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Surrogate based sensitivity analysis of process equipment

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ABSTRACT

The computational cost associated with the use of high-fidelity computational fluid dynamics (CFD) models poses a serious impediment to the successful application of formal sensitivity analysis in engineering design. Even though advances in computing hardware and parallel processing have reduced costs by orders of magnitude over the last few decades, the fidelity with which engineers desire to model engineering systems has also increased considerably. Evaluation of such high-fidelity models may take significant computational time for complex geometries.

In many engineering design problems, thousands of function evaluations may be required to undertake a sensitivity analysis. As a result, CFD models are often impractical to use for design sensitivity analyses. In contrast, surrogate models are compact and cheap to evaluate (order of seconds or less) and can therefore be easily used for such tasks.

This paper discusses and demonstrates the application of several common surrogate modelling techniques to a CFD model of flocculant adsorption in an industrial thickener. Results from conducting sensitivity analyses on the surrogates are also presented.

1. Introduction

For many industrial fluid dynamics problems, it is impractical to perform experiments on the physical world directly. Instead, complex, physics-based simulation codes are used to run experiments on computer hardware. Accurate, high-fidelity computational fluid dynamics (CFD) models are typically time consuming and computationally expensive, this poses a serious impediment to the successful application of formal sensitivity analysis in engineering design. While advances in High Performance Computing and multi-core architectures have helped, routine tasks such as visualisation, design space exploration, sensitivity analysis and optimisation quickly become impractical [1,2]. As a result, researchers have turned to various methods to mimic the behaviour of the simulation model as closely as possible, while being computationally cheaper to evaluate. This work concentrates on the use of data-driven, global approximations using compact surrogate models in the context of computer experiments. The objective is to construct a surrogate model that is as accurate as possible over the complete design space of interest using as few simulation points as possible. Once constructed, the global surrogate model is reused in other stages of the computational engineering pipeline, such as sensitivity analysis.

Sensitivity analysis of model output aims to quantify how a model depends on its input factors. Global sensitivity determines the effect on model output of all the input parameters acting simultaneously over their ranges. Most global sensitivity

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techniques are variance-based methods and determine the fractional contribution of each input factor to the variance of a model output. The main difficulty with global sensitivity analysis is that the number of model evaluations required is often large. As a result, CFD models are often impractical to use for design sensitivity analyses.

The objective of this paper is to discuss and demonstrate the application of several common surrogate modelling techniques to a case study of a CFD model of flocculant adsorption in an industrial thickener. A sensitivity analysis is then conducted on the produced surrogate models.

2. Surrogate modelling

2.1. Radial basis functions

Radial basis function (RBF) models use linear combinations of radially symmetric functions to interpolate samples data points. The simplest form of these models is

$$\tilde{y}(x) = \beta_0 + \sum_{i=1}^{N} \beta_i \|x - x_i\|, \tag{1}$$

where $\| \bullet \|$ is the Euclidean distance, N is the total number of sample points, x_i is the ith sample point, and the β's are model parameters found solving a linear system of N equations. RBF models are shown to produce a good fit for arbitrary contours [3].

2.2. Artificial neural networks

Artificial neural networks (ANN) are massively parallel highly interconnected simple processors (neurons). A typical ANN structure consists of an input layer into which the independent variables are fed, the output layer that produces the dependent variables and one or more hidden layers. The hidden layers link the input and output layers together and allow for complex, nonlinear mapping from the input to the output. The mapping is not specified but is learned. An artificial neural network can be described in terms of the individual neurons, the network connectivity, the weights associated with the interconnections between neurons, and the activation function of each neuron. A typical architecture, known as the multilayer feed-forward network, is shown in Fig. 1 and is used in the simulations in this work. In this figure the lines represent the unidirectional feed-forward communication links between the neurons. A weight associated with each of these connections controls the output passing through a connection. The output of a neuron for the feed-forward network shown in Fig. 1 may be represented as [4]:

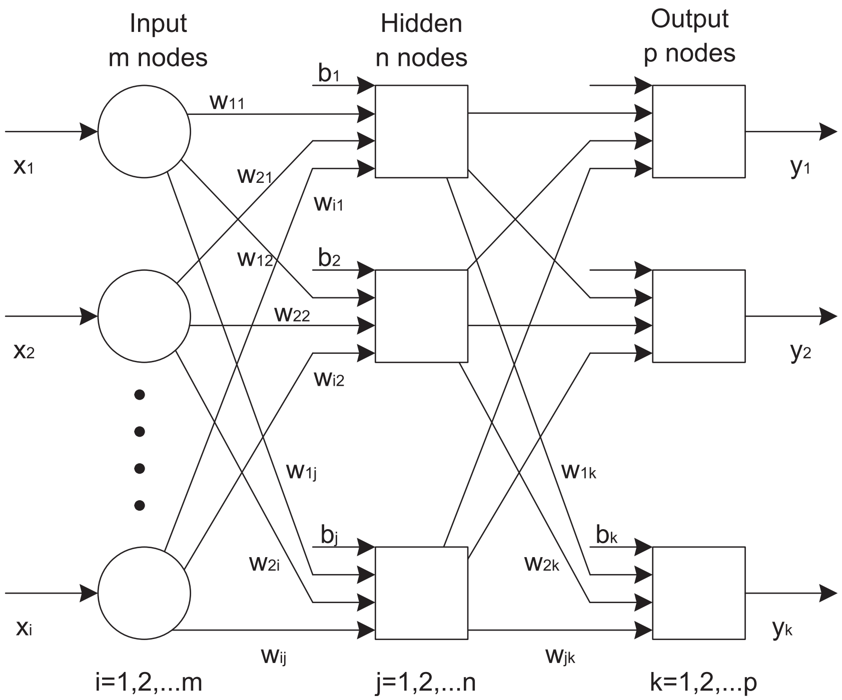

Fig. 1. Multilayer feed-forward artificial neural network (ANN).