A MATLAB Toolbox for Surrogate-Assisted Multi-Objective Optimization: A Preliminary Study

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Motivation

Multi-objective Optimization Problems (MOPs) involve a set of **conflicting** objectives that are to be optimized **simultaneously**.

It is common that derivatives of the objectives **f** are neither **symbolically** nor **numerically** available.

Evaluating **f** is typically **expensive** requiring some computational resources (e.g., a computer code or a laboratory experiment).

Solve using a **finite budget** of function evaluations.

Motivation

Surrogate modeling: a powerful ingredient for **computationally-expensive** Single-objective Optimization Problems (SOPs) (Jones et al., JOPT, 1998).

Readily **available** **well-benchmarked** software libraries for surrogate-assisted SOPs (Mueller, arXiv, 2014).

MOPs: growing community efforts towards

- consolidating—e.g., the recent SAMCO workshop[1].
- benchmarking surrogate-assisted algorithms (on different problems independently (Akhtar & Shoemaker, JOPT, 2015)).

[1] http://samco.gforge.inria.fr/doku.php

Objective

Add a brick to the ongoing efforts

- **Multi-objectifying** `MATSuMoTo`: a surrogate-assisted library for SOPs (Mueller, arXiv, 2014).
- **Validate** its performance on the Bi-objective Black Box Optimization Benchmarking (Tusar et al., arXiv, 2016).

Surrogate-Assisted Optimization

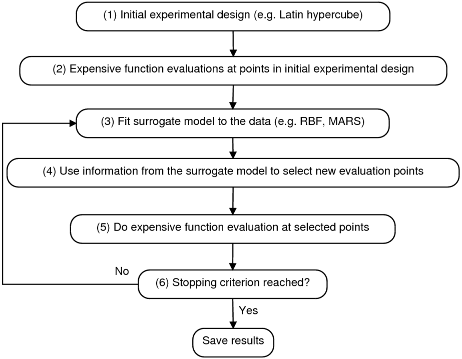

Figure: Surrogate-assisted optimization framework.

For MOPs: **exploration-exploitation-diversification** is sought.

Two approaches for Step 4:

- *A*1 Using the surrogate model indirectly to generate a set of candidate points: the selected points for evaluation are the optimizers of a measure derived from the surrogate model (e.g., Emmerich et al., IEEE CEC, 2011).
- *A*2 Using the surrogate model directly to generate a set of candidate points: a subset of these points are then selected for evaluation based on a set of rules (e.g., Akhtar & Shoemaker, JOPT, 2015).

Surrogate-Assisted Optimization

- The first approach has been the focus of several optimization software packages (e.g., Binois & Picheny, GPareto, 2016).
- The second approach lends itself naturally to the framework of the `MATSuMoTo` library for SOPs (Mueller, arXiv, 2014).
- In this paper:
  * incorporate a variant of Approach A2 (`GOMORS` by Akhtar & Shoemaker, JOPT, 2015) into the `MATSuMoTo` library.
  * assess its strength and weakness vs. a variant of Approach A1: GPareto package: `SMS-EGO`, `EHI-EGO`, `EMI-EGO`, `SUR-EGO` by Binois & Picheny, GPareto, 2016.

Surrogate-Assisted Optimization

Table: Possible feature choices for the individual steps of MATSuMoTo. Highlighted choices: new features supporting multi-objective optimization problems.

Algorithm Step	Choice Name	Description
(1) Initial design	CORNER	Corner points of the hypercube
	SLHD	Symmetric Latin hypercube
	lhd	Latin hypercube
(3) Surrogate model	RBFcub	Cubic RBF
	RBFgauss	Gaussian RBF
	RBFtps	Thin-plate spline RBF
	RBFlin	Linear RBF
	MARS	Multivariate adaptive regression spline
	POLYlin	Linear regression polynomial
	POLYquad	Quadratic regression polynomial
	POLYquadr	Reduced quadratic regression polynomial
	POLYcub	Cubic regression polynomial
	POLYcubr	Reduced cubic regression polynomial
	MIX_RcM	Mixture of RBFcub and MARS
	MIX_RcPc	Mixture of RBFcub and POLYcub
	MIX_RcPcr	Mixture of RBFcub and POLYcubr
	MIX_RcPq	Mixture of RBFcub and POLYquad
	MIX_RcPqr	Mixture of RBFcub and POLYquadr
	MIX_RcPcM	Mixture of RBFcub, POLYcub, and MARS
(4) Sampling strategy	CANDloc	Local candidate point search
	CANDglob	Global candidate point search
	SurfMin	Minimum point of surrogate model
	SurfPareto	Pareto front of surrogate model (currently employs GOMORS)

Assessment

- Interfacing the Comparing Continuous Optimizer (COCO) platform with GPareto R package (too slow, weeks for $n = 20$!).
- Preliminary results qualified SMS-EGO
- Within MO-MATSuMoTo, SMS-EMOA (Beume et al., EJOR, 2007) and MO-DIRECT (Al-Dujaili & Suresh, CEC, 2016) used.[2]
- SMS-EGO vs. MAT-SMS vs. MAT-DIRECT.

[2] Available at http://ash-aldujaili.github.io/projects.html

Experimental Setup

COCO guidelines : data profiles and statistical test

55 problems based on bi-combinations of 24 noiseless functions :

- f_1-f_5 : separable functions
- f_6-f_9 : functions with low or moderate conditioning
- f_{10}-f_{14} : functions with high conditioning and unimodal
- f_{15}-f_{19} : multi-modal functions with adequate global structure
- f_{20}-f_{24} : multi-modal functions with weak global structure

dimensionality : 5-D, 10-D, 20-D, 40-D

evaluation budget : $75 \cdot n$ (time limitation & slow `GPareto`)

Performance Results

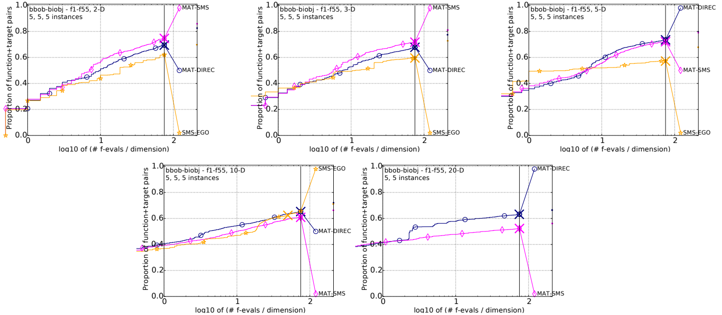

Figure: Bootstrapped empirical cumulative distribution of the number of objective function evaluations divided by dimension (FEvals/DIM) for 121 targets with target precision in $\{0, 10^{-0.19}, 10^{-0.18}, \ldots, 10^{0.98}, 10^{0.99}, 10^{1}\}$ over all the problems in $n \in \{2, 3, 5, 10, 20\}$.

Performance Results

- Given this expensive budget setting, `MAT-DIRCT` and `MAT-SMS` show a comparable performance, outperforming `SMS-EGO`.
- With more function evaluations, `SMS-EGO`'s performance stagnates.
- On the other hand, `MAT-DIRCT` and `MAT-SMS` exhibit a gradual progress with more evaluations.

Insights & Issues

- Limited evaluation budget ($75 \cdot n$) makes it difficult to reach a **conclusive statement**.
- **GPareto** R package:
  1. Extremely **slow** in higher dimension: R–MATLAB communication.
  2. Several run instances exited with **run-time errors** (error in `optim` function)
- Multi-objectifying **MATSuMoTo** with `GOMORS` (Akhtar & Shoemaker, JOPT, 2015):
  1. Ill-condition behavior after a batch of sampled points.
  2. Re-think about what kind of points are used to build the models.

BMOBench

- Inspired by COCO, we built `BMOBench`
- a platform with 100 MOPs.
- data profiles generated in terms of 4 quality indicators.
- Special session at SSCI'2016, Greece.[3] (Deadline: 15-August-2016)
- We invite the multi-objective community to test their published/novel algorithms on these problems.

[3] `http://ash-aldujaili.github.io/BMOBench/`

Thank you