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Citation for published version (APA):

Schoofs, A. J. G., Klink, M. B. M., & Campen, van, D. H. (1992). Approximation of structural optimization problems by means of designed numerical experiments. *Structural Optimization*, 4(3-4), 206-212.
<https://doi.org/10.1007/BF01742746>

DOI:

[10.1007/BF01742746](https://doi.org/10.1007/BF01742746)

Document status and date:

Published: 01/01/1992

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
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Approximation of structural optimization problems by means of designed numerical experiments*

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Abstract In this paper we describe an approach in which the Experimental Design Theory (EDT) (see Montgomery and Wiley 1984; Kiefer and Wolfowitz 1959; Fedorov 1972) is used as a tool in building approximate analysis models to be applied in structural optimization problems. This theory has been developed for the planning and analysis of comprehensive physical experiments in order to reduce the number of required experiments while preserving the amount of information that can be extracted from them. This situation is very similar to that of structural optimization, where the number of expensive finite element (FEM) analyses has to be minimized (Schoofs 1987). FEM computations can be regarded as numerical experiments, where the design variables are treated as input quantities. All computable properties of the structure, such as weight, displacements, stresses, etc. can be regarded as response quantities of the numerical experiment. The approximating models will be derived for these responses by using regression techniques, and they can be substituted in the optimization problem for the definition of the objective and the constraint functions. The application of the proposed method is illustrated with two case studies.

1 Experimental design theory

1.1 Regression model

EDT consists of two main parts. The first part concerns the planning of experiments and ends up with a list of experiments to be carried out. This list is called the experimental design (ED). In the second part the experimental results are analysed and fitted to some mathematical relationship: the regression model.

We use the following notations:

\mathbf{x} is a column matrix,

$\underline{\mathbf{x}}$ is a stochastic variable,

$\hat{\mathbf{x}}$ is an estimated variable.

When a structure is determined by n design variables, denoted by the column, \mathbf{x} , we may search for t functions describing the response quantities

$$y_j = y_j(\mathbf{x}), \quad j = 1, \dots, t, \quad (1)$$

in a certain limited area according to the bounds of the design variables given by

$$x_i^l \leq x_i \leq x_i^u, \quad i = 1, \dots, n. \quad (2)$$

In the sequel we will consider only one response quantity, y_j , and for brevity we omit the index j . To find the relation

$y = y(\mathbf{x})$ we assume a mathematical model. Mostly a linear model will apply of the form

$$\underline{y} = \mathbf{f}^T(\mathbf{x})\boldsymbol{\beta} + \underline{\epsilon} = \beta_1 f_1(\mathbf{x}) + \dots + \beta_k f_k(\mathbf{x}) + \underline{\epsilon}, \quad (3)$$

where the components β_1, \dots, β_k of the column $\boldsymbol{\beta}$ are unknown parameters; the model is linear in the components of $\boldsymbol{\beta}$. The functions $f_1(\mathbf{x}), \dots, f_k(\mathbf{x})$ are the components of the column $\mathbf{f}(\mathbf{x})$. We can choose both linear and non-linear functions for them; in most cases, a polynomial is chosen for (3). The variable $\underline{\epsilon}$ accounts for the stochastic or deterministic model error that is inherent in every model assumption.

1.2 Parameter and response estimation

An allowable point in the design variable space is characterized by specific values of all design variables within the bounds given by (2). The formulation of an ED implies the choice of a certain number, say N , of such points. For a proper estimation of $\beta_i, i = 1, \dots, k$, see (3), the number N should exceed the number k .

Now we assume that somehow an ED has been determined consisting of N points, represented by the sets of design variables $\mathbf{x}_1, \dots, \mathbf{x}_N$. If we analyse the structure at these points yielding the column of response quantities $\mathbf{y} = [y_1 y_2 \dots y_N]^T$, then by using a least-squares technique the unknown parameters $\boldsymbol{\beta}$ can be estimated from

$$\hat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T \mathbf{y}, \quad (4)$$

where X is the $(N \times k)$ "design matrix", which is given by

$$X = [\mathbf{f}(\mathbf{x}_1) \mathbf{f}(\mathbf{x}_2) \dots \mathbf{f}(\mathbf{x}_N)]^T. \quad (5)$$

Subsequently, for an arbitrary design point, \mathbf{x} , within the bounds (2) the response variable can be estimated from the explicit approximation

$$\hat{y}(\mathbf{x}) = \mathbf{f}^T(\mathbf{x})\hat{\boldsymbol{\beta}}. \quad (6)$$

It is our purpose to use regression models of the type of (6) to formulate and solve optimization problems.

1.3 Use of sensitivities

Differentiation of the mathematical model (3) with respect to the design variable x_i gives

$$\frac{\partial y}{\partial x_i} = \beta_1 \frac{\partial f_1}{\partial x_i} + \dots + \beta_k \frac{\partial f_k}{\partial x_i} + \frac{\partial \underline{\epsilon}}{\partial x_i}, \quad i = 1, \dots, n. \quad (7)$$

In FEM-formulations such sensitivities of y can be efficiently computed and thus (7) can be used with advantage, together with (3), to estimate the parameters $\boldsymbol{\beta}$. Furthermore, the accuracy of partial derivatives of the resulting regression models will then be increased, which is advantageous for use of the regression models in optimization algorithms.

* Presented at NATO ASI "Optimization of Large Structural Systems", Berchtesgaden, Sept. 23 - Oct. 4, 1991

1.4 Accuracy of the estimates

A measure for the accuracy of $\hat{\beta}$ is the variance-co-variance matrix $V(\hat{\beta})$, which is defined as

$$V(\hat{\beta}) = E[(\hat{\beta} - \beta)(\hat{\beta} - \beta)^T] = (X^T X)^{-1} \sigma^2, \quad (8)$$

where E is the expected value operator, and σ^2 is the variance of the response variable y . For the response estimator $y(\mathbf{x})$ the variance $V[\hat{y}(\mathbf{x})]$ is used as a measure for its accuracy. From (6) and (8) it follows:

$$V[\hat{y}(\mathbf{x})] = \mathbf{f}^T(\mathbf{x})(X^T X)^{-1} \mathbf{f}(\mathbf{x}) \sigma^2. \quad (9)$$

1.5 Planning of the experiments

The first part of EDT concerns the determination of the list of experiments to be carried out, the experimental design (ED), in such a way that model parameters and responses can accurately be estimated. For this purpose several, more or less classical methods are available (Montgomery 1984; Box *et al.* 1978). We will treat a relatively recently developed method: the optimal experimental design theory (see Kiefer and Wolfowitz 1959; Fedorov 1972).

1.6 Optimal experimental design

The formulation of an ED implies the choice of a certain number, N , of points in the design variable space limited by the bounds given by (2). The objective in optimal experimental design is to determine these N points, in general, from a much larger set of so-called candidate points, in such a way that the variances of the estimated parameters, or the variance of the estimated response quantity, are minimized.

1.7 Discrete levels of design variables

In principle all real design variable values within the bounds are allowed for a candidate point. For the purpose of efficiency, however, we only allow a very limited number of discrete values, called levels, of every design variable.

The choice of the number of levels for a certain design variable depends on the order of the variable in the assumed mathematical model [see (3)]. A linear effect can be estimated by means of at least two levels. A quadratic effect needs at least three levels, and so on. For function types other than polynomial terms, for example trigonometric functions, similar considerations can be applied.

1.8 The set of candidate points

The set of candidate points is composed by choosing a relatively large number of discrete points. A quite commonly used set of candidate points comprises all possible combinations of the levels of the variables. This builds a so-called "complete" design. If the number of the design variables and/or the number of levels increases, a complete design may be too large a set of candidate points. Classical experimental design methods (Montgomery 1984; Box *et al.* 1978) provide methods to determine a fraction of the complete design, which can be used as a reasonable set of candidate points.

1.9 Optimality criteria

As mentioned above, experimental designs can be evaluated, using the variances of the parameter estimators $V(\hat{\beta})$ or the variance of the response estimator $V[\hat{y}(\mathbf{x})]$ as a measure, see

(11) and (12), respectively. In both cases the quality of the ED is a function of the matrix $(X^T X)^{-1}$ and the objective is to determine that ED among all possible N -point designs which makes $(X^T X)^{-1}$ minimal. However, the minimum of a matrix is not a well-defined concept and a number of operational criteria have been developed. The most important of these criteria are

D-optimality: minimize $\det(X^T X)^{-1}$, (10)

G-optimality: minimize the maximum response variance, (11)

V-optimality: minimize the average response variance. (12)

Mitchell (1974) developed an efficient algorithm called DETMAX as the most popular in optimal experimental design. The algorithm starts with an initial ED. During each iteration step, the candidate point which results in the largest increase of $\det(X^T X)$ is added to the design, and subsequently the point which results in the smallest decrease of $\det(X^T X)$ is removed from the design. The algorithm generates high quality EDs at relatively low computing costs.

Optimal experimental design is useful in those situations where classic designs are unsuitable or unavailable, that is when

- the experimental region is irregularly shaped due to constraints on the variables,
- it is necessary to augment an existing design,
- the number of levels of the variables varies considerably,
- designs must be constructed for special models, i.e. other than polynomial models,
- designs must be constructed for simultaneous observation of several responses.

2 Model building

The building of an accurate regression model for a given system or structure is an iterative process. Initially the following questions must be resolved to some degree:

- which variables play a role and what is their range of interest,
- which form of functions $f_i(\mathbf{x})$, see (3), may be suitable to describe the relationship searched for.

A good strategy is to begin with moderate model demands, thus reducing the initial computing costs. The iterative model building process is able to enhance models in a cost efficient way, see Fig. 1.

At the start of each iteration step a model assumption of the type of (3) must be available. The iteration step then involves generation of an ED, collection of data, followed by estimation of the parameters from the collected data, and the evaluation of the model. Evaluation implies answering questions like

- Is the model valid?
- Are the estimated parameters accurate enough?
- Are the response predictions accurate enough for all relevant values of \mathbf{x} ?

If the results of the testing require further model improvement, it is necessary to perform another model building cycle consisting of experimental design, data collection, parameter estimation, and retesting.

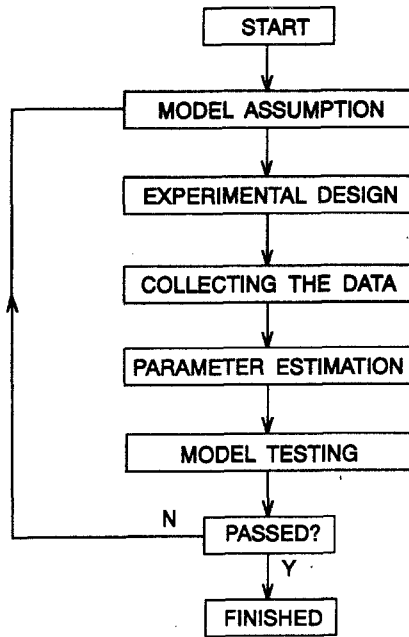


Fig. 1. Scheme for model building

3 Computer program for model building and optimization

Nagtegaal (1978) developed an interactive computer program called CADE (Computer Aided Design of Experiments). Apart from experimental design, facilities for the analysis of experiments have also been implemented. For the experimental design part, the core of the program ACED (Welch 1985) has been used. In CADE the optimality criteria and algorithms of ACED have been generalized to the case of simultaneous observation of several response quantities.

CADE has been coded in Fortran 77 and runs on Apollo D3000 work-stations, Vax systems and an Alliant FX40 computer. The program originally consisted of three main modules, being model input, design of experiments and parameter estimation.

In the model input module all kinds of linear models can be entered, stored in a file or read from a previously prepared file without the need for user supplied subroutines.

The experimental design module offers the following facilities.

- Optimal design for a single and for several simultaneous responses.
- Implementation of the D-, G- and V-optimality criteria.
- Implementation of several optimization algorithms, including DETMAX.
- Determination of the characteristics of user-supplied designs.
- Augmentation of existing experimental designs.
- Generation of some classical designs (fractional 2^n -designs).

Finally, the main characteristics of the parameter estimation module are as follows:

- parameters can be selected by means of stepwise regression, backward elimination and forward selection; they can also be selected "by hand";
- parameters can be protected against removal from the model;

- parameters are estimated accurately by means of QR-decomposition, followed by an iterative refinement procedure.

Recently, Klink (1991) added a fourth module to CADE. Using this module, several regression models can be composed to formulate an objective function and constraint functions defining a (structural) optimization problem. Subsequently, the optimization problem is solved using CADE by means of an SQP algorithm. The second application in the next section illustrates this feature.

4 Applications

The procedures described in the preceding sections have been applied to several mechanical engineering problems. In this section two applications are presented.

4.1 Stress concentration problem

Van Campen *et al.* (1990) applied the method to a stress concentration problem in a chain link of a continuous variable transmission system, see Fig. 2a. Each section of the chain contains a number of links of about 0.5 mm in thickness. The pins transmitting the driving force to conical discs are locked up by the links in subsequent sections of the chain. Only a symmetric loading case was considered, allowing us to use only one quarter of the link in the FEM model. Figure 2b shows the geometry of the link. The loading force $F/2$ is 134 N.

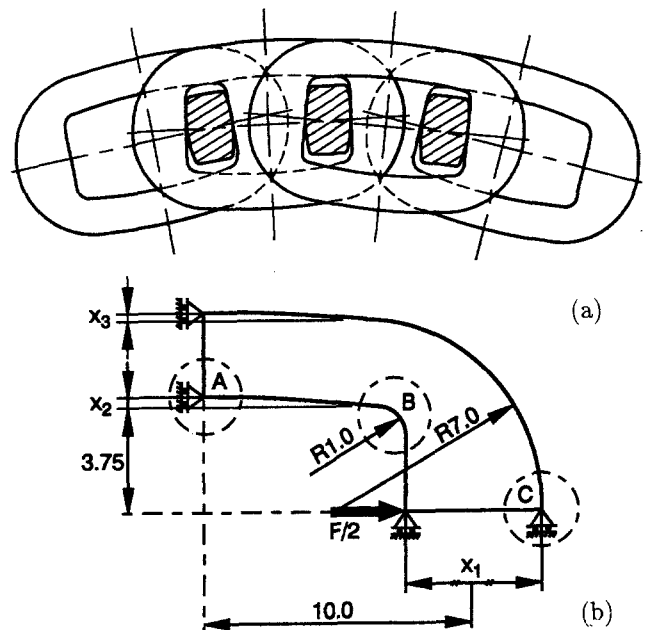


Fig. 2. (a) View of the chain, (b) one quarter of the link

In Fig. 2b three areas, A, B, and C are indicated with potentially high tensile stresses along the contour of the link. The maximum tensile stresses are denoted by σ_A , σ_B , and σ_C , respectively, and the objective was to derive regression models for these quantities. The level of the stresses can be influenced by variation of the geometry parameters x_1 , x_2 and x_3 . Hence these parameters were used as design variables.

The design variables are subject to the constructive constraints

$$4.5 \leq x_1 \leq 6.0, \quad 0.0 \leq x_2 \leq 0.6, \quad 0.0 \leq x_3 \leq 0.6. \quad (13)$$

Each design variable was varied on four levels. For the set of candidate points from which the experimental design had to be selected, all possible combinations of the levels were used resulting in $4 \times 4 \times 4 = 64$ candidate points. For each stress area a mathematical model was assumed containing 11 unknown parameters. One FEM analysis provides 4 observations, namely one value of the stress and three values of its partial derivatives

$$\sigma_i, \quad \frac{\partial \sigma_i}{\partial x_1}, \quad \frac{\partial \sigma_i}{\partial x_2}, \quad \frac{\partial \sigma_i}{\partial x_3}, \quad i = A, B, C. \quad (14)$$

Hence; a minimum of 3 ($\sim 11/4$) FEM runs was required. The number of design points, N , was chosen as 5. These 5 points were selected from the 64 candidate points using the optimal experimental design module of CADE.

The model fitting process resulted in the following regression models for the three stress quantities:

$$\begin{aligned} \sigma_A = & 540.3 - 110.1x_1 + 7.7x_1^2 + 201.6x_2 + 10.5x_2^2 - \\ & -76.3x_3^2 - 17.1x_1x_2 - 3.0x_1x_2x_3 + 12.6x_1x_3, \end{aligned} \quad (15a)$$

$$\begin{aligned} \sigma_B = & 870.9 - 199.3x_1 + 15.2x_1^2 - 263.6x_2 - \\ & -46.1x_2^2 + 41.2x_1x_3 + 3.1x_1^2x_2 - 7.0x_1^2x_3, \end{aligned} \quad (15b)$$

$$\begin{aligned} \sigma_C = & 1311.6 - 335.9x_1 + 23.7x_1^2 + 44.2x_2 + \\ & +7.7x_2^2 - 39.2x_3^2 - 0.9x_1^2x_2 + 6.0x_1x_3^2. \end{aligned} \quad (15c)$$

In order to test the capability of the procedure one hundred test points were chosen in the design space at random. The FEM observations in these points were compared with the predictions of the models (15). Figure 3 shows the distributions of the residuals.

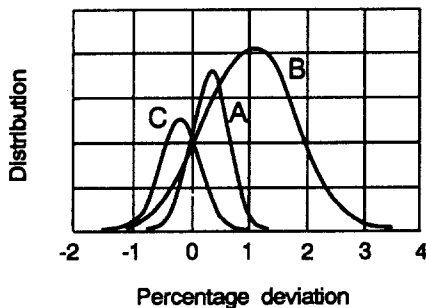


Fig. 3. Distribution of residuals of 100 random test points for the approximations in the areas A, B, and C

We may conclude that, based on as little as five FEM analyses (and using partial derivatives), regression models of good overall fit could be derived.

4.2 Optimization of a child's car seat

4.2.1 Introduction

Figure 4 shows a child strapped in a child's car seat; the seat in turn is fastened onto the back seat of the car. The child's seat and its suspension on the car seat has to be designed such that, in the case of a crash, the child is protected as much as possible.



Fig. 4. Child in a child's car seat

4.2.2 Design variables

In the present case study (Klink 1991), the design variables in Table 1 and Fig. 5 are relevant.

Table 1. Design variables of the child's seat problem

x_1	mass of child's seat
x_2	moment of inertia of child's seat
x_3	y -coordinate of center of gravity of child's seat
x_4	z -coordinate of center of gravity of child's seat
x_5	angular position of child's seat
x_6	stiffness of contact of child's seat versus car seat
x_7	hysteresis of the contact x_6
x_8	stiffness of the car seat belt
x_9	stiffness of the child's seat belt
x_{10}	backlash child's seat belt
x_{11}	junction of shoulder segment of child's seat belt
x_{12}	junction of hip segment of child's seat belt

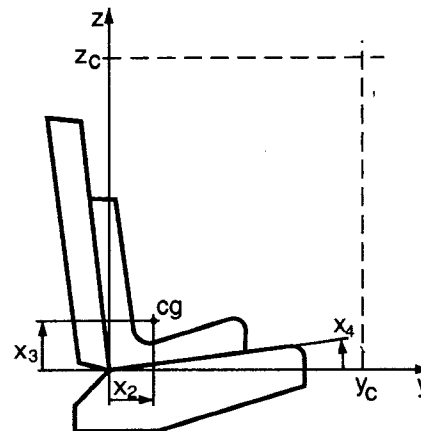


Fig. 5. Definition of some design variables

4.2.3 Crash simulations

Specifications for the design problem are extracted from the behaviour of, and the loads on a standardized child dummy, resulting from crash experiments. Because such experiments are very expensive and time-consuming, numerical crash simulations are applied. The crash simulation program MADYMO (1990) has been developed to analyse the response of the human body to a dynamic impact (Wismans 1988), and is well-suited to carry out the numerical crash simulations of the dummy in the child's seat. Figure 6 shows a sequence of situations during a specific crash simulation.

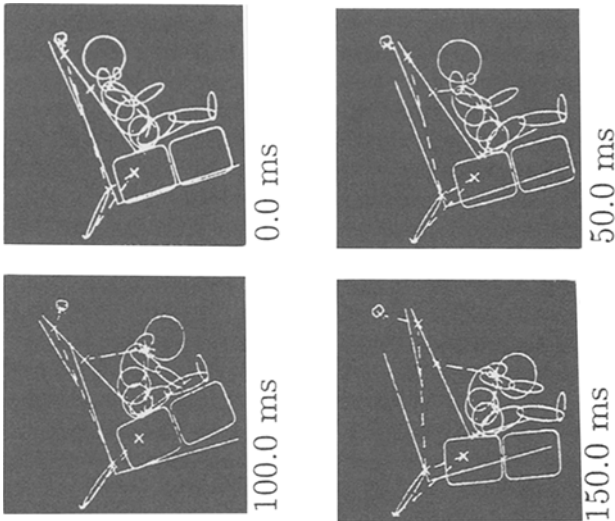


Fig. 6. Sequence of situations during a crash simulation (Courtesy of TNO Road-Vehicles Research Inst., Delft)

4.2.4 Injury parameters

Several simulation results can be applied as injury parameters. In this case study the following maximum (in the absolute sense) internal dummy loads during the simulation are used as injury parameters, see Table 2 and Fig. 7.

Table 2. Injury parameters

A1	the maximum axial force in the torso-neck joint
S1	the maximum shear force in the torso-neck joint
A2	the maximum axial force in the neck-head joint
S2	the maximum shear force in the neck-head joint
M1	the maximum bending moment in the torso-neck joint
M2	the maximum bending moment in the neck-head joint

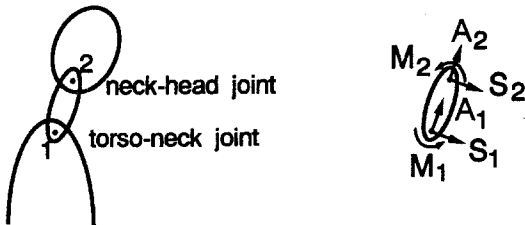


Fig. 7. Internal dummy loads used as injury parameters

4.2.5 Multi-objective function

In the design process the injury parameters have to be minimized, and therefore they serve as separate objective functions for the optimization process. However, for a reasonable design the injury parameters have to be used as the components of a multi-criterion objective function. This is accomplished in the following way.

For each injury parameter an injury probability function is defined as (see also Fig. 8)

$$p_i(q_i) = [1 + \exp(\alpha_i - \beta_i q_i)]^{-1}, \quad i = 1, \dots, 6. \quad (16)$$

The parameters α and β are thus chosen that the chance of injury at $q_i = q_{i1}$ is p_{i1} , and at $q_i = q_{i2}$ is p_{i2} , where $p_{i2} = 1 - p_{i1}$. A typical value of p_{i1} is 25%. In other words

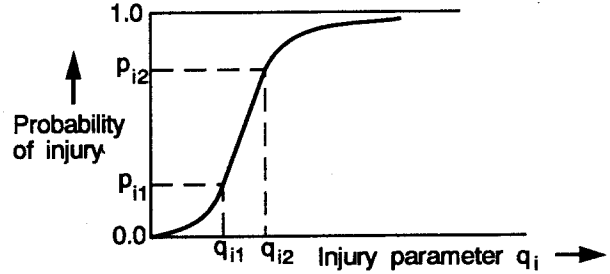


Fig. 8. Injury probability function

- if $q_i < q_{i1}$ the probability of injury $\leq 25\%$ and
- if $q_i > q_{i2}$ the probability of injury $\geq 75\%$.

Using (16), the multi-criterion objective function is simply defined as

$$F_m = \sum_{i=1}^6 p_i(q_i). \quad (17)$$

4.2.6 Constraints

In the optimization process the following constraints have to be applied.

1. The acceleration of the dummy's chest is not allowed to exceed the 55 g-level for more than 3 ms.
2. The position of the dummy's head has to stay within the bounds $y_c = 550$ mm and $z_c = 800$ mm, see Fig. 5.

4.2.7 Experimental design

To solve the optimization problem, regression models were derived for the injury parameters and for the constraints, as functions of the design variables. For all these quantities the same first order model was assumed of the form

$$q_i(\mathbf{x}) = \beta_0 + \beta_1 x_1 + \dots + \beta_{12} x_{12} + \beta_{13} x_1 x_2 + \dots + \beta_{78} x_{11} x_{12}. \quad (18)$$

For such a model it is sufficient to vary all the design variables on two levels. The set of candidate points was composed of all possible combinations of the levels, giving a number of $2^{12} = 4096$ candidate points.

Because the program MADYMO has no facilities to compute sensitivities of the response quantities, we have to select a number of design points from the set of candidate points which is larger than the number of unknown parameters, here 79 [see (18)]. It was decided to use 100 design points, defining 100 simulations to be performed using MADYMO. The program CADE was used to finding an optimal set of 100 design points.

4.2.8 Model fitting and optimization

After the simulations were carried out, the regression models were fitted using CADE. Next, the injury parameters were minimized as separate objective functions. The constraints always proved to be passive. Table 3 shows the optimization results.

From Table 3 it can be seen that the first order regression models show considerable deviations from direct MADYMO results. Therefore it was decided to perform a second model building cycle, using quadratic regression models.

Table 3. Single objective optima versus direct MADYMO results, using first order regression models

Injury parameter	Single objective optima predicted by regression models	MADYMO results for the predicted optimum point
A1 [N]	1246.00	1391.0
S1 [N]	209.00	260.0
A2 [N]	719.00	788.0
S2 [N]	999.00	1195.0
M1 [Nm]	44.00	55.0
M2 [Nm]	2.24	6.9

4.2.9 Second model building cycle

For a quadratic model the design variables have to be varied on (at least) three levels. With 12 design variables a complete design would give a far too large set of candidate points. Therefore, using the results of the first model building cycle, six design variables were fixed on favourable values. The six variables which were still allowed to vary are (see Table 1): x_2, x_3, x_4, x_5, x_8 and x_9 . Here, the following type of regression model was used:

$$q_i(x) = \beta_0 + \beta_1 x_2 + \dots + \beta_6 x_9 + \beta_7 x_2^2 + \dots + \beta_{12} x_9^2 + \beta_{13} x_2 x_3 + \dots + \beta_{27} x_8 x_9 + \beta_{28} x_2^2 x_3 + \dots + \beta_{58} x_8 x_9^2. \quad (19)$$

The set of candidate points was now chosen a complete 3^6 -design, giving 729 candidate points. Again using CADE, an optimal experimental design was selected consisting of 100 design points. Next, in these points simulations were carried out using MADYMO. The subsequent model fitting and optimization (by means of CADE) of the child's seat problem gave the results shown in Table 4.

Table 4. Single objective optima versus direct MADYMO results, using quadratic regression models

Injury parameter	Single objective optima predicted by regression models	MADYMO results for the predicted optimum point
A1 [N]	1380.0	1364.0
S1 [N]	617.0	610.0
A2 [N]	771.0	780.0
S2 [N]	1146.0	1150.0
M1 [Nm]	47.0	51.0
M2 [Nm]	7.3	7.6

Comparing Tables 3 and 4 it can be concluded that the quadratic models are much more accurate than the first order models. However, the need for quadratic models is somewhat more open to question if we consider the results of multi-objective optimization, see Table 5.

Table 5. Comparison of initial and final designs in the first and the second model building cycle using the multi-objective function

Injury parameter	Initial design	Multi-objective optimum first cycle	Initial design	Multi-objective optimum second cycle
	first cycle		second cycle	
A1 [N]	1678	1433.0	1378	1379
S1 [N]	626	548.0	767	540
A2 [N]	1009	848.0	767	769
S2 [N]	1365	1166.0	1168	1165
M1 [Nm]	71	53.0	51	51
M2 [Nm]	15	5.7	10	11

- From Table 5 the following conclusions may be derived.
- The final design in the second cycle is considerably improved compared to the initial design of the first cycle.
- The improvement in the second cycle is almost accomplished at the beginning of that cycle. Only the injury parameter S1 is substantially improved (767→540) during the multi-objective optimization run.
- The second cycle optimum is a moderate improvement compared to the first cycle optimum.

5 Conclusions

We described a method for deriving approximate analysis models as a substitute for time-consuming numerical analyses in solving structural optimization problems. Those analyses are regarded as numerical experiments from which data is extracted as input for the model building process by means of linear regression techniques. The resulting regression models can be used to define the objective function and the constraint functions of the structural optimization problem. Regression models and their use for solving an optimization problem are implemented in the program CADE.

Due to the iterative character of the model building process, regression models can be created in a cost effective way.

The proposed method has been tested and illustrated by two practical examples. The stress concentration problem is described by three design variables. Due to the application of sensitivities, accurate regression models could be derived from very few (five) FEM analyses. The child's car seat problem showed 12 design variables. Through the use of regression models an optimization problem could be defined and solved using the program CADE, whereas the crash simulation program MADYMO does not have optimization facilities such as computation of sensitivities.

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Received Oct. 4, 1991