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Optimal Design of Computer Experiments for the Generation of Microsystem Macromodels Using IMSET™ and Non-Parametric Fitting

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ABSTRACT

We present a new and unique software program, IMSET, capable of finding optimal designs for computer experiments. A finite-element simulation of a micro-machined flow sensor was used to illustrate macromodel generation and to compare the quality of the IMSET design with other approaches. Coupled with an appropriate analysis, IMSET provides a highly efficient means of non-parametric macromodel generation. IMSET is available on the World-Wide Web.

Keywords: MEMS, I-optimality, I-OPT, silicon flow sensor, design of experiments

INTRODUCTION

The design and optimization of microsystems can require large numbers of computationally intensive simulations, such as discretized approximations of partial differential equations (finite-element or boundary-element analyses) or systems of coupled ordinary differential equations. Often it would be convenient if a simpler, but still reasonably accurate, functional approximation could be found that could be evaluated orders of magnitude more rapidly than the systems of equations it is replacing. Such surrogate functions, which we call macromodels, could represent components of a MEMS system and could be used effectively in design synthesis to allow for the rapid trial evaluation and then selection of components in a system. Alternatively, such macromodels could be used for rapid optimization, since the functional evaluations that normally dominate such optimization would be computed very rapidly.

In earlier work, we demonstrated two *parametric* methods for designing experiments for macromodel generation in the context of MEMS, namely I-optimal, single-domain, response-surface methodology [**1**] and an algorithm for patch-wise functional approximation [**2**]. These methods required the specification of either a model function or a set of basis functions prior to the search for a suitable designed experiment. By contrast, in this paper we draw upon a fairly recent methodology from the field of statistics to demonstrate a *non-parametric* method [**3-6**] that does not require such specification. There are both advantages and disadvantages to the method presented here, and these will be discussed in the IMSET section, below.

This approach has been demonstrated previously [**7-9**] with considerable success. In an early chemical-kinetics example with two salient factors, Sacks et al. [**3**] compared the new approach with that of a traditional response-surface method (3x3 factorial design and least-squares fitting analysis was performed in [**10**]) and demonstrated a remarkable 8- to 10-fold reduction in the variance of prediction of the fitting function. The approach has also been applied to computationally intensive problems in marine science and semiconductor engineering.

Our work followed the Sacks et al. paper [**3**] closely, and we were able to duplicate much of their work on a demonstration MEMS example. However, there were also notable differences. The most important of these were that we were able to find superior designs to those published in their paper and that our design software is available to the public.

IMSET

Briefly, IMSET is a single program, compiled from both FORTRAN and C source code, that finds optimal designs minimizing the expected integrated mean-squared error of prediction (IMSE) of a macromodel, where the model function can contain an unknown part. For example, in two-factors the model function may be the following:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2 + Z(x_1, x_2), \quad (1)$$

where $Z(x_1, x_2)$, the departure from the second-degree model, is modeled as a stochastic process with covariance given by

$$\mathrm{cov}[Z(s_1, s_2), Z(t_1, t_2)] = \sigma_z^2 \exp\{-[\theta_1 (s_1-t_1)^2 + \theta_2 (s_2-t_2)^2]\} ,$$

with θ_1 , θ_2 , and σ_z^2 being parameters that must be set prior to the search for the optimal design. The setting of the θ's and σ_z^2 can be accomplished in one of the following three ways: (1) through a set of preliminary simulations and a fitting using maximum likelihood, (2) through a so-called "robustness study," or (3) in the course of sequential computer experimentation, again using maximum likelihood. Standard statistical methods are used to find the best linear unbiased predictor (BLUP) fit to the data.

One advantage of the method is that the error is not assumed to be random upon repetition of an experiment, as in more traditional approaches to design of experiments, including D-, G-, and I-optimality. Rather, the generally correct assumption is made that the differences between responses of replicated computer experiments are zero. This is consistent with the concept of deterministic computer experiments, although there are situations in which computer experiments give different results for the same inputs [**1**]. A second advantage of the method is that the form of the model function need not be specified prior to finding a design and initiating simulations. There is, however, the burden of establishing appropriate values for the θ's and σ_z^2.

Readers are referred to the literature for the mathematical background of the method [**3-6**].

EXAMPLE

To compare the quality of an IMSET design with other experimental-design approaches, a test case involving a micromachined flow sensor was chosen.

Description of the Flow Sensor

Flow sensors find applications in many fields, including industrial process control, automotive applications, security, and biomedical instrumentation [**11**]. There are many flow measurement principles, but most silicon flow sensors are based on thermal effects. Figure 1 is a photomicrograph of a thermal anemometer developed by Leister Process Technologies in Switzerland. A silicon nitride membrane (0.3 μm thick) is fabricated by anisotropic backside etching of silicon (0.5 mm thick). Three nickel-film thermoresistors are structured on the dielectric membrane and covered with a silicon nitride passivation layer (0.2 μm). The package includes a channel (3 mm deep and 0.8 mm high) so that gas flows perpendicularly to the thermoresistors.

The principle of a hot wire anemometer is based on correlating the heat transfer from a heated wire to a fluid with the rate of flow. The energy losses due to a moving fluid increase with fluid velocity. In the device described above, the center wire is the heating element and the outside wires are resistive temperature sensors. An electronic circuit establishes the average temperature of the upstream and downstream thermoresistors and maintains the heater at a constant temperature above this average. Such a sensor can detect flows from less than 0.10 ml/min up to 20 ml/min, the

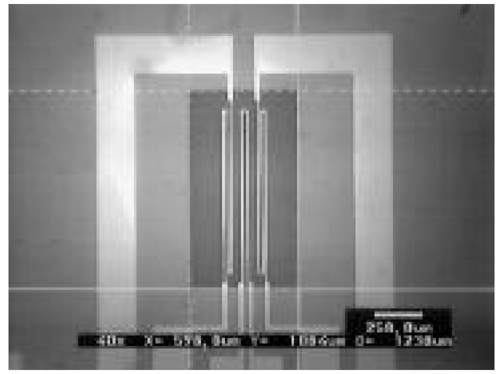


Figure 1: Photomicrograph of the gas flow sensor. The three serpentine thermoresistors are show on the (dark) membrane region.

time constant is less than 1 ms, and the power consumption of the sensor is 200 mW.

Modeling

A two-dimensional, finite-element model of the cross section perpendicular to the thermoresistors in the direction of flow was developed, and the ANSYS commercial finite-element package was used to simulate the thermal behavior of the sensor. The model contained the silicon-nitride membrane with its passivation layer, supported at both ends by the anisotropically etched silicon. The flow to be measured passes above the membrane, enters at ambient temperature, and is considered fully developed in a parabolic profile. The air that is trapped below the membrane and between the silicon walls is modeled as stationary. The outside edges of the bulk silicon are kept at ambient temperature. The nickel film thermoresistors are not included in the model, so the appropriate heating boundary conditions (either heat flux or constant temperature) are applied directly to the silicon nitride membrane. An example of a simulated temperature distribution (logarithmic scale), for a specific flow rate, membrane thickness, and a heater temperature of 50°C above ambient is shown in Fig. 2.

Optimal Experimental Designs and IMSET

For our example, we chose to build a macromodel in two factors, namely the membrane thickness and the thermoresistor sensor separation. The response chosen was the temperature difference between the upstream and downstream wires.

We used the search capability of IMSET to find the optimal two-factor design on the square $[-1,1]^2$, with θ_1, θ_2, and σ_z^2 taken as unity, following the robustness study of Sacks et al. [**3**]. The design is shown on the right-hand side of Fig. 3 below and differs somewhat from the design given in Sacks et al. [**3**] for the same problem. Specifically, we

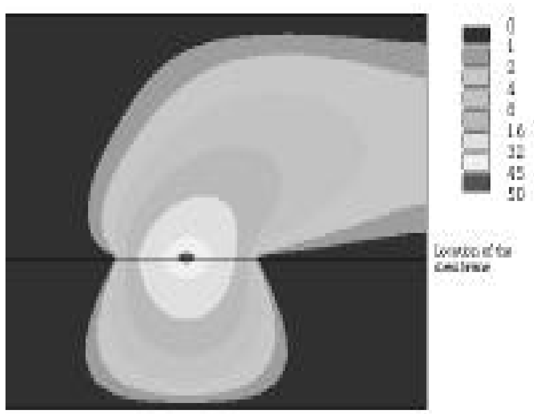
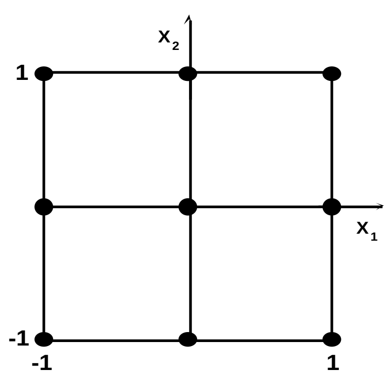


Figure 2: An example of the above-ambient temperature distribution, as determined by FEA. The heater is located at the middle of the membrane, and flow is present above the membrane.

obtained the putatively optimal design given in Table 1, with normalized integrated variance NIV=0.04650. We also used IMSET to evaluate the NIV of the design from the Sacks et al. paper [**3**], obtained by picking off points from their Fig. 1a. This gave NIV=0.04878 for the design given in Table 2.

Because of the discrepancy between our putatively optimal design and that of the earlier paper, we sought an independent check of the numerical correctness of IMSET. We wrote a complete IMSE-evaluation program in a commercial, symbolic-manipulation software system (Maple V, Release 5) that performed all the needed matrix operations and evaluated all the required moment integrals of gaussian functions, thus obviating the need for tables of integrals. The numerical evaluations of the IMSE's as computed by IMSET were confirmed.



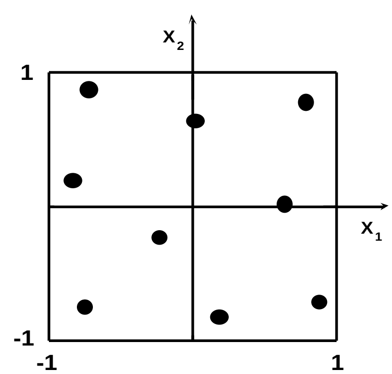


Table 1: IMSET-generated, nine-point, putatively optimal design for model (1) and 9 points, assuming $\theta_1=\theta_2=1$

x_1	x_2
-0.719	0.874
0.013	0.642
0.782	0.782
-0.830	0.189
0.642	0.013
-0.236	-0.236
-0.753	-0.753
0.189	-0.830
0.874	-0.719

As a further check on the correctness of IMSET, we made comparison with the design given by Sacks et al. [**3**] in their Fig. 1b for the identical problem specification, but with $\theta_1=\theta_2=100$ instead of unity. That design contains 9 points, all of which are nearly on a 3x3 grid. We found a very different design, using IMSET, as given in Table 3.

While this latter design has 8 points spread out approximately on a 3x3 grid, one point in the middle of one side is missing, and there is, instead, a second centrally located point (centrally located points are denoted by asterisks). While this design may seem unusual, this type of design has been seen in earlier work on I-optimal designs generated using both I-OPT [**12**] and Gosset [**13**]. The second centrally located point is understood as providing additional support in the central region, where the prediction

Figure 3: The 3^2 factorial design, which is also S-optimal and maximin,
is shown on the left, and the new design found with IMSET is shown on the right.
The thickness axis is horizontal and the distance-between-sensors axis is vertical.

Table 2: Nine-point design for model (1), assuming $\theta_1=\theta_2=1$, from Sacks et al. [**3**]

x_1	x_2
-0.74	0.90
0.00	0.66
0.80	0.80
-0.86	0.27
0.66	0.00
-0.34	-0.34
-0.78	-0.78
0.27	-0.86
0.90	-0.74

Table 3: IMSET-generated, nine-point, putatively optimal design for model (1), assuming $\theta_1=\theta_2=100$

x_1	x_2
1.000	0.984
1.000	-0.121
0.749	-1.000
0.018	0.924
-0.952	-0.043
-0.869	-1.000
-1.000	1.000
*-0.008	0.103
*-0.017	-0.165

would be weak without it. Specifically, the N=9 point putatively I-optimal design on the two-unit square for the model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2 \qquad (2)$$

is as given in Table 4, and this design has exactly one replicated point, which is in the central region.

We made the plausible conjecture that as θ grows significantly larger than unity the IMSET designs increasingly resemble I-optimal designs. Runs of IMSET for larger and larger values of θ provided anecdotal confirmation of this conjecture. Subsequently we proved that in the limit $\theta \to \infty$ the optimal IMSET design is I-optimal. The mathematical proof will be given elsewhere. (A proof that D-optimal designs for models of the type given in (1) are maximin in this limit was presented by Mitchell et al. [**14**].)

Table 4: I-OPT-generated, nine-point, putatively optimal design for model (2)

x_1	x_2
0.837	-1.000
-0.837	-1.000
-1.000	-0.044
1.000	-0.044
1.000	1.000
-1.000	1.000
0.000	1.000
*0.000	-0.045
*0.000	-0.045

World-Wide-Web Presence

IMSET was confirmed to be correct for several additional anecdotal cases in one and two factors using symbolic-manipulation software. This evidence, along with the demonstration of the correct asymptotics as $\theta \to \infty$ provide the basis for the University of Michigan authors to place and maintain a demonstration version of IMSET on the World-Wide Web by April 19, 1999, the starting day of this Conference. The planned URL is the following: http://www-personal.engin.umich.edu/~crary/iopt

Simulations

For this test example, the thickness of the membrane varied from 0.1 μm to 0.5 μm, and the distance of the thermoresistors from the heater varied from 60 μm to 140 μm. For each computer experiment, the flow medium was considered to be air with a constant flow rate of 2.88 ml/min, and the heater temperature was kept at a constant 50°C above ambient. The temperature difference between the centers of the upstream and downstream wires was computed.

Simulations were run at the nine optimal-design points found with IMSET, the nine points picked off Fig. 1a of the Sacks et al. paper [**3**], the 3^2 factorial-design points shown on the left-hand side of Fig. 3, as well as on a 11x11 regular grid covering the square, for validation. In all, we ran 139 distinct simulations. It is noted that the 3^2 factorial design is also the maximin (maximizes the minimum Cartesian distance between any pair of points) and S-optimal (maximizes the geometric mean of the Cartesian distances to near neighbors) designs.

Analyses

The data were fit using the best linear unbiased predictor (BLUP), as described in the Sacks et al. paper [**3**]. The fit function can be rapidly evaluated. It is as follows:

$$
\begin{aligned}
Y = {} & \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2 + \beta_5 x_1 x_2 + \\
& \gamma_1 \exp(-(x_1 - s^{(1)}{}_1)^2 - (x_2 - s^{(1)}{}_2)^2) + \\
& \gamma_2 \exp(-(x_1 - s^{(2)}{}_1)^2 - (x_2 - s^{(2)}{}_2)^2) + \\
& \gamma_3 \exp(-(x_1 - s^{(3)}{}_1)^2 - (x_2 - s^{(3)}{}_2)^2) + \\
& \gamma_4 \exp(-(x_1 - s^{(4)}{}_1)^2 - (x_2 - s^{(4)}{}_2)^2) + \\
& \gamma_5 \exp(-(x_1 - s^{(5)}{}_1)^2 - (x_2 - s^{(5)}{}_2)^2) + \\
& \gamma_6 \exp(-(x_1 - s^{(6)}{}_1)^2 - (x_2 - s^{(6)}{}_2)^2) + \\
& \gamma_7 \exp(-(x_1 - s^{(7)}{}_1)^2 - (x_2 - s^{(7)}{}_2)^2) + \\
& \gamma_8 \exp(-(x_1 - s^{(8)}{}_1)^2 - (x_2 - s^{(8)}{}_2)^2) + \\
& \gamma_9 \exp(-(x_1 - s^{(9)}{}_1)^2 - (x_2 - s^{(9)}{}_2)^2) , \qquad (3)
\end{aligned}
$$

where the β's and γ's are given in Table 5, and the $s^{(i)}{}_1$ and $s^{(i)}{}_2$ are the x_1 and x_2 coordinates of the i'th design point, respectively, as given in Table 1 (e.g., $s^{(1)}{}_1 = -0.719$ and $s^{(1)}{}_2 = 0.874$). Equation (3) can be rapidly evaluated in its present form or can be rearranged to be evaluated with fewer numerical operations.

Table 5: Coefficients of fitting equation (3)

Index	β	γ
1	0.2106770747	-0.009605485034
2	-0.09530174386	-0.004860289369
3	0.03642619705	0.006245066892
4	0.08068649057	0.02836365714
5	-0.01950666427	0.002709677889
6	-0.02939317575	-0.02528060233
7		-0.01439878125
8		0.03129878818
9		-0.01447203137

The BLUP passes through all of the data and provides an interpolation elsewhere.

The root mean squared error of the BLUP fits using the Sacks et al. design [**3**] and the IMSET-generated design were both 4 milliKelvin, and the variance of the fit to the IMSET-generated design was 1.35 x 10^{-5} $(mK)^2$. Using the 3^2 factorial design and fitting with ordinary least squares (OLS) fitting gave a variance 2.4 times larger (3.26 x 10^{-5} $(mK)^2$). Thus, we observed a factor of 2.4 reduction in variance of the fit using the IMSET design and BLUP fit, compared to the 3^2 factorial design and OLS fit. This improvement is similar in character to the factor of 8 to 10 reduction in prediction variance observed by Sacks et al. [**3**].

There was evidence of a synergistic coupling between design and fitting improvements. Using OLS fitting, the reduction in variance due to changing solely the design from the factorial design to the IMSET-generated design was 16%. For the factorial design, the reduction in variance due to changing solely the fitting method from OLS to BLUP was 21%. Together the reduction was 59%.

ACKNOWLEDGMENTS

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