MascotNum2017 conference - RBF-based multifidelity metamodeling for the optimization of a photoacoustic gas sensor

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Abstract:

Numerical simulation is widely employed in engineering to study the behavior of a device and optimize its design. Nevertheless, each computation is often time consuming and, during an optimization sequence, the simulation code is evaluated a large number of times. An interesting way to reduce the computational burden is to build a metamodel (or surrogate model) of the simulation code. Sometimes, models having different levels of complexity are available and can be hierarchically ranked in terms of accuracy. In this case, multifidelity surrogate modeling aims at efficiently combining information from the different levels of approximation in order to build a metamodel at a reduced cost.

Here the system studied is a photoacoustic (PA) gas sensor employed to detect gas traces with a high sensitivity. The principle of PA spectroscopy relies on the excitation of a molecule of interest by a light source emitting at the wavelength of an absorption line of the molecule. The light source, usually a laser in the mid-infrared range, is modulated at the acoustic frequency of a resonant cell, containing the gas mixture. During the molecules collisional relaxation, the kinetic energy exchange with the surrounding gas creates local temperature modulation, and thus acoustic waves in the chamber [3]. On the one hand, the linearized Navier-Stokes equations constitute the high fidelity model of this process. On the other hand, the coarse model consists in the decomposition of the pressure field onto the acoustic modes basis, obtained by solving the homogeneous Helmholtz equation. The cell resonance frequency and the maximum photoacoustic signal detected are the two outputs used in the design.

A study has been initiated to compare the prediction accuracy of two metamodel types, Kriging and RBF, on the two outputs of both the high fidelity and coarse model. The purpose was to select the best metamodel for our test case and use it in an optimization sequence. Results are given in Table 1, where the high fidelity and coarse model have been evaluated using a maximin optimized latin hypercube sampling (LHS) of respectively 20 points and 100 points. The prediction accuracy of metamodels are assessed using the root mean squared error with 10 test points chosen by LHS.

Output	Model	High fidelity model	Coarse model
Resonance frequency	RBF	41.7±18.7	5.6±2.1
	Kriging	242.7±62.3	35.2±14.7
Signal	RBF	0.08±0.09	$9 \times 10^{-4} \pm 8 \times 10^{-4}$
	Kriging	0.06±0.02	0.005±0.001

Table 1: Prediction error comparison on both output of the PA sensor models over 5 initial designs

The prediction error for the RBF is lower than that of the Kriging on 3 out of 4 cases. The approximation of the signal using the high fidelity dataset is the only case where Kriging is

superior in terms of accuracy. This result motivates the development of a RBF-based multidelity metamodel: the co-RBF. The formulation of the proposed method is based on the auto-regressive model of Kennedy and O'Hagan [2]. At present, co-kriging (the multifidelity version of kriging) is widely used when fast approximation of a complex code is available. The new method offers an alternative to co-kriging that might be interesting in high dimensional optimization problem, as stated by Regis and Shoemaker on single fidelity problems [4].

In a first stage, the performances of the proposed method are compared to co-kriging on analytic test cases. Different combinations between the number of expensive and coarse evaluations are analyzed. The accuracy of each metamodel is assessed by averaging on multiple samples. On a eight parameters function (borehole model), the co-RBF appears to have a lower prediction error than co-kriging. Concerning the PA sensor model outputs depending on three parameters, results are available in Table 2, with 100 points of the coarse model in the training dataset and between 5 to 20 points of the high fidelity model. Prediction error is lower with co-RBF for the resonance frequency. Co-kriging performed better on the approximation of the signal.

Output	Model	5 points	10 points	15 points	20 points
Resonance	co-RBF	16±5	18±6	17±5	12±3
frequency	co-kriging	33±27	86±2	20±18	28±18
Signal	co-RBF	0.08±0.04	0.08±0.05	0.05±0.02	0.08±0.06
	co-kriging	0.04±0.01	0.04±0.02	0.02±0.06	0.06±0.04

Table 2: Prediction error comparison on both output over 5 initial designs of expensive evaluations. Multi-fidelity metamodels results are obtained with 100 coarse evaluations.

Finally, an adaptive sampling method for co-RBF is proposed. It is based on the bumpiness criterion from Gutmann [1] and used to enrich the co-RBF training dataset towards the global optimum. The signal of the PA cell is then maximized with this method and the result is similar to the one obtained with the classical EGO algorithm based on co-kriging.

References

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Short biography – Cedric Durantin holds an engineering degree in advanced mechanics from the Institut Français de Mécanique Avancée (IFMA). He is currently a PhD student at CEA LETI in Grenoble on a subject entitled 'Metamodel and optimization of nanophotonics devices', which consists in developing and applying numerical methods to design and optimize photonic component.