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Abstract

Optimization of simulated systems is tackled by many methods, but most methods assume known environments. This article, however, develops a 'robust' methodology for uncertain environments. This methodology uses Taguchi's view of the uncertain world, but replaces his statistical techniques by Response Surface Methodology (RSM). George Box originated RSM, and Douglas Montgomery recently extended RSM to robust optimization of real (non-simulated) systems. We combine Taguchi's view with RSM for simulated systems, and apply the resulting methodology to classic Economic Order Quantity (EOQ) inventory models. Our results demonstrate that in general robust optimization requires order quantities that differ from the classic EOQ.

Key words: Pareto frontier, bootstrap, Latin hypercube sampling

1 Introduction

The importance of *optimizing* engineered systems (artifacts) is emphasized in the 2006 NSF panel reported in Oden (2006). That report also points out the crucial role of *simulation* in engineering science. The simulation model may

be either deterministic or random (stochastic, discrete event). In this article, however, we focus on deterministic simulation. Nevertheless, we expect that our new methodology can also be applied to find the optimal inputs for random simulation models and real-world systems.

In practice, some inputs of the given simulation model are uncertain so the optimum solution that is derived—ignoring these uncertainties—may be completely wrong. In a different context—namely Linear Programming (LP)—Ben-Tal mentions that 13 of the approximately 100 LP models in the NETLIB Library give constraint violations (infeasibility) when perturbing the input data by only 0.01% (see also Ben-Tal and Nemirovski (2008)). Simulation models are more difficult compared with LP and Non-Linear Programming (NLP) models:

- Simulation models treated as black boxes imply *implicit* functions for the goal and constrained outputs.
- Simulation models are *dynamic* (whereas LP and NLP models are usually static).

A well-known distinction in the management literature (see the many references in Kleijnen (1980)) is

- Operational decisions: repetitive decisions (e.g., daily inventory management)
- Strategic decisions: one-shot decisions (e.g., designing a computerized inventory management system).

We focus on strategic decisions (for operational decisions, Control Theory seems more appropriate). These decisions may concern the design of either products or processes (for manufacturing these products). *Robust design* is important for engineers, in many disciplines. Actually, these engineers should work together, which results in *Multidisciplinary Design Optimization* (MDO); see Alexandrov and Hussaini (1997) and Beyer and Sendhoff (2007). Products of *Computer Aided Design* (CAD) and *Computer Aided Engineering* (CAE) are airplanes, automobiles, TV sets, chemical plants, computer chips, etc.—developed at companies such as Boeing, General Motors, and Philips. Recent surveys are Chen et al. (2003), Chen et al. (2006), Meckesheimer et al. (2001), Oden (2006), and Simpson et al. (2001).

Furthermore, we focus on decision variables that are continuous (like Myers and Montgomery (1995, p. 486) do for RSM); i.e., we do not consider integer (discrete) or qualitative decision variables (e.g. priority rules).

The literature (see Beyer and Sendhoff (2007) and Kleijnen (2008)) distinguishes the following two approaches to strategic decision-making in an uncertain world (Park et al. (2006) also detail the first approach, and discuss

more approaches):

- *Taguchi*'s approach, originally developed to help Toyota design 'robust' cars; i.e., cars that perform reasonably well in many circumstances (from the snows in Alaska to the sands in the Sahara). Taguchi is a Japanese engineer and statistician; see Taguchi (1987) and Wu and Hamada (2000).
- *Robust Optimization* (RO)—developed by Ben-Tal, Nemirovsky, Bertsimas and others—to make the original Mathematical Programming (MP) solutions less sensitive to perturbations in the coefficients of the MP models; see Ben-Tal and Nemirovski (2008) and also Beyer and Sendhoff (2007) and Greenberg and Morrison (2008). (Stochastic MP is a related yet different approach; see Mulvey, Vanderbei, and Zenios (1995) and also Beyer and Sendhoff (2007), Greenberg and Morrison (2008), and Sahinidis (2004).)

We do not use RO in the sense of Ben-Tal et al.; instead, we adapt Taguchi's approach and combine it with RSM. This RSM uses low-order polynomial regression metamodels (metamodels are also called response surfaces, surrogates, emulators, auxiliary models, repromodels, etc.). These metamodels run much faster than the—possibly computationally expensive—simulation models. RSM was introduced by Box and Wilson (1951) as an iterative heuristic for optimizing real (non-simulated) systems. RSM was further developed for robust optimization of such systems by Myers and Montgomery (1995). In this article, we further develop RSM for RO of simulated systems, including bootstrapping for a simple statistical analysis of the estimated Pareto frontier.

Note: In practice, classic (standard) optimization may be counterproductive! Indeed, the French say (in translation): 'the best is the enemy of the better'; and Marczyk (2000, p. 3) states: 'Optimization is actually just the opposite of robustness'.

The rest of this article is organized as follows. Section 2 summarizes Taguchi's worldview. Section 3 summarizes and extends Myers and Montgomery (1995)'s approach that uses RSM for robust optimization. Section 4 illustrates the new methodology through the classic EOQ simulation (which is closely related to the Economic Production Quantity or EPQ—see Darwish (2008)—and is a building block for more complicated and realistic supply chain simulations). Section 5 presents our conclusions and possible topics for future research. Appendices gives technical details. An extensive list of references enables the reader to study robust simulation-optimization in more detail. Hasty readers may skip appendices and paragraphs that start with 'Note:' (an example is the immediately preceding paragraph).

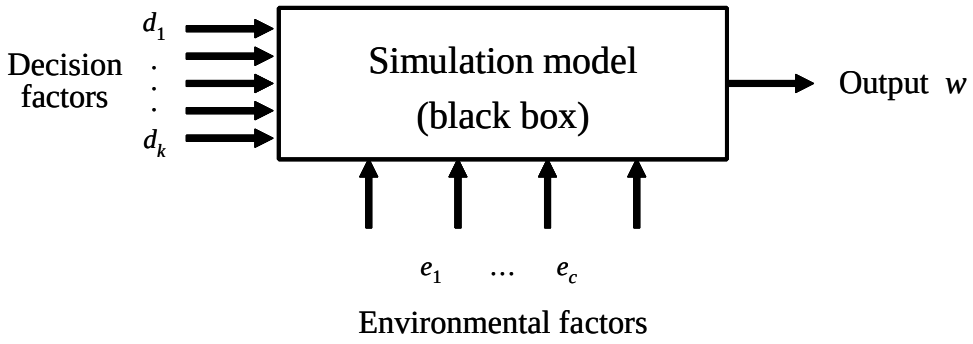

Fig. 1. Taguchi's view

2 Taguchi's worldview

Based on Kleijnen (2008, pp. 130-137), we summarize *Taguchi*'s view (but not his techniques, which include experimental designs such as 'orthogonal arrays') as follows. As Figure 1 illustrates, Taguchi distinguishes between two types of variables:

- Decision (or control) factors, which we denote by d_j $(j = 1, \ldots, k)$.
- Environmental (or noise) factors, which we denote by e_g $(g = 1, \ldots, c)$.

Taguchi assumes a single output, which we denote by w. Taguchians focus on the mean and the variance of this output (see below).

The first type of factors are under the control of the users; e.g., in inventory management, the Order Quantity (OQ) may be controllable. The second type of factors are not controlled by the users; an example is the demand rate in inventory management. In practice, the controllability of a factor depends on the specific situation; e.g., the users may change the demand rate through an advertising campaign.

Note: Other authors distinguish between environmental uncertainty (e.g., demand uncertainty) and system uncertainty (e.g., yield uncertainty); see Mula et al. (2006) and also Beyer and Sendhoff (2007). Implementation errors may also be a source of uncertainty. These errors occur whenever recommended (optimal) values of control factors are to be realized in practice; see Stinstra and Den Hertog (2007). Continuous values are hard to realize in practice, because only limited accuracy is then possible; e.g., the EOQ turns out to be the square root of some expression, but in practice only a discrete number of units can be ordered. Besides implementation errors, there are validation errors of the simulation model (compared with the real system) and the metamodel (compared with the simulation model); see Kleijnen and Sargent (2000).

As we mentioned above, we do not use Taguchi's statistical methods. Our main reason is that simulation experiments enable the exploration of many more factors, factor levels, and combinations of factor levels than real-life (physical) experiments do. Moreover, we do not use Taguchi's scalar output (such as the signal-to-noise or mean-to-variance ratio); instead we allow each output to have a statistical distribution (or density function), which we characterize through its mean and standard deviation; also see Beyer and Sendhoff (2007), Lee and Nelder (2003), and Myers and Montgomery (1995, p. 491). So we feel that a *Taguchian loss function* (see, e.g., Park et al. (2006)) is too restrictive. We solve the resulting bi-objective problem through the Pareto-optimal efficiency frontier—briefly called the *Pareto frontier*.

Note: The relevant problem formulation depends on the risk attitude of the users (they might be risk-seeking optimists), which may vary with the application. We conjecture that our heuristic also applies to alternative problem formulations, but in this article we do not investigate these alternatives. Many references on supply-chain risk-management are given in Wu et al. (2008), who focus on the mean-variance trade-off in the newsvendor's inventory problem. The mean-variance trade-off for simulation models is also examined by Apley, Liu, and Chen (2006) and Chen, Jin, and Sudjianto (2006).

3 RSM and robust optimization

To design and analyze our simulation experiments; we use RSM following Myers and Montgomery (1995). RSM extends Taguchi's simpler statistical techniques. The simplest RSM metamodel is a polynomial of a degree as low as possible:

- Because we wish to estimate the optimal combination(s) of the decision factors d_j ($j = 1, \ldots, k$), we fit a *second-order* polynomial for these factors.
- Moreover, we wish to model possible effects of the environmental factors e_g ($g = 1, \ldots, c$); we fit a first-order polynomial for these factors.
- Finally, we wish to estimate interactions between the two types of factors, so we fit *'control-by-noise' two-factor interactions*. (Interaction between d_j and e_g implies nonparallel response surfaces for d_j—given different values for e_g.)

Altogether we fit the following metamodel proposed by Myers and Montgomery (1995, p. 218, 492):

$$\begin{aligned} y &= \beta_0 + \sum_{j=1}^{k} \beta_j d_j + \sum_{j=1}^{k} \sum_{j' \geq j}^{k} \beta_{j;j'} d_j d_{j'} + \sum_{g=1}^{c} \gamma_j e_j + \sum_{j=1}^{k} \sum_{g=1}^{c} \delta_{j;g} d_j e_g + \epsilon \\ &= \beta_0 + \boldsymbol{\beta}'\mathbf{d} + \mathbf{d}'\mathbf{B}\mathbf{d} + \boldsymbol{\gamma}'\mathbf{e} + \mathbf{d}'\boldsymbol{\Delta}\mathbf{e} + \epsilon, \end{aligned} \tag{1}$$

where y denotes the regression predictor of the simulation output w, ϵ denotes the residual with $E(\epsilon) = 0$ if this metamodel has no *lack of fit* (this zero mean should be tested; see cross-validation below) and constant variance σ_ϵ^2 (an unrealistic assumption in simulation experimentation), and the bold symbols are the vectors and matrices that are defined in the obvious way (e.g., $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_k)'$ and $\mathbf{B}$ denotes the $k \times k$ symmetric matrix with main-diagonal elements $\beta_{j;j}$ and off-diagonal elements $\beta_{j;j'}/2$).

It is convenient and traditional in Design Of Experiments (DOE) to use *coded*—also called *standardized* or *scaled*—factor values. Let the experiment consist of n factor combinations of the 'original' factors z_j (z_j corresponds with d_j or e_g in (1)); furthermore, let l_j denote the lowest value of z_j in the experiment, and u_j the highest ('upper') value. Then the coded variable x_j use the linear transformation

$$x_j = a_j + b_j z_j \text{ with } a_j = \frac{l_j + u_j}{l_j - u_j} \text{ and } b_j = \frac{2}{u_j - l_j}. \tag{2}$$

The term $(u_j - l_j)$ is the *range* of input j. If z is a random variable (like e), then this coding implies $var(x) = b^2 var(e)$. The numerical accuracy of the estimates may be affected by coding; we focus on the estimated effects of the coded variables. Coding is further discussed by Kleijnen (2008, p. 29).

Assuming a model like (1), Myers and Montgomery (1995, p. 493-494) derive the mean and the variance of y (the regression predictor of the simulation output w), after averaging over the noise factors—and assuming that the environmental variables $\mathbf{e}$ satisfy

$$E(\mathbf{e}) = \mathbf{0} \text{ and } \mathbf{cov}(\mathbf{e}) = \sigma_e^2 \mathbf{I}. \tag{3}$$

Obviously, assuming zero means and constant variances is unrealistic, so we shall replace (3) by (11). Given (3), they derive

$$E(y) = \beta_0 + \boldsymbol{\beta}'\mathbf{d} + \mathbf{d}'\mathbf{B}\mathbf{d} \tag{4}$$

and

$$var(y) = \sigma_e^2(\boldsymbol{\gamma}' + \mathbf{d}'\boldsymbol{\Delta})(\boldsymbol{\gamma} + \boldsymbol{\Delta}'\mathbf{d}) + \sigma_\epsilon^2 = \sigma_e^2 \mathbf{l}'\mathbf{l} + \sigma_\epsilon^2, \tag{5}$$

where $\mathbf{l} = (\boldsymbol{\gamma} + \boldsymbol{\Delta}'\mathbf{d}) = (\partial y/\partial e_1, \ldots, \partial y/\partial e_c)'$; i.e., $\mathbf{l}$ is the gradient with respect to the environmental factors—which follows directly from (1). So, the larger

the gradient's elements are, the larger the variance of the predicted simulation output is—which stands to reason. Furthermore, if $\mathbf{\Delta} = \mathbf{0}$ (no control-by-noise interactions), then $var(y)$ cannot be controlled through the control variables $\mathbf{d}$.

Equation (5) implies that the predicted simulation output y has heterogeneous variances—even if σ_e^2 and σ_ϵ^2 were constants—because changing the control factors $\mathbf{d}$ changes $var(y)$. Whereas Myers and Montgomery (1995, p. ...) present examples with $\sigma_e^2 = \sigma_\epsilon^2/2$, Kleijnen (2008, p. 136) gives a supply-chain simulation with $\sigma_e^2 = 10\sigma_\epsilon^2$. Most important is the gradient $\mathbf{l}$, because it shows the key role played by the control-by-noise interactions; i.e., to reduce the predicted output's variance $var(y)$(or σ_y^2) the analysts should take advantage of the interactions $\mathbf{\Delta}$; they cannot control the main effects of the noise factors ($\boldsymbol{\gamma}$) and the variances of the noise factors and the residuals (σ_e^2 and σ_ϵ^2). For example, if a particular decision factor (say, d_1) has no effects on the mean output (so $\beta_1 = \beta_{1;1} = \beta_{1;2} = \ldots = \beta_{1;k} = 0$) but has important interactions with the noise factors (e.g., $\delta_{1;2} >> 0$), then this interaction can be utilized to decrease the output variance (e.g., decrease σ_y^2 by decreasing d_1). If there are multiple decision factors, then the following solution method may be tried:

(1) select the values of some decision factors such that $\mathbf{l} = \mathbf{0}$, so $var(y)$ in (5) is minimized;
(2) select the remaining decision factors such that the predicted mean output $E(y)$ in (4) gets the desired value.

Myers and Montgomery (1995, p. 495) also discuss *constrained optimization*, which minimizes (e.g.) the variance (5) subject to a constraint on the mean (4). Often those authors simply superimpose contour plots for the mean and variance, to select an appropriate compromise or 'robust' solution. We shall use Mathematical Programming, which is more general and flexible.

To *estimate* the unknown (regression) parameters in (1)—which also gives the parameters in the mean and variance equations (4) and (5)—we reformulate (1) as the following *linear regression model*:

$$y = \boldsymbol{\zeta}'\mathbf{x} + \epsilon \tag{6}$$

with $\boldsymbol{\zeta} = (\beta_0, \boldsymbol{\beta}, \mathbf{b}, \boldsymbol{\gamma}, \boldsymbol{\delta})'$ where $\mathbf{b}$ denotes the vector with the $k \times (k-1)/2$ interactions between the decision factors plus their k purely quadratic effects, and $\boldsymbol{\delta}$ denotes the $k \times c$ control-by-noise interactions; $\mathbf{x}$ is defined in the obvious way (e.g., the element corresponding with the interaction effect $\beta_{1;2}$ is $d_1 d_2$).

If we use the Least Squares (LS) criterion, then (6) gives the Ordinary LS (OLS) estimator

$$\widehat{\boldsymbol{\zeta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{w}, \tag{7}$$

where $\mathbf{X}$ is the $n \times q$ matrix of explanatory variables with n denoting the number of scenarios (combinations of decision and environmental factors) determined by DOE that are actually simulated, and q denotes the number of parameters collected in $\boldsymbol{\zeta}$; this $\mathbf{X}$ is assumed not to be collinear (otherwise, $(\mathbf{X}'\mathbf{X})^{-1}$ would not exist). So a necessary but not sufficient condition for $\mathbf{X}$ is $n > q$. The vector $\mathbf{w}$ consists of the n simulation outputs.

The covariance matrix of the OLS estimator, $\mathbf{cov}(\widehat{\boldsymbol{\zeta}})$, is needed to test the importance of the estimated effects. If σ_w^2 were constant, then (7) would imply

$$\mathbf{cov}(\widehat{\boldsymbol{\zeta}}) = (\mathbf{X}'\mathbf{X})^{-1}\sigma_w^2. \tag{8}$$

Note: We might use this equation to find a design that is 'D-optimal'; i.e., a design that minimizes the determinant of $\mathbf{cov}(\widehat{\boldsymbol{\zeta}})$; see Chung, Goldfarb, and Montgomery (2007).

In order to apply classic OLS results, we assume that σ_w^2 is constant, the outputs for different scenarios are independent, and the environmental factors are fixed (Myers and Montgomery (1995, p. 490) do not make these assumptions explicit; in our EOQ application we can derive the true Pareto optimum, so we can verify how sensitive our analysis is to these assumptions). Then the classic estimator of σ_ϵ^2 is the Mean Squared Residuals (MSR)

$$MSR = \frac{(\widehat{\mathbf{y}} - \mathbf{w})'(\widehat{\mathbf{y}} - \mathbf{w})}{n - q} \tag{9}$$

where $\widehat{\mathbf{y}} = \widehat{\boldsymbol{\zeta}}'\mathbf{x}$; also see Kleijnen (2000, p. 23). Note that σ_e^2 is known because the environmental factors are sampled from a known distribution. So $var(y)$ can be estimated through substitution of the estimator MSR for σ_ϵ^2 into (5).

Moreover, we assume that the simulation outputs $\mathbf{w}$ are *normally* distributed; i.e., we assume that the environmental variables $\mathbf{e}$ and the noise ϵ in (1) are normally distributed. The OLS estimator $\widehat{\boldsymbol{\zeta}}$ in (7) is then also normally distributed. Consequently, the individual estimated regression parameters $\widehat{\zeta_j}$ may be tested through the following t statistic with $n - q$ degrees of freedom:

$$t_{n-q} = \frac{\widehat{\zeta_j} - \zeta_j}{s(\widehat{\zeta_j})} \text{ with } j = 1, \ldots, q \tag{10}$$

where $s(\widehat{\zeta_j})$ is the square root of the j^{th} element on the main diagonal of the covariance matrix for $\widehat{\boldsymbol{\zeta}}$ given in (8) with σ_w^2 estimated through the MSR defined in (9). It is well-known that the t statistic is not very sensitive to nonnormality; see Kleijnen (1987).

Myers and Montgomery (1995, p. 488) keep only the significant effects in their response model. We agree that when estimating the robust optimum, we should use the *reduced* metamodel, which eliminates all non-significant effects in the full model—except for those non-significant effects that involve factors that have significant higher-order effects; e.g., if the estimated main effect $\widehat{\beta_1}$ is not significant but the estimated quadratic effect $\widehat{\beta_{1;1}}$ is, then $\widehat{\beta_1}$ is not set to zero. We point out that the (possibly non-significant) OLS estimator is the Best Linear Unbiased Estimator (BLUE) so we must have good reasons to replace it by zero (also see the 'strong heredity' assumption in Wu and Hamada (2000)). The reduced metamodel may imply a unique optimum, whereas the full metamodel may suggest (say) a saddlepoint. To find the unimportant effects, Myers and Montgomery (1995, p. 487) use ANalysis Of VAriance (ANOVA). Note that $t^2_{n-q} = F_{1;n-q}$; the F statistic is used in ANOVA.

To construct *confidence intervals* for the robust optimum Myers and Montgomery (1995, p. 498) assume normality, which results in an F statistic. Myers and Montgomery (1995, p. 504) notice that the analysis becomes complicated when the noise factors do not have constant variances. We shall therefore use *parametric bootstrapping* for RSM applied to the EOQ examples; by definition, parametric bootstrapping assumes that the distribution of the relevant random variable is known (in the EOQ examples, we assume that the distribution is Gaussian). In general bootstrapping is a simple numerical/computerized method for obtaining the Estimated Density Function (EDF) of a—possibly complicated—statistic for a—possibly non-Gaussian—parent distribution. Examples are the well-known Student statistic for a non-Gaussian parent distribution, and the statistic that is formed by the solution of a Nonlinear Programming problem with Gaussian inputs (as is the case for our study). More details are given by Efron and Tibshirani (1993), Kleijnen (2008, p. 86), and Kleijnen, Van Beers, and Van Nieuwenhuyse (2008).

Note: Myers and Montgomery (1995, p. 508) discuss the use of transformations of the dependent variable, before performing the regression analysis; also see Kleijnen (2008, p. 98).

Finally, we replace Myers and Montgomery's assumption formulated in (3) by

$$E(\mathbf{e}) = \boldsymbol{\mu}_{\mathbf{e}} \text{ and } \mathbf{cov}(\mathbf{e}) = \boldsymbol{\Omega}_{\mathbf{e}}. \tag{11}$$

Then (4) becomes

$$E(y) = \beta_0 + \boldsymbol{\beta}'\mathbf{d} + \mathbf{d}'\mathbf{B}\mathbf{d} + \boldsymbol{\gamma}'\boldsymbol{\mu}_{\mathbf{e}} + \mathbf{d}'\boldsymbol{\Delta}\boldsymbol{\mu}_{\mathbf{e}} \tag{12}$$

and (5) becomes

$$var(y) = (\boldsymbol{\gamma}' + \mathbf{d}'\boldsymbol{\Delta})\boldsymbol{\Omega}_{\mathbf{e}}(\boldsymbol{\gamma} + \boldsymbol{\Delta}'\mathbf{d}) + \sigma^2_\epsilon = \mathbf{l}'\boldsymbol{\Omega}_{\mathbf{e}}\mathbf{l} + \sigma^2_\epsilon. \tag{13}$$

To estimate the left-hand side of (12), we simply plug in the estimators for β_0, $\boldsymbol{\beta}$, $\mathbf{B}$, $\boldsymbol{\gamma}$, and $\boldsymbol{\Delta}$ in the right-hand side (the factors $\mathbf{d}$ and $\boldsymbol{\mu}_{\mathbf{e}}$ are known). To estimate the left-hand side of (13), we again use plug-in estimators—now for $\boldsymbol{\gamma}$, $\boldsymbol{\Delta}$, and σ_ϵ^2 (the factor $\boldsymbol{\Omega}_{\mathbf{e}}$ is known); see Myers and Montgomery (1995, p. 495). However, we point out that (13) has products of unknown parameters, so it implies a *nonlinear estimator* $\widehat{\sigma_y^2}$ (we are also interested in $\widehat{\sigma_y} = \sqrt{\widehat{\sigma_y^2}}$, a nonlinear transformation of $\widehat{\sigma_y^2}$) so this plug-in estimator is certainly biased; this bias we ignore when estimating the Pareto frontier that balances $\widehat{y}$ and $\widehat{\sigma_y}$. To study the variability of this estimated Pareto frontier (caused by the noise following from estimating the regression parameters), we use bootstrapping.

The estimation of the mean and variance of the simulation output through (12) and (13) raises the following crucial question (also raised by Myers and Montgomery (1995, pp. 41-54), but assuming a constant output variance): Is the underlying RSM model (1) an *adequate approximation*? The linear regression literature presents several methods for answering this question; see Kleijnen (2008, p. 54). We focus on a method that is also applied outside linear regression (e.g. in Kriging), namely cross-validation. There are several variations on cross-validation (see Iooss, Ribatet, and Marrel (2007) and Meckesheimer et al. (2001)), but the most popular variant is *leave-one-out cross-validation*. Following Kleijnen (2008, p. 57), we define this cross-validation as follows.

(1) Delete I/O combination i from the complete set of n combinations, to obtain the remaining I/O data set—denoted by $(\mathbf{X}_{-i}, \mathbf{w}_{-i})$. Assume that this step results in an $(n-1) \times q$ noncollinear matrix $\mathbf{X}_{-i}$ $(i = 1, \ldots, n)$; a necessary condition is $n > q$. Obviously, $\mathbf{w}_{-i}$ denotes the $(n-1)$-dimensional vector with the remaining $(n-1)$ simulation outputs.
(2) Recompute the OLS estimator of the regression parameters in (7):

$$\widehat{\boldsymbol{\zeta}_{-i}} = (\mathbf{X}'_{-i}\mathbf{X}_{-i})^{-1}\mathbf{X}'_{-i}\mathbf{w}_{-i}. \tag{14}$$

(3) Use $\widehat{\boldsymbol{\zeta}_{-i}}$ (recomputed regression parameters) to compute $\widehat{y_{-i}}$, which denotes the regression predictor of the simulation output generated by $\mathbf{x}_i$ (which corresponds with the simulation input of the combination deleted in step 1):

$$\widehat{y_{-i}} = \mathbf{x}'_i\widehat{\boldsymbol{\zeta}_{-i}}. \tag{15}$$

(4) Repeat the preceding three steps, until all n combinations have been processed. This results in n predictions $\widehat{y_{-i}}$ $(i = 1, \ldots, n)$.
(5) Use a scatterplot with the n pairs $(w_i, \widehat{y_{-i}})$ to judge whether the metamodel is valid.
(6) Because the scaling of this scatterplot may give the wrong impression, we also evaluate the relative prediction errors $\widehat{y_{(-i)}}/w_i$.
(7) A valid regression model also implies that the estimated regression coefficients do not change much when deleting an I/O combination; i.e., there

is not much change in $\widehat{\boldsymbol{\zeta}_{-i}}$ with $(i = 0, 1, \ldots, n)$ where $\widehat{\boldsymbol{\zeta}_{-0}}$ denotes the estimator when zero combinations are deleted, so $\widehat{\boldsymbol{\zeta}_{-0}} = \widehat{\boldsymbol{\zeta}}$.

Our final goal in robust optimization is to minimize the estimated mean $\widehat{y}$—which assumes that (12) is an adequate approximation—while keeping the estimated standard deviation $\widehat{\sigma_y}$—which assumes that (13) is adequate—below a given Threshold (say) T. We solve this constrained minimization problem through Matlab's 'fmincon', which gives the values of the 'estimated robust decision variables' (say) $\widehat{\mathbf{d}^+}$ and its corresponding mean $\widehat{y}$ and standard deviation $\widehat{\sigma_y}$. Next, we vary the threshold value T (say) 100 times, which may give a different solution $\widehat{\mathbf{d}^+}$ with its corresponding $\widehat{y}$ and $\widehat{\sigma_y}$. Then, we collect the 100 pairs $(\widehat{y}, \widehat{\sigma_y})$ to estimate the Pareto frontier. Finally, we estimate the variability of this frontier curve through bootstrapping of the estimated regression estimates that gave $\widehat{y}$ and $\widehat{\sigma_y}$. We shall illustrate our methodology in the next section.

4 EOQ inventory simulation

We apply our methodology to the simulation optimization of the classic EOQ inventory model, which is often used in practical supply chain management. First, we define the EOQ model, including symbols and assumptions; also see Pentico, Drake, and Toews (2008) and Teng (2008). Following Zipkin (2000, pp. 30-39), we use the following assumptions:

(1) The demand is known and constant, say a units per time unit.
(2) The order quantity is Q units.
(3) No shortages are allowed.
(4) Delivery lead time is zero; i.e., the order arrives into inventory as soon as the order is placed.
(5) Review is continuous; i.e. an order is placed as soon as the inventory level drops to the reorder point, which is set to zero because of assumptions 1 and 4.
(6) Total costs has the following components:
   - setup cost per order, K
   - cost per unit purchased or produced, c
   - holding cost per inventory unit per time unit, h.

Defining a 'cycle' as the period between two consecutive replenishments, the cycle length is obviously Q/a. The cost per time unit is simply the total cost over one cycle divided by the cycle length. The goal is to minimize the costs per time unit (say) C, over an infinite time horizon.

This problem has an *analytical* solution, which we shall use to check our simulation results. The (analytical or simulated) cost C is

$$C = \frac{aK}{Q} + ac + \frac{hQ}{2}. \tag{16}$$

So the EOQ is

$$Q_o = \sqrt{\frac{2aK}{h}}, \tag{17}$$

which is known as the *square-root EOQ formula.* The corresponding minimum cost is

$$C_o = C(Q_o) = \sqrt{2aKh} + ac. \tag{18}$$

4.1 Simulation optimization of the EOQ model

Obviously, the EOQ simulation is deterministic. Because all cycles are identical, we simulate a single cycle only. We start this cycle with an inventory of Q units. We copy the following parameter values from Hillier and Lieberman (2001, pp. 936-937, 942-943): $a = 8000$, $K = 12000$, $c = 10$, and $h = 0.3$. Hence (17) and (18) imply that the true optimal input is $Q_o = 25298$ and the corresponding output is $C_o = 87589$; of course, this optimum input remains unknown to our procedure, and we use it only to guide our design of the simulation experiment and to verify its results.

Our simulation experiment consists of the following four steps.

(1) *Design*: We assume that in practice the analysts have some knowledge about the location of the relevant experimental area. To select the experimental area, we therefore start with the interval $[0.5\,Q_o, 1.5\,Q_o]$. This selection, however, would imply that the midpoint coincides with the true optimum input ($Q_o = 25298$)—which rarely occurs in practice. We therefore shift the interval a little bit (namely, by less than 5000 units) to the right so that it is centered at the 'round' value $Q = 30000$. Furthermore, we pick five equally spaced points (a Central Composite Design or CCD would also have five points, albeit not equally spaced; see Myers and Montgomery (1995, p. 55) and Table 5), including the extreme points, $0.5 \times 30000 = 15000$ and $1.5 \times 30000 = 45000$; see row 1 of Table 1 below. The input parameters are fixed to their base (nominal) values ($a = 8000$, $K = 12000$, $c = 10$, $h = 0.3$).

(2) *Simulation Model:* We program the simulation model in Arena; see Kelton, Sadowski, and Sturrock (2007). Next we run this simulation, and obtain $C(Q_i) = C_i$, which denotes the cost corresponding with input value i ($i = 1, \ldots, 5$) selected in step 1; see the Input/Output (I/O) combinations (Q_i, C_i) displayed in Table 1.

Q	15000	22500	30000	37500	45000
C	88650	87641.66	87700	88185	88883.34

Table 1
I/O data of EOQ simulation

i	$\widehat{\beta_{0(-i)}}$	$\widehat{\beta_{1(-i)}}$	$\widehat{\beta_{1;1(-i)}}$	$\widehat{y_{(-i)}}$	$\widehat{y_{(-i)}}/C_i$
0	87663.4257	202.004	1097.15		
1	87731.998	522.008	640	87849.94	0.991
2	87769.82	139.94	1008.49	87952.11	1.004
3	87628.88	202.004	1137.79	87628.92	0.999
4	87583.63	155.46	1163.64	87951.95	0.997
5	87603.997	479.34	1493.34	89576.98	1.008

Table 2
Cross-validation of EOQ regression metamodel

(3) *RSM Metamodel:* Based on these I/O data, we estimate a second-order polynomial regression metamodel, using OLS. We could use either the original or the coded factor values; see again (2). However, we focus on the estimated effects of the coded decision variable, because these effects (say) $\widehat{\boldsymbol{\beta}}$ show their relative importance; moreover, their numerical accuracy is better: the condition number for $\mathbf{X}$ is 3.08, whereas it is $1.07 \cdot 10^{10}$ when using the original Q. This $\widehat{\boldsymbol{\beta}}$ is displayed in the row with $i = 0$ (zero I/O data eliminated) in Table 2. (We also compute the estimated effects of the original variable; e.g., the estimated quadratic effect is then of order 10^{-6}, so it seems unimportant; however, Q^2 is $30298^2 = 9 \times 10^8$ so their joint effect is of order 10^2.)

(4) *Metamodel cross-validation:* The remaining rows of Table 2 display the re-estimated regression parameters following from (14), and the re-estimated regression prediction following from (15). This table also presents the relative prediction errors $\widehat{y_{(-i)}}/C_i$, which supplement the scatterplot in Figure 2. The estimated regression coefficients in different rows remain more or less the same. Anyhow, we decide to accept the regression metamodel because we think it is an approximation that is adequate enough for our goal, which is the illustration of robust optimization through the EOQ model (for the roles of different goals in simulation see Kleijnen and Sargent (2000)). Comparing Figures 2 and 3 suggests that the first figure is much worse; however, using the same scale in both figures (not displayed) changes that impression.

Note: Table 2 implies that the estimated main effect is not significantly different from zero, whereas the quadratic effect is; see the t statistic in (10). As we discussed below (10), we do not replace the estimated main effect by zero. We

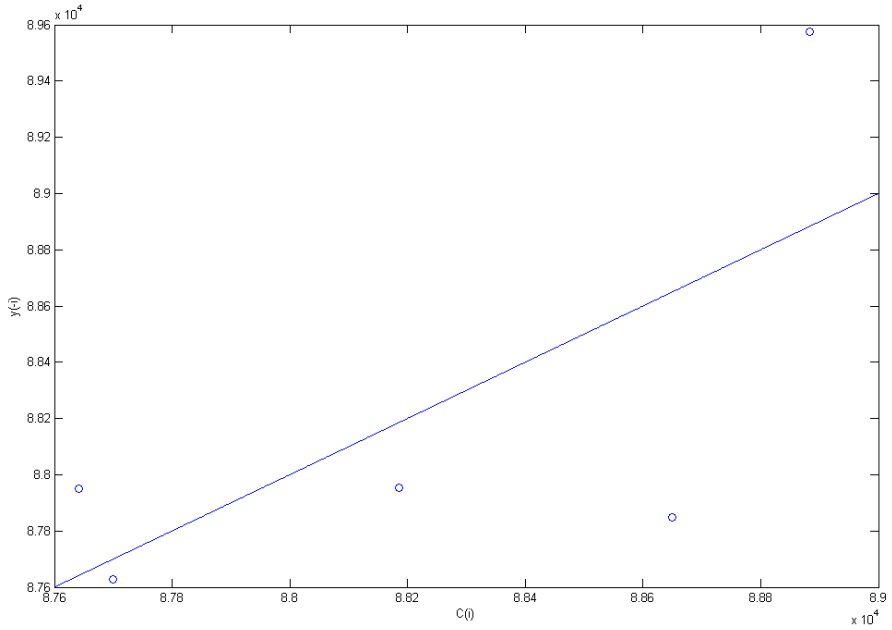

Fig. 2. Scatterplot for regression metamodel of EOQ simulation model

point out that the estimated effects are not independent, because $(\mathbf{X}'\mathbf{X})^{-1}$ in (8) is not diagonal.

The estimated optimum (say) $\widehat{Q_o}$ follows from the first-order optimality condition $\partial\widehat{C}/\partial Q = \widehat{\beta_1} + 2\widehat{\beta_{1;1}}x_1 = 0$, where x_1 is the coded variable corresponding with Q, which gives $\widehat{Q_o} = 28636$. This $\widehat{Q_o}$ gives the estimated minimal cost $\widehat{C_o} = 87654$. In this example, we know the true optimum so we can easily verify the estimated optimum: $\widehat{Q_o}/Q_o$ =28636/25298 = 1.13 and $\widehat{C_o}/C_o$ = 87654/87589 = 1.001 so the cost virtually equals the true minimum, even though the input is 13% off. This illustrates the well-known insensitivity property of the EOQ formula.

Note: We also experiment with a smaller experimental area; i.e., a smaller Q range. We assume that the center of this new area is still close to the true optimum. The Taylor series argument suggests that this smaller area gives a better approximation locally. Appendix 1 shows that the smaller Q range indeed gives a more accurate metamodel; the resulting estimated optimum is only 1% below the true EOQ and the corresponding cost virtually equals the true cost.

4.2 Robust optimization of EOQ model

Next, we drop Assumption 1 in Section 4, which stated that the demand is a known constant a. We still assume that the demand per time unit is constant, but this constant is unknown. Many references on inventory management with uncertain parameters are given by Borgonovo and Peccati (2007).

Note: Yu (1997) also assumes an uncertain demand rate, but uses other criteria than we do: he either minimizes the maximum costs or minimizes the maximum percentage deviation from the optimal cost. Moreover he does not assume a probability function for the various scenarios (demand rate values), but uses 'a discrete scenario set'. Altogether, his approach resembles that of Ben-Tal et al., which we discussed in the Introduction.

Note: The assumption of uncertain constants is often made in deterministic simulation of physical systems; e.g., a nuclear waste-disposal simulation may assume that the permeability of a specific area is constant but unknown; see Kleijnen and Helton (1999). An economic example is the exchange rate between the US dollar and the euro exactly one year from today: that rate is a constant but unknown.

We may collect historical data to infer the probability of the true value of the parameter a. If there is no such data, then we may ask experts for their opinion on the true value of the parameter. This *knowledge elicitation* results in an input distribution (say) $F(a)$. In practice, several distribution types are used, such as normal, lognormal, and uniform; see Kleijnen and Helton (1999). In our experiments we assume—without loss of generality—that a has a Normal (Gaussian) distribution with mean μ_a and standard deviation σ_a:

$$a \sim N(\mu_a, \sigma_a). \tag{19}$$

More specifically, we assume that μ_a denotes the 'base' or 'nominal' value that was used in the simulation optimization of the EOQ model in Section 4.1, and σ_a quantifies the uncertainty about the true input parameter. We experiment with a 'low' and 'high' uncertainty: $\sigma_a = 0.10\mu_a$ and $\sigma_a = 0.50\mu_a$. Because these standard deviations can give a negative value for a, we resample until we get non-negative values only; i.e., we adjust the normal distribution in (19) slightly. However, we ignore this adjustment in our further analysis.

Following Myers and Montgomery (1995, pp. 463-534), we select 'a few' values (levels) for the environmental factors. Those authors use only two values per environmental factor (which suffices to estimate its main effect and its interactions with the decision factors). We, however, use *Latin Hypercube Sampling* (LHS) to select 'a few' values for the environmental factors (because LHS is popular in risk and uncertainty analysis; see Kleijnen 2008), which runs as

$Q \setminus a$	4530,34	5478,85	7687,37	9329,26	11559,02
15000	51177,72	61421,54	85273,65	103006	127087,4
22500	51094,63	61085,52	84348,68	101643,2	125130
30000	51615,59	61480	84448,7	101524,3	124713,8
37500	52378,16	62166,7	84958,71	101902,9	124914,1
45000	53261,54	62999,49	85673,71	102530,4	125422,6

Table 3
I/O simulation data for EOQ model with uncertain demand rate

follows.

Let n_e denote the number of combinations of the environmental factors e. Then LHS splits the admissible (experimental) range of each factor e_g into n_e subranges such that each subrange has an equal probability $1/n_e$. More specifically, our EOQ simulation has a single environmental factor, denoted by a. So, LHS splits the range of possible a values ($0 < a < \infty$) into $n_e = 5$ equally likely subranges, namely $(0, \mu_a - 0.85\sigma_a]$, $(\mu_a - 0.85\sigma_a, \mu_a - 0.73\sigma_a]$, $(\mu_a - 0.73\sigma_a, \mu_a + 0.73\sigma_a]$, $(\mu_a + 0.73\sigma_a, \mu_a + 0.85\sigma_a]$, $(\mu_a + 0.85\sigma_a, \infty)$. Notice that the 'base' value μ_a has zero probability, but a value 'close' (namely less than $0.73\sigma_a$ away) has 20% probability. We use *lhsnorm* from the Matlab Statistics Toolbox to select five values from $N(\mu_a, \sigma_a)$; see The MathWorks Inc. (2005). This gives the a values in Table 3, which uses the relatively high uncertainty $\sigma_a = 0.50\mu_a$. Appendix 2 shows the results for the smaller uncertainty $\sigma_a = 0.10\mu_a$.

For the decision variable Q we select the five values that we also used in Table 1 (Appendix 1 also considers a smaller Q-range). We *cross* the two designs for a and Q respectively, as is usual in a Taguchian approach. However, we could also have used LHS to get a combined design for a and Q. We also use a CCD instead of LHS (see Table 5); Myers and Montgomery(1995, p. 487) also discuss designs more efficient than crossed designs.

We run the EOQ simulation model for all 5×5 combinations of the inputs (decision and environmental inputs), which gives Table 3.

We again code the inputs; see (2). So x_1 corresponds with Q and x_2 with a; e.g., $a = 7687{,}37$ corresponds with $x_2 = -0.1017$ (not exactly zero, because of the sampling that LHS does). Furthermore, if $\sigma_a = 0.50\mu_a = 4000$ and $b_2 = 2.85 \times 10^{-4}$, then the standard deviation of x_2 is $\sigma_2 = 4000 \times 2.85 \times 10^{-4} = 1.14$.

To analyze these I/O data, we might compute the estimated *conditional* variance $\widehat{var(C|Q_i)}$ from the row with Q_i ($i = 1, \ldots, 5$) in Table 3; also see Lee and Nelder (2003). Instead we follow Myers and Montgomery (1995) and es-

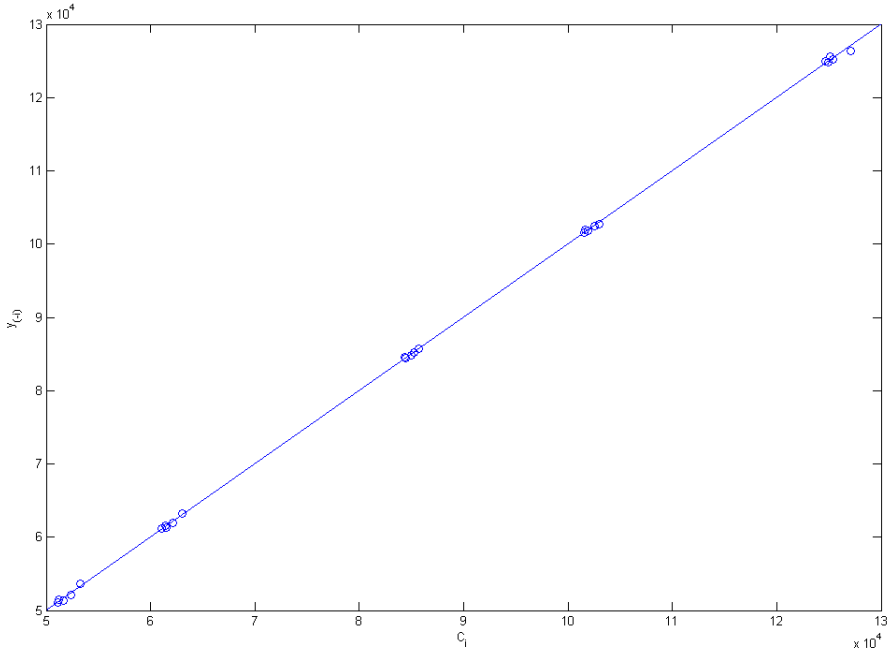

Fig. 3. Scatterplot of regression metamodel for RO of EOQ

timate the variance using all the elements in this table; also see (13). The latter approach gives a better estimator, provided the RSM metamodel (1) is correct.

To compute the OLS estimates, we must re-arrange the 5×5 elements of Table 3 into the $n \times q$ **X**-matrix of (7) where now $n = 25$ and $q = 5$; **w** now becomes a vector with the 25 simulation outputs C. This gives the estimated intercept $\widehat{\beta_0}$, the estimated first-order effect $\widehat{\beta_1}$ and second-order effect $\widehat{\beta_{1;1}}$ of Q, the estimated first-order effect $\widehat{\gamma_1}$ of a, and the interaction $\widehat{\delta_{1;1}}$, which are displayed in the row denoted by 0 (zero rows eliminated) in Table 4. The rest of this table displays the cross-validation results (analogous to Table 2). This table gives the scatterplot in Figure 3. This table and this figure suggest that this metamodel is adequate for robust optimization through RSM.

Note: Appendices 1 and 2 give results for a smaller range of the decision variable Q and the environmental variable a. These results show even better fit.

Note: To check the negative sign of $\widehat{\delta_{1;1}}$ (interaction between Q and a), we use the analytical solution (16) to derive $\partial^2 C/\partial Q \partial a = -K/Q^2$, which is indeed negative.

Using a RSM metamodel like the one in the first row of Table 4, Myers and Montgomery (1995, p. 501) derive *contour plots* for the mean and variance. Be-

i	$\widehat{\beta_{0(-i)}}$	$\widehat{\beta_{1(-i)}}$	$\widehat{\beta_{1;1(-i)}}$	$\widehat{\gamma_{1(-i)}}$	$\widehat{\delta_{1;1(-i)}}$	$\widehat{y_{(-i)}}$	$\widehat{y_{(-i)}}/C_i$
0	88150.40	190.56	1058.33	36774.03	-899.67		
1	88144.21	172.94	1088.31	36755.96	-863.54	51440.09	1.005
2	88147.70	181.73	1072.54	36768.01	-887.64	61545.93	1.002
3	88152.19	198.89	1046.41	36774.09	-899.80	85169.34	0.999
4	88154.29	214.81	1026.29	36764.26	-880.14	102725.72	0.997
5	88157.15	259.16	976.22	36714.38	-780.37	126368.95	0.994
6	88150.48	190.51	1058.24	36773.93	-899.57	51096.08	1.000
7	88154.53	188.27	1054.63	36770.90	-896.54	61150.15	1.001
8	88164.19	182.52	1046.82	36773.90	-899.54	84550.05	1.002
9	88172.91	177.00	1040.41	36784.95	-910.59	101956.72	1.003
10	88190.37	165.55	1028.40	36817.51	-943.16	125653.78	1.004
11	88124.57	190.56	1090.86	36793.63	-899.67	51330.94	0.994
12	88131.43	190.56	1081.72	36783.93	-899.67	61275.30	0.997
13	88146.40	190.56	1063.03	36774.05	-899.67	84407.52	1.000
14	88158.08	190.56	1049.58	36776.69	-899.67	101600.85	1.001
15	88177.60	190.56	1028.69	36795.56	-899.67	124973.16	1.002
16	88136.05	182.81	1071.52	36789.93	-883.77	52147.29	0.996
17	88137.51	183.42	1069.82	36783.76	-889.94	61965.54	0.997
18	88139.92	184.45	1067.07	36774.13	-899.57	84805.76	0.998
19	88141.21	185.03	1065.63	36769.57	-904.12	101775.07	0.999
20	88142.70	185.75	1064.09	36765.65	-908.04	124813.22	0.999
21	88140.63	218.39	1105.69	36745.49	-956.75	53675.97	1.008
22	88144.24	210.75	1090.83	36760.27	-927.18	63283.89	1.005
23	88148.76	198.15	1069.18	36773.97	-899.79	85768.71	1.001
24	88150.72	188.53	1055.65	36773.21	-901.30	102506.95	1.000
25	88152.94	164.73	1027.41	36751.56	-944.60	125152.04	0.998

Table 4
Cross-validation of regression metamodel for RO of EOQ

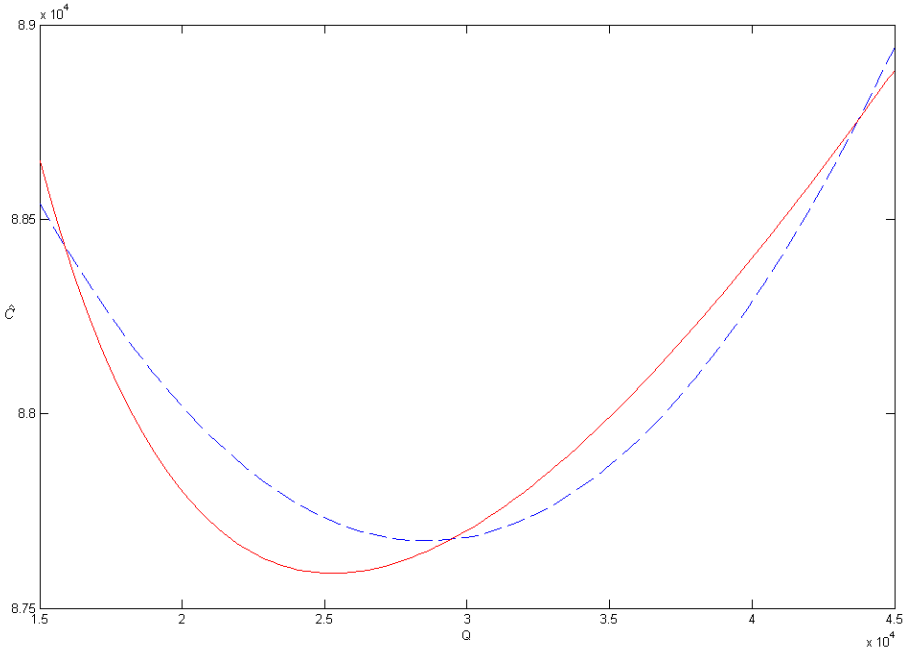

Fig. 4. Estimated (dashed) curve and true (solid) curve for mean cost versus order quantity

cause our EOQ example has a single decision variable, we do not superimpose contour plots but present the following two plots:

- Figure 4 shows the plot for Q (the decision variable) versus $\widehat{C}$ (mean output, estimated through regression analysis); see (12) with the regression parameters β_0, $\boldsymbol{\beta}$, $\mathbf{B}$, $\boldsymbol{\gamma}$, and $\boldsymbol{\Delta}$ replaced by their estimates. Indeed, $E(a)$ in (12) is a known input value: it is not exactly equal to μ_a in (19) because we resample negative a values, which have a probability of nearly 2% for high σ_a and virtually zero for small σ_a; we could also have estimated $E(a)$ through $\overline{a} = \sum_{1}^{5} a_i/5$ where a_i is shown in Table 3.
- Figure 5 shows Q versus $\widehat{\sigma_C}$, the estimated standard deviation of C predicted through the RSM metamodel. We prefer the standard deviation over the variance because the former uses the same scale as the simulated cost C and its regression estimate $\widehat{C}$. We use (13) with $\boldsymbol{\gamma}$, $\boldsymbol{\Delta}$, and σ_ϵ^2 replaced by their estimates, including the MSR estimator (9) of σ_ϵ^2. Notice that σ_a^2 is a known input value, so we also know the variance of the corresponding coded variable x_2, namely $\sigma_2^2 = 1.14^2 = 1.3$). Altogether we obtain $\widehat{\sigma_C} = [(\widehat{\gamma_1} + \widehat{\delta_{1;1}} x_1)^2 \sigma_2^2 + \widehat{\sigma}_\epsilon^2]^{1/2} = [(36755.96 - 863.54 x_1)^2 \times 1.3 + 4.6224 \times 10^4]^{1/2}$. Figure 5 shows this second-order polynomial, which actually resembles a linearly decreasing function in the relatively small domain of Q that is pictured; also see the next Note.

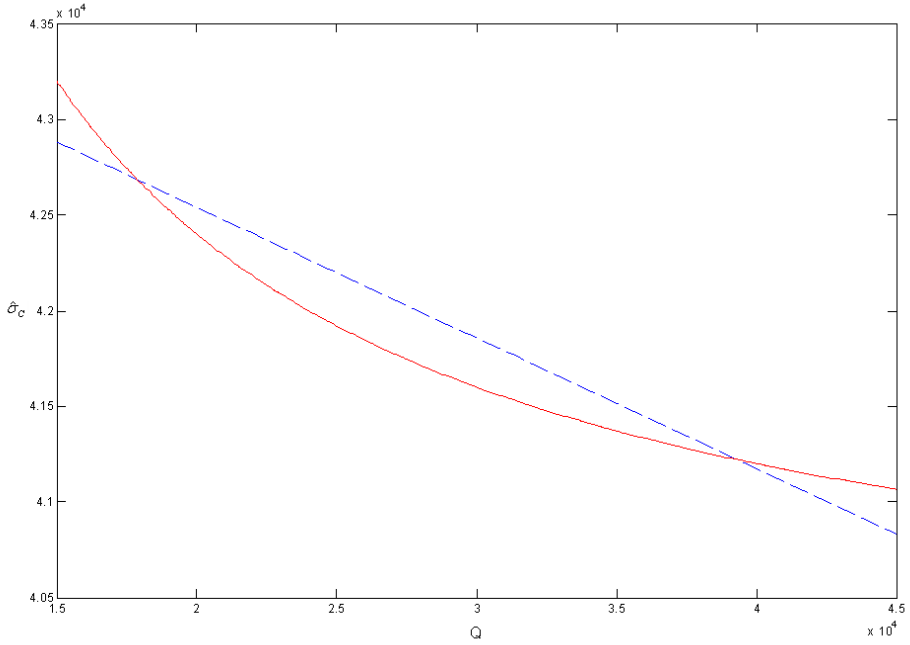

Fig. 5. Estimated (dashed) curve and true (solid) curve for standard deviation of cost versus order quantity

Note: For this simple example we know the true I/O function of the simulation model, namely (16). So the true standard error of the cost C is

$$\sigma_C = \sigma\left(\frac{aK}{Q} + ac + \frac{hQ}{2}\right) = \sigma\left(\frac{hQ}{2} + [\frac{K}{Q} + c]a\right) = \left(\frac{K}{Q} + c\right)\sigma_a = c\sigma_a + \frac{K\sigma_a}{Q}. \tag{20}$$

We also plot this σ_C against Q in Figure 5 (assuming fixed cost parameters K and c, and demand variance σ_a^2). Comparing the two curves in Figure 5 shows that the estimated curve is an adequate approximation.

From Figures 4 and 5 we derive the 'estimated robust optimal' order quantity (say) $\widehat{Q^+}$, which we define as the quantity that minimizes the estimated mean $\widehat{C}$ while keeping the estimated standard deviation $\widehat{\sigma_C}$ below a given threshold T. We solve this constrained minimization problem through Matlab's fmincon. For example, if $T = 4.25 \times 10^4 = 42500$, then Figure 5 implies $\widehat{Q^+} = 2.8568 \times 10^4 = 28568$. However, let T become smaller, e.g., $T = 4.15 \times 10^4 = 41500$. Then Figure 5 implies $\widehat{Q^+} = 3.5222 \times 10^4 = 35222$; see Figure 6, in which the curve becomes a horizontal line with 'height' $\widehat{Q^+}$ if the threshold is high enough.

We point out that Section 4.1 gave the classic EOQ $\widehat{Q_o} = 28636$, assuming the demand rate equals the nominal value. Now we use a different model, assuming different demand rates. The latter model gives an estimated optimal order quantity $\widehat{Q^+}$ that differs from $\widehat{Q_o}$. This difference is nearly 25% if the managers are risk-averse (high threshold T).

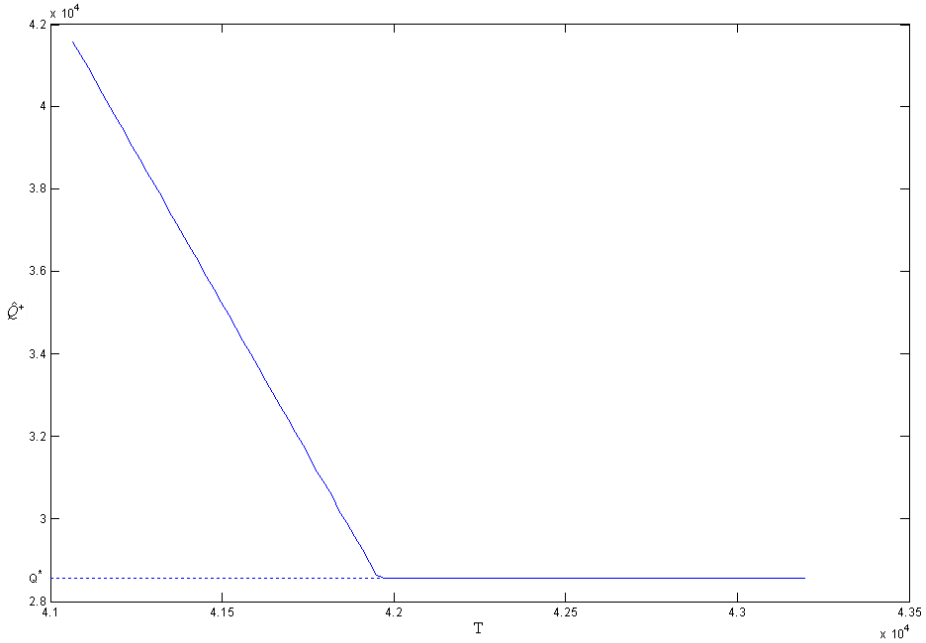

Fig. 6. Estimated robust optimal value for EOQ against threshold for standard deviation of cost

We assume that management cannot give a single, fixed value for the threshold, so we vary the threshold over the interval [41067,43200]. This interval gives the estimated *Pareto frontier* in Figure 7. This figure demonstrates that if management prefers low costs variability, then they must pay a price; i.e., the expected cost increases.

We repeat the experiment with a smaller σ_a (lower demand variability), which implies a less volatile environment. Some reflection shows that we cannot keep the threshold values T the same in environments with different magnitudes of *volatility*. The new threshold values give the estimated Pareto frontier of Figure 8. Comparing the estimated Pareto frontiers of Figures 7 and 8 demonstrates that a less volatile world gives lower mean cost. Moreover, this comparison quantifies the benefits of obtaining more information on the uncertain demand rate (e.g., a marketing survey may decrease the standard deviation of the demand rate).

The estimated Pareto frontier is built on the estimates $\widehat{\boldsymbol{\zeta}}$, so we further analyze this frontier. Whereas Myers and Montgomery (1995, pp. 496-503) use rather complicated confidence intervals, we use *parametric bootstrapping*. More specifically, we sample—via the Monte Carlo method, using pseudo-random numbers—(say) B times from the multivariate—namely q-variate—normal distribution with mean vector and covariance matrix given by (7) and (8):

$$\widehat{\boldsymbol{\zeta}}^* \sim N_q(\widehat{\boldsymbol{\zeta}}, (\mathbf{X}'\mathbf{X})^{-1}\widehat{\sigma_w^2}) \tag{21}$$

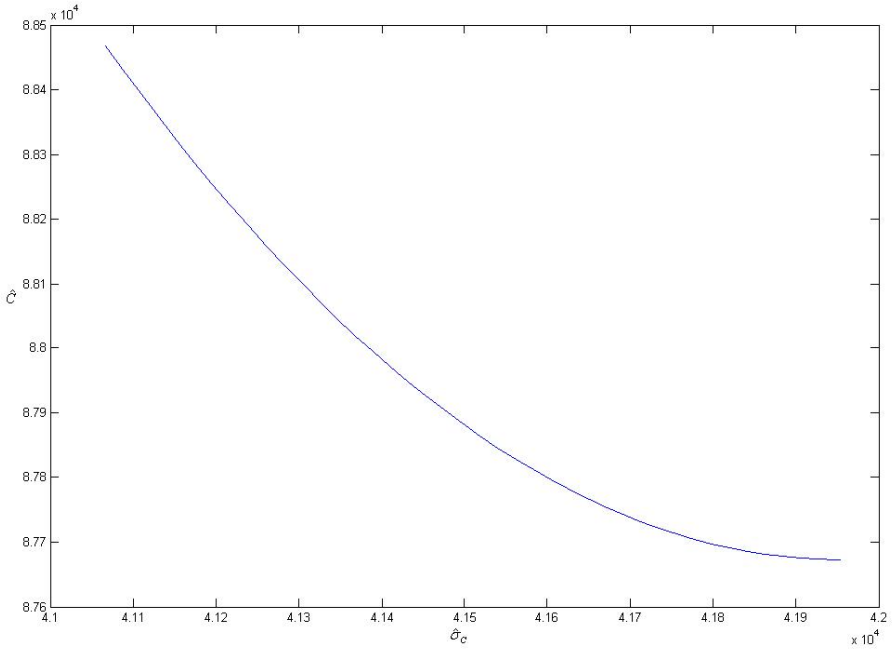

Fig. 7. Estimated Pareto frontier for EOQ simulation with threshold for standard deviation of cost

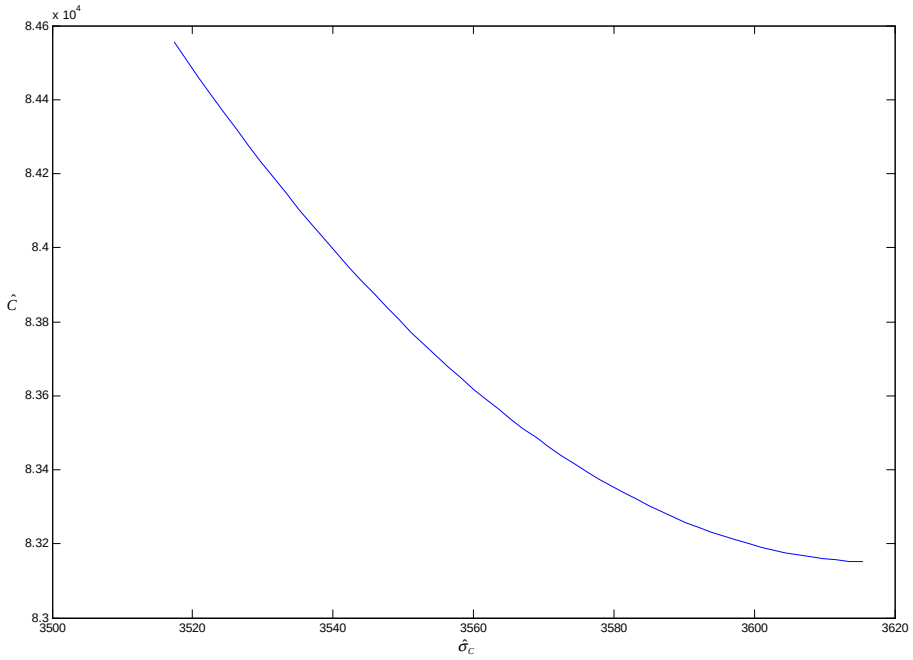

Fig. 8. Less volatile world: estimated Pareto frontier for EOQ simulation with threshold

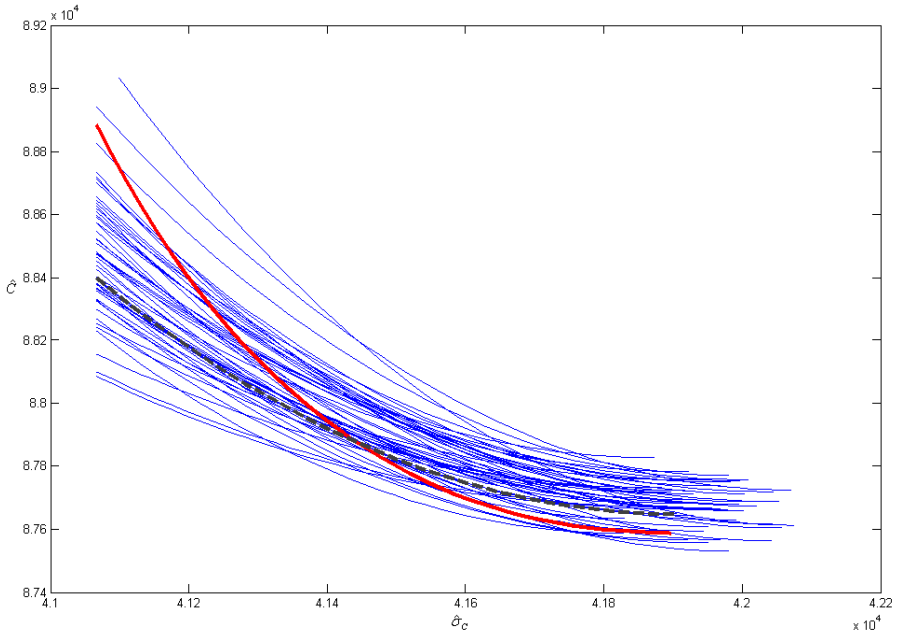

Fig. 9. Bootstrapped Pareto frontiers, original estimated frontier (dashed curve), and true frontier (heavy curve)

where the superscript $*$ is the usual symbol for bootstrapped values. This sampling gives $\widehat{\boldsymbol{\zeta}}_b^*$ $(b = 1, \ldots, B)$. This $\widehat{\boldsymbol{\zeta}}_b^*$ gives $\widehat{C_b^*}$; see (12) with β_0, $\boldsymbol{\beta}$, $\mathbf{B}$, $\boldsymbol{\gamma}$, and $\boldsymbol{\Delta}$ replaced by their bootstrapped estimates (i.e., estimates computed from the bootstrapped $\widehat{C_b^*}$). It also gives $\widehat{\sigma_{C_b^*}}$; see (13) where σ_ϵ^2 is replaced by the estimate computed from the bootstrapped parameters. These two bootstrapped variables $\widehat{C_b^*}$ and $\widehat{\sigma_{C_b^*}}$ give the bootstrapped optimal decision variable $\widehat{Q_b^{+*}}$, which are computed through Matlab's fmincon. This bootstrap sample gives the B estimated Pareto frontiers of Figure 9, where we select $B = 50$ and derive the true Pareto frontier from the analytical costs (16) and its standard deviation (20) and we also display the original estimated frontier of Figure 7. This figure demonstrates that bootstrapping gives a good idea of the variability of the estimated Pareto frontier; the bundle of bootstrapped curves 'envelop' the original estimated curve and the true curve. We observe that the bundle of bootstrapped estimated costs does not completely envelop the true curve; neither does the bundle for the bootstrapped standard deviations; see Figures 10 and 11.

Note: Though we focus on estimating the variability of the Pareto curve, we could also have estimated the variability of the solution of the robust optimum problem. So the B bootstrap regression parameters ζ^* gives B values for Q^+ and the corresponding C^+ and $s(C)^+$. These B values can be used to derive a CI; see Efron and Tibshirani (1993).

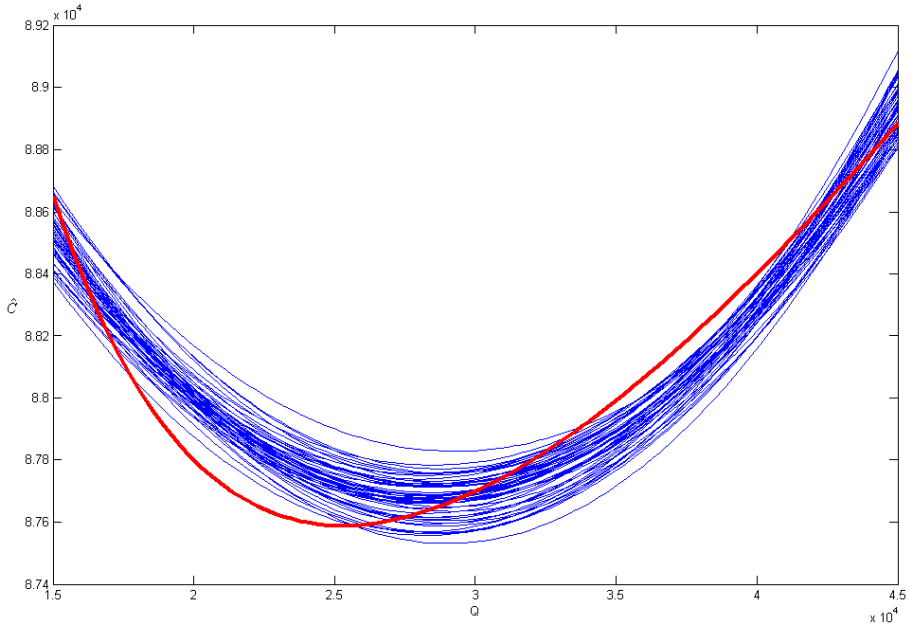

Fig. 10. Bootstrapped estimated costs, and true cost (heavy curve)

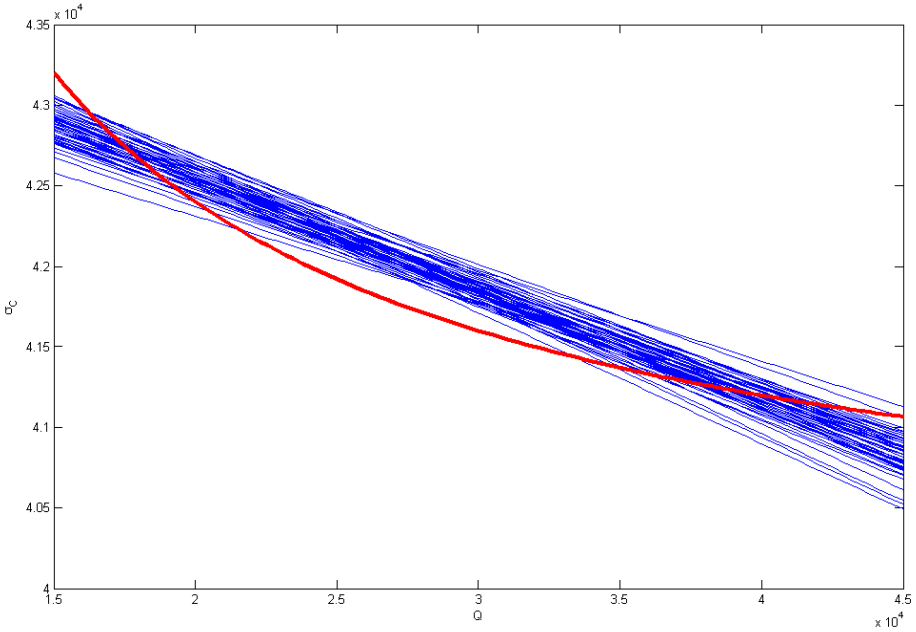

Fig. 11. Bootstrapped standard deviations of the cost, and true standard deviation of the cost (heavy curve)

Note: Actually, we can validate our (fast) bootstrap procedure as follows Our EOQ simulation is the opposite of *expensive simulation*: some realistic simulations take hours or weeks for a single run, whereas bootstrapping this simulation's results still takes only seconds. So we repeat our LHS sample (say) L times; i.e., we sample the demand rate a from the normal distribution in (19) cut-off at zero, while keeping the five Q values in Table 3 fixed. This sample of L *macroreplicates* gives the regression estimate $\widehat{\boldsymbol{\zeta}}_l$ with $l = 1, \ldots, L$. This $\widehat{\boldsymbol{\zeta}}_l$ gives $\widehat{C_l}$ (costs estimated through RSM metamodel) and $\widehat{\sigma_{C_l}}$ (corresponding standard deviation). Together with the threshold T this gives the estimated Pareto frontier. Repeating this LHS L times gives a set of L estimated Pareto frontiers; see Figure 12 with $L = 50$. This figure suggests that these estimated curves all intersect near the point $(4.11, 8.83)$, but zooming-in around this point reveals that the 50 curves do not intersect in a single point. Appendix 3 also displays the 50 $\widehat{C}$-curves and the 50 $\widehat{\sigma_C}$-curves. These curves results in 50 Pareto curves estimated from 50 macroreplicates; see again Figure 12. This figure assumes that a second-order polynomial is a perfect approximation of the true I/O function, whereas the true EOQ formulas in (16) and (20) show that this assumption is false Comparing this figure and Figure 9 shows that the macroreplicates give a tighter bundle. Appendix 3 shows that this phenomenon is explained by the negative correlations between estimated regression coefficients in the macroreplicates. In general, we could argue that —compared with bootstrapping—macroreplicates use much more computer time, and provide more information so the spread in the estimated Pareto curves is smaller. Appendix 3 also shows that if we replace LHS by crude sampling in the macroreplicates, then a bigger spread is the result; i.e., LHS is indeed a variance reduction technique.

Finally, we compare the (traditional Taguchian) crossed design in Table 3 with a CCD. A CCD for two factors (Q and a) consists of a 2^2 design (the four combinations of the two extreme values per factor -1 and 1), the four 'axial' points $((0, -\sqrt{2}), (0, \sqrt{2}), (-\sqrt{2}, 0), (\sqrt{2}, 0))$, and the central point $((0, 0))$ in coded values; the value $\sqrt{2}$ is selected to make the CCD 'rotatable' (see Myers and Montgomery (1995, p. 299)) The original input values plus the corresponding output values are displayed in Table 5.

Note: A CCD is not a subset of Table 3, because a CCD does not sample any factor value, whereas Table 3 uses LHS for the environmental factor a. Consequently, Table 3 does not have (say) coded values -1 and 1 for a, which are at exactly the same distance from 0.

We again validate the resulting metamodel through cross-validation; see Appendix 4 for details. We repeat our analysis for this CCD. This gives the Pareto frontier of Figure 13. Comparison of Figures 7 and 13 shows that the CCD with its nine combinations gives a better estimate of the true frontier (the heavy curve in Figure 9) than the 5×5 crossed-design does. We con-

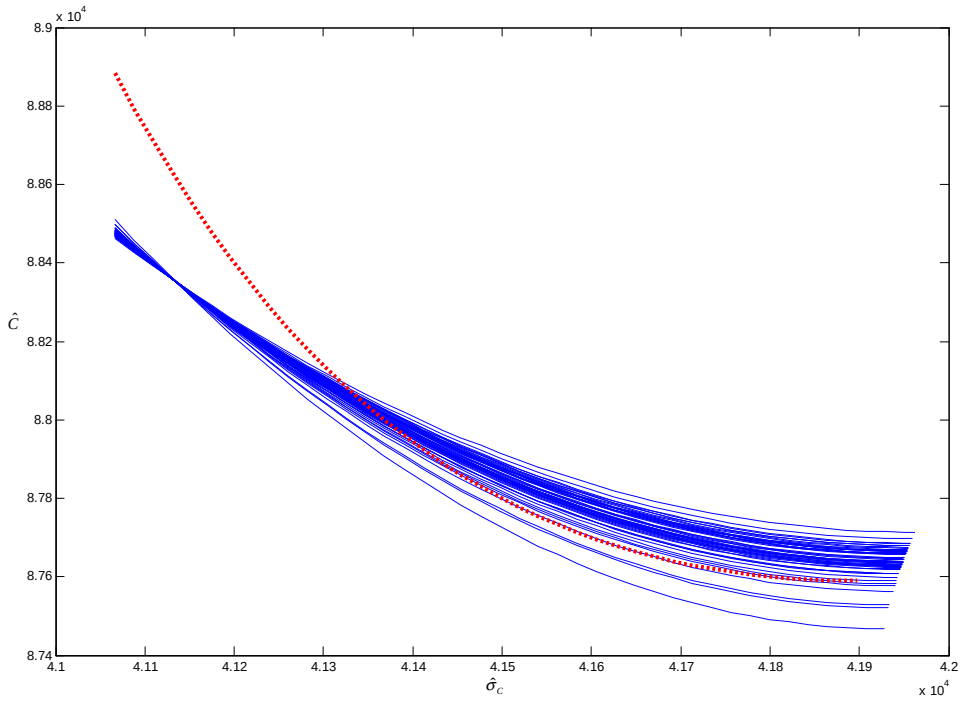

Fig. 12. Pareto frontiers estimated from 50 macroreplicates, and true frontier (dotted curve)

Q	a	C
19393.40	5559.67	61945.81
19393.40	10529.69	114721.4
40606.60	5559.67	63330.64
40606.60	10529.69	114499.6
15000	8044.68	89132.55
45000	8044.68	89342.05
30000	4530.34	51615.54
30000	11559.02	124713.8
30000	8044.68	88164.67

Table 5
I/O simulation data for EOQ model with CCD design

jecture that the bigger design gives a more accurate OLS estimator $\widehat{\boldsymbol{\zeta}}$ of the *wrong* (misspecified) metamodel (namely, a second-order polynomial) for the true I/O function implied by the EOQ simulation model.

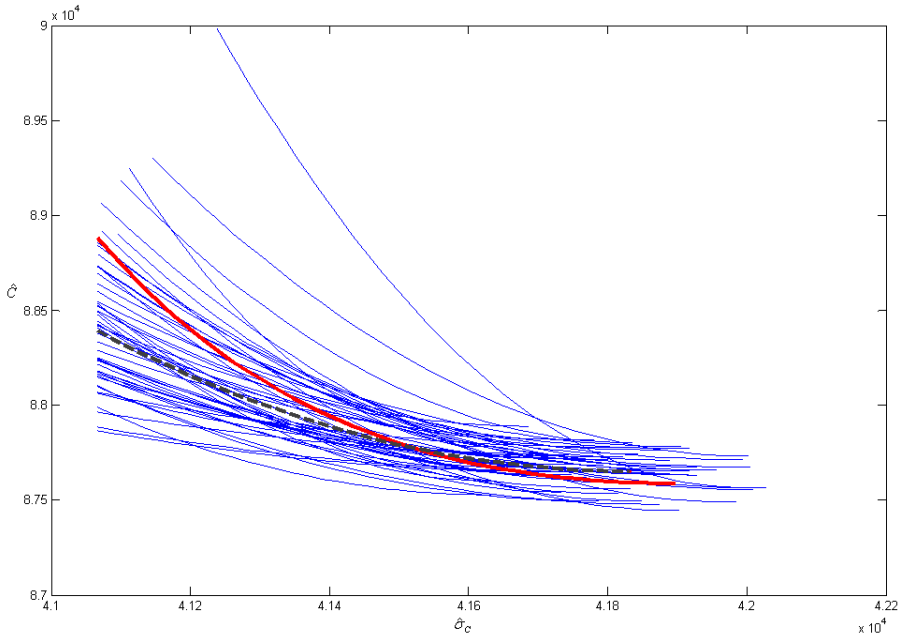

Fig. 13. Bootstrapped Pareto frontiers, original estimated frontier (dashed curve) and true Pareto frontier (heavy curve) based on CCD

5 Conclusions and future research

This article leads to the following conclusions:

(1) Robust optimization of simulated systems may use *Taguchi*'s worldview, which distinguishes between decision variables to be optimized and environmental variables that remain uncertain.
(2) Taguchi's statistical techniques may be replaced by *RSM*.
(3) Myers and Montgomery (1995)'s RSM developed for Taguchian optimization may be further adapted such that it results in *bootstrapped Pareto frontiers*, which better enable management to make the final compromise decision.
(4) Application of this new methodology to the classic *EOQ* model shows that—for a certain (known) environment—the methodology gives a good estimate of the true EOQ, and—for an environment with a demand rate that has a known distribution—the classic EOQ and the robust EOQ differ.

Future research may address the following issues.

- We conjectured that the bigger crossed design gave a more accurate OLS estimator $\widehat{\boldsymbol{\zeta}}$ of a misspecified metamodel. This is a good reason for using a better type of metamodel, namely a *Kriging* model (Generalized Linear

Q	22500	26250	30000	33750	37500
C	87641.66	87594.64	87700	87906.95	88185

Table 6
I/O data for EOQ simulation with smaller experimental area

Models or GLMs are proposed by Lee and Nelder (2003)) as alternatives for RSM models; also see Iooss et al. (2007). In a next article we shall present Kriging for RO.

- We shall also adjust our methodology for *random* simulation models, namely (s, S) models, with either explicit out-of-stock costs so the model has a scalar output or a service constraint so the model has vector output. Notice that the difference $S - s$ is often based on the EOQ model.
- We shall consider *integer* constraints on some input variables: Lodree (2007) studies the EOQ, assuming an integer order size. Kleijnen et al. (2008) use the Matlab code 'bnb20' to estimate the optimum accounting for integer input constraints.
- We may consider *qualitative* decision variables. If the number of combinations of qualitative variables is small, then we may fit metamodels for each combination, and still apply our methodology.
- We hope to apply our methodology to complex *supply chain* models.
- We might try to derive an *optimal design* for our RO. Chung et al. (2007) use a Genetic Algorithm to find a D-optimal design.

Acknowledgements

Carlo Meloni wishes to thank CentER for the financial support when he visited Tilburg University. We thank Wim van Beers (Tilburg University) for helpful discussions on our research.

Appendix 1: Smaller Q-range

Row 1 of Table 6 shows the Q values in the smaller experimental area; row 2 gives the corresponding simulation outputs.

Regression analysis of the I/O data in Table 6 gives Table 7 and the scatterplot of Figure 14. Comparison with Table 2 and Figure 2 shows that the smaller Q-range gives a more accurate metamodel. The new estimated optimum $\widehat{Q_o}$ is 25115, which gives $\widehat{C_o} = 87607$ so $\widehat{Q_o}/Q_o = 25115/25298 = 0.99$ and $\widehat{C_o}/C_o = 87618/87589 = 1.0003$. Comparison with the old results ($\widehat{Q_o}/Q_o = 1.13$ and $\widehat{C_o}/C_o = 1.001$) shows that the smaller Q range improves the estimated optimum.

Appendix 2: Smaller uncertainty $\sigma_a = 0.10\mu_a$

i	$\widehat{\beta_{0(-i)}}$	$\widehat{\beta_{1(-i)}}$	$\widehat{\beta_{1;1(-i)}}$	$\widehat{y_{(-i)}}$	$\widehat{y_{(-i)}}/C_i$
0	87698.26	279.798	214.78		
1	87704.57	309.26	172.69	87633.242	0,999
2	87707.76	274.26	206.86	87612.056	1,000
3	87696.62	279.798	216.71	87698.26	0,9999
4	87690.03	274.99	221.64	87891.854	0,9997
5	87692.38	307.23	253.97	88192.838	1,001

Table 7
Cross-validation of EOQ regression metamodel with smaller range

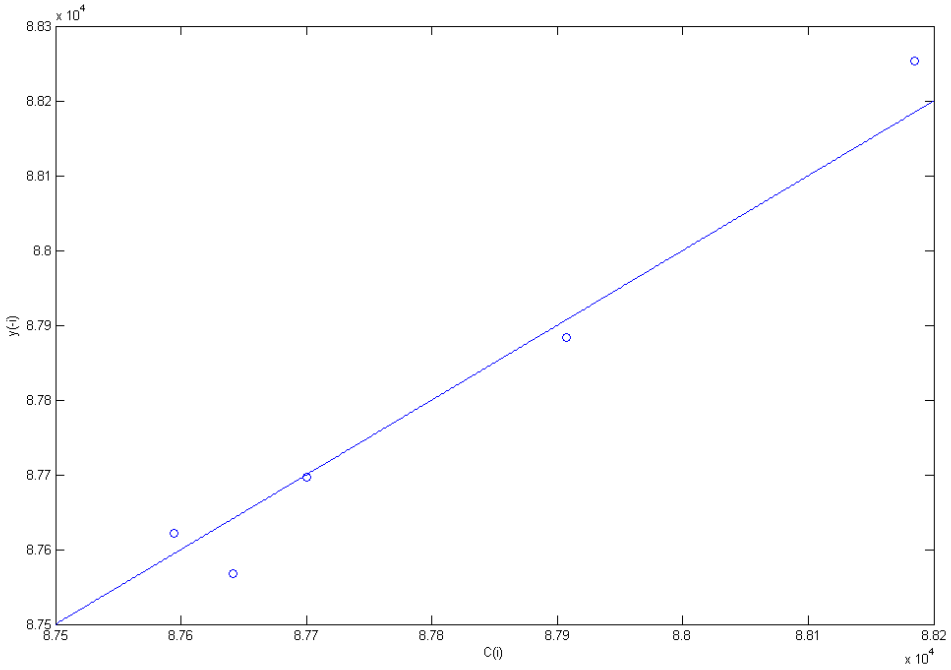

Fig. 14. Scatterplot of the EOQ regression metamodel for smaller Q-range

Tables 8 and 9 and Figure 15 give results for smaller uncertainty in the demand rate.

Appendix 3: Macroreplicates

Figures 16 and 17 display the 50 $\widehat{C}$-curves and the 50 $\widehat{\sigma_C}$-curves respectively, computed from 50 macroreplicates. Note that the latter figure suggests that the 50 estimated curves coincide, but zooming-in reveals that the 50 curves do not coincide: these curves have little spread; see Figures 18 and 19. We point out that each macroreplicate gives a different mean and standard deviation for

$Q \setminus a$	6076.55	7438.96	7.832.04	8595.36	9101.10
15000	67876.77	82590.79	86836.02	95079.90	111541.90
22500	67381.35	81732.06	85872.48	93912.80	99239.95
30000	67696.14	81865.20	85953.20	93891.76	99151.47
37500	68335.02	82395.09	86451.64	94329.13	99548.38
45000	69135.94	83123.34	87158.94	94995.71	100188

Table 8
I/O simulation data for EOQ model with smaller a-range

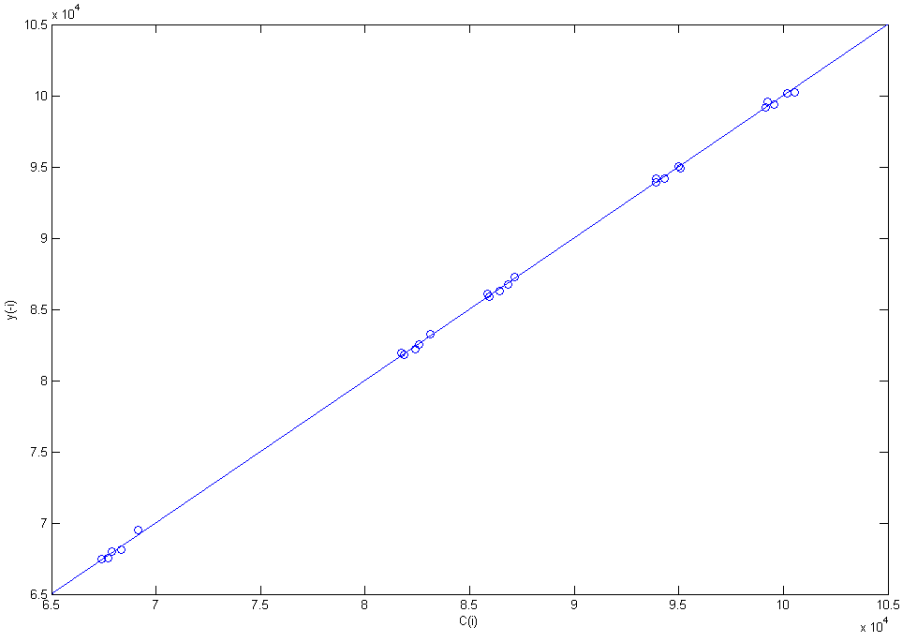

Fig. 15. Scatterplot of the EOQ regression metamodel for smaller a-range

the coded variable x_2; e.g., $x_{2;l} = min_k a_{l;k}$ with $l = 1, \ldots, 50$ and $k = 1, \ldots, 5$.

There is no solution for the constrained optimization problem if the LHS happens to result in an extremely high $\widehat{\sigma}(C)$. Actually this happened once in our 50 macroreplicates; we simply threw away this macroreplicate, and sampled again.

Figure 20 shows that if we replace LHS by crude sampling in the macroreplicates, then bigger spread results. This bigger spread is caused by a bigger spread in the estimated regression coefficients; e.g. Figure 21 shows the Box plot for the estimated interaction $\widehat{\delta_{1;1}}$.

It is interesting that the spread of the estimated regression coefficients is smaller for the bootstrap than for the macroreplicates using LHS; nevertheless,

i	$\widehat{\beta_{0(-i)}}$	$\widehat{\beta_{1(-i)}}$	$\widehat{\beta_{1;1(-i)}}$	$\widehat{\gamma_{1(-i)}}$	$\widehat{\delta_{1;1(-i)}}$	$\widehat{y_{(-i)}}$	$\widehat{y_{(-i)}}/C_i$
0	83374.03	307.26	1070.93	15824.45	-387.14		
1	83373.72	296.40	1082.41	15814.75	-367.74	67977.23	1.001
2	83375.07	313.61	1062.48	15825.97	-390.18	82516.93	0.999
3	83375.95	316.08	1058.27	15824.30	-386.85	86725.30	0.999
4	83378.77	320.83	1047.87	15815.61	-369.45	94878.21	0.998
5	83382.36	325.08	1036.43	15802.71	-343.66	100240.08	0.997
6	83383.68	300.95	1064.25	15813.17	-375.86	67498.17	1.002
7	83387.18	299.36	1060.43	15820.66	-383.35	81915.79	1.002
8	83388.19	299.02	1059.09	15824.72	-387.41	86079.62	1.002
9	83390.53	298.34	1055.76	15836.08	-398.77	94178.12	1.003
10	83392.58	297.83	1052.67	15847.45	-410.14	99559.36	1.003
11	83353.46	307.26	1092.07	15842.31	-387.14	67511.15	0.997
12	83367.41	307.26	1078.48	15825.81	-387.14	81799.08	0.999
13	83370.36	307.26	1075.25	15824.40	-387.14	85915.31	1.000
14	83375.54	307.26	1069.02	15825.18	-387.14	93908.39	1.000
15	83378.87	307.26	1064.54	15828.47	-387.14	99207.34	1.001
16	83355.49	295.13	1083.75	15846.11	-365.47	68110.62	0.997
17	83362.44	300.30	1080.18	15827.79	-383.80	82233.12	0.998
18	83363.51	301.14	1079.72	15824.25	-387.34	86297.79	0.998
19	83364.95	302.35	1079.27	15818.05	-393.54	94183.08	0.998
20	83365.52	302.94	1079.30	15813.89	-397.69	99401.86	0.999
21	83372.90	346.65	1112.57	15789.26	-457.51	69500.37	1.005
22	83372.29	317.81	1084.94	15821.92	-392.19	83245.96	1.001
23	83372.43	314.61	1081.48	15824.57	-386.90	87251.28	1.001
24	83373.06	310.04	1075.65	15826.26	-383.51	95037.07	1.000
25	83373.96	307.40	1071.20	15824.62	-386.79	100190.39	1.000

Table 9
Cross-validation of regression metamodel for RO of EOQ with smaller a-range

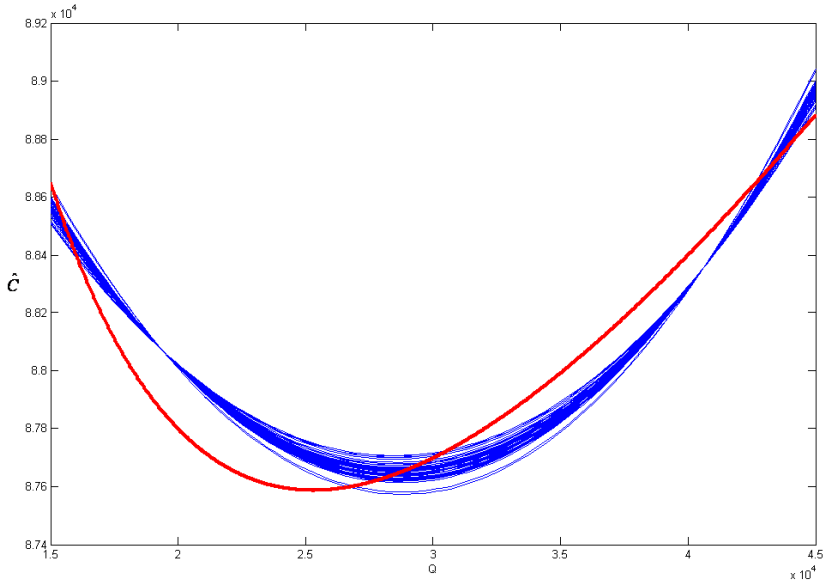

Fig. 16. Replicated estimated costs, and true cost (heavy curve)

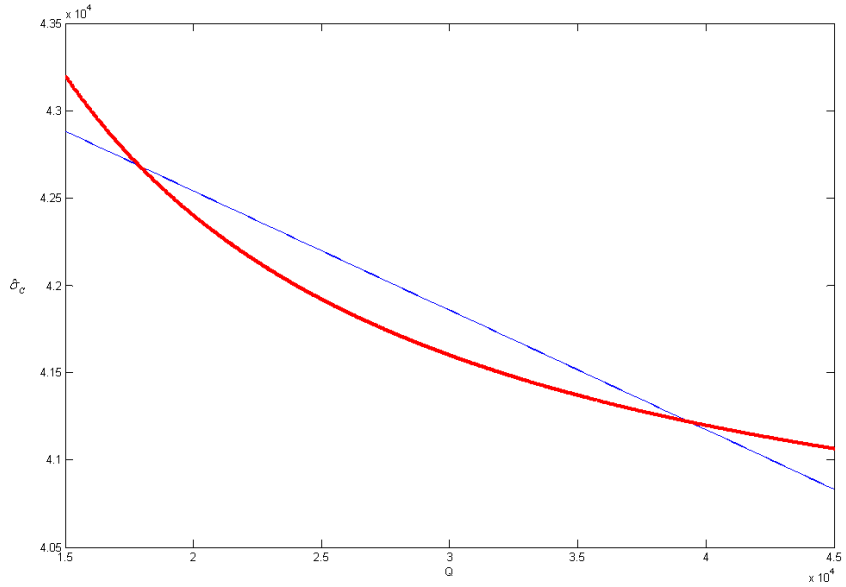

Fig. 17. Replicated standard deviations of the cost, and true standard deviation (heavy curve)

the bootstrap gives more spread in the Pareto curves! The explanation is that the estimated regression coefficients in the metamodel for the standard deviation are negatively correlated (so they compensate variations in each other's values) in the macroreplicates, whereas they are independent in the bootstrap. More precisely, the covariance matrix in (21) implies that in our experiment $cov(\widehat{\gamma^*_{1(-i)}}, \widehat{\delta^*_{1;1(-i)}}) = 0$; for the macroreplicates we use Matlab's 'Symbolic

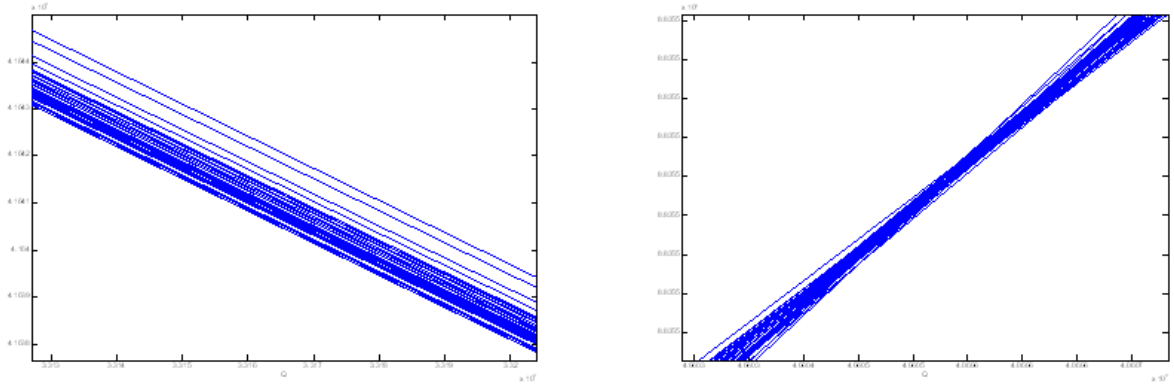

Fig. 18. Zoom: Mean Cost, estimated through 50 macroreplicates

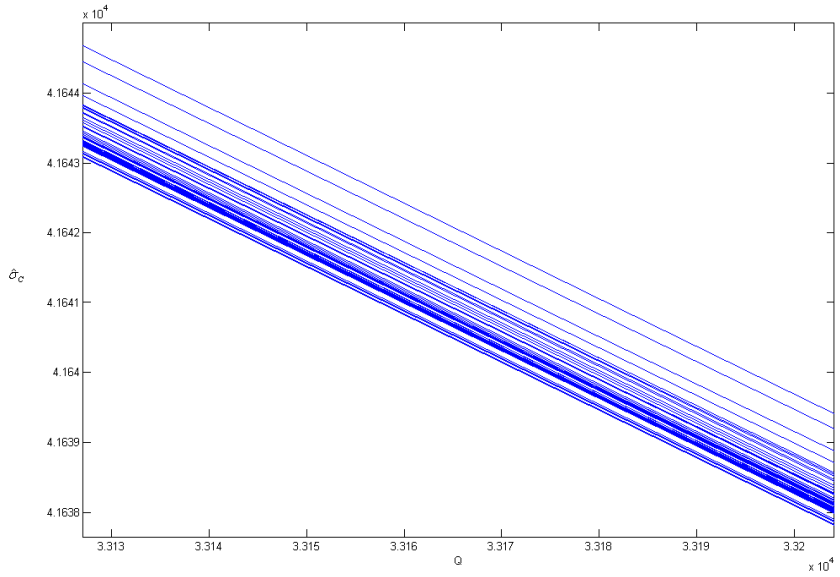

Fig. 19. Zoom: Standard deviation of Cost, estimated through 50 macroreplicates

Math Toolbox' to derive that the correlation coefficient $cor(\widehat{\gamma_{1(-i)}}, \widehat{\delta_{1;1(-i)}})$ is -1; see Figure 22.

Appendix 4: CCD experiment

Table 10 and Figure 23 give details on our CCD experiment.

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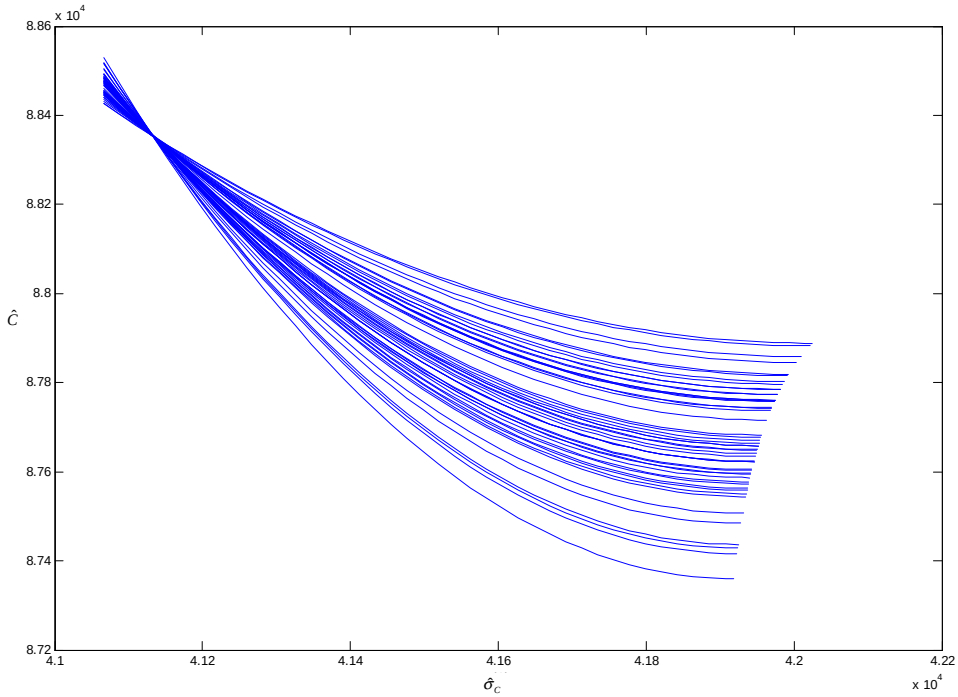

Fig. 20. Crude sampling: replicated estimated Pareto frontiers

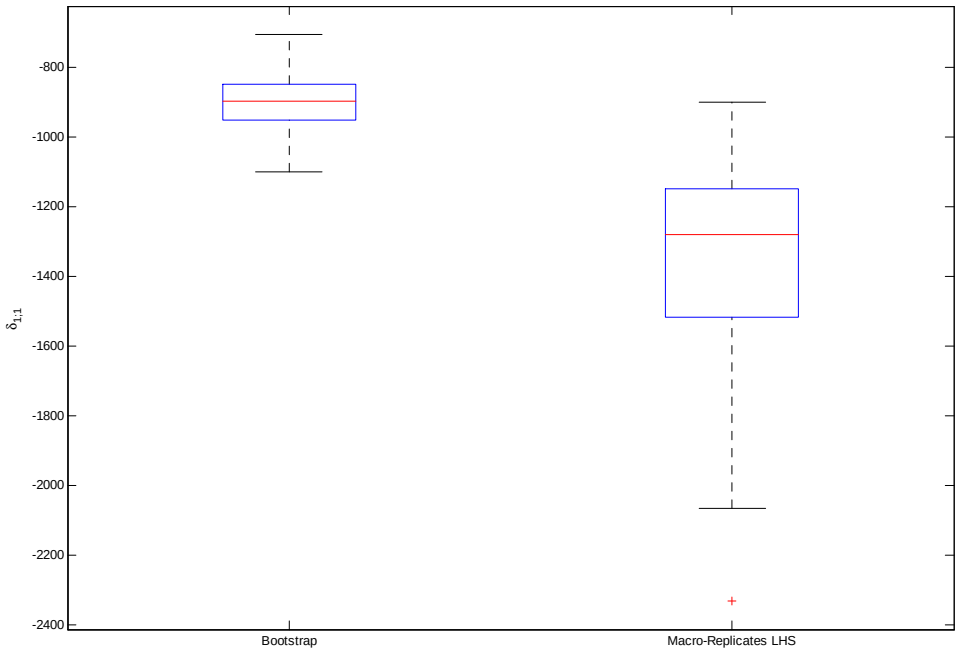

Fig. 21. Box plot for the estimated interaction $\delta_{1;1}$

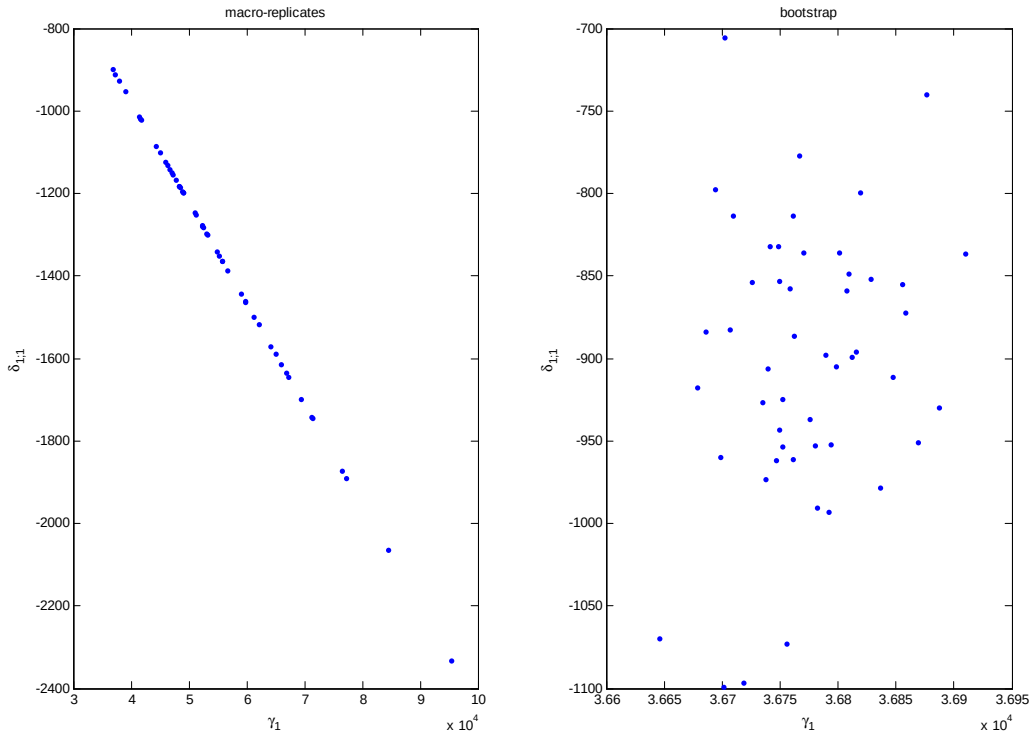

Fig. 22. Scatterplot of $\widehat{\gamma_1}$ and $\widehat{\delta_{1;1}}$ in macro-replicates (left-hand side) and bootstrap (right-hand side)

i	$\widehat{\beta_{0(-i)}}$	$\widehat{\beta_{1(-i)}}$	$\widehat{\beta_{1;1(-i)}}$	$\widehat{\gamma_{1(-i)}}$	$\widehat{\delta_{1;1(-i)}}$	$\widehat{y_{(-i)}}$	$\widehat{y_{(-i)}}/C_i$
0	88136.81	182.41	529.35	25915.14	-401.66		
1	88188.84	110.87	542.36	25843.59	-258.57	62518.17	1.0092
2	88155.43	156.81	534.00	25940.74	-452.86	114926.23	1.0018
3	88137.85	183.85	529.61	25913.70	-404.54	63342.16	1.0002
4	88104.44	137.91	521.26	25870.64	-490.66	114143.59	0.9969
5	88182.69	271.64	414.63	25915.14	-401.66	88627.80	0.9943
6	88110.59	233.40	594.89	25915.14	-401.66	89630.45	1.0032
7	88063.51	182.41	578.21	25962.65	-401.66	51346.78	0.9948
8	88178.26	182.41	501.71	25942.01	-401.66	124865.80	1.0012
9	88126.36	182.41	536.32	25915.14	-401.66	88126.36	0.9996

Table 10
Cross-validation of regression metamodel for RO of EOQ, based on CCD

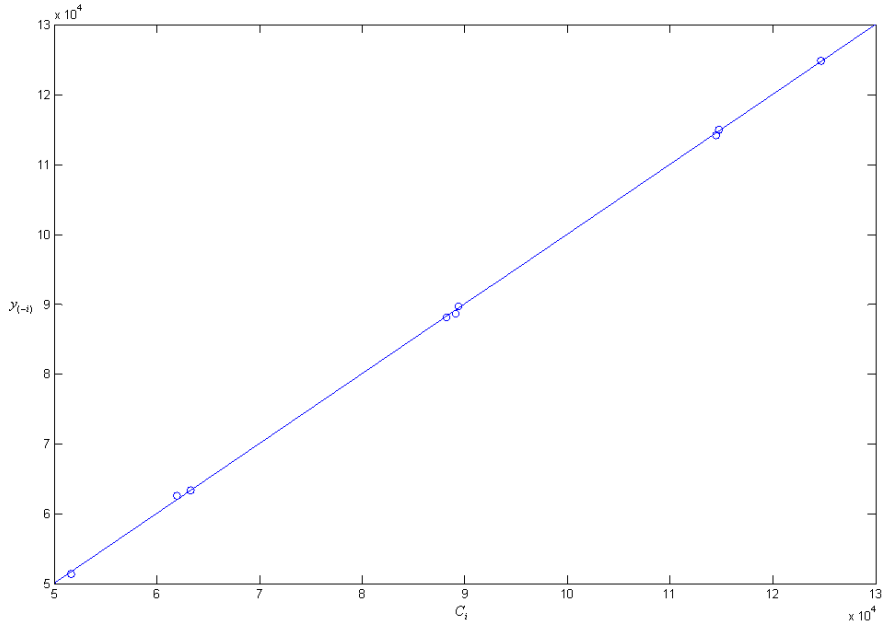

Fig. 23. Scatterplot of the EOQ regression metamodel for CCD

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Vitae

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