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USING BAYESIAN MODELS IN PRELIMINARY DESIGN

Susan Finger, Jorge Pacheco and Cristina Amon

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1. Introduction

We are developing analytical methods that will enable designers to create models with different levels of detail and accuracy depending on the current state of the design. During preliminary design, many parameters are not known with great precision. Additionally, the design requirements are often vague and change frequently, so single point solutions are not the best approach. Instead, we propose to create models that allow for the incorporation of new information as the design progresses [Osio and Amon 1996]. A major advantage of these models is that they can be continuously refined. Thus, an approximate model developed for preliminary design can evolve throughout the design process. By the time the final design stage is reached, the model can be highly accurate in the reduced region of the design space close to the optima. We believe that having a methodology that allows designers to create models at any desired level of accuracy will improve the selection of initial ideas at the conceptual design stage, decrease design cycle time, and reduce costs in optimisation.

Our methodology creates surrogate models using a Bayesian framework. The surrogate is an analytical model of the expected response for a set of design parameters. This methodology does not require the assumption of any specific form of the response; instead, models are defined in terms of the correlation between sampling sites, assuming the response is a realization of a stochastic process. We do assume that the designer is able to evaluate the system response for a set of design parameters using analysis, computation models, or physical experiments.

1.1 Bayesian Framework

In the Bayesian framework, the initial knowledge of the response is represented by an *a priori* distribution. *A priori* information refers to information obtained before data collection begins. *A priori* information can come from first principles, application of physical laws to simplified systems, or empirical correlations obtained from experiments. The prior distribution is updated as data is collected at sampling points. This new data can come from numerical simulations, physical experiments, or other sources. The updated prior mean, called the posterior mean, forms the surrogate model. Bayesian analysis offers a mathematically rigorous framework in which information is updated based on the outcomes from previous stages.

Our approach of collecting data in stages was developed by Osio and Amon [1996]. This approach has several advantages because it allows for the integration of new information as the model is refined, reduces the optimisation burden, and allows changes in the design region as well as changes in the parameters as the model is updated.

1.2 Previous Work

Sacks *et al.* [1989] identified requirements for models of computer experiments. They proposed a statistical approach to create a response that interpolates the observations at the sampling points. These models are based on an approximation scheme called kriging [Cressie 1991]. This scheme is based on the existence of a covariance structure that models a response as the addition of a prior expected value plus a deviation term that updates this prior expectation. Yesilyurt *et al.* [1996] and Otto *et al.* [1995] developed Bayesian validated computer simulation surrogates, which use a first stage of sampling points to generate the surrogate and a second stage to generate uncertainty measures for the surrogate prediction. Osio and Amon [1996] started the development of the multistage Bayesian surrogate methodology (MBSM). Leoni [1999] developed the covariance-based framework to incorporate *a priori* information into the surrogates. This method of using physical bounds showed improvements on the accuracy of the models created with a given number of sampling points and stages. Other approaches, such as neural networks and response surface methodologies, can also be used to build surrogate models; however, neural networks generally require a large number of experiments to calibrate the response [Hertz *et al*. 1991]. In contrast, our methodology is designed for use in preliminary design, when the number of experiments must be small. Response surface methodologies require *a priori* assumption on the form of the response. Bayesian surrogates are based only on the correlation between sampling points; it requires no assumptions about the form of the response.

2. Surrogate Framework

The response variable of interest $y(\mathbf{x})$ in a multi-stage Bayesian surrogate model is expressed as a realization of a Gaussian stochastic process $Y(\mathbf{x})$ where $\mathbf{x}$ is a K-dimensional vector representing a design point in the K -fold space of control parameters.

$$Y(\mathrm{x}) = \mu_0 + Z(\mathbf{x}) \tag{1}$$

In Equation 1, μ_0 is a constant representing an initial guess of the response. $Z(\mathbf{x})$ is itself a stochastic process with mean zero and covariance matrix V that depends on the distance between two design points $\mathbf{x}_1$ and $\mathbf{x}_2$ and, as suggested in Sacks et *al.* [1989], it can be modelled as:

$$V(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 R(\mathbf{x}_1, \mathbf{x}_2) = \sigma^2 \prod_{j=1}^{K} \exp\{-\theta(\mathrm{x}_{1(j)} - \mathrm{x}_{2(j)})^2\} \tag{2}$$

The correlation matrix $R(\mathbf{x}_1, \mathbf{x}_2)$ is the product of one-dimensional correlations expressed through a correlation constant θ and the squared distance between the values of control parameters at any two design sites. This form of correlation matrix is computationally convenient and allows the response to be a smooth surface. The stochastic process $Z(\mathbf{x})$ can be regarded as a Bayesian prior distribution on the response function while μ_0 is the prior mean for $Y(\mathrm{x})$.

At each stage *p,* the response variable $y(\mathrm{x})$ is evaluated at m_p design sites. For the first stage, either maximin orthogonal array of strength one or two [Osio and Amon 1996; Morris and Mitchell 1995] or Latin Hypercubes [Park 1994] can be used. For the following stages, an estimate of the correlation parameter θ can be computed, together with posterior mean and covariance matrix of the process. New design points will be found that minimize either the trace or the determinant of the posterior covariance matrix. This last criterion has been shown to be equivalent to maximize the information to be gained from the next stage of the process.

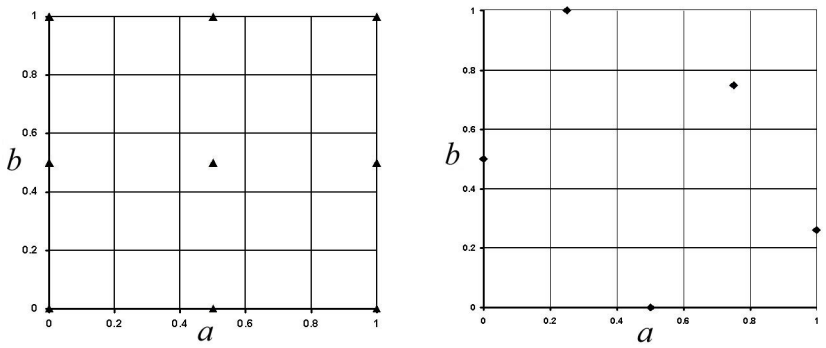


Figure 1. Sample Points a) standard factorial design, b) Latin hypercube

To illustrate the Bayesian methodology, we carry out a set of hypothetical experiments on a system with two variables. To simulate the results of each experiment, we have constructed an analytical function that returns the system response given the values of the two variables. The function used is $f(a,b)= 2.4 -0.8ab^2 + cos(1.22a) -0.5\ sin(5.5b + 2.2)$.

Using Bayesian methods, we show how the results of experiments can be used to construct a surrogate of the system response. We sample 5 different combinations of the two variables *a* and *b*. We use a Latin hypercube to select 5 experimental points that are distributed evenly through the sample space (Figure 1b). This design is more parsimonious than a standard factorial design (Figure 1a), that would have selected low, medium and high values for each variable and then performed experiments for each combination.

To construct the surrogate, we evaluate the function at the 5 sample points in Figure 2a**.** These values are used to compute the correlation parameter θ from Equation 2 using maximum likelihood estimation. The correlation matrix, *R*, between points can also be estimated and the first stage surrogate can be constructed as shown in Figure 2b**.** This approximates the response function evaluated at the design points of Figure 2a. The surface shows approximate values of outcomes for each combination of *a* and *b*.

First Stage Experimental Outcomes			
	a	***b***	***f***
1	0.00	0.50	2.85036
2	0.25	1.00	2.68591
3	0.55	0.00	2.69501
4	0.75	0.75	3.92131
5	1.00	0.25	2.93767

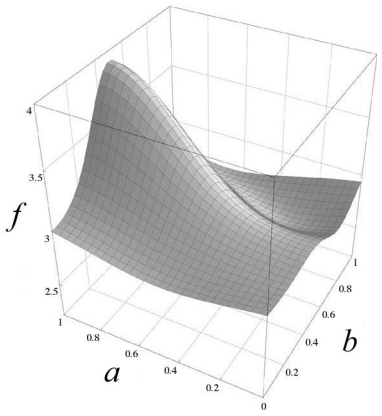


Figure 2. a) Experimental outcomes **b) First stage surrogate**

Based on the outcomes of the first set of experiments, we select a second set of sample points using an optimal sampling strategy that maximizes the amount of information obtained from the next set of experiments. The points sampled are given in Figure 3a**.** To simulate running the experiments, we again evaluate the function at each sample point. A new maximum likelihood estimate of the correlation parameter θ is found with maximum likelihood. Using the first stage surrogate as our prior estimate, we construct the second stage surrogate. From the ten sample points shown in the tables in Figures 2 and 3, we construct a surrogate function that approximates the analytical function (Figure 3a) used to simulate the experiments. The surrogate is shown in Figure 3b. The expected outcome for any combination of *a* and *b* can be found from this surrogate model.

From ten sample points, we have constructed a surrogate function that approximates the analytical function (shown in Figure 3c) that was used to simulate the experiments. For a discussion of the errors in the approximation, see [Osio 1996]. The surrogate is illustrated in Figure 3b**.** The expected outcome for any combination of *a* and *b* can be found from this surrogate model.

Second Stage Experimental Outcomes			
	a	***b***	***f***
6	0.99928	0.99961	1.48577
7	0.000203	0.13394	3.33363
8	0.000937	0.76794	3.36488
9	0.472746	0.34241	3.63317
10	.9983035	0.52097	3.03204

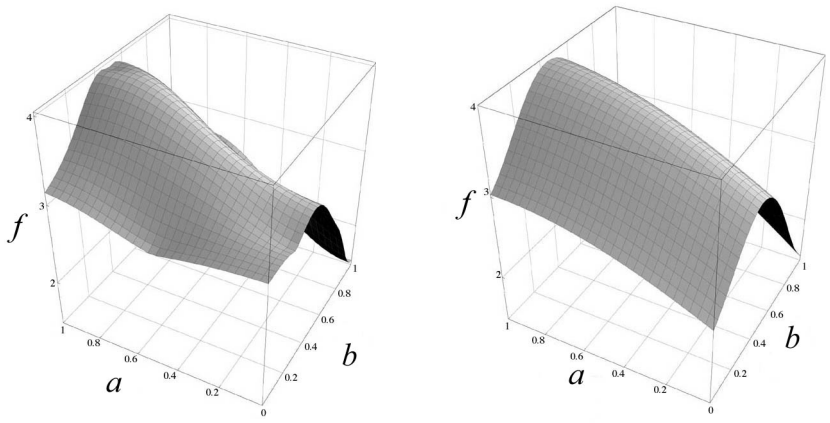


Figure 3. a) Experimental outcomes b) Second stage surrogate c) Analytic function

3. Design problem

A designer may know that a small change in a parameter may make large changes in the overall behaviour of the system, yet be at a stage in the design where it is not yet possible to specify those parameters. For example, we have studied the problem of cooling electronic components in wearable computers. We are experimenting with a cooling strategy that involves pumping dielectric fluids to decrease the temperature of electronic components by direct contact. In some applications, the pipes must run through internal structural supports within the wearable computers. Because the pipes that transport the dielectric fluid are small, the designer must consider the counter-intuitive phenomenon in which surrounding material may enhance rather than inhibit heat transfer. While it is possible to perform detailed numerical simulations for particular choices of design parameters or to run experiments to determine critical values, these tend to be expensive and time-consuming. In addition, during the preliminary stages, the designer often only needs to know which factors dominate in the region of interest and how these factors interact.

In the design of a wearable computer, a pipe, which contains a dielectric fluid, passes through a plastic structure that is used to increase the rigidity and provide mechanical support of the computer assembly. The design requirement is to maximize the heat transferred from the pipe, since the dielectric fluid is circulating in a closed-loop for cooling other components. The design variables include the length and height of the plastic support structure, shown in Figure 4.

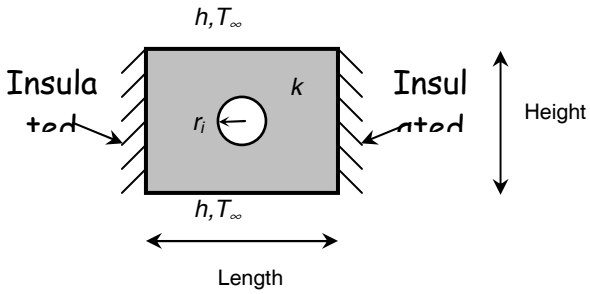


Figure 4. Thermal design problem for a support structure that maximizes heat transfer

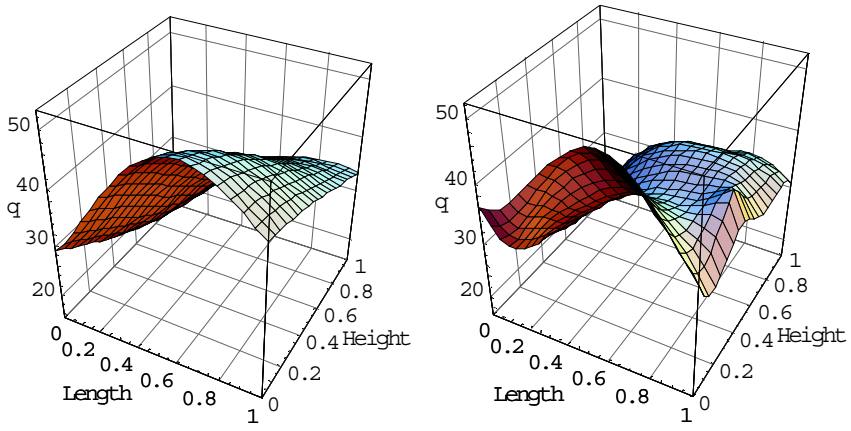
The radius of circular pipe, r_i, has been set at 0.005 m and the pipe must be in the centre of the support structure. Both the height and the width are in the range of 0.015 to 0.05 m. Two of the walls are modelled as thermally insulated due to contact with the computer structure, which has a much lower thermal conductivity. The remaining two walls are subject to a convective airflow, at temperature T_∞= 303.15 K and with a convective heat transfer coefficient h = 10 W/m^{2}K. The average temperature of the fluid entering the pipe is T_i = 423.15 K. This problem can be solved through numerical simulations of the governing energy equations using commercially available codes [Jaluria 1987]. To construct the surrogate model, five simulations using a spectral element code are run for the first stage and five more are added in a second stage. Table 1 presents the values of both parameters in each simulation.

Table 1. Design parameters for each numerical simulation

1st stage	Length (m)	Height (m)
1	0.048	0.030
2	0.02	0.022
3	0.03	0.015
4	0.015	0.04
5	0.04	0.05

2nd stage	Length (m)	Height (m)
1	0.032	0.02
2	0.024	0.015
3	0.015	0.03
4	0.04	0.04
5	0.05	0.05

The first and second stage surrogates, shown in Figure 5, is a function of non-dimensional length and height. While it would be possible for the designer to perform multiple numerical simulations to determine the optimum, during the preliminary design stage, when the design is in flux, this effort is not warranted. Moreover, even though the surrogate requires effort to construct, once it has been constructed, it can continue to evolve with the design.



a) First stage surrogate **b) Second stage surrogate**

Figure 5. Heat transfer, q, versus non-dimensional length and height of the plastic support

4. Conclusions

Using surrogate models enables designers to develop models of the interactions among design parameters even when they have little *a priori* knowledge about the response of the system. This multi-stage Bayesian approach results in surrogates that accurately model the system response. The ability to refine models and increase their accuracy in stages is valuable in the design process since it allows the models to evolve with the design. Thus, in the early design stages, approximate models that cover a large design space can be developed. As the design is refined, and new points in the design space are sampled, the scope of the model can be reduced and its accuracy increased without discarding the earlier information. We are currently implementing the framework with an interface that will make it easy for designers to step through constructing and using a surrogate.

Acknowledgments

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Susan Finger, Associate Professor
Civil and Environmental Engineering
Carnegie Mellon University
Pittsburgh, PA 15213, USA
Telephone: +1 412 268-8828; Telefax: +1 412 268-7813; e-mail: sfinger@cmu.edu