

An Experimental Investigation of Model-Based Parameter Optimization: SPO and Beyond

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Motivation for Parameter Optimization

Genetic Algorithms & Evolutionary Strategies are

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- Tedious to configure for a new domain
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 - ▶ Hybridizations, ...

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Automated parameter optimization can help

- ▶ High-dimensional optimization problem
- ▶ Automate \rightsquigarrow saves time & improves results

Parameter Optimization Methods

- ▶ Numerical parameters
 - See Blackbox optimization workshop (this GECCO)
 - Algorithm parameters: CALIBRA [Adenso-Diaz & Laguna, '06]

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 - Genetic algorithms [Terashima-Marín, Ross & Valenzuela-Réndon, '99]
 - Iterated Local Search
[Hutter, Hoos, Leyton-Brown & Stützle, '07-'09]
 - ↪ Dozens of parameters (e.g., CPLEX with 63 parameters)
 - ↪ For many problems: SAT, MIP, time-tabling, protein folding, MPE, ...

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Model-free Parameter Optimization

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 - Fractional factorial designs [e.g., Ridge & Kudenko, '07]
 - Sequential Parameter Optimization (SPO)
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 - Sequential Parameter Optimization (SPO)
[Bartz-Beielstein, Preuss, Lasarczyk, '05-'09]
- ▶ Can use model for more than optimization
 - Importance of each parameter
 - Interaction between parameters

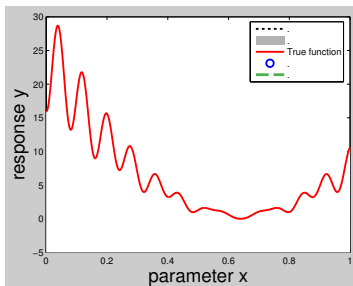
Outline

1. Sequential Model-Based Optimization (SMBO): Introduction
2. Comparing Two SMBO Methods: SPO vs SKO
3. Components of SPO: Model Quality
4. Components of SPO: Sequential Experimental Design
5. Conclusions and Future Work

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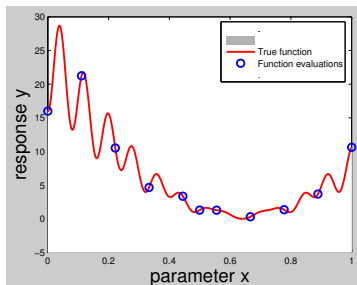
SMBO: Introduction



First step of SMBO

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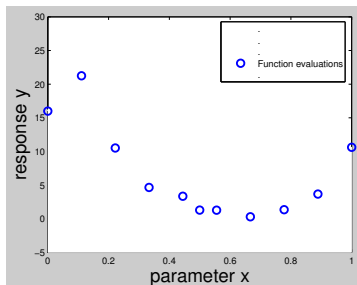
1. Get response values at initial design points



First step of SMBO

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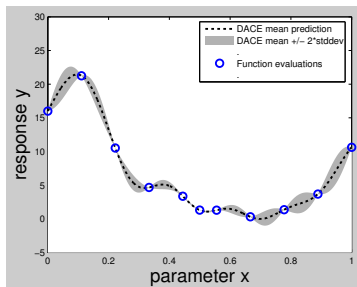
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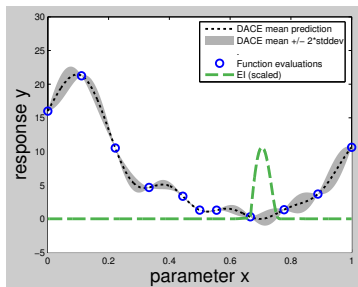
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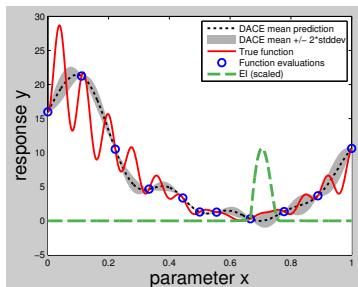
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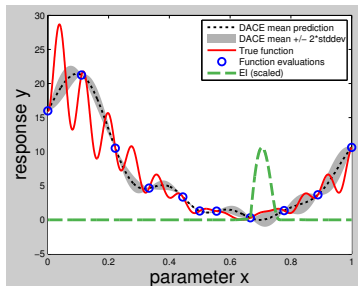
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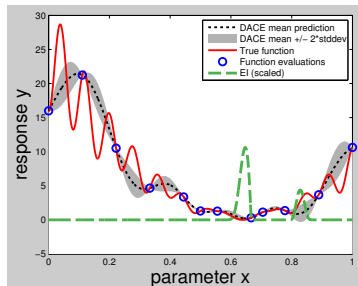
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SMBO: Introduction

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2. Fit a model to the data
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4. Repeat 2. and 3. until time is up



First step of SMBO



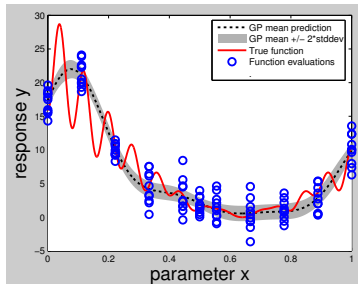
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Dealing with Noise: SKO vs SPO

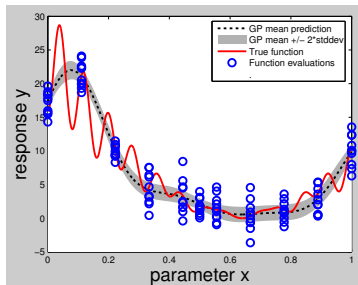
- ▶ Method I (used in SKO) [Huang, Allen, Notz & Zeng, '06.]
 - Fit standard GP assuming Gaussian observation noise
 - Can only fit the mean of the responses



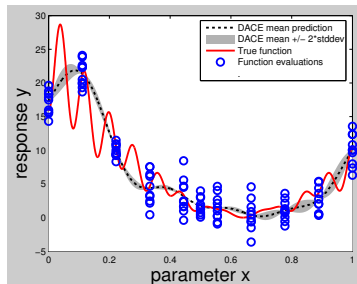
Method I: noisy fit of original response

Dealing with Noise: SKO vs SPO

- ▶ Method I (used in SKO) [Huang, Allen, Notz & Zeng, '06.]
 - Fit standard GP assuming Gaussian observation noise
 - Can only fit the mean of the responses
- ▶ Method II (used in SPO) [Bartz-Beielstein, Preuss, Lasarczyk, '05-'09]
 - Compute *statistic of empirical distribution of responses* at each design point
 - Fit noise-free GP to that



Method I: noisy fit of original response



Method II: noise-free fit of cost statistic

Experiment: SPO vs SKO for Tuning CMA-ES

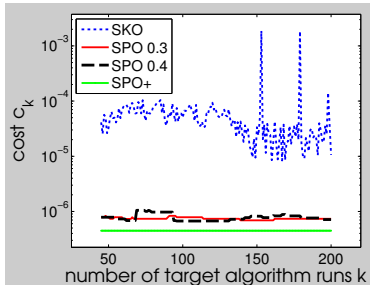
- ▶ CMA-ES [Hansen et al., '95-'09]
 - Evolutionary strategy for global optimization
 - State-of-the-art (see BBOB workshop this GECCO)
 - Parameters: population size, number of parents, learning rate, damping parameter

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 - Solution cost: best function value found in budget
 - Here: Sphere function
 - Minimize mean solution cost across many runs

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Components of SPO: initial design

- ▶ Fixed number of initial design points (250) and repeats (2)
 - Size of initial design studied before [Bartz-Beielstein & Preuss, '06]
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 - SPO's standard LHD
- ▶ Result: no significant difference
 - Initial design not very important
 - Using cheap random LHD from here on

Components of SPO: Transformations

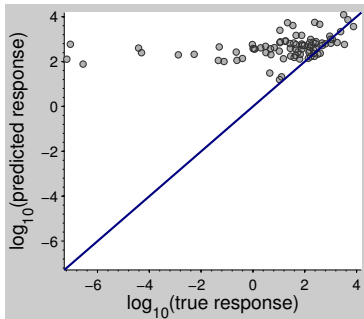
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 - Training: 250 · 2 data points as above
 - Test: 250 new points, sampled uniformly at random

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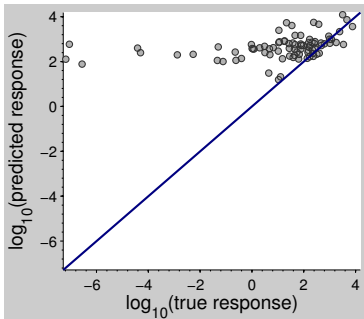
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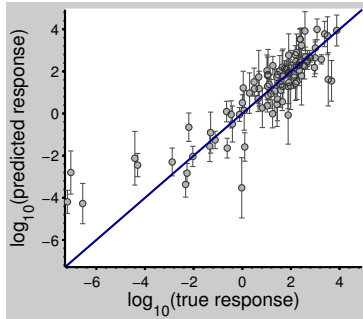
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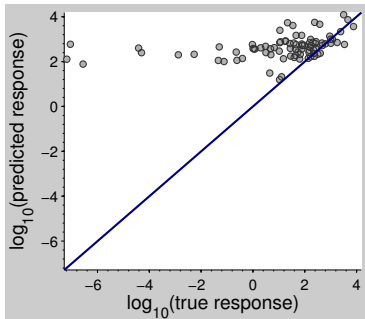
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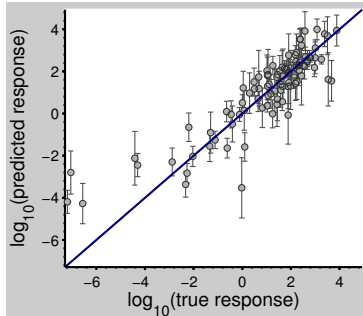
Log transformation

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Log transformation

Note: In newer experiments, SKO with log models was competitive

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User wants to optimize some objective c

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Some algorithm runs can be lucky

- ~> need extra mechanism to ensure incumbent is really good
- ~> SPO increases number of repeats over time

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 - Increase R over time
- ▶ But what if it doesn't perform well?
 - Then a different incumbent is picked in the next iteration
 - That might also turn out not to be good...

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Simple fix

- ▶ Iteratively perform runs for single most promising θ_{new}
 - ▶ Compare against current incumbent θ_{inc}
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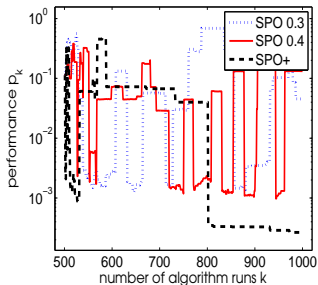
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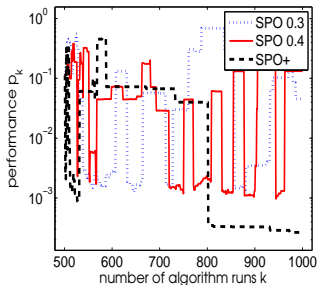


Tuning CMA-ES on Griewangk

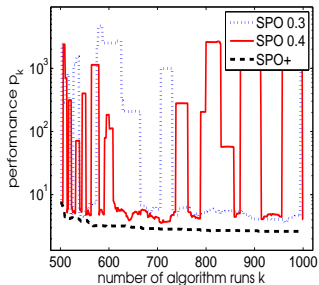
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Tuning CMA-ES on Griewangk



Tuning CMA-ES on Rastrigin

Summary of Study of SPO components & Definition of SPO⁺

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 - ↪ use simple random LHD in SPO⁺
- ▶ Log-transforms sometimes improve model quality a lot
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Sequential Experimental Design

- ▶ Expected improvement criterion
 - ↪ New one that's better in theory but not in practice
 - ↪ Use original one in SPO⁺
- ▶ New mechanism for increasing #runs & selecting incumbent
 - ↪ substantially improves robustness
 - ↪ Use it in SPO⁺

Comparison to State of the Art for tuning SAPS

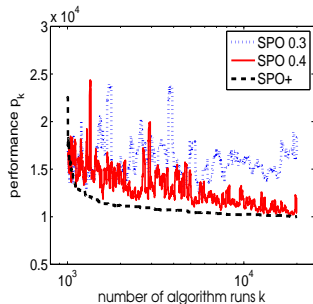
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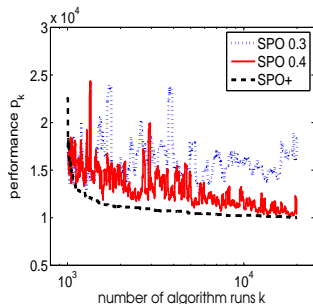
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Comparison to SPO variants,
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Procedure	SAPS median run-time/ 10^3
SAPS default	85.5
CALIBRA(100)	10.7 ± 1.1
BasicILS(100)	10.9 ± 0.6
FocusedILS	10.6 ± 0.5
SPO 0.3	18.3 ± 13.7
SPO 0.4	10.4 ± 0.7
SPO ⁺	10.0 ± 0.4

With budget of 20000 runs of SAPS

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- ▶ SMBO can help design algorithms
 - ▶ More principled, saves development time
 - ▶ Can exploit full potential of flexible algorithms
- ▶ Our contribution
 - ▶ Insights: what makes a popular SMBO algorithm, SPO, work
 - ▶ Improved version, SPO⁺, often performs better than SPO

Ongoing & Future Work

Ongoing Extensions of Model-Based Framework

- ▶ Use of different models in SPO⁺ framework
- ▶ Dealing with categorical parameters
- ▶ Optimization for Sets/Distributions of Instances

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Use of models for scientific understanding

- ▶ Interactions of instance features and parameter values
- ▶ Can help understand and hopefully improve algorithms

Thanks to

- ▶ Thomas Bartz-Beielstein
 - SPO implementation & CMA-ES wrapper
- ▶ Theodore Allen
 - SKO implementation