Model-Based Optimization Revisited: Towards Real-World Processes
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- Introduction
- Design of Experiments
- A Benchmark of Modeling Techniques
- Model-Based Optimization of a Novel Turning Process
- Summary and Outlook
Introduction

Real-World Manufacturing Processes
- Expensive to evaluate
- Inexact evaluations
- A moderate number of decision parameters
Design of Experiments

Response Surface Method (RSM)
- Least-squares fit of a given functional
- Residuals are assumed to be uncorrelated
- Uncertainty of predictions depends on the fit of the model

Design and Analysis of Computer Experiments (DACE)
- Additional modeling of the spatial residual correlations
- Uncertainty of prediction also depends on the exploration of the search space

Neural Networks, Radial Basis Functions
Survey of Jin, Soft Computing 9 (2005) 1
Allowing for Noise in DACE Models

Nugget Factor (Sasena, PhD thesis, 2002)

- Downscaling of the correlation

\[ R(w, x) = (1 - \text{nugget}) \prod_{k=1}^{d} e^{-\theta \| w^k - x^k \|^2} \]

\[ s^2(x^*) = \sigma^2 \left[ 1 - \mathbf{r}' \mathbf{R}^{-1} \mathbf{r} + \frac{(1 - \mathbf{1}' \mathbf{R}^{-1} \mathbf{1})^2}{\mathbf{1}' \mathbf{R}^{-1} \mathbf{1}} \right] \]

- No interpolation
- Even observed parameter vectors have a non-zero uncertainty
DACE-Based Approaches for Noisy Data

Sequential Parameter Optimization (SPO)
(Bartz-Beielstein, Lasarczyk, Preuβ, CEC 2005)
- Replicate all design points and use expected value in an interpolating DACE model
- Increase the number of replications during the optimization
- Second order polynomial regression and Gaussian correlation model

Fixed Nugget Optimization (FINO)
- Estimate nugget factor by replicating the median design
  \[(1 - \text{nugget}) = \frac{\hat{\sigma}^2}{\sigma^2 + \hat{\sigma}^2}\]
  - Closely related to the central composite design in classical DOE
  - Only one design is repeated
Research Question

Is it possible to improve the prediction quality of classic DOE regression models by using DACE models for noisy data?

Pre-Experimental Planning

- Implementation of the approaches using the MATLAB® toolbox DACE
- Extending the `dacefit` routine by using Hansen’s CMA-ES implementation

Task

Statistical testing of three hypotheses:

H1: DACE provides more precise models whenever the regression functional is not completely adequate, even for noisy data.

H2: It is better to test different designs than replicating single ones

H3: The use of nugget factors improves the robustness of the models
Benchmark

Setup

- Test functions (2-6 dim.) with non-uniform noise (3% const. + 5% var.)
  - Weighted sphere
  - Hartman
  - Rastrigin

- Modeling approaches
  - DOE (linear and quadratic regression functions)
  - SPO (quadratic regression function and Gaussian correlation model)
  - EGO (constant regression function and kriging correlation model)
    - One to three evaluations of each design
  - FINO (EGO including a nugget factor)
  - The number of evaluations is derived from the central composite design

Tobias Wagner (wagner@isf.de)
Experimentation (Normalized Root Mean Squared Prediction Error)

**Sphere**

- $d = 2, n = 16$
- $d = 4, n = 36$
- $d = 6, n = 59$

**Hartman**

**Rastrigin**

<table>
<thead>
<tr>
<th>DOE</th>
<th>SPO</th>
<th>EGO</th>
<th>FINO</th>
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Experimentation (Normalized Accuracy in Detecting the Optimum)

H1 accepted
H3 rejected

Sphere
Hartman
Rastrigin

\[ d = 2, n = 16 \]
\[ d = 4, n = 36 \]
\[ d = 6, n = 59 \]
Benchmark

Visualization

Test function

Sphere  Hartman  Rastrigin

DOE

EGO

FINO
Effect of Design Replications Within EGO

H2 accepted
Model-Based Optimization

Turning of Functional Graded Workpieces

- Decision variables
  - Cutting speed $v_c$
  - Feed $f$
  - Cutting depth $a_p$

- Objectives
  - Production time $t$
  - Surface roughness $R_z$
    - Hard region
    - Ductile region
  - Width of flank wear length
    - Major cutting edge
    - Minor cutting edge

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Model-Based Optimization

NSGA-II Optimization Based on EGO Models of the Objectives

Validation Experiment
Production time: 37 min

Surface roughness Rz:
2.76 µm in the ductile region
1.79 µm in the hard region

Width of flank wear length VB\textsubscript{max}:
78.3 µm at the major cutting edge
86.4 µm at the minor cutting edge
Summary

- Refutation of the universally assumed sensitivity of interpolating DACE models to noise
- Introduction of methods to allow for noise in DACE
- Empirically derived suggestions on the choice of regression functions, correlation models, and replications of designs
- Successful real-world application

Outlook

- Incorporation of methods to detect outliers in the data
- Advancements of single- and multi-objective optimizers based on DACE

Ponweiser, W.; Wagner, T.; Vincze, M.

Clustered Multiple Generalized Expected Improvement: A Novel Infill Sampling Criterion for Surrogate Models (EC0755)

Hybrid Algorithms IV, June 4, 9:30 -11:30, Room 603

Thank you for your attention!