search for constrained black box optimization.* Optimization Methods and Software, 2013.

▶ S. Kodiyalam: *Multidisciplinary aerospace systems optimization.* NASA/Lockheed Martin Technical Report, 2001.

▶ S. Le Digabel: *Algorithm 909: NOMAD: Nonlinear optimization with the MADS algorithm.* ACM Transactions on Mathematical Software, 2011.

▶ M.A. Taddy, R.B. Gramacy, and N.G. Polson: *Dynamic trees for learning and design.* Journal of the American Statistical Association, 2011.

▶ B. Talgorn, S. Le Digabel, and M. Kokkolaras: *Problem Formulations for Simulation-based Design Optimization using Statistical Surrogates and Direct Search.* Technical report, Les Cahiers du GERAD G-2014-04.