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Multi-fidelity modeling and optimization of biogas plants

Martin Zaefferer*, Daniel Gaida, Thomas Bartz-Beielstein

Faculty of Computer Science and Engineering Science, TH Köln (University of Applied Sciences), Steinmüllerallee 1, 51643 Gummersbach, Germany

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ABSTRACT

An essential task for operation and planning of biogas plants is the optimization of substrate feed mixtures. Optimizing the monetary gain requires the determination of the exact amounts of maize, manure, grass silage, and other substrates. For this purpose, accurate simulation models are mandatory, because the underlying biochemical processes are very slow. The simulation models may be time-consuming to evaluate, hence we show how to use surrogate-model-based approaches to optimize biogas plants efficiently. In detail, a Kriging surrogate is employed. To improve model quality of this surrogate, we integrate cheaply available data into the optimization process. To this end, multi-fidelity modeling methods like Co-Kriging are applied. Furthermore, a two-layered modeling approach is used to avoid deterioration of model quality due to discontinuities in the search space. At the same time, the cheaply available data is shown to be very useful for initialization of the employed optimization algorithms. Overall, we show how biogas plants can be efficiently modeled using data-driven methods, avoiding discontinuities as well as including cheaply available data. The application of the derived surrogate models to an optimization process is only partly successful. Given the same budget of function evaluations, the multi-fidelity approach outperforms the alternatives. However, due to considerable computational requirements, this advantage may not translate into a success with regards to overall computation time.

1. Introduction

Optimizing the operation of biogas plants is and will be one of the main challenges in the field of *anaerobic digestion* (AD) in the near future. Due to a steady decrease in funding and increasing substrate costs only optimal operating biogas plants will be economically advantageous.

The operation of biogas plants is very sensitive to the mixture of the used substrates. Hence, optimizing the mixture is an important task to run or plan such plants efficiently. Due to the very slow processes involved, optimizing the plants in real-time would consume too much time. Models like the *Anaerobic Digestion Model No. 1* (ADM1) allow to compute a good prediction of biogas plant's process variables, based on the used substrates [7]. Thus, ADM1 can be used as a substitute in the optimization process instead of a real plant.

While such models are much cheaper to evaluate than their real-world counter-part, they do take some time to evaluate. Hence, methods that use the smallest amount of evaluations possible are of interest. This situation motivated the central question that will be tackled in this study:

(Q-1) How can the precision of simulation models be improved without increasing the number of evaluations?

Surrogate modeling techniques are therefore a promising choice. Besides the expensive information derived from ADM1, additional performance information is available. A rough performance estimate can be determined based on the biogas potential of the used substrates and their associated costs. This additional knowledge can be integrated into the optimization process, by bolstering the quality of the chosen surrogate-modeling technique. This approach of integrating different levels of granularity or cost has previously been called multi-fidelity optimization [19]. It is worth investigating whether these approaches are applicable to real-world settings. This can be formulated as the second question to be analyzed in this study:

(Q-2) What are the benefits and limitations of multi-fidelity modeling approaches?

* Corresponding author.
E-mail addresses: martin.zaefferer@th-koeln.de (M. Zaefferer), daniel.gaida@th-koeln.de (D. Gaida), thomas.bartz-beielstein@th-koeln.de (T. Bartz-Beielstein).

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In this paper, several multi-fidelity modeling approaches are compared, and the best are tested for their performance in an optimization process.

Section 2 gives an overview of relevant previous work. The specific problem to be solved is introduced in Section 3. In Section 4, methods that were used in this study are described. Section 5 presents experiments, in which various multi-fidelity approaches are tested for their modeling quality, whereas Section 6 tests the best of these for their success in solving the actual optimization problem. A concluding summary of findings as well as an outlook on future research is given in Section 7.

2. Former research

2.1. Biogas plant simulation

Islam et al. [28] analyze the impact of different factors on production of biogas in different biogas plants of Bangladesh. The data was collected from 18 poultry farms. Their analysis is based on collected data from survey, Internet, and other sources. To obtain further insight in the behavior of biogas plants, simulation models such as the ADM1 can be used. ADM1 is very popular and the nowadays most complex mathematical model used to simulate the anaerobic digestion process (for a review see [6]). In several publications it is utilized to dynamically model full-scale agricultural and industrial biogas plants [8,33,47]. ADM1 is a structured model incorporating disintegration and hydrolysis, acidogenesis, acetogenesis, and methanogenenesis steps. The ADM1 is implemented as a stiff differential equation system in a MATLAB® toolbox for biogas plant modeling, optimization and control published by Gaida et al. [23]. In this toolbox, a model of a full-scale agricultural biogas plant is developed that is used in the empirical part of this publication. The simulation model of the biogas plant includes the ADM1 and furthermore models of electrical and thermal energy sinks and sources as well as models for performance and stability criteria. Typical criteria include cost versus benefit (with respect to the Renewable Energy Sources Act (EEG 2009) in Germany [9]), stability of substrate degradation processes and operating constraints such as upper and lower pH limits, maximum VFA/TA [52] value, maximum total solids content in the digester, and minimum methane concentration of the biogas.

2.2. Biogas substrate feed optimization

Biogas plant substrate feed mixtures have previously been optimized with a Genetic Algorithm and Particle Swarm Optimization by Wolf et al. [56]. More recently Ziegenhirt et al. [60] used state of the art evolution strategies like *Covariance Matrix Adaption Evolution Strategy* (CMAES) [27,26] or *Differential Evolution* (DE) [54] to reduce the number of needed simulations. They also used the *Sequential Parameter Optimization Toolbox* (SPOT) [5] to tune the employed algorithms. In our work, we directly use SPOT on the substrate feed optimization problem. That is, we support the optimization procedure with surrogate-models.

Both previous studies used a biogas plant model based on the MATLAB® Simulink® Toolbox SIMBA, developed by ifak system GmbH[1]. The herein presented research on the other hand is based on the MATLAB® Toolbox for Biogas Plant Simulation [23]. In contrast to earlier works by Wolf et al. [56] and Ziegenhirt et al. [60] our approach is not limited to the ADM1. A simple estimate of a substrate mixtures quality is derived from the biogas potential of each ingredient.

2.3. Surrogate modeling in optimization

Especially when the evaluation of target functions is expensive, it is a well established approach to exploit surrogate models of the target function to save expensive function evaluations.

A methodical framework for surrogate model based optimization of noisy and deterministic problems is *Sequential Parameter Optimization* (SPO) introduced by Bartz-Beielstein et al. [5]. SPO has been developed for solving expensive algorithm tuning problems but can be directly employed for solving real world engineering problems as well.

One of the most often used surrogate-models is Kriging, which is an especially promising model for continuous, smooth problem landscapes. Besides its prediction performance, it is often employed because it provides an estimator of the local certainty of the model, which can be used to calculate the *Expected Improvement* (EI) of a new sample over the best known sample. Jones et al. [32] introduced this concept to balance exploitation and exploration in expensive optimization, terming it *Efficient Global Optimization* (EGO).

Other models include *Artificial Neural Networks* (ANN) or *Support Vector Regression* (SVR) [14]. Non-continuous problem landscapes, or problems which are not that expensive, may be tackled with approaches like *Random Forest* (RF) [11] or *Multivariate Adaptive Regression Splines* (MARS) [20].

A comprehensive overview of surrogate model assisted optimization was provided by Jin [30], focusing on single objective problems.

Extensions of the above concepts to multi-objective problems are available (e.g., multi objective EGO [35,48,16] and SPO [58,59]). Since multi-objective problems are not in the focus of this paper, we refer to the overview by Knowles and Nakayama [36] for further information.

2.4. Multi-fidelity

Multi-fidelity optimization [19] deals with problems where the target function can be evaluated at different levels of fidelity. That is, the actual target function represents the highest level of fidelity, yielding the most accurate but also most expensive fitness estimate. At the same time, one or several cheaper, less accurate estimates can represent the lower fidelity levels. The actual, expensive target function will be referred to as the *fine function*, whereas the cheaper and less accurate function will be referred to as *coarse function*, respectively. Note, that in this study, multi-fidelity will usually refer to the case where in fact at least three levels of fidelity exist: fine function, coarse function and surrogate model. Only the first two are inherent to the problem, the third is learned based on collected data.

Such situations often arise, especially in engineering problems. There, the evaluation of the actual problem may be an expensive real-world evaluation measurement, or a time consuming *Computational Fluid Dynamics* (CFD) simulation. In these cases, a simplified physics-based model may yield an inexpensive but less accurate quality estimate. For some models, fidelity may even be scalable. For instance, simplified meshes with less density can be employed with CFD, or if available pre-converged simulation results may be harnessed.

2.4.1. Multi-fidelity modeling

To exploit information from different fidelity levels in surrogate modeling, several methods exist, including Co-Kriging. Forrester et al. [19] show how this can be applied to engineering problems. Co-Kriging exploits correlation between coarse and fine function to generate a better surrogate model of the fine function.

[1] www.ifak-system.com.