European Journal of Operational Research xxx (2008) xxx–xxx

Contents lists available at ScienceDirect

European Journal of Operational Research

journal homepage: www.elsevier.com/locate/ejor

Stochastics and Statistics

Using subsystem linear regression metamodels in stochastic simulation

Pedro M. Reis dos Santos [a,*], M. Isabel Reis dos Santos [b]

[a] Department of Computer Science and Engineering, INESC-ID, Technical University of Lisbon (IST), Av. Rovisco Pais, 1, 1049-001 Lisbon, Portugal
[b] Department of Mathematics, Centre for Management Studies, Technical University of Lisbon (IST), Av. Rovisco Pais, 1, 1049-001 Lisbon, Portugal

ARTICLE INFO

Article history:
Received 19 January 2008
Accepted 7 May 2008
Available online xxxx

Keywords:
Simulation
Subsystem metamodels
Linear regression
Validation
Integrated simulation

ABSTRACT

This article explores the use of metamodels as simulation building blocks. The metamodel replaces a part of the simulation model with a mathematical function that mimics the input–output behavior of that part, with respect to some measure of interest to the designer. The integration of metamodels as components of the simulation model simplifies the model and reduces the simulation time. Such use of the metamodels also gives the designer a better understanding of the behavior of those parts of the model, making the simulation model as a whole more intelligible. The metamodel-based simulation model building process is examined, step by step, and the designer options are explored. This process includes the identification of the metamodel candidates and the construction of the metamodels themselves. The assessment of the proposed approach includes the evaluation of the integration effort of the metamodel into the metamodel-based simulation model, and the accuracy of the output data when compared to the original system.

A metamodel-based simulation model validation test, based on a simulation model validation test, is developed to ensure that the response conforms to the original simulation model. The proposed test comprises the cases when the simulation response variance varies with the experimental point and when it is constant. A message routing and processing example, with a fourth-degree polynomial regression metamodel, is used to illustrate the proposed procedure. An integrated simulation system is used to integrate the metamodel-based simulation model as well as the original simulation model.

1. Introduction

Simulation is a very commonly used technique of designing a model of a real or proposed system and conducting experiments with this model. Frequently, the purpose of the experiments is to estimate the effects on system performance due to changes to a set of controllable input variables. However, the simulation model may be quite complex and the use of metamodels is often an alternative. A simulation metamodel is a simple mathematical function intended to mimic the behavior of the large complex simulation model (Barton, 1998). Blanning (1975) proposed the use of metamodels to obtain useful sensitivity information with a significant reduction in the computation time. Kleijnen (1975) suggested some statistical tools to lead metamodels into common use in stochastic simulation. When a system is very complex, several separate simulation models are built. Each simulation model represents an aspect of performance. In this case, it may be possible to build a metamodel for each simulation model and the combination of the resulting metamodels yields a system-level simulation (Barton, 1997); see also Chambers and Mount-Campbell (2002). The most popular metamodels can be represented as a linear combination of basis functions from a parametric family. In particular, linear regression models have been intensively used because they are relatively simple to construct and use; see Kleijnen and Sargent (2000) and Cheng and Kleijnen (1999). However, in some situations we obtain a poor approximation when using linear regression metamodels, and we must look for a more precise and flexible models (Barton, 1992) like, for example, nonlinear regression metamodels (Santos and Porta Nova, 2006, 1999), Kriging metamodels (Kleijnen and van Beers, 2005) or neural nets (Badiru and Sieger, 1998).

A metamodel can be reused stand-alone as a surrogate for a complete simulation model or may be reused as a building block in a larger simulation model (Santos and Santos, 2007). Frequently, for complex simulation models, no simple metamodel exists. However, we could use metamodels for some, or all, of the components of the simulation model. Each component represents a different subsystem of the original system. The use of metamodels is particularly useful when the simulation models are impractically slow and/or large. The strategy proposed in this paper consists of estimating and validating linear regression metamodels for each subsystem and of integrating the metamodels with the simulation

* Corresponding author. Tel.: +351 214233297.
E-mail addresses: pedro.reis@tagus.ist.utl.pt (P.M. Reis dos Santos), maria.santos@tagus.ist.utl.pt (M. Isabel Reis dos Santos).
URLs: http://web.tagus.ist.utl.pt/~pedro.reis (P.M. Reis dos Santos), http://web.tagus.ist.utl.pt/~maria.santos (M. Isabel Reis dos Santos).

0377-2217/$ - see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.ejor.2008.05.005

model. Our focus will be on the commonly used linear regression metamodels as, in many situations, linear regression offers a good approximation. The integration consists of replacing the original subsystem simulation elements by the correspondent metamodels.

This paper is organized as follows: In Section 2 the formulation of models is presented, including the subsystem metamodel's construction and their validation. The design procedure for metamodel-based simulation model is explained in Section 3, including the validation of the resulting model with respect to the original simulation model. A motivating example explores, in Section 4, the use of metamodels as building blocks of metamodel-based simulation model. Section 5 is reserved for conclusions.

2. Problem formulation

Consider a simulation model that models a real system. Suppose that the response of the real system is modeled by the output variable of the simulation program. So the simulation model can be represented by

$$S = \phi(\mathbf{Z}, \mathbf{r}), \tag{1}$$

where S is the response, $\mathbf{Z} = (Z_1, \ldots, Z_k)^{\mathrm{T}}$ is a vector of input variables and $\mathbf{r}$ is a vector of random numbers or randomly selected seeds of the pseudo-random number generators. The simulation model can be seen as an aggregate of connected blocks with contractually specified interfaces and explicit context dependencies, or components (Oses et al., 2004). Assume that some components of the simulation model can be represented by metamodels. Such metamodels can be deployed independently and may be used for composition by third parties. That is, the original simulation model can be represented by the metamodel-based simulation model

$$R = \eta(\mathbf{Z}, \mathbf{r}) + \varepsilon, \tag{2}$$

with ε representing the inadequacy of η as representant of ϕ. The metamodel that models the component k of the original simulation model (that is, the kth metamodel) is given by

$$Y_k = f_k(\mathbf{X}_k; \boldsymbol{\theta}_k) + \epsilon_k, \quad k = 1, \ldots, h, \tag{3}$$

where $\mathbf{X}_k = (X_{k1}, \ldots, X_{ku})$ is a vector of u explanatory variables, $\boldsymbol{\theta}_k = (\theta_{k0}, \theta_{k1}, \ldots, \theta_{kq-1})^{\mathrm{T}}$ represents a vector of unknown parameters, ϵ_k represents the error, and f_k is a mathematical function. The variable X_{ki} may be a transformation of one or more Z_j or the response of some other metamodel (that is, $X_{ki} = Y_{k'}$ with $k' \neq k$), or originate from a part of the original simulation model that has not been substituted by a metamodel. For instance, the utilization factor $X_1 = \rho = \lambda/\mu$ may be a better explanatory variable than the arrival rate $Z_1 = \lambda$ and the service rate $Z_2 = \mu$ (Santos and Porta Nova, 2006). The example of Fig. 1 illustrates the relation between explanatory variables, subsystem metamodels and the output variable R (response).

The validity of the metamodel-based simulation model depends on the validity of the subsystem metamodels. In addition, the validity of each metamodel depends on the metamodel type, on the experimental design selected for estimating the unknown parameters of the metamodel, on the goal of the metamodel, etc.; see Kleijnen and Sargent (2000), Sargent (1991) and Santos and Porta Nova (2005). In the following subsections, we present the formulation of linear regression metamodels used for the construction of a metamodel-based simulation model, and the validity measures used to determine the validity of each fitted metamodel.

2.1. Linear regression metamodels

Consider a simulation experiment, for each component k of the simulation model, based on some experimental design fixed by the simulation analyst: $\{D_{il} : i = 1, \ldots, n; l = 1, \ldots, d\}$, where n is the number of experimental points and d is the number of factors. For simplicity's purpose we will omit the subscript k in the notation. Moreover, we assume that each experimental point i is replicated r_i times, that is, we simulate r_i times the same experimental point i using different pseudo-random numbers. The simulation experiment produces

$$\{Y_{ij} : i = 1, \ldots, n, j = 1, \ldots, r_i\},$$

that allow us to obtain

$$\hat{\sigma}_i = \left[\frac{1}{r_i - 1}\sum_{j=1}^{r_i}(Y_{ij} - \bar{Y}_{i.})^2\right]^{1/2}, \tag{4}$$

the estimated standard deviation of Y_{ij}, with $\bar{Y}_{i.} = \sum_{j=1}^{r_i} Y_{ij}/r_i$ and Y_{ij} denoting the response of interest observed in the replication j of the ith experimental point.

Denoting the additive error term correspondent to the jth replication of the experimental point i as ϵ_{ij}, we propose to express the metamodel (3) as the general linear regression model

$$Y_{ij} = \theta_0 + \sum_{l=1}^{q-1}\theta_l X_{il} + \epsilon_{ij}, \tag{5}$$

where $\epsilon_{ij} \sim N(0, \sigma_i^2)$, $\sigma_i > 0$, θ_0 is the overall response level, θ_l $(l = 1, \ldots, q-1)$ is the first order approximation effect of X_l, and X_i is identical to D_j, or may be a transformation of one or more D_j's.

When the purpose is to use metamodels with pth order approximation effects $(p \geqslant 2)$ or/and interactions, the linear regression model still applies. For example, consider the following regression model:

$$Y_{ij} = \theta_0 + \theta_1 X_{i1} + \theta_2 X_{i1}^2 + \theta_3 X_{i2} + \theta_4 X_{i2}^2 + \theta_5 X_{i1} X_{i2} + \epsilon_{ij}. \tag{6}$$

If we define $Z_{i1} = X_{i1}$, $Z_{i2} = X_{i1}^2$, $Z_{i3} = X_{i2}$, $Z_{i4} = X_{i2}^2$, and $Z_{i5} = X_{i1}X_{i2}$, we can then write the regression model (6) which is linear in the parameters $\boldsymbol{\theta}$.

The unknown parameters of the metamodel (5) may be estimated using the method of linear least squares. Kleijnen (1987),

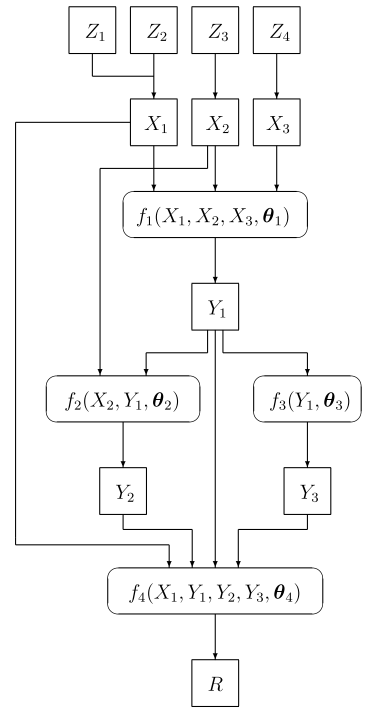

Fig. 1. Explanatory variables, subsystem metamodels and output variable.

Please cite this article in press as: Reis dos Santos, P.M., Isabel Reis dos Santos, M., Using subsystem linear regression metamodels in stochastic simulation, European Journal of Operational Research (2008), doi:10.1016/j.ejor.2008.05.005

p. 195, proves that fitting the regression model to the individual responses Y_{ij} is equivalent to fitting the model to the averages $\bar{Y}_{i.} = \sum_{j=1}^{r_i} Y_{ij}/r_i$ with weights r_i. Therefore, we simplify the estimation procedure: instead of problem (5), we consider the equivalent least squares problem in which the individual observations, at each design point, are replaced by their averages across simulation runs

$$\bar{Y}_{i.} = \theta_0 + \sum_{l=1}^{q-1} \theta_l X_{il} + \bar{\epsilon}_{i.}, \tag{7}$$

with $\bar{\epsilon}_{i.} \sim \mathrm{N}(0, \sigma_i^2/r_i)$.

In matrix terms, the general linear regression model (7) can be expressed by

$$\bar{\mathbf{Y}} = \mathbf{X}\boldsymbol{\theta} + \bar{\epsilon},$$

where $\bar{\mathbf{Y}} = (\bar{Y}_{1.}, \bar{Y}_{2.}, \ldots, \bar{Y}_{n.})^{\mathrm{T}}$, $\bar{\boldsymbol{\epsilon}} = (\bar{\epsilon}_{1.}, \bar{\epsilon}_{2.}, \ldots, \bar{\epsilon}_{n.})^{\mathrm{T}}$, $\boldsymbol{\theta} = (\theta_0, \theta_1, \ldots, \theta_{q-1})$ and $\mathbf{X}$ is $n \times q$ matrix where the row i, corresponds to the experimental point i and is given by the scalar 1 followed successively by the $X_{i1} \ldots X_{iq-1}$:

$$\mathbf{X} = \begin{bmatrix} 1 & X_{11} & X_{12} & \ldots & X_{1q-1} \\ 1 & X_{21} & X_{22} & \ldots & X_{2q-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & X_{n1} & X_{n2} & \ldots & X_{nq-1} \end{bmatrix}.$$

In the estimation of the parameter vector $\boldsymbol{\theta}$, we considered the weighted least squares method that yield the following estimator:

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}^{\mathrm{T}}\mathbf{V}_{\bar{Y}}^{-1}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{V}_{\bar{Y}}^{-1}\bar{\mathbf{Y}},$$

where $n \geqslant q = \mathrm{rank}(\mathbf{X})$, $\mathbf{V}_{\bar{Y}} = \mathrm{diag}(\sigma_1^2/r_1, \sigma_2^2/r_2, \ldots, \sigma_n^2/r_n)$ is a $n \times n$ diagonal matrix. If $\bar{\epsilon}_{i.} \sim N(0, \sigma^2/r_i)$, $\sigma > 0$, then $\hat{\boldsymbol{\theta}} = (\mathbf{X}^{\mathrm{T}}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{W}\bar{\mathbf{Y}}$, with $\mathbf{W} = \mathrm{diag}(r_1, r_2, \ldots, r_n)$.

In most applications the variances are unknown and $\mathbf{V}_{\bar{Y}}$ must be replaced by

$$\widehat{\mathbf{V}}_{\bar{Y}} = \mathrm{diag}(\hat{\sigma}_1^2/r_1, \ldots, \hat{\sigma}_1^2/r_2, \ldots, \hat{\sigma}_n^2/r_n),$$

in the weighted least squares estimation of $\boldsymbol{\theta}$ yielding the estimated weighted least squares estimator

$$\tilde{\boldsymbol{\theta}} = (\mathbf{X}^{\mathrm{T}}\widehat{\mathbf{V}}_{\bar{Y}}^{-1}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\widehat{\mathbf{V}}_{\bar{Y}}^{-1}\bar{\mathbf{Y}}.$$

This estimator is nonlinear because the transformation of $\bar{\mathbf{Y}}$ involves the random variables $\widehat{\mathbf{V}}_{\bar{Y}}$. Its covariance matrix is approximately

$$\mathrm{cov}[\tilde{\theta}] = (\mathbf{X}^{\mathrm{T}}\mathbf{V}_{\bar{Y}}^{-1}\mathbf{X})^{-1},$$

when $N = \sum_{i=1}^{n} r_i \to \infty$ (Kleijnen and van Groenendaal, 1992, p. 141).

2.2. Metamodel validation

In order to use the kth estimated metamodel as a surrogate of the component k of the simulation model, we must verify the metamodel adequacy and the validity with respect to that component. Since the responses are Gaussian, we use the lack of fit F test that compares two variance estimators, one based on residuals and the other based on replications (Kleijnen, 1987, p. 286):

$$F = \frac{N-n}{n-q} \frac{\sum_{i=1}^{n} r_i(\bar{Y}_i - \widehat{Y}_i)^2}{\sum_{i=1}^{n}\sum_{j=1}^{r_i}(Y_{ij} - \bar{Y}_{i.})^2},$$

with $N = \sum_{i=1}^{n} r_i$ and $\widehat{Y}_i$ is the fitted value for the i-th experimental point ($\widehat{Y}_i = \bar{Y}_{i.} = \widehat{Y}_{ij}, j = 1, \ldots, r_i$). The variance estimator based on replications does not depend on the regression model. The metamodel is rejected if $F > F(n-q, N-n; 1-\alpha)$. This test is based on the classical assumption where ϵ_{ij} are assumed to be i.i.d. $N(0, \sigma^2)$. Ideally the residuals are null and, in this case, the F test's value is null, and we do not reject the metamodel as a substitute for the component k of the original simulation model.

If the responses have different variances and ϵ_{ij} are i.i.d. $N(0, \sigma_i^2)$ then a rough test of the adequacy of the model can be made using the following F test:

$$F_w = \frac{N-n}{n-q} \frac{\sum_{i=1}^{n} r_i(\bar{Y}_{i.} - \widehat{Y}_i)^2/\hat{\sigma}_i^2}{\sum_{i=1}^{n}\sum_{j=1}^{r_i}(Y_{ij} - \bar{Y}_{i.})^2/\hat{\sigma}_i^2},$$

with $\hat{\sigma}_i$ given by (4). This is only an approximate test because the estimation of the variances σ_i^2 introduces another source of variability. However, this approximation is frequently quite good when N is not too small, since r_i must be large in order to ensure an acceptable weight estimation (Panis et al., 1994). If different design points use the same seed, then $\mathbf{V}_{\bar{Y}}$ is no longer diagonal. Although, we can estimate appropriately the elements of this symmetric matrix and, assuming a constant number of replications $r_i = r$, we may use the Rao's lack of fit test (Kleijnen and van Groenendaal, 1992, p. 158).

The validation with respect to the component k of the simulation model can be tested using double cross-validation (Friedman and Friedman, 1985). In double cross-validation, data is randomly divided in two equal size parts, or split-halves. A metamodel is constructed for each of the split-halves and if the regression coefficients are very different, especially with respect to sign, the metamodel lacks internal consistency or reliability. If the split-half metamodels are reliable, each one is used on the other half of the data for predicting the response variable. As a result, two R^2 values are determined for each split-half metamodel, one for the data used in the metamodel construction R^2_{bui} and the other for the holdout data R^2_{val}, the data used for the construction of the other metamodel. The metamodel is probably not valid if the homologous values from both split-half metamodels differ substantially.

3. Metamodel-based simulation model building

A metamodel-based integration procedure may simplify the optimization and/or investigation of the system performance. Also, in some situations, it may allow the analytical combination of several metamodels in order to build a system metamodel. For the construction of a metamodel-based simulation model we identified five major steps, depicted in Fig. 2, each of these steps will be subsequently analyzed in the next five sections.

3.1. Definition of the simulation purpose

The construction of a metamodel-based simulation model, as addressed in this paper, assumes the existence of a previously validated simulation model. In this context, the designer must determine the conditions under which the model will be used, or domain of applicability. Namely, the designer must determine if the inputs are deterministic or random, and a measurement scale must be selected. While input variables are directly observable, random parameters are subjected to statistical inference. These conditions, also defined in the metamodeling process proposed by Kleijnen and Sargent (2000), will influence the characteristics of the metamodels. The designer specifies the inputs of the model, such as the number of servers and their service rate, and the output of interest or goal, such as customer time in the system or average delay in queue. Some of these inputs are considered to be fixed for the purpose at hand. The other inputs are variable and can take values from a range of interest, or experimental region.

3.2. Identification of possible metamodels

The construction of a metamodel-based simulation model from a validated simulation model requires the identification of which

Please cite this article in press as: Reis dos Santos, P.M., Isabel Reis dos Santos, M., Using subsystem linear regression metamodels in stochastic simulation, European Journal of Operational Research (2008), doi:10.1016/j.ejor.2008.05.005

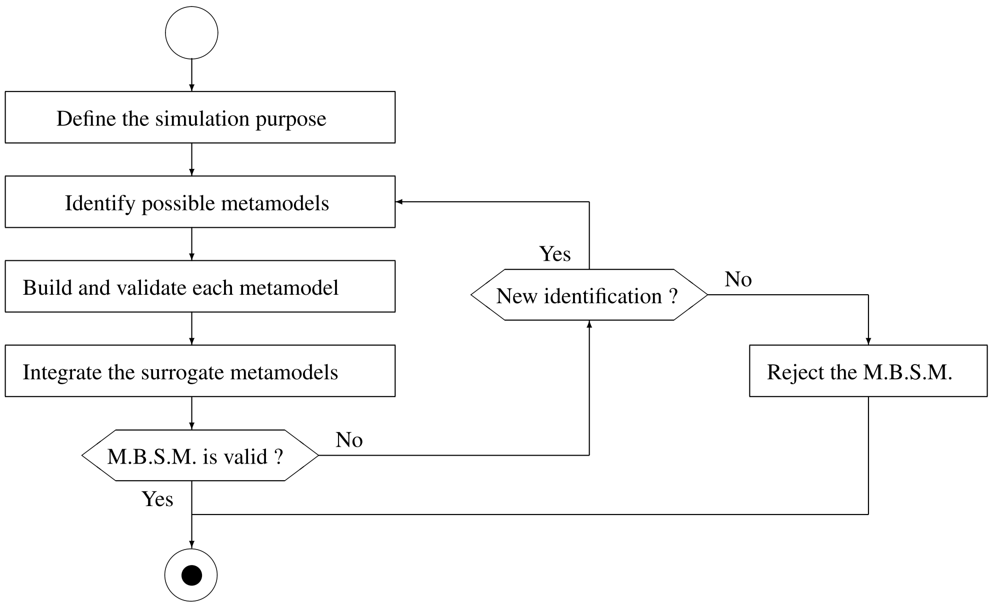

Fig. 2. Building a valid metamodel-based simulation model.

subsystems are candidates to be replaced by metamodels; see Fig. 3. Some systems exhibit parts with specific purposes and well defined interfaces that represent good candidates for metamodels. Examples range from front-end and back-end services to specific tasks within an organization, such as stock-management or distribution. As a general rule of thumb, parts of the system with low structural connectivity are, frequently, good candidates due to smaller interfaces and less constraints (Oses et al., 2004).

From a simulation point of view, when a model of a system is built up by connecting some existing models, each of the previous models can also be a metamodel candidate. The designer may also have specific reasons to evaluate the independent behavior of some part of the system and then use it as a metamodel candidate.

The identification of a metamodel candidate also requires the determination of its independent variables, and the respective experimental regions, as well as the dependent variable. These experimental regions depend on the experimental region previously defined for the original simulation model. This means that the metamodel independent variables are, in fact, dependent on the original simulation model's inputs. To assess the limits of the experimental region of each candidate metamodel, some executions of the simulation model must be performed, unless the designer has some insight into the situation at hand. Since, in most cases, these variables have a monotonic behavior, only the extreme values of the simulation model inputs need to be assessed. Such an approach requires a safety trigger, in the metamodel, to detect any possible violation of this premise; that is, if any of the metamodel independent variables take values outside the assumed experimental region.

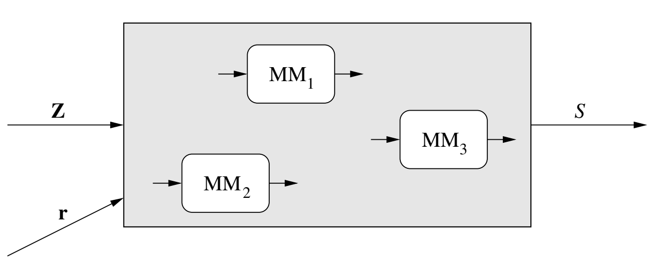

Fig. 3. Identification of metamodels within the simulation model.

3.3. Build and validate each metamodel

Each of the metamodel candidates must be individually built to fit the input–output characteristics of the subsystem it is intended to replace. Then it must be validated to ensure that it accurately mimics those characteristics; see Fig. 4.

First, the type of each metamodel must be selected depending on the input–output transfer function that the metamodel is intended to mimic. In our case, the goal of each metamodel is the *prediction* of the simulation output. That is, each metamodel is used repeatedly instead of the subsystem simulation code that originated it (Kleijnen and Sargent, 2000). The type of the metamodel must be carefully selected because the input–output relation to be approximated is usually complex and a very high accuracy is needed. If the metamodel is a polynomial function, then, in general, its degree is not low. Cheng and Kleijnen (1999) use, for example, polynomials of degree four and six. Although, in some cases, it is possible to use low order polynomials if good transformations of data are encountered; see also Cheng and Kleijnen (1999).

After determining a metamodel type, we must choose an experimental design. In this step, we determine the type of experimental design to be utilized and the set of design points for which simulation data must be collected, for constructing the kth metamodel. This initial design is used for estimating the hypothetical metamodel's unknown parameters and depends on the metamodel type that represents the subsystem k. If the metamodel is rejected by the validity test, he may improve or substitute the design in order to construct some other metamodel of either the same or other type. For example, he may start with a construction of a first order metamodel with two explanatory variables. If the resulting metamodel is rejected, then he may enlarge the design (that is, augments the matrix $\mathbf{X}$) in such a way that he can construct another metamodel with interaction effect of the explanatory variables. The analyst should select a design for the k metamodel estimation and, sometimes, the same design is used for $k-1$ metamodel estimation. Possible designs include 2^{h-p} designs, central composite designs, sequential bifurcation and Latin hypercube sampling; see Kleijnen et al. (2005) for details on the selection of appropriate designs in simulation.

Please cite this article in press as: Reis dos Santos, P.M., Isabel Reis dos Santos, M., Using subsystem linear regression metamodels in stochastic simulation, European Journal of Operational Research (2008), doi:10.1016/j.ejor.2008.05.005

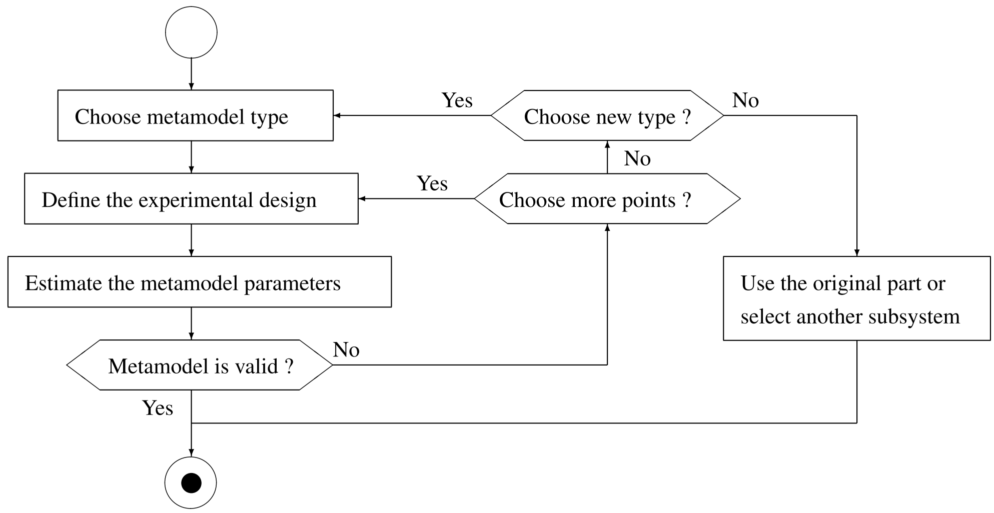

Fig. 4. Construction of a surrogate metamodel.

After estimating metamodel's unknown parameters, using linear least squares method, the metamodel must be validated within the domain of applicability (current experimental region of interest). The domain of applicability may be, for example, the rectangular region bounded by the maximum and minimum values of each factor. The metamodel is validated using the validation tests described in Section 2.2. In general, the experimental region does not cover the entire area in which the simulation model is valid. When it happens, then other metamodels, that permit global approximations, become significant. For example, Kleijnen and van Beers (2005) discover that a Kriging metamodel may yield a global approximation that is more accurate than a second-order polynomial. Also, Santos and Nova (2001) discuss a case where several linear regression polynomials do not permit an acceptable fit, whereas a nonlinear regression metamodel provide an adequate fit.

3.4. Integration of the surrogate metamodels

The integration process consists of incorporating the validated metamodel into the metamodel-based simulation model, resulting in a graphical representation of the simulation that resembles the sketch outlined in Fig. 3. Most simulation systems provide facilities to integrate user written code into the simulation model; see Kelton et al. (1998), Pritsker et al. (1997) and Hauge and Paige (2004). This code can be used to set up inputs, gather output data or even to access entities and schedule events. For instance, a queue is an already written piece of code that is distributed with the simulator and inserted into the simulation model with a textual or graphical editor. The metamodel as a simulation building block is another type of entity that can be parameterized and inserted into a simulation model, called metamodel-based simulation model to distinguish from the original model without the metamodels. The particular mechanics of the integration of the user code into the simulation model is dependent on the software under use. As far as the simulation tool under use provides facilities for user code inserts, the integration process is quite straightforward and simpler than we have anticipated.

For each metamodel previously identified and validated, a piece of code implementing the input–output transfer function, usually a simple mathematical expression, must be written. Then it is connected to the adjacent elements within the simulation model, in such a way that every entity arriving to the metamodel is supplied to the user written code. The user code must extract the required characteristics of the arriving entity in order to evaluate the mathematical function. Frequently, the code is even simpler, since it does not depend on the characteristics of the arriving entities, but on fixed or global values, such as the simulation clock. The evaluation of the mathematical function must then be fed into the simulation model by scheduling the departure instant of the entity. The departure instant is determined by adding the arriving instant with the evaluation of the metamodel for the design point under examination.

The resulting simulation model will enclose all the originally modeled nodes except the ones replaced by the black box approach that implements the metamodel. The resulting model will contain less nodes, or the same number of nodes in the extreme case when a single node is replaced by the metamodel, thus making the model simpler and the simulations run faster.

3.5. Validation of the metamodel-based simulation model

The resulting metamodel-based simulation model must finally be validated to ensure that it accurately substitutes the original simulation model. The validity of a metamodel-based simulation model depends on the validity of the original simulation model and the validity of the metamodel-based simulation model with respect to the original simulation model. In this paper, it is assumed that the original simulation model is valid, that is, 'the conceptual simulation model is an accurate representation of the system under study' (Law and Kelton, 2000). Also, it is assumed that the simulation program is correctly implemented, so it works as intended.

As a result, we are concerned whether, or not, the metamodel-based simulation model gives a good representation of the original simulation model. In order to validate the metamodel-based simulation model, we execute both the metamodel-based simulation model and the original simulation model at a new set of experimental points, and then compare the results; see Fig. 5. The results are compared using a statistical test specifically developed and presented below. It is desirable to use a set of experimental points, that do not overlap with the ones used for the construction of the metamodels, in order to make the test more reliable.

In the context of validation of simulation models, Kleijnen et al. (1998) consider a simulation model valid if the real system and the simulation model have identical means, identical variances, and positively correlated real and simulated responses; see also Kleijnen et al. (2000). In order to test this composite hypothesis, the

Please cite this article in press as: Reis dos Santos, P.M., Isabel Reis dos Santos, M., Using subsystem linear regression metamodels in stochastic simulation, European Journal of Operational Research (2008), doi:10.1016/j.ejor.2008.05.005

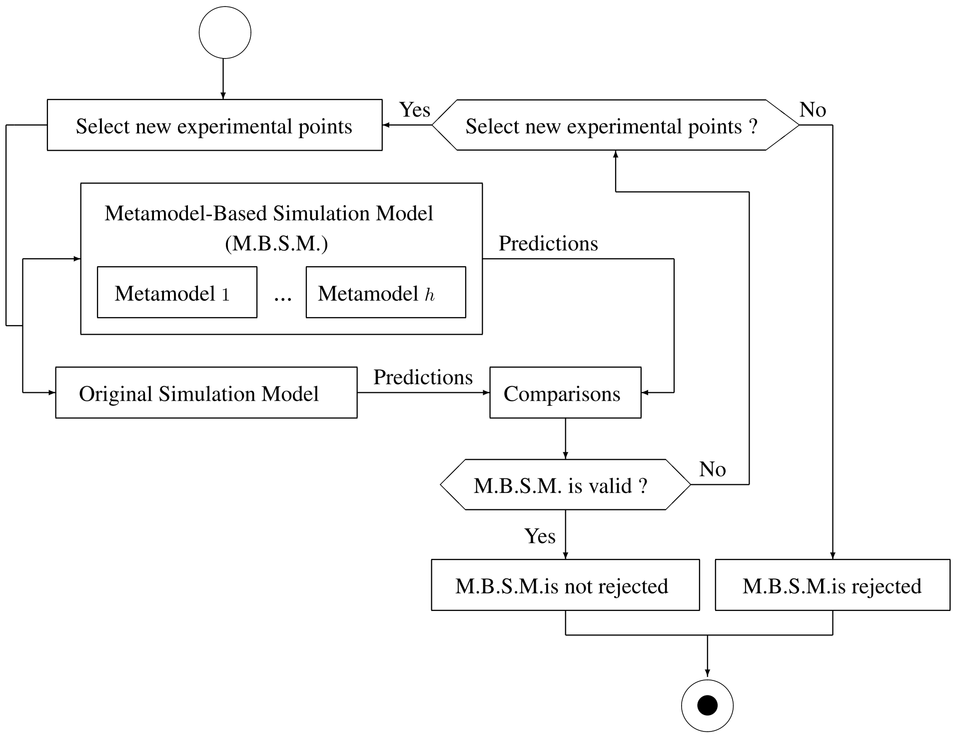

Fig. 5. Validating and comparing a metamodel-based simulation model.

authors use a test regressing differences of simulated and real responses on sums. In this paper, we use the same perspective when comparing the simulation model and the metamodel-based simulation model. However, we use independent replications on both models as a basis for the comparison, since in well-designed experiments it is convenient to replicate the factor combinations, and in simulation it is not difficult to do this (compared with the design of experiments in real problems). Also, these replications allow the estimation of the weights in the test statistic (12).

Let S_{ij} and R_{ij} denote the simulated output and the metamodel-based simulated output respectively in replicate j of the experimental point i, $i = 1,\dots,v$, $j = 1,\dots,m$. The set of experimental points used for the metamodel-based simulation model validation should be, preferably, different from the sets selected in the estimation of subsystem metamodels, although within the experimental region. The use of experimental points outside the metamodels tuning points weakens the comparison of the two systems, improving the rejection possibility.

We assume that the simulation model and the metamodel-based simulation model are run under the same conditions; this idea is similar to the use of common random numbers in the variance reduction techniques context (Law and Kelton, 2000, Section 11.2). As a result, S_{ij} and R_{ij} are dependent. Since the objective is to test the validity of the metamodel-based simulation model, we assume that S_{ij} and R_{ij} are positively correlated, that is, $0 < \rho_{sr} \leqslant 1$; in order that this assumption holds, it is sufficient that S and R are monotonically decreasing functions of their common random input data, while the remaining input data of S are independent of the remaining inputs of R Kleijnen et al. (1998).

We also assume that the pairs (S_{ij}, R_{ij}) are independent and identically distributed and have a bivariate normal distribution

$$\begin{bmatrix} S_{ij} \\ R_{ij} \end{bmatrix} \sim N_2\left(\begin{bmatrix} \mu_s \\ \mu_r \end{bmatrix}, \begin{bmatrix} \sigma_s^2 & \sigma_{sr} \\ \sigma_{rs} & \sigma_r^2 \end{bmatrix}\right).$$

Under these hypotheses, we consider that a metamodel-based simulation model is valid with respect to the simulation model if and only if the metamodel-based simulation model and the original simulation model have identical means, and identical variances

$$H_0 : \mu_s = \mu_r \wedge \sigma_s^2 = \sigma_r^2. \tag{8}$$

Based on the regression test proposed by Kleijnen et al. (1998) we regress $\bar{D}$ on $\bar{Q}$, where $\bar{D} = \bar{S} - \bar{R}$ and $\bar{Q} = \bar{S} + \bar{R}$, that is

$$E[\bar{D}|\bar{Q} = \bar{q}] = \beta_0 + \beta_1 \bar{q}.$$

Testing $\sigma_{\bar{s}}^2 = \sigma_{\bar{r}}^2$ is equivalent to testing whether $\bar{Q}$ and $\bar{D}$ are uncorrelated, that is, $\rho_{\bar{d}\bar{q}} = 0$ (Kleijnen, 1987, p. 99). Moreover, $\sigma_{\bar{s}}^2 = \sigma_{\bar{r}}^2 \iff \sigma_s^2 = \sigma_r^2$. As a result, S and R have equal variances if and only if $\bar{D}$ and $\bar{Q}$ are uncorrelated. If $\rho_{\bar{d}\bar{q}} = 0$, then $\beta_1 = 0$ $(\beta_1 = \rho_{\bar{d}\bar{q}}\sigma_{\bar{q}}/\sigma_{\bar{d}})$. If the means of S and R are equal, $\mu_s = \mu_r$, then $\mu_{\bar{d}} = \mu_{\bar{s}} - \mu_{\bar{r}} = \mu_s - \mu_r = 0$ $(\beta_0 = \mu_{\bar{d}} - \beta_1 \mu_{\bar{q}})$. Consequently, if S and R have common means and variances, then $\beta_0 = 0$. So, the hypothesis (8) results in

$$H_0 : \beta_0 = 0 \wedge \beta_1 = 0. \tag{9}$$

Applying a general linear test approach, described in Neter et al. (1996, Chapter 2), we follow the basic three steps:

(i) Fit the *full* or unrestricted model and obtain the error sum of squares. In this case, the full model is

$$\bar{D}_{i.} = \beta_0 + \beta_1 \bar{Q}_{i.} + \tau_i,$$

$i = 1,\dots,v$. If the errors τ_i have constant variances, we fit this model using the ordinary least squares method and we obtain the estimators $\hat{\beta}_0$ and $\hat{\beta}_1$. So, the error sum of squares can be calculated by

$$\mathrm{SSE}(F) = \sum_{i=1}^{v} (\bar{D}_{i.} - \widehat{D}_i)^2,$$

where $\widehat{D}_i = \hat{\beta}_0 + \hat{\beta}_1 \bar{Q}_{i.}$. If $\tau_i \sim \mathrm{N}(0, 1/w_i)$ (non constancy of error variance), then

$$\mathrm{SSE}_w(F) = \sum_{i=1}^{v} w_i (\bar{D}_{i.} - \widetilde{D}_i)^2, \tag{10}$$

with $\widetilde{D}_i = \tilde{\beta}_0 + \tilde{\beta}_1 \bar{Q}_{i.}$, where $\tilde{\beta}_0$ and $\tilde{\beta}_1$ are the weighted least squares estimators.

(ii) Fit the model under H_0, named *reduced* or restricted model, and obtain the error sum of squares SSE(R). In this case, if $\beta_0 = 0$ and $\beta_1 = 0$, then

$$\bar{D}_{i.} = \tau_i,$$

and the correspondent error sum of squares is given by

$$\mathrm{SSE}(R) = \sum_{i=1}^{v} \bar{D}_{i.}^2,$$

if the errors τ_i have constant variances. If $\tau_i \sim \mathrm{N}(0, 1/w_i)$, then

$$\mathrm{SSE}_w(R) = \sum_{i=1}^{v} w_i \bar{D}_{i.}^2. \tag{11}$$

(iii) If the errors τ_i have constant variances, use the following test statistic:

$$F^* = \frac{\mathrm{SSE}(R) - \mathrm{SSE}(F)}{v - (v-2)} \div \frac{\mathrm{SSE}(F)}{v-2},$$

that is

$$F^* = \frac{(\mathrm{SSE}(R) - \mathrm{SSE}(F))/2}{\mathrm{SSE}(F)/(v-2)},$$

and we reject H_0 if $F^* > F(2, v-2; 1-\alpha)$; F^* follows the F distribution when H_0 holds.

In the error variance is not constant over all cases, then use

$$F_w^* = \frac{(\mathrm{SSE}_w(R) - \mathrm{SSE}_w(F))/2}{\mathrm{SSE}_w(F)/(v-2)}. \tag{12}$$

The hypothesis H_0 is rejected if $F_w^* > F(2, v-2; 1-\alpha)$. In practice, the weights w_i's are unknown and they must be estimated. The estimates of the variances, $\hat{\sigma}_i^2 = 1/\hat{w}_i$, can be obtained using different methods (Neter et al., 1996, pp. 403–406). Since independent replications are available, we use the estimates $\hat{\sigma}_i^2 = \sum_{j=1}^{m} (D_{ij} - \bar{D}_{i.})^2 / [m(m-1)]$. A rough test for testing the hypothesis (9) can be made also using (12), with w_i replaced by $\hat{w}_i$. Since the weights are based on the estimated variances, the distribution of F_w^* under H_0 is only approximately an F distribution with 2 and $v-2$ degrees of freedom (Neter et al., 1996).

4. Motivating example

Consider a messages routing and processing system depicted in Fig. 6, where the messages arrive through a network of 3 limited capacity queues. Each message requires a fixed basic processing time followed by a sorting process that reprocesses some of the messages.

Our goal is to express the routing part of the system as a surrogate linear regression metamodel and then to compare the metamodel-based simulation model with the original simulation model. The analysis is performed in terms of the average time in the system (response S), in relation to the mean interarrival time (decision variable μ). The relevant mean interarrival time considered is in [1; 2] interval (experimental region).

4.1. Metamodel construction and validation

The surrogate metamodel is built in terms of the same response (average time in the system, Y), decision variable (mean interarrival time, $X = \mu$), and experimental region [1; 2]. We considered $n = 14$ design points $\{X_i : i = 1, 14\} = \{1.0, 1.05, 1.1, 1.15, 1.2, 1.25, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0\}$, with smaller steps where the output variation rate is higher. The number of replications is $r_i = r = 15 > 9$ in order to obtain an appropriate estimate for $\hat{\sigma}_i, i = 1, \ldots, n$ (Santos and Porta Nova, 2006) (see Fig. 7).

The warm-up period at each point was evaluated with the Welch's procedure and, due to small differences between the points, an equal 300 initial observations were removed from every simulation run; see Law and Kelton (2000). The total number of observations in each run is 2000, making the removed observation account for 15% of the total.

In the metamodel building process we used polynomial functions of the second to seventh degree. Since we have heterogeneous variances the weighted least squares method is used

$$H = \frac{\max_{i=1,n} \hat{\sigma}_i^2}{\min_{i=1,n} \hat{\sigma}_i^2} = 97.719 > H(14, 14; 0.95) \approx 6.71,$$

where $H(14, 14; 0.95)$ is the $(1-0.05)100$ percentile of the H statistic distribution, with $n = 14$ populations and $r - 1 = 14$ degrees of freedom associated with each sample variance (Neter et al., 1996, pp. 764–766); see also Conover et al. (1981). We used the Hartley test because this test is simple to carry out, the number of replications are equal, and the error terms are normally distributed; if the number of replications is unequal but do not differ greatly this test may still be used as an approximate test. When substantial departures from normality exit, the Hartley test should not be used because it is quite sensitive to departures from the assumption of normal populations. In this case, we may use the modified Levene test, since it has been shown to be robust to departures from normality and number of replications need not be equal (Neter et al., 1996, p. 766–768).

The estimated linear regression metamodels resulted in a rejection of the second, third and seventh degree polynomials

$$\begin{aligned} Y &= 34.7262 - 31.3308X + 8.38289X^2 Y \\ &= 103.519 - 164.74X + 92.7217X^2 - 17.4401X^3 Y \\ &= 403.98 - 1342.52X + 2250.22X^2 - 2445.86X^3 + 1774.96X^4 \\ &\quad - 810.053X^5 + 206.847X^6 - 22.3553X^7, \end{aligned}$$

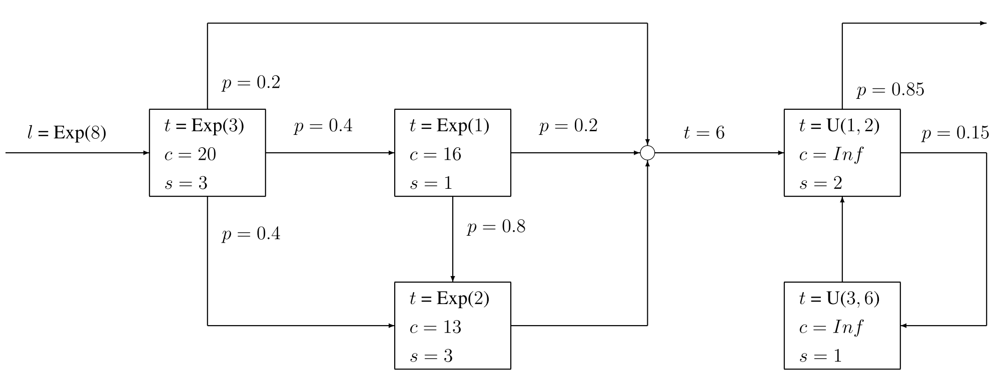

Fig. 6. Messaging routing and processing system: c = queue capacity, s = number of servers, t = processing time, l = time between arrivals, and p = path probability.

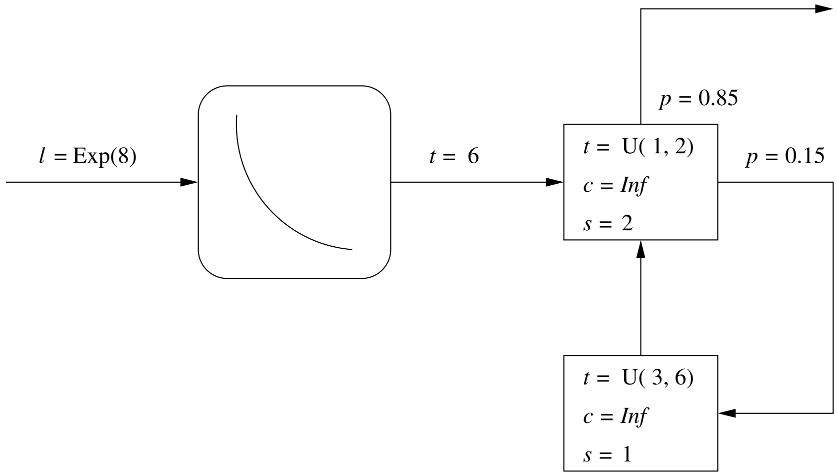

Fig. 7. Model with a surrogate metamodel.

and a non rejection of the fourth, fifth and sixth degree polynomials

$$
\begin{aligned}
Y &= 240.887 - 532.48X + 455.638X^2 - 174.099X^3 + 24.9857X^4 Y \\
&= 407.101 - 1096.6X + 1210.45X^2 - 672.188X^3 + 187.214X^4 \\
&\quad - 20.8807X^5 Y \\
&= 36.5894 + 430.197X - 1380.14X^2 + 1645.4X^3 - 966.255X^4 \\
&\quad + 282.079X^5 - 32.8224X^6,
\end{aligned}
$$

using the lack of fit F test as depicted in Table 1.

In order to gain additional knowledge into the predictive validity of the non rejected metamodels, we performed the double cross-validation test depicted in Table 2. The resulting values, correspondent to the polynomials of degrees 4 and 5, can be considered similar since the interval under consideration is small [1,2], and some variation can be accepted. The polynomial of degree 6 may lack reliability since the coefficients for the two regression models are very different, both in magnitude and in sign (Friedman and Friedman, 1985). Since the non-rejected polynomials of degree 4–6 are metamodel candidates we must select the best. The three sets of estimated parameters of each polynomial can be used to measure the discrepancy between the sets. A small discrepancy emphasizes a low sensitivity to the set of replications used for the parameter's estimation. This discrepancy can be evaluated using the mean relative difference

$$\frac{1}{s}\sum_{i=1}^{s}\frac{|\hat{\theta}_i^{(1)} - \hat{\theta}_i^{(2)}|}{|\hat{\theta}_i|},$$

where $\hat{\theta}_i^{(j)}$ is the ith estimated parameter based on the subset j, $\hat{\theta}_i$ is the ith estimated parameter based on all available data ($\hat{\theta}_i \neq 0$), and s is the number of estimated parameters. We selected the polynomial of degree 4 based on the values displayed in Table 3.

4.2. Integration and validation of the metamodel-based simulation model

In order to integrate the validated surrogate metamodel into the metamodel-based simulation model, each arriving entity is de-

Table 1
Lack of fit F test of the metamodels

Metamodel	F_w	Critical value
Pol2	15.905	$F(11, 196; 0.95) = 1.8378$
Pol3	2.739	$F(10, 196; 0.95) = 1.8793$
Pol4	0.62807	$F(9, 196; 0.95) = 1.9279$
Pol5	0.58880	$F(8, 196; 0.95) = 1.9859$
Pol6	0.65890	$F(7, 196; 0.95) = 2.0565$
Pol7[a]	731.631	$F(6, 196; 0.95) = 2.1451$

[a] We obtain matrices close to singular or badly scaled.

Table 3
Relative difference

Coefficient	Pol4	pol5	pol6
$\hat{\theta}_0$	0.19077	0.43538	103.0799
$\hat{\theta}_1$	0.21131	0.51618	35.7536
$\hat{\theta}_2$	0.21892	0.59244	18.7406
$\hat{\theta}_3$	0.21930	0.67279	13.9556
$\hat{\theta}_4$	0.21390	0.75977	11.7504
$\hat{\theta}_5$		0.85539	10.5121
$\hat{\theta}_6$			9.7386
Mean relative difference	0.21084	0.63866	29.076

Table 2
Double cross-validation test

Coefficient	Pol4		Pol5		Pol6	
	Subset 1	Subset 2	Subset 1	Subset 2	Subset 1	Subset 2
$\hat{\theta}_0$	214.626	260.581	410.701	587.945	−1410.2	2361.43
$\hat{\theta}_1$	−468.638	−581.157	−1131.75	−1697.79	6335.43	−9045.67
$\hat{\theta}_2$	399.38	499.129	1283.75	2000.87	−11328.4	14536.2
$\hat{\theta}_3$	−152.705	−190.885	−734.581	−1186.82	10501.0	−12461.6
$\hat{\theta}_4$	22.0149	27.3593	211.052	353.292	−5359.62	5994.3
$\hat{\theta}_5$			−24.2788	−42.14	433.94	−1531.3
$\hat{\theta}_6$					−157.523	162.122
R^2_{bui}	0.992536	0.996993	0.991832	0.997112	0.992785	0.997503
R^2_{val}	0.993415	0.992567	0.993748	0.991449	0.993312	0.990346

Please cite this article in press as: Reis dos Santos, P.M., Isabel Reis dos Santos, M., Using subsystem linear regression metamodels in stochastic simulation, European Journal of Operational Research (2008), doi:10.1016/j.ejor.2008.05.005

layed by the metamodel. The evaluation of the estimated fourth degree polynomial yields the value of the delay imposed on the entity. As stated above, the analysis of the metamodel-based simulation model uses the same response, decision variable and experimental region. The experimental points should differ from the ones used for the construction of the metamodel. We considered $v = 12$ design points $\{Z_i : i = 1, 12\} = \{1.06, 1.1, 1.14, 1.18, 1.22, 1.3, 1.38, 1.46, 1.52, 1.65, 1.78, 1.91\}$ and $m = 20$ replications were selected. However, since the output variation rate of the metamodel is higher in the first half of the interval, it induces high variations on the message processing part. Although the outputs are different, the variation rate is alike.

The validation of the metamodel-based simulation model requires its comparison with the original simulation model. The proposed method compares the simulated output S_{ij} with the metamodel-based simulated output R_{ij}, depicted in Fig. 8. As both responses (time in system) are monotonically decreasing functions of their common input (mean interarrival time), thus the responses S_{ij} and R_{ij} are positively correlated. Furthermore, the correlation is high ($\widehat{\mathrm{corr}} = 0.9983$). So, we regress their differences $\bar{D}_{i.} = \bar{S}_{i.} - \bar{R}_{i.}$ against their sums $\bar{Q}_{i.} = \bar{S}_{i.} + \bar{R}_{i.}$. Since the variances of the sums $\bar{D}_{i.}$ varies with the experimental point ($H = 65.28 > H(12, 19; 0.95) = 4.86$ Neter et al. (1996)) the estimated weighted least squares is used, resulting in the first degree polynomial

$$\bar{D} = -0.00671231 - 0.170106\bar{Q}.$$

To test the similarity of the means and variances of both outputs, we evaluated $\mathrm{SSE}_w(F)$, $\mathrm{SSE}_w(R)$ and F^*_w. This lead to the non rejection of the hypothesis H_0 in (9) since the critical value $F(2, 10; 0.95) > F^*_w$; see Table 4. We conclude that the response of the metamodel-based simulation model conforms to the original simulation model, providing a better perception of the system's behavior and requiring less computational effort.

All the simulations performed in this article used the AweSim 3.0 integrated simulation system (Pritsker et al., 1997) using the

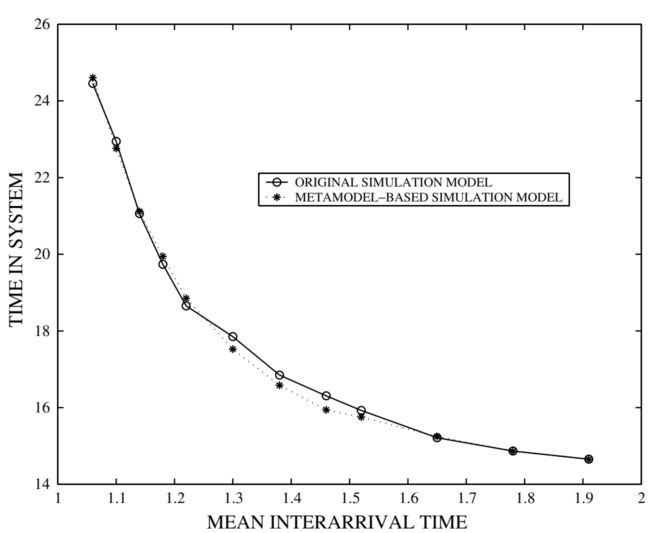

Fig. 8. System output with and without the metamodel surrogate.

Table 4
Metamodel-based simulation model validation

$\mathrm{SSE}_w(F)$	0.607365
$\mathrm{SSE}_w(R)$	0.693176
F^*_w	0.847705
$F(2, 10; 0.95)$	4.10

INTLC to control the simulation parameters for every run of each design point. The routines OTPUT and EVENT were used to gather output simulation data, and the implementation of the surrogate metamodel is easily performed by the routine:

```
#define X XX[1]
double USERF(int IFN, ENTITY *ent) {
double X2 = X*X, X3 = X2*X, X4=X3*X;
if (X < 1.0 || X > 2.0) MSTOP = -1;
return 240.887 -532.48 * X + 455.638 * X2
- 174.099 * X3 + 24.9857 * X4;
}
```

where the parameter XX[1] is the metamodel input variable by the INTLC routine. The regression and all statistical computations were performed in Matlab 6.5 using custom made and library routines. Simulations and computations were performed in a PENTIUM M 715 at 1.5 GHz with 1 Gb of RAM. The 20 replications, for each Z_i, took between 21.672*s* and 22.552*s* for the simulation model and between 12.794*s* and 14.387*s* for the metamodel-based simulation model, corresponding to a reduction in simulation time between 41.8% and 34.6%.

5. Conclusions

This article explores the use of metamodels as simulation building blocks. Such approach requires the identification of complex components of the system that are analyzed independently for later use as surrogate metamodels. The metamodels must be estimated and validated before they can be used as acceptable surrogates. As linear regression metamodels are some of the most widely diffused for metamodel building, we applied them in our study. Once the metamodel's parameters are estimated, the implementation of the metamodel consists of a piece of code that schedules the departure instant of every arriving entity. The resulting model, with the metamodel surrogates, is then compared with the original model to ensure that the simulation output, with respect to the input data, has the same behavior. The assessment of the proposed approach included the evaluation of the integration effort of the metamodel and the accuracy of the output data when compared to the original system.

The resulting metamodel-based simulation model can be used as a replacement of the simulation model, providing simpler and straightforward models, and faster simulations. It provides higher abstractions for a better understanding of the internal behavior of the system being analyzed, and can be used as an optimization tool of a specific observable output. Our approach allows the use of metamodels, not only as an analysis tool of the fundamental nature of the system input–output relationships, but as modeler custom made building block. This metamodel can, in fact, be used to mimic the real system's expected behavior, even if no model was identified. The use of metamodels as building blocks allows the use of higher abstractions (higher-resolution models) and reduces the simulation time. This creates a compromise between the designers of the original simulation model and the overall subsystem behavior, as both approaches intend to mimic the real system. High-resolution models are important, since if a high-level decision maker does not fully understand a model, then he avoids making decisions based on this model. This is specially true if they know that uncertainties abound. Frequently, high-level decision makers try to discover a robust correct reason or argument that they can easily understand and can be easily explained to others. Often, they also appreciate to have an analytic comprehension, such as a connection of crude simple mathematical formulas that gives information about the issues.

This paper introduces the concept of using metamodels as accurate simulation building blocks and a respective development methodology. To achieve statistical accuracy of the metamodel-based simulation model with respect to the simulation model, a test is proposed for equal and unequal variances using replication, based on a test that compares the real world with the simulation model. To select the best of the non-rejected metamodel candidates, we propose a mean relative difference method to quantify the lack of reliability.

Additional areas of interest include the use of wider experimental regions with more complex input–output functional relationships and the application to more elaborate subsystem compositions. This may require the use of rational or nonlinear metamodels instead of the presented linear approach.

References

Badiru, A.B., Sieger, D.B., 1998. Neural network as a simulation metamodel in economic analysis of risky projects. European Journal of Operational Research 105, 130–142.

Barton, R.R., 1992. Metamodels for simulation input–output relations. In: Swain, J.J., Goldsman, D., Crain, R.C., Wilson, J.R. (Eds.), Proceedings of the Winter Simulation Conference. IEEE, pp. 289–299.

Barton, R.R., 1997. Design of experiments for fitting subsystem metamodels. In: Andradóttir, S., Healy, K.J., Withers, D.H. (Eds.), Proceedings of the Winter Simulation Conference. IEEE, pp. 303–310.

Barton, R.R., 1998. Simulation metamodels. In: Medeiros, D.J., Watson, E.F., Carson, J.S., Manivannan, M.S. (Eds.), Proceedings of the Winter Simulation Conference. IEEE, pp. 167–174.

Blanning, R.W., 1975. The construction and implementation of metamodels. Simulation, 177–183.

Chambers, M., Mount-Campbell, C.A., 2002. Process optimization via neural network metamodeling. International Journal of Production Economics 79, 93–100.

Cheng, R.C.H., Kleijnen, J.P.C., 1999. Improved design of queueing simulation experiments with highly heteroscedastic responses. Operations Research 47 (5), 762–777.

Conover, W.J., Johnson, M.E., Johnson, M.M., 1981. A comparative study of tests for homogeneity of variances with applications to the outer continental shelf bidding data. Technometrics 23 (4), 351–361.

Friedman, L.W., Friedman, H.H., 1985. Validating the simulation metamodel: Some practical approaches. Simulation 45 (3), 144–146.

Hauge, Jaret W., Paige, Kerrie N., 2004. Learning SIMUL8: The Complete Guide, second ed. Plain Vu Publishers.

Kelton, W.D., Sadowski, R.P., Sadowski, D.A., 1998. Simulation with Arena. McGraw-Hill, New York.

Kleijnen, J.P.C., 1975. A comment on blanning's "metamodel for sensitivity analysis: The regression metamodel in simulation". Interfaces 5 (3), 21–23.

Kleijnen, J.P.C., 1987. Statistical Tools for Simulation Practitioners. Marcel Dekker, New York.

Kleijnen, J.P.C., Bettonvil, B., Groenendaal, W.V., 1998. Validation of trace-driven simulation models: A novel regression test. Management Science 44 (6), 812–819.

Kleijnen, J.P.C., Cheng, R.C.H., Bettonvil, B., 2000. Validation of trace-driven simulation models: More on bootstrap tests. In: Joines, J.A., Barton, R.R., Kang, K., Fishwick, P.A. (Eds.), Proceedings of the Winter Simulation Conference. IEEE, pp. 882–892.

Kleijnen, J.P.C., Sanchez, S.M., Lucas, T.W., Cioppa, T.M., 2005. A user's guide to the brave new world of designing simulation experiments. INFORMS Journal on Computing 17 (3), 263–289.

Kleijnen, J.P.C., Sargent, R.G., 2000. A methodology for fitting and validating metamodels in simulation. European Journal of Operational Research 120, 14–29.

Kleijnen, J.P.C., van Beers, W.C.M., 2005. Robustness of kriging when interpolating in random simulation with heterogenous variances: Some experiments. European Journal of Operational Research 165 (3), 826–834.

Kleijnen, J.P.C., van Groenendaal, W., 1992. Simulation, A Statistical Perspective. John Wiley and Sons, New York, NY, USA.

Law, A.M., Kelton, W.D., 2000. Simulation Modeling and Analysis, third ed. McGraw-Hill, New York, NY, USA.

Neter, J., Kutner, M.H., Nachtsheim, C.J., Wasserman, W., 1996. Applied Linear Statistical Models, fourth ed. Mc-Graw-Hill, New York, NY, USA.

Oses, N., Pidd, M., Brooks, R., 2004. Critical issues in the development of component-based discrete simulation. Simulation Modeling Practice and Theory 12, 495–514.

Panis, R., Myers, R., Houck, E., 1994. Combining regression diagnostics with simulation metamodels. European Journal of Operational Research 73 (1), 85–94.

Pritsker, A., O'Reilly, J., LaVal, D., 1997. Simulation with Visual SLAM and AweSim. John Wiley and Sons, New York, NY, USA.

Santos, M.I., Porta Nova, A.M., 1999. The main issues in nonlinear simulation metamodel estimation. In: Farrington, P.A., Nembhard, H.B., Sturrock, D.T., Evans, G.W. (Eds.), Proceedings of the Winter Simulation Conference. IEEE, pp. 502–509.

Santos, M.I., Porta Nova, A.M., 2001. Validation of nonlinear simulation metamodels. In: Hamza, M.H. (Ed.), Proceedings of Applied Simulation and Modeling Conference. IASTED, pp. 421–425.

Santos, M.I., Porta Nova, A.M., 2005. Estimation of nonlinear simulation metamodels using control variables. Journal of Statistical Computation and Simulation 75 (12), 959–973.

Santos, M.I., Porta Nova, A.M., 2006. Statistical fitting and validation of nonlinear simulation metamodels: A case study. European Journal of Operational Research 171 (1), 53–63.

Santos, M.I., Santos, P.M., 2007. Simulation metamodels for modeling output distribution parameters. In: Henderson, S.G., Biller, B., Hsieh, M.-H., Shortle, J., Tew, J.D., Barton, R.R. (Eds.), Proceedings of the Winter Simulation Conference. IEEE, pp. 910–918.

Sargent, R.G., 1991. Research issues in metamodeling. In: Nelson, B.L., Kelton, W.D., Clark, G.M. (Eds.), Proceedings of the Winter Simulation Conference. IEEE, pp. 888–893.

Please cite this article in press as: Reis dos Santos, P.M., Isabel Reis dos Santos, M., Using subsystem linear regression metamodels in stochastic simulation, European Journal of Operational Research (2008), doi:10.1016/j.ejor.2008.05.005