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Switching regression metamodels in stochastic simulation

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ABSTRACT

Simulation models are frequently analyzed through a linear regression model that relates the input/output data behavior. However, in several situations, it happens that different data subsets may resemble different models. The purpose of this paper is to present a procedure for constructing switching regression metamodels in stochastic simulation, and to exemplify the practical use of statistical techniques of switching regression in the analysis of simulation results. The metamodel estimation is made using a mixture weighted least squares and the maximum likelihood method. The consistency and the asymptotic normality of the maximum likelihood estimator are establish. The proposed methods are applied in the construction of a switching regression metamodel. This paper gives special emphasis on the usefulness of constructing switching metamodels in simulation analysis.

1. Introduction

Linear regression analysis plays an important role in many fields. A regression metamodel may be used for interpreting the input/output of a simulation model and, consequently, for analysing the real world data. A simulation metamodel, usually a simple mathematical function, is an approximation of the input/output function that is defined by the underlying simulation model (Kleijnen, 2008). Kleijnen (1975) proposed some statistical tools for making the regression metamodels commonly usable, and the most popular methods for constructing simulation metamodels are the polynomial regression ones; see also (Biles, 1974). The construction and use of metamodels continues today and comprises several types of metamodels like, for example, linear regression metamodels (Kleijnen, 1992), nonlinear regression metamodels (Santos & Nova, 2006; Santos & Santos, 2008), Kriging metamodels (Kleijnen, 2009) among others. A metamodel may be used with different purposes; for example, it may be used as a surrogate of a simulation model or as a building block inside a simulation model (Santos & Santos, 2009).

However, in simulation practice sometimes we may obtain a poor fit when a single regression metamodel is used. It happens when simulation model behavior isn't likely to follow one unique regime, and that different subsets of the input/output data may favor different submodels. A different approach may be using switching regression techniques for constructing metamodels in stochastic simulation. A switching regression model assumes that we have a random variable y such that $\mathrm{E}[y]$ is a linear function of explanatory variables with $y \sim \mathrm{N}(\mathbf{x}^T\boldsymbol{\theta}_s, \sigma_s^2)$ with probability λ_s, $s = 1, \ldots, S$. So, there are a set of S regression models characterized by the parameters $(\boldsymbol{\theta}_1, \sigma_1^2), \ldots, (\boldsymbol{\theta}_S, \sigma_S^2)$, and for each observation pair $(y_i, \mathbf{x}_i)$ the indicator λ_{si} chooses one among several models to obtain y_i; the unknown parameters $\boldsymbol{\theta}_1, \sigma_1^2, \ldots, \boldsymbol{\theta}_S, \sigma_S^2$ are estimated from the data.

Switching regression models are dated to at least (Quandt, 1958), and find applications in a wide variety of areas such as economics (Chen, 2007; McKenzie & Takaoka, 2008), finance (Fukuda, 2009), and marketing (DeSarbo & Cron, 1988). Goldfeld and Quandt (1973) introduced the Markov-switching models, in which a latent state variable (instead of a fixed probability) following a Markov-chain controls regime shifts, meanwhile (Quandt, 1972) studies a mixture of normal linear regression models where the choice between regimes is based on fixed probabilities. In the clusterwise linear regression context, Späth (1979) considers the regression problem where the error sums of squares is computed over all regimes (referred by clusters) is minimized using an exchange algorithm. Lau, Leung, and Tse (1999) propose a programming procedure to estimate clusterwise linear regression models based on combinatorial optimization problems; see also Carbonneau, Caporossi, and Hansen (2011). Quandt (1972) proposed the maximum likelihood method for estimating switching regressions, and Kiefer (1978) studied the problem of data covering two regression regimes and maximum likelihood methods for unknown parameters estimation. In the maximum likelihood context, DeSarbo and Cron (1988) generalize the Quandt (1972) and Hosmer (1974) stochastic switching regression models to more than two regimes. This article extend these developments to the construction of simulation switching regressions metamodels, where the unknown

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Table 1
Illustrative data.

x_i	y_{ij}		
1	8.705	8.105	5.200
2	8.760	9.160	3.700
3	9.715	9.115	3.100
4	9.670	10.170	1.500
5	10.725	10.425	1.000

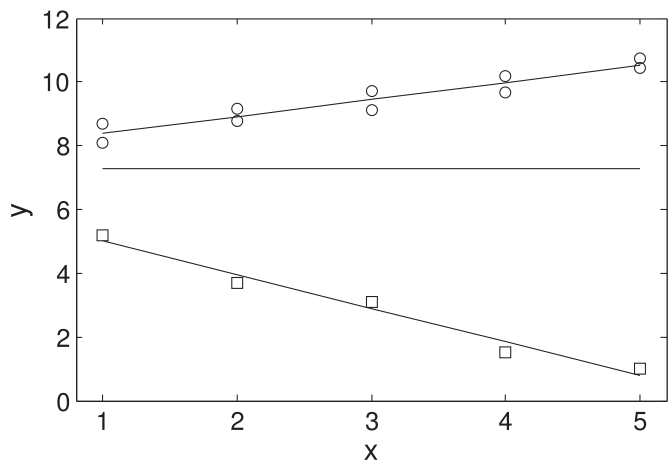

Fig. 1. Graphical representation of data from Table 1.

variances are estimated using the replications available from a simulation experiment and the switching probabilities may vary with the experimental points, and are also estimated from de data.

This paper is organized as follows. A framework of the metamodel with relation to simulation metamodels and switching regression models is described in Section 2. In Section 3 the estimation procedure for constructing switching regression metamodels is presented. Section 4 describes an application example related to a simple manufacturing process. The conclusions are presented in Section 5.

2. Simulation metamodels

A simulation model viewed as a black-box may be represented trough a mathematical function $\mathbf{g}(.,.)$ as

$$\mathbf{y} = \mathbf{g}(\mathbf{d}, \mathbf{r}_0)$$

where, $\mathbf{y}$ is a vector of simulation outputs, $\mathbf{d}$ is the vector of input factors of the simulation model and $\mathbf{r}_0$ is a vector of pseudo-random seeds. Typically, one metamodel is constructed for each component of $\mathbf{y}$, so we consider metamodels where $\mathbf{y}$ has one component

$$y = f(\mathbf{x}; \boldsymbol{\theta}) + \epsilon$$

where $\boldsymbol{\theta}$ is the unknown metamodel parameters, and $\mathbf{x}$ is a vector of metamodel inputs; for example, in the simulation of the M/M/1 system we may choose $x_1 = d_1/d_2 = \lambda/\mu$, where λ is the arrival rate and μ is the service rate. If f is a linear regression function, then a common set of regression parameters is enough for describing the input/output characteristics of the simulation program and, consequently, the simulation data may be described with only one regime. However, sometimes the input/output data exhibit some heterogeneity which produces the variation of the set of regression parameters over the data and, consequently, one regime may not be adequate for approximating the simulation input/output data. Switching regression metamodels (mixture of linear regressions) may help to overcome the lack-of-fit problem in these situations.

An illustrative example, where the usual regression leads to misleading results, is given in Table 1 and is depicted in Fig. 1. The adjusted metamodel based on all data points is

$$\hat{y} = 0\,x + 7.270$$

and we may observe that this line poorly approximates the data. If the observations are split into two subsets then the following metamodel, which allows a good fit, is obtained

$$\hat{y} = \begin{cases} -1.06\,x + 6.080, & \text{with probability} \quad \hat{\lambda}_1 = 2/3 \quad \text{(subset 1)} \\ 0.53\,x + 7.865, & \text{with probability} \quad \hat{\lambda}_2 = 1/3 \quad \text{(subset 2)} \end{cases}$$

3. Switching regression metamodels in stochastic simulation

Consider an experimental design consisting of n different design points, $\{x_{il} : i = 1, \ldots, n; l = 1, \ldots, p\}$, with p explanatory variables. For each design point i, r independent replications of the simulation model are carried out and the experiment yields $\Omega_{ij} = \{\tilde{z}_{ijk} : i = 1, \ldots, n, j = 1, \ldots, r, k = 1, \ldots, o\}$, where $\tilde{z}$ is the relevant system response, with o observations per replication. For each experimental point i and replicate j the observations $(\tilde{z}_{ij1}, \tilde{z}_{ij2}, \ldots \tilde{z}_{ijo})$ are split into S regimes sequentially ordered:

$$\begin{array}{ll}
\text{regime 1:} & \Omega_{1ij} = \{z_{i,j,1}, z_{i,j,2}, \ldots, z_{i,j,t_{1ij}}\} \\
\text{regime 2:} & \Omega_{2ij} = \{z_{i,j,t_{1ij}+1}, z_{i,j,t_{1ij}+2}, \ldots, z_{i,j,t_{1ij}+t_{2ij}}\} \\
\text{regime 3:} & \Omega_{3ij} = \{z_{i,j,t_{1ij}+t_{2ij}+1}, z_{i,j,t_{1ij}+t_{2ij}+2}, \ldots, z_{i,j,t_{1ij}+t_{2ij}+t_{3ij}}\} \\
\vdots & \vdots \\
\text{regime } S\text{:} & \Omega_{Sij} = \{z_{i,j,t_{1ij}+t_{2ij}+\cdots+t_{ijS-1}+1}, z_{i,j,t_{1ij}+t_{2ij}+\cdots+t_{ijS-1}+2}, \ldots, z_{i,j,t_{1ij}+t_{2ij}+\ldots+t_{Sij}}\}
\end{array}$$

where

$$\Omega_{ij} = \bigcup_{s=1}^{S} \Omega_{sij}$$

The probability associated with each set Ω_{sij} is estimated by

$$\hat{\lambda}_{si\cdot} = \frac{1}{r}\sum_{j=1}^{r} \hat{\lambda}_{sij} \quad \text{where} \quad \hat{\lambda}_{sij} = \frac{\#\Omega_{sij}}{\#\Omega_{ij}} = \frac{t_{sij}}{o} \qquad (1)$$

where $\#\Omega$ represents the number of elements belonging to the set Ω.

If $\hat{\lambda}_{si} \approx 1$ for some i and $s = 1, \ldots, S$, then we may assume one regime only at experimental point i. Since λ_s may depend on the experimental point, when predicting the response at $\mathbf{x}$ between $\mathbf{x}_i$ and $\mathbf{x}_{i+1}$ the corresponding probabilities may be computed using, for example, interpolation of first degree. For a single input:

$$\hat{\lambda}_s(x) = \hat{\lambda}_{si} + \frac{x - x_i}{x_{i+1} - x_i}(\hat{\lambda}_{s,i+1} - \hat{\lambda}_{s,i})$$

For each regime $s = 1, \ldots, S$, and replication j of each design point i a measure of interest y_{sij} is determined from $z_{i,j,k}$. For instance, the mean value for each regime is

$$y_{sij} = \frac{1}{t_{sij}} \sum_{k=k_{1ij}}^{k_{2ij}} z_{i,j,k}$$

where

$$k_{1ij} = 1 + \sum_{m=1}^{s-1} t_{mij} \quad \text{and} \quad k_{2ij} = \sum_{m=1}^{s} t_{mij}$$

For each experimental point i the mean and variance values of the measure of interest each regime can now be computed

$$\bar{y}_{si\cdot} = \frac{1}{r}\sum_{j=1}^{r} y_{sij}$$

$$\hat{\sigma}_{si}^2 = \frac{1}{r-1}\sum_{j=1}^{r} (y_{sij} - \bar{y}_{si\cdot})^2 \qquad (2)$$