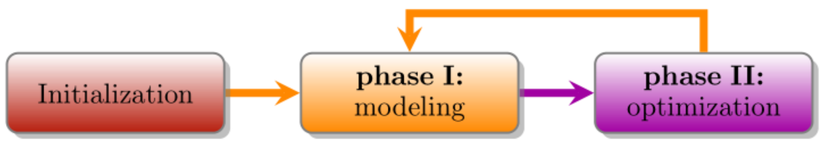
Online Whitening for High Conditioning Optimization Problems

Samineh Bagheri, Wolfgang Konen and Thomas Bäck
TH Köln – University of Applied Sciences
Leiden University, LIACS

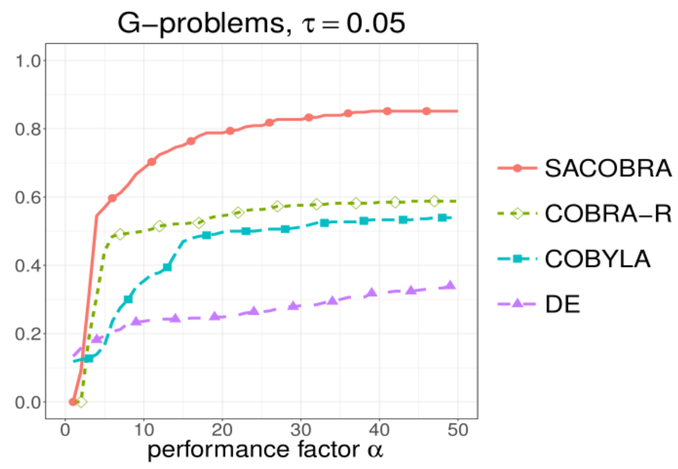
SACOBRA

SACOBRA (**S**elf-**A**djusting **C**onstrained **O**ptimization **By** **RA**dial Basis Function Inteprolation) : a surrgate-assisted optimization framework for handling **expensive** high-dimensional **black box constrained** optimization problems (COP)

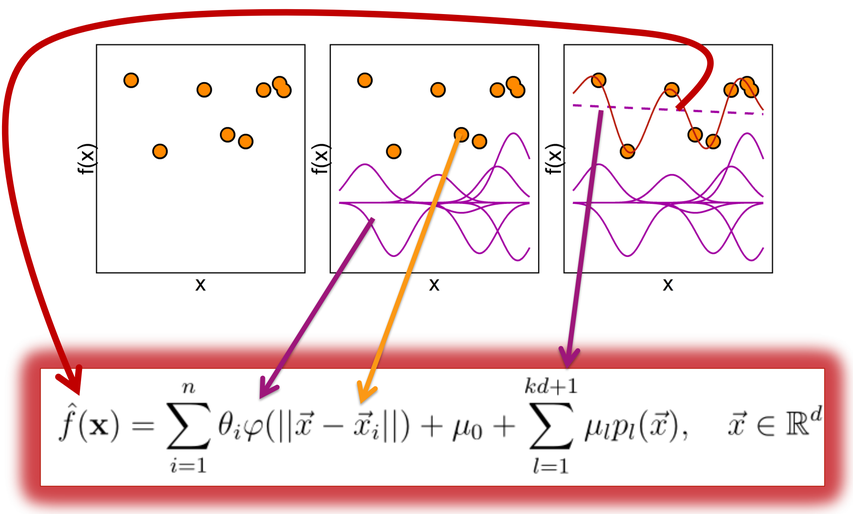


SACOBRA Highlights :

- Self-adjusting elements:
  - Automatic transformation of the objective and constraint functions
  - Parameter selection to control the exploration/exploitation rate
- Repair functionality
- Online model selection
- Handling equality and inequality constraints
- State-of-the-art in efficiently solving a large set of COPs (G-functions, MOPTA08)



RBF Interpolation

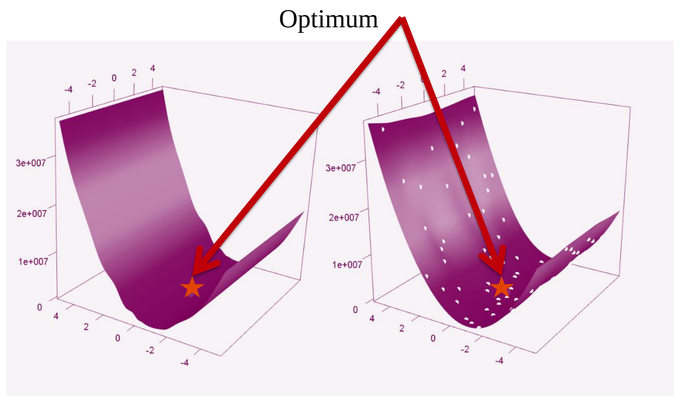


Different basis functions: Gaussian, Cubic, Multiquadric, …

- Easy and fast to train
- Require very few points
- Efficient in high dimensions
- ….

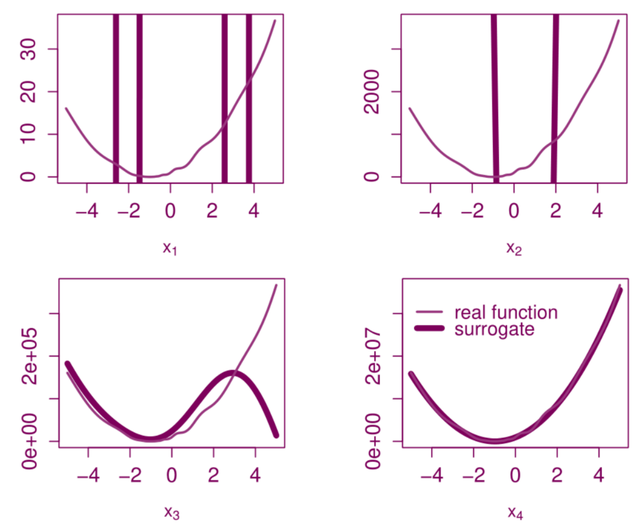
MOTIVATION

- SACOBRA can address unconstrained problems
- But RBFs fail to deliver useful models for **functions with high conditioning:** high ratio of steepest slope in one direction to flattest slope in another direction



F02-2D function from the BBOB benchmark (ellipsoidal function). Left: The real function. Right: RBF model for F02-2D built from 60 points.

- Condition number: ratio of the largest to smallest singular value of the Hessian matrix.



Four cuts at the optimum of F02-4D along each dimension. The model follows the real function only in the 'steep' dimension x_4 (and to some extent in dimension x_3).

- RBF models have many misleading local minima along the shallow directions

Online Whitening

The main idea is to transform a function with high conditioning $f(\vec{x})$ into an easier-to-model function $g(\vec{x})$.

$$g(\vec{x}) = f(\boldsymbol{M}(\vec{x} - \vec{x}_c))$$

M: a linear transformation matrix
$\vec{x}_c$: transformation center

M is found in such a way that the Hessian matrix of the new function becomes the identity matrix

$$\frac{\partial^2 g(\vec{x})}{\partial \vec{x}^2} = \boldsymbol{I}$$

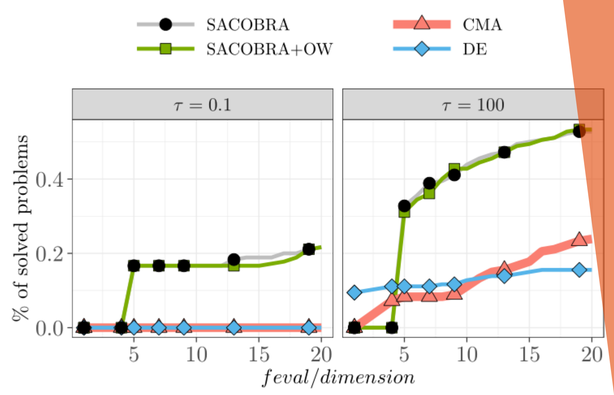
As shown in our paper, a solution for the equations above, is as follows:

$$\boldsymbol{M} = \boldsymbol{H}^{-0.5}$$

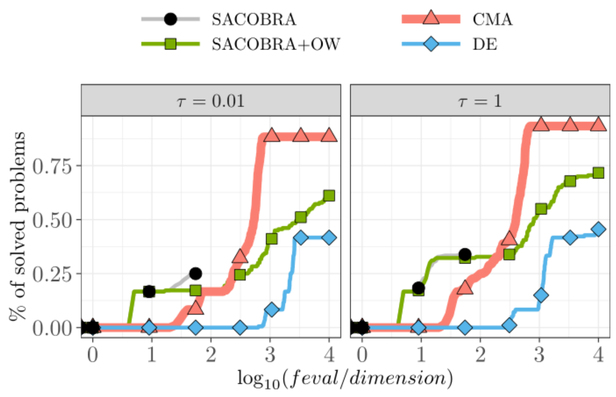
$\boldsymbol{H}$: Hessian Matrix

- Estimating the Hessian matrix numerically imposes $4D^2+4D$ function evalutions
- Online Whitening is applied after every 10 iterations

Results



Comparing the overall performances of SACOBRA, SACOBRA+OW, DE and CMA-ES, on 12 BBOB problems with D = 10, for very limited function evaluations.



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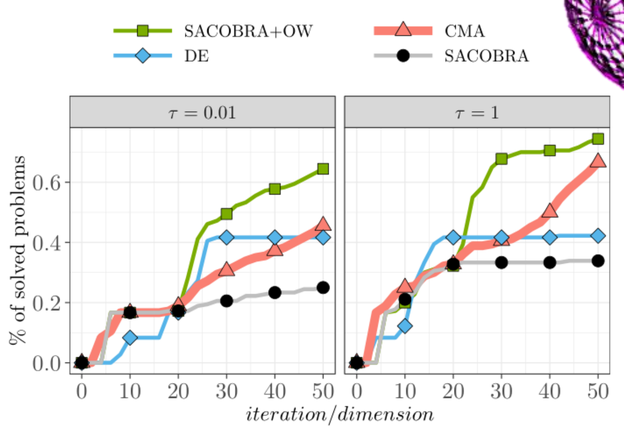

Ideally parallelizable scenario

SACOBRA Framework

- SACOBRA framework can be found on **CRAN**
- The detailed mathematical derivation of online whitening algorithm can be found in our **technical report**
- A series of publications related to **SACOBRA** and the most recent news about our work can be found on the **CIOP** blog

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