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A Modular Algorithm for Dynamic Design of Large-Scale Experiments

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Abstract: Large-scale experiments usually run on carriers (e.g., test benches in technical industry) which may have individual limitations concerning the setting of certain design factors. Consequently, this leads to restricted factor ranges for single realizations of the experiment. This article discusses a modular algorithm for the generation of a D-optimal design based on the point exchange principle. For single experiments, fixed and partly fixed factor settings can be considered. The term *dynamic* refers to the possibility of experiment-specific design adaptations.

Zusammenfassung: Aufwendige technische Versuche laufen üblicherweise auf Trägern (z.B. Prüfständen), welche hinsichtlich der Einstellbarkeit von zu studierenden Faktoren individuell eingeschränkt sind. Die Menge der möglichen Positionen im Faktorraum variiert von Träger zu Träger. Dieser Artikel diskutiert einen modularen Austausch-Algorithmus für das Erstellen eines D-optimalen Designs. Dabei können Experimente mit fixierten und teilweise fixierten Faktoreinstellungen berücksichtigt werden. Die Bezeichnung *dynamic* bezieht sich auf die Möglichkeit der versuchsspezifischen Designerweiterung.

Keywords: Computer Generated Designs, Adaptive Optimal Design, Life Time Experiments.

1 Introduction

A large-scale experiment usually is carried out to investigate several properties of a complex object. E.g., the automotive industry provides typical practical problems.

1. The wear behavior of an engine at several positions (piston, cylinder head, bushings etc.) has to be compared with the performance of the forerunner model.
2. A validation program for a vehicle should be designed. The experiments have to be carried out under (multivariate) customer-representative load. Various requirements regarding several subsystems have to be considered.
3. The functionality of an exhaust gas aftertreatment system has to be optimized. A couple of component variants are available, several critical usage conditions have to be borne in mind. Existing experiment carriers dedicated to engine testing should be used as far as possible.
4. A number of physical parameters cause various failure modes of a sensor system during usage. Per mode, a *damage model* should be created dependent on real-world stress conditions spanning the *usage space.*

Such experimental programs are expensive in terms of time and money. Several simultaneous targets, individual restrictions of experiment carriers as well as limited resources of different parts or components of the object require design of large-scale experiments to

- provide designs with a given number of (initial) experiments,
- inspect factors which may not be varied independently,
- examine experiments already carried out before creating the design,
- consider experiments with a subset of factor settings a priori fixed,
- adapt the design during the experimentation.

These requirements demand rather computer generated designs than classical designs as described in textbooks like Montgomery (2005). Relevant concepts for computer-generation of designs are *point exchange algorithms* (see, e.g., Dykstra, 1971, Mitchell, 1974a, Mitchell, 1974b, Cook and Nachtsheim, 1980, Galil and Kiefer, 1980, Johnson and Nachtsheim, 1983) and *genetic algorithms* (compare Heredia-Langner, Carlyle, Montgomery, Borror, and Runger, 2003).

We found that the point exchange approach is very flexible to be suitable for designs with fixed and partly fixed experimental settings. Therefore, it will be used as basis for the development of the dynamic design algorithm.

In Section 2 we introduce the general notation, the classical linear model, the accelerated failure time model, a general life time model, and mention also some design criteria. The modular algorithm for dynamic design of experiments (DDoE) is established in Section 3 and specific recommendations concerning configuration matters are given in Section 4. In Section 5, our proposed algorithm is compared with standard DoE tools and finally, in Section 6, applied to life time experiments motivated by practical requirements.

2 Concepts for Experimental Design

2.1 Notation

Suppose $g(\mathbf{x}) = (g_1(\mathbf{x}), \dots, g_m(\mathbf{x}))'$ to be m linear independent functions on a compact space $\Omega_\mathbf{x}$ which is a compact set in the Euclidean space of dimension $m_0 \leq m$. A design measure or weight is a probability measure $\chi(\mathbf{x})$ on $\Omega_\mathbf{x}$ with $\int_{\Omega_\mathbf{x}} \chi(d\mathbf{x}) = 1$. A finite design is given as

$$\begin{pmatrix} g(\mathbf{x}_1) & \dots & g(\mathbf{x}_n) \\ \chi(\mathbf{x}_1) & \dots & \chi(\mathbf{x}_n) \end{pmatrix} ,$$

where $\mathbf{x}_1, \dots, \mathbf{x}_n \in \Omega_\mathbf{x}$. If $n\chi(\mathbf{x}_j) \in \mathbb{N} \; \forall \; j \in \{1, \dots, n\}$, the design is discrete and will be denoted as $(n \times m)$-matrix $\mathbf{X}$ containing the series of experiments $g'(\mathbf{x}_j)$ with $(\mathbf{x}_j : j = 1, \dots, n)$. To find a design providing maximum information under given boundary conditions, first let

$$\mathbf{M}(\chi) = \left(\int_{\Omega_\mathbf{x}} g_i(\mathbf{x}) g_k(\mathbf{x}) \chi(d\mathbf{x}) \right)_{i,k=1,\dots,m} .$$

In the special case of a discrete design we have $\chi_n = 1/n$ for each experiment or point $\mathbf{x}_j$ and hence $\mathbf{M}(\chi_n) = \mathbf{X}'\mathbf{X}/n$, where $\mathbf{M}$ is the moment matrix.

2.2 Model Assumptions

Consider the linear model $y = g'(\mathbf{x})\boldsymbol{\theta}_{\mathbf{x}} + \varepsilon$ with response $y \in \mathbb{R}$ and m_0-vector $\mathbf{x}$ of factors extended by the function g carrying the structure of m effects. $\boldsymbol{\theta}_{\mathbf{x}} = (\theta_1, \ldots, \theta_m)'$ is the m-parameter vector and $\varepsilon \sim \mathbf{P}_\varepsilon(0, \sigma)$ is the error term following a known location-scale distribution with unknown scale σ. The corresponding matrix notation for n independent realizations of y, $\mathbf{y} = \mathbf{X}\boldsymbol{\theta}_{\mathbf{x}} + \boldsymbol{\varepsilon}$, contains the discrete design $\mathbf{X}$ as $(n \times m)$-model matrix with $n \geq m$ and rank$(\mathbf{X}) = m$.

The Classical Linear Model

Let $\mathbf{P}_\varepsilon = \mathbf{N}(0, \sigma^2)$, i.e. a normal distribution with variance σ^2 independent of $\mathbf{x}$. For $\mathbf{X}$ and an uncensored response $\mathbf{y}$ we have $\boldsymbol{\varepsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}_{\mathbf{x}})/\sigma$ with the total likelihood $L(\boldsymbol{\theta}_{\mathbf{x}}, \sigma) \propto \prod_{j=1}^{n} f(\varepsilon_j)/\sigma$ where $f(\varepsilon_j)$ is the p.d.f. of the error term. In this case, the maximum likelihood estimator for $\boldsymbol{\theta}_{\mathbf{x}}$ is identical to the ordinary least squares estimator $\hat{\boldsymbol{\theta}}_{\mathbf{x}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ with $\mathrm{E}(\hat{\boldsymbol{\theta}}_{\mathbf{x}}) = \boldsymbol{\theta}_{\mathbf{x}}$ and covariance matrix $\boldsymbol{\Sigma}_{\hat{\boldsymbol{\theta}}_{\mathbf{x}}} = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$ where its inverse is known as the information matrix $\mathbf{I}_{\boldsymbol{\theta}_{\mathbf{x}}} = (\mathbf{X}'\mathbf{X})/\sigma^2$ (see, e.g., Fahrmeir, Hamerle, and Tutz, 1996).

The Accelerated Failure Time Model

If the response is a life time random variable $t \in \mathbb{R}^+$, we may observe also incomplete, i.e. right-censored, data. Then, for a maximum possible duration of the experiment $t_r > 0$, we observe $y_j = \min(\tau(t_r), \tau(t_j))$ with $\delta_j = 1$ if $t_j \leq t_r$ and $\delta_j = 0$ otherwise, where τ is a monotonically increasing transformation. In general, the correlation between the parameter estimators increases with increasing proportion of censored data. Haselgruber (2007) investigated this property in detail for the intercept model ($y = \theta + \varepsilon$) with different distributions $\mathbf{P}_\varepsilon$. Assuming a sufficient proportion of exact life time data, the total likelihood is

$$L(\boldsymbol{\theta}_{\mathbf{x}}, \sigma) \propto \prod_{j=1}^{n} \left(\frac{1}{\sigma} f(\varepsilon_j)\right)^{\delta_j} S(\varepsilon_j)^{1-\delta_j}$$

with $\boldsymbol{\varepsilon} = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}_{\mathbf{x}})/\sigma$ and survival function $S(\varepsilon) = \int_\varepsilon^\infty f(\varepsilon)d\varepsilon$. The information matrix of $\boldsymbol{\theta}_{\mathbf{x}}$ is

$$\mathbf{I}_{\boldsymbol{\theta}_{\mathbf{x}}} = \mathrm{E}\left(-\frac{\partial^2 \log L(\boldsymbol{\theta}_{\mathbf{x}}, \sigma)}{\partial\boldsymbol{\theta}_{\mathbf{x}}\partial\boldsymbol{\theta}'_{\mathbf{x}}}\right) = \mathrm{E}\left(\frac{1}{\sigma^2}\sum_{j=1}^{n} a_j \mathbf{x}_j \mathbf{x}'_j\right) \tag{1}$$

with $a_j = \delta_j \partial^2 \log h(\varepsilon_j)/(\partial\varepsilon)^2 - \partial h(\varepsilon_j)/\partial\varepsilon$ and $h(\varepsilon) = f(\varepsilon)/S(\varepsilon)$.

Note that here $\mathbf{P}_\varepsilon$ could be any location-scale distribution with σ independent of $\mathbf{x}$. Expression (1) is equal to $\mathrm{E}(a)(\mathbf{X}'\mathbf{X})/\sigma^2$ if $a = a_j \,\forall\, j \in \{1, \ldots, n\}$. If there is no a priori knowledge on the relation between y and $\mathbf{x}$ – which is usually the case for large-scale experiments – we assume $g_1(\mathbf{x}) = 1$ and the null hypothesis $H_0 : \theta_2 = \cdots = \theta_m = 0$. Then we have $a_j = a \,\forall\, j$ and $\mathbf{I}_{\boldsymbol{\theta}_{\mathbf{x}}} \propto \mathbf{M}$. For $\mathbf{P}_\varepsilon = \mathbf{N}(0, \sigma^2)$, the transformed response $y = \tau(t) = \log(t)$ leads to a log-normal distribution of t. For $\mathbf{P}_\varepsilon = \mathbf{sEv}(0, \sigma)$, i.e. a smallest extreme value distributed error variable ε and $y = \log(t)$, we have a Weibull distribution for t. The book of Fahrmeir et al. (1996) contains further details on accelerated failure time models.

A General Life Time Model

For known distributions $\mathbf{P}_\varepsilon$ with some unknown parameters, the maximum likelihood method provides minimum-variance estimators. If $\mathbf{P}_\varepsilon$ is not known at all or the data contain unobserved heterogeneity, the maximum likelihood method is not applicable. In these cases, least squares estimation provides robust results and should be used therefore. Buckley and James (1979) propose least squares estimation for right-censored response variables. They define the pseudo random variable

$$y_j^* = \delta_j y_j + (1-\delta_j)\mathrm{E}(\tau(t_j)|\tau(t_j) > y_j)\,,$$

describe the iterative estimation of $\mathrm{E}(\tau(t_j)|\tau(t_j) > y_j)$, and propose $\hat{\boldsymbol{\theta}}_{\mathbf{x}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}^*$. Smith (2002) describes the estimation procedure and gives further references. As far as there is no a priori information on the distribution of the censored data on $\Omega_{\mathbf{x}}$ and thus, their influence on the information of the design is unknown for a given t_r, we will assume complete data for optimizing a design. At least in this case we have with $\mathbf{I}_{\boldsymbol{\theta}_{\mathbf{x}}} \propto (\mathbf{X}'\mathbf{X})$.

2.3 Design Criteria

Important contributions to the theory of optimum designs are due to Fedorov (1972), Wynn (1972), and Kiefer (1974). Chernoff (1962) proposes a method to design accelerated life time experiments for univariate parameter estimation. Additionally, the books of Pukelsheim (1993), Schwabe (1996), and the monograph of Fedorov and Hackl (1997) extend the theory to more general models and criteria. The moment matrix $\mathbf{M}$ of a discrete design as introduced above is a suitable basis for design criteria, because it is proportional to the information matrices discussed in this chapter. Subsequently, the widely-used determinant criterion $D = \det(\mathbf{M}^{-1})^{1/m}$, measuring the generalized variance of $\hat{\boldsymbol{\theta}}_{\mathbf{x}}$, will be applied. Another criterion of interest is $G = \sup_{\mathbf{x}\in\Omega_{\mathbf{x}}} \mathbf{x}'\mathbf{M}^{-1}\mathbf{x}/n$ which quantifies the maximum prediction variance in $\Omega_{\mathbf{x}}$. Pukelsheim (1993) shows the theoretical optimum of G as m/n which leads to the definition of G-efficiency as $G_e = m/(nG)$.

3 An Algorithm for Dynamic Design of Experiments

The requirements regarding fixed and partly fixed experiment settings demand the use of the point exchange concept with the focus of optimization on discrete designs. To evaluate their performance they will be compared with continuous optimal designs. In general, the latter designs have better performance since they are not limited to design weights with restrictions $n\chi \in \mathbb{N}$, although in applications the weights have to be rounded correspondingly.

Our DDoE algorithm consists of four modules which will be, by default, performed sequentially and iteratively:

- Module 1, **design space:** creating the set of candidate points
- Module 2, **initialization:** setting up the start design matrix
- Module 3, **optimization:** finding an initial D-optimal design
- Module 4, **adaptation:** extending the design

The advantage of the modular concept is that the algorithm may be started with any module. The following sections describe the individual modules in detail.

3.1 The Set of Candidates

The set of candidates $\Xi_{\mathbf{x}}$ consists of $\nu \geq m$ points representing experiment settings distributed on the design space $\Omega_{\mathbf{x}}$. The required density of the points depends on the model assumed. At least all corner points of $\Omega_{\mathbf{x}}$ should belong to $\Xi_{\mathbf{x}}$. The density in dimension j of $\Omega_{\mathbf{x}}$, $j = 1, \ldots, m_0$, depends on the level of measurement of factor x_j. For quantitative factors x_j there have to be at least $(d_{m,j} + 1)$ different points if $d_{m,j}$ denotes the highest degree of x_j in the model. Here, they will be equidistant on the interval $[x_{\min}; x_{\max}]$ occupying the interval bounds. For the investigation of polynomial models, a non-uniform pattern of points may be considered (compare, e.g., Wynn, 1972).

In addition, a $(\nu \times 1)$-candidate alternative group vector $\boldsymbol{\xi}_A$ has to be established. Exactly one member from each alternative group has to be included in the optimized design. In $\boldsymbol{\xi}_A$, each alternative group will be identified by a unique integer value. The $(\nu \times 1)$-candidate status vector $\boldsymbol{\xi}_S$ indicates whether a certain experiment $\mathbf{x}_k$, $k = 1, \ldots, \nu$, has to be a member of the optimized design (i) obligatory ($\xi_{Sk} = 1$) or (ii) if it may be replaced during the exchange algorithm ($\xi_{Sk} = 0$) by any of the candidates. For each member of an alternative group, the candidate status is 1.

DDoE Algorithm Module 1: Creating the Set of Candidate Points

1. Create exchangeable candidates
   (a) Define the mesh density ρ_j for each factor x_j, $j = 1, \ldots, m_0$. This is the maximum number of different attitudes per factor investigated in the design. For qualitative factors, it is the number of levels, for quantitative factors x_j, a lower bound for ρ_j is $d_{m,j} + 1$.
   (b) Create a full factorial design based on the mesh densities ρ_j. If there are $m_n \geq 0$ quantitative and $m_l \geq 0$ qualitative factors, the full factorial design contains $\nu_0^+ = \prod_{j=1}^{m_0} \rho_j$ experiments (points) where $m_0 = m_n + m_l > 0$.
2. Set restrictions
   (a) If there are any multiple factor restrictions, remove all ν_r points outside the restricted design space. Then, the number of candidates in the set $\Xi_{\mathbf{x}}$ changes to $\nu_0 = \nu_0^+ - \nu_r$ candidates. If there are no multiple restrictions, consequently $\nu_r = 0$.
   (b) If there are any experiments with partly fixed factor settings to consider in the optimized design, i.e. $n_f > 0$, each of them may be varied in a subspace $\Omega_{\mathbf{x}_{\mathbf{k}_j}} \subset \Omega_{\mathbf{x}}$, $j = 1, \ldots, n_f$. $\mathbf{k}_j$ denotes the index set of factors which are not fixed for experiment j. Add per experiment j all distinct candidate points $\nu_{fj} \geq 2$ in $\Omega_{\mathbf{x}_{\mathbf{k}_j}}$ to $\Xi_{\mathbf{x}}$ which sum up to $\nu_f = \sum_{j=1}^{n_f} \nu_{fj} \geq 2n_f$ candidates.
   (c) If there are any experiments mandatory for the optimized design , i.e. $n_e > 0$ fixed experiments, add them to the set of candidates such that $\Xi_{\mathbf{x}}$ contains $\nu = \nu_0 + \nu_f + n_e$ runs.
3. Identify properties of candidates

(a) Set up the $(\nu \times 1)$-alternative group vector $\boldsymbol{\xi}_A$ which contains a unique integer value for each candidate except those in an alternative group $1, \ldots, n_f$. Assign one integer value to all candidates within the same alternative group. For computational purposes, the integer values should be assigned in ascending order.

(b) Set up the $(\nu \times 1)$-status vector $\boldsymbol{\xi}_S$ which contains value 1 for each of the ν_f and n_e experiments and value 0 for all other candidates.

4. According to the model $y = g'(\mathbf{x})\boldsymbol{\theta}_{\mathbf{x}} + \varepsilon$, use g to extend the candidate set such that each of the m model effects will be represented by a column of $\Xi_{\mathbf{x}}$.

Module 1 provides a set of candidate points fulfilling the boundary conditions and ready to be selected for the initial design.

3.2 An Initial Design

Module 2 contains the search for a design with a non-singular moment matrix as starting point for the subsequent optimization module. After selecting n_e mandatory and n_f partly fixed candidates, n_0 points out of $\Xi_{\mathbf{x}}$ will randomly be selected such that $(m \leq n_e + n_f + n_0 \leq n)$. If $n_e + n_f + n_0 < n$, the remaining $n - (n_e + n_f + n_0)$ points are the results of a systematic selection due to optimizing the determinant criterion. The design size n depends on the model and has as lower bound m since the model matrix $\mathbf{X}$ requires full column rank.

DDoE Algorithm Module 2: Setting up the Start Design

1. Select constrained candidates

   (a) If $n_e > 0$, initialize the start model matrix $\mathbf{X}$ with the n_e fixed (mandatory) experiments, initialize the design status vector $\boldsymbol{\zeta}_S = \mathbf{1}_{n_e}$ and the alternative group vector $\boldsymbol{\zeta}_A$ with corresponding values of $\boldsymbol{\xi}_A$.

   (b) If $n_f > 0$, select one candidate randomly from each alternative group $1, \ldots, n_f$ and concatenate it to the model matrix $\mathbf{X}$. Extend the design status vector as $\boldsymbol{\zeta}_S = \mathbf{1}_{n_e+n_f}$. Extend $\boldsymbol{\zeta}_A$ by the group identifications contained in $\boldsymbol{\xi}_A$.

2. Select exchangeable candidates and check design

   (a) Add $n_0 \leq n - n_e - n_f$ randomly selected points from the ν_0 exchangeable points of $\Xi_{\mathbf{x}}$ to $\mathbf{X}$ and extend the design status vector to $\boldsymbol{\zeta}_S = \begin{pmatrix} \mathbf{1}_{n_e+n_f} \\ \mathbf{0}_{n_0} \end{pmatrix}$ as well as $\boldsymbol{\zeta}_A$ by the corresponding n_0 group identifications of $\boldsymbol{\xi}_A$.

   (b) Ensure that $n_e + n_f + n_0 \geq m$, compute $\mathbf{M}_n = \mathbf{X}'\mathbf{X}$, and check whether $\mathbf{M}_n$ is regular. In case of singularity, repeat the random sampling of n_0 points until $\mathbf{M}_n$ becomes regular. If necessary, increase n_0 (and possibly n) or go back to module 1 and adapt the candidate set.

3. Fill up to design size required

   (a) Compute $\det(\mathbf{M}_n)$ and $\mathbf{M}_n^{-1}$. If $n_e + n_f + n_0 = n$, terminate this module.

   (b) Add the candidate $\mathbf{x}'_k$, $k = 1, \ldots, \nu_0$, from $\Xi_{\mathbf{x}}$ which maximizes $\mathbf{x}'_k\mathbf{M}_n^{-1}\mathbf{x}_k$.

   (c) Set $\mathbf{X} = \begin{pmatrix} \mathbf{X} \\ \mathbf{x}'_k \end{pmatrix}$, $\boldsymbol{\zeta}_S = \begin{pmatrix} \boldsymbol{\zeta}_S \\ 0 \end{pmatrix}$, and $\boldsymbol{\zeta}_A = \begin{pmatrix} \boldsymbol{\zeta}_A \\ \xi_{Ak} \end{pmatrix}$.

4. Repeat step 3 until the design size n is reached.

Based on the start design, the optimum will be searched by point exchange. This algorithmic principle concentrates only on candidates j with $\zeta_j = 0$, i.e. exchangeable candidates, or members of an alternative group. In the latter case, only candidates within the same alternative group will be considered as exchangeable candidates.

The Exchange Delta Function

To save computation time in the optimization routine, Fedorov (1972) proposed an iterative computation of $\det(\mathbf{M}_n)$ and $\mathbf{M}_n^{-1}$. If $\mathbf{x}$ is a point to be augmented to $(+)$ or removed from $(-)$ $\mathbf{X}$, then

$$\begin{aligned} \det(\mathbf{M}_n \pm \mathbf{x}'\mathbf{x}) &= \det(\mathbf{M}_n)(1 \pm \mathbf{x}'\mathbf{u}) , \\ (\mathbf{M}_n \pm \mathbf{x}'\mathbf{x})^{-1} &= \mathbf{M}_n^{-1} \mp \mathbf{u}\mathbf{u}'/(1 \pm \mathbf{x}'\mathbf{u}) \end{aligned}$$

and $\mathbf{u} = \mathbf{M}_n^{-1}\mathbf{x}$. Let $\mathbf{x}_0$ be the point taken out and $\mathbf{x}_1$ be the point taken into the design, then

$$\begin{aligned} \det(\mathbf{M}_n + \mathbf{x}_1\mathbf{x}_1' - \mathbf{x}_0\mathbf{x}_0') &= \det(\mathbf{M}_n)(1 + \Delta(\mathbf{x}_0, \mathbf{x}_1)) \qquad \text{where} , \\ \Delta(\mathbf{x}_0, \mathbf{x}_1) &= \mathbf{x}_1'\mathbf{u}_1 - \mathbf{x}_0'\mathbf{u}_0 + (\mathbf{x}_1'\mathbf{u}_0)^2 - \mathbf{x}_1'\mathbf{u}_1\mathbf{x}_0'\mathbf{u}_0 . \end{aligned} \tag{2}$$

DDoE Algorithm Module 3: Finding a D-Optimal Design

1. Initialize optimization measures
   (a) Compute $\det(\mathbf{M}_n)$ and $\mathbf{M}_n^{-1}$ for the given model matrix $\mathbf{X}$.
   (b) $\forall\, \mathbf{x}_k : k = 1, \ldots, \nu - n_e$, initialize the information factor $\omega_k = \mathbf{x}_k'\mathbf{M}_n^{-1}\mathbf{x}_k$.
2. Find most efficient point exchange
   (a) Find simultaneously a point $\mathbf{x}_j$ in the current n-point design $\mathbf{X}$ and a point $\mathbf{x}_k$ in the candidate set $\Xi_{\mathbf{x}}$ which maximize $\Delta(\mathbf{x}_j, \mathbf{x}_k)$ calculated by (2). The index j refers to points of the design $\mathbf{X}$, the index k to that of the candidate set $\Xi_{\mathbf{x}}$.
      i. Set $\Delta_{\text{act}} = 0$.
      ii. $\forall\, \mathbf{x}_j : j = n_e + 1, \ldots, n$, compute the information factor $w_j = \mathbf{x}_j'\mathbf{M}_n^{-1}\mathbf{x}_j$.
      iii. $\forall\, j \in (n_e + 1, \ldots, n)$
         - Set $\mathbf{k} = (1, \ldots, \nu_0)$
         - If $(\exists\, k \in (1, \ldots, \nu) : \xi_{Ak} = \zeta_{Aj}\ \&\ \mathbf{x}_j \neq \mathbf{x}_k)$, set $\mathbf{k} = (k : \xi_{Ak} = \zeta_{Aj})$
         - $\forall\, k \in \mathbf{k}$
           – If $\omega_k - w_j > \Delta_{\text{act}}$, compute $\Delta(\mathbf{x}_j, \mathbf{x}_k)$
           – If $\Delta(\mathbf{x}_j, \mathbf{x}_k) > \Delta_{\text{act}}$, set $\Delta_{\text{act}} = \Delta(\mathbf{x}_j, \mathbf{x}_k)$, $j_{\text{out}} = j$, $k_{\text{in}} = k$.
   (b) Replace $\mathbf{x}_{j_{\text{out}}}$ by $\mathbf{x}_{k_{\text{in}}}$ in $\mathbf{X}$ and update $\boldsymbol{\zeta}_A$.
   (c) Update $\det(\mathbf{M}_n)$, $\mathbf{M}_n^{-1}$, and $\omega_k : k = 1, \ldots, \nu - n_e$.
3. Repeat step 2 until $\Delta(\mathbf{x}_j, \mathbf{x}_k)$ is less than ϵ (e.g., $\epsilon = 10^{-5}$).
4. Compute D based on $\mathbf{X}$ and export the results.

The evaluation of $\Delta(\mathbf{x}_j, \mathbf{x}_k)$ is required only in those cases where the sum of its first two terms is larger than Δ_{act}, the currently largest value of $\Delta(\mathbf{x}_j, \mathbf{x}_k)$ obtained at a particular point. The *Cauchy-Schwarz inequality* shows that the sum of the last two terms of (2) is always less than or equal to 0.

Following a recommendation of Nguyen and Piepel (2005), the modules 2 and 3 should be repeated several times to reduce the risk of reaching a sub-optimal solution caused by the n_0 randomly selected points.

3.3 Extension of an Existing Design

This routine extends an existing design of size n by $n_a \geq 1$ experiments such that the new design of size $(n + n_a)$ is D-optimal regarding the existing design and $\Xi_{\mathbf{x}}$.

A specific part of the point exchange principle is also suitable for the dynamic extension of the design. Then, the objective may be to add a new experiment to the existing design under given boundary conditions to reach a new D-optimal design.

DDoE Algorithm Module 4: Extending the Design

1. Identify boundary conditions for design extension
   (a) Identify the experiment $\mathbf{x}_j$ to be replaced and the restrictions for the extension. If the design has to be extended without any specific replacement of a point, the number of experiments n_a to add has to be defined.
   (b) Identify the index set $\mathbf{k}$ of all candidate experiments appropriate for extension or for replacing $\mathbf{x}_j$, i.e. $\mathbf{k} = (k : \xi_{Ak} = \zeta_{Aj}) \Leftrightarrow (\exists\, k \in (1, \ldots, \nu) : \xi_{Ak} = \zeta_{Aj} \;\&\; \mathbf{x}_j \neq \mathbf{x}_k)$. By default, $\mathbf{k} = (1, \ldots, \nu_0)$. For single candidates $k \in \mathbf{k}$ not appropriate, set $\xi_{Sk} = \xi_{Sk} - 2$.
2. Initialize optimization measures
   (a) Compute $\mathbf{M}_n^{-1}$ for the existing design $\mathbf{X}$.
   (b) $\forall\, \mathbf{x}_k : k \in \mathbf{k} \;\&\; \xi_{Sk} \geq 0$, compute the information factor $\omega_k = \mathbf{x}_k' \mathbf{M}_n^{-1} \mathbf{x}_k'$.
3. Extend the design
   (a) Select the candidate $\mathbf{x}_{\text{opt}}$ with $\omega_{\text{opt}} = \max_{k \in \mathbf{k} \;\&\; \xi_{Sk} \geq 0}(\omega_k)$.
   (b) Set $\mathbf{X} = \begin{pmatrix} \mathbf{X} \\ \mathbf{x}_{\text{opt}}' \end{pmatrix}$, build the new corresponding model matrix $\mathbf{X}$, and update $\boldsymbol{\zeta}_A$ as well as $\boldsymbol{\zeta}_S$. If any values $\xi_{Sk} < 0$, $k \in \mathbf{k}$, replace them by $\xi_{Sk} = \xi_{Sk} + 2$.
   (c) If $n_a > 1$, repeat steps 1 (b) to 3 until the model matrix $\mathbf{X}$ has $n + n_a$ rows.
4. Compute D based on $\mathbf{X}$ and export the results.

All requirements stated in the introduction can be handled with the algorithm presented above. For the dynamic aspects of enlarging the design by rows (i.e. additional experiments) or by columns (i.e. additional factors), the candidate set has to be adapted accordingly.

4 Configuration

To apply the dynamic design algorithm, several parameters have to be set in advance. These are not only controllable algorithmic parameters but also parameters driven by properties of the specific application. Thus, the configuration of the DDoE algorithm is a robust design problem. The target is to provide optimal designs with respect to given boundary conditions, as far as possible independent of the properties of the specific application.

Computer simulation experiments (CSE) have been carried out to find an optimal configuration of the DDoE algorithm. Due to the random selection of n_0 points in module 2, the simulation experiments are stochastic rather than deterministic. For the CSE parameters, Table 1 shows the ranges defined due to practical relevance and experience. A lower bound for the number of experiments n is n_m dependent on m_0 (m_n, m_l) and d_m. Usually, also an upper bound for n is given by economical reasons. As a consequence, the number of factors and the degree of the statistical model (degree 1 for linear models and degree 2 for linear models with second order interactions) are restricted. Three levels are assumed for each qualitative factor. Since the influence of partly fixed points on the design quality is between that of fixed and fully exchangeable candidates, in this study we use no fixed candidates ($n_f = 0$). In case of no multiple factor restrictions we set $r_m = 0$. Otherwise, for $r_m = 1$, the area $x_1 + x_2 > 1$ of the standardized factors x_1, x_2 will be excluded from $\Omega_{\mathbf{x}}$.

Table 1: Ranges of the CSE parameters for configuration of the dynamic design algorithm. Note that n, n_e, and n_0 are dependent factors.

Label	CSE Parameter	Type	Controllable	Range
m_0	no. of factors	quant.	no	$\{2; 4\}$
m_l	no. of qualitative factors	quant.	no	$\{0; 1\}$
r_m	multiple factor restrictions	qual.	no	$\{0; 1\}$
d_m	degree of model	qual.	no	$\{1; 2\}$
ρ_n	mesh density	quant.	yes	$\{3; 5\}$
n	no. of experiments	quant.	yes	$\{n_m; 2n_m\}$
n_e	no. of fixed experiments	mixture	no	$\{0; n_m/2\}$
n_0	no. of randomly selected points	mixture	yes	$\{n_m/2 \dots 2n_m\}$
n_{rep}	no. of repetitions	quant.	yes	$\{2^4; 2^8\}$

Table 2 shows six different decompositions of n which have been investigated for all combinations of the CSE parameters $\rho_n, n_{\text{rep}}, m_0, m_l, r_m$, and d_m. This leads to $n_{\text{CSE}} = 384$ simulation experiments, i.e., generate 384 times either 16 or 256 designs and compute for each optimized design a desirability value $W \in (0; 1)$ as a function of D and G to consider also the aspect of prediction variance. In each simulation experiment select the design with maximum W. The DDoE module 4 will not be investigated in this study since its optimization part is similar to that of module 3. Haselgruber (2007) contains a detailed description of this CSE study.

Linear models including interactions between controllable parameters and noise factors have been fitted for desirability expectation $\mathrm{E}(W)$ and variance $\mathrm{V}(W)$. The robust

Table 2: Decomposition of n into n_e, n_0, and points to be added systematically to the start design in module 2. For odd n_m use $n_e = \lfloor n_m/2 \rfloor$ and complement n_0 correspondingly.

n	n_e	n_0	$n - n_e - n_0$
n_m	$n_m/2$	$n_m/2$	0
n_m	0	n_m	0
$2n_m$	$n_m/2$	$3n_m/2$	0
$2n_m$	$n_m/2$	$n_m/2$	n_m
$2n_m$	0	n_m	n_m
$2n_m$	0	$2n_m$	0

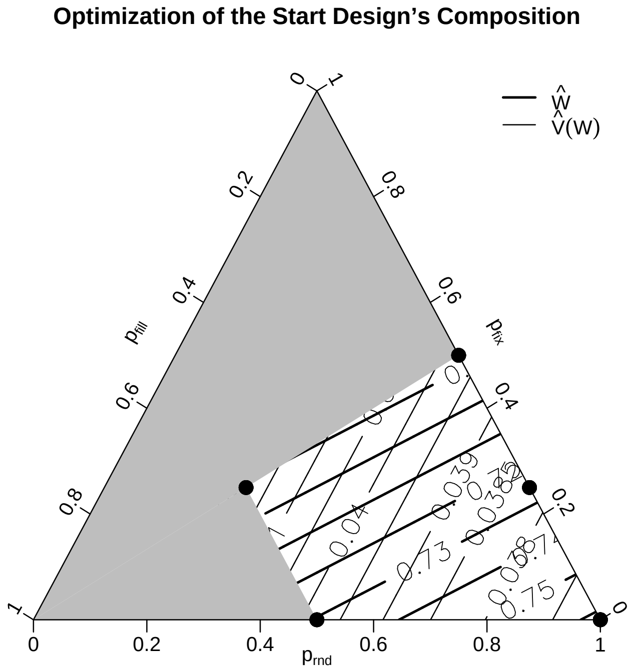

Figure 1: Estimated desirability $\hat{W}$ and estimated variance of W for the design size n decomposed into n_e, n_0, and $n - n_e - n_0$ expressed as $p_{\text{fix}} = n_e/n$, $p_{\text{rnd}} = n_0/n$, and $p_{\text{fill}} = 1 - p_{\text{fix}} - p_{\text{rnd}}$ in a trilinear coordinate system. All other CSE parameters have been set to 0 in their standardized form. Compare also Table 2.

setting of the CSE parameters will be found by a simultaneous search for $\sup_\Omega W$ and $\inf_\Omega \mathrm{V}(W)$ in the CSE parameter space Ω. The results show how to calibrate the dynamic design algorithms by the controllable parameters.

All noise factors investigated have influence on the desirability and interact with controllable factors. E.g., as expected, a qualitative factor (m_l), multiple factor restrictions (r_m), and a higher degree (d_m) of the assumed model have a negative influence on W. The impact of these noise factors m_l, r_m, and d_m on the response can be reduced by an increased number of experiments n. The number of randomly selected points n_0 in DDoE module 2 should be as high as possible to increase the expectation of the desirability as well as to minimize its variance (compare Figure 1).

5 Comparison of the DDoE with other Algorithms and some DoE Software Tools

In general, the results of any optimization algorithm may be influenced by its fine tuning and coding, so this section has not to be interpreted as a benchmark between DoE software tools. The aim is to validate the results of the DDoE algorithm for one representative example.

Without claim of completeness, the following tools and algorithms have been compared with the DDoE algorithm modules 2 and 3: DesignExpert version 7.0.1, MATLAB version 6.5, Minitab version 14.13, MODDE version 7.0.0.1, SAS/QC version 6.1, STATISTICA version 7.1, a fast Fedorov exchange algorithm (FFEA, see Nguyen and Piepel, 2005), a genetic algorithm (see Heredia-Langner et al., 2003), and the design package AlgDesign version 1.0.7 of the statistical programming language R, which provides continuous designs (see Wheeler, 2004).

The modules 1 and 4 of the DDoE algorithm provide the flexibility required for the design of large-scale life time experiments and are not of interest here. For the comparison, a well-known example mentioned by Heredia-Langner et al. (2003) as well as Nguyen and Piepel (2005) has been used. There are two quantitative factors x_1 and x_2, both scaled to $[-1; 1]$ and restricted by

I: $x_1 + x_2 \leq 1$ and

II: $x_1 + x_2 \geq -\frac{1}{2}$.

The candidate set has a mesh density $\rho_n = 21$, i.e. 21 levels per factor in the unrestricted design space. The statistical model is $y = \theta_1 x_1 + \theta_2 x_2 + \theta_{12} x_1 x_2 + \theta_{11} x_1^2 + \theta_{22} x_2^2 + \varepsilon$ with $\varepsilon \sim \mathbf{P}_\varepsilon$. The design should contain $n = 12$ experiments.

The DDoE algorithm (modules 2 and 3) has been repeated $n_{\text{sim}} = 1,000$ times. For each trial it reached the optimal design provided by the FFEA algorithm presented in Nguyen and Piepel (2005) and shown in Figure 2.

As the DDoE algorithm, the software packages MATLAB and STATISTICA as well as the FFEA algorithm reach $D = 4.5836$ in the first trial. Note that the loss of information of these discrete designs compared to the continuous D-optimal design is smaller

Table 3: Continuous D-optimal design from R AlgDesign.

p	x_1	x_2
0.1216	0.5	−1.0
0.1231	1.0	−1.0
0.0517	−0.3	−0.2
0.1529	1.0	0.0
0.1552	0.1	0.1
0.1182	−1.0	0.5
0.1246	−1.0	1.0
0.1528	0.0	1.0

Table 4: Criteria of different designs declared as D-optimal.

Tool	D	D_{ec}	G	G_e
R AlgDesign[1]	4.4947	1.0000	0.6667	0.7500
DesignExpert	5.1925	0.8656	0.8952	0.5585
MATLAB	4.5836	0.9806	0.6754	0.7403
Minitab	4.5887	0.9795	0.6761	0.7395
MODDE	4.7501	0.9462	0.6848	0.7301
SAS	4.7185	0.9462	0.7105	0.7037
STATISTICA	4.5836	0.9806	0.6754	0.7403
FFEA	4.5836	0.9806	0.6754	0.7403
GA	4.6856	0.9593	0.8497	0.5885
DDoE algorithm	4.5836	0.9806	0.6754	0.7403

[1]R AlgDesign creates a continuous, all other tools discrete designs.

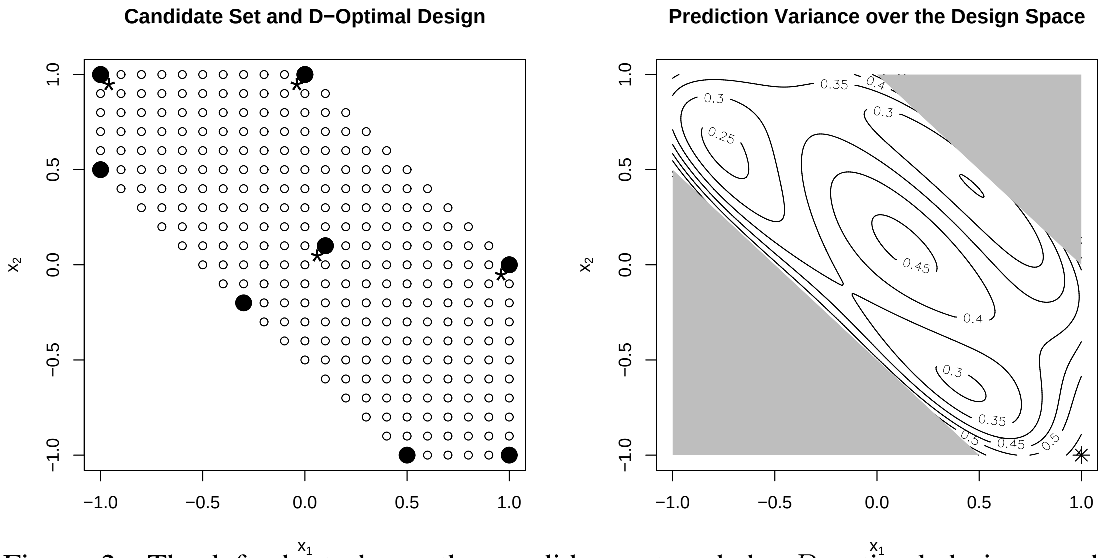

Figure 2: The left chart shows the candidate set and the D-optimal design reached $n_{\text{sim}} = 1,000$ times by the DDoE algorithm. Points marked with an asterisk represent two experiments with equal factor settings. The right chart shows the prediction variance factor $\mathbf{x}'\mathbf{M}^{-1}\mathbf{x}/n$ over the design space with the supremum of around 0.6754 at $(x_1 = 1, x_2 = -1)$ determining G.

than 2% as indicated by D_{ec} in Table 4. All other tools and the GA algorithm have an information loss smaller than 15%. Similar results for G are reached by scaling the continuous design accordingly for $n = 12$. Rounding the weights p of the continuous design (see Table 3) leads to the discrete design as shown in Figure 2. All tools and algorithms have been used with the same candidate set which might influence the potential of the genetic algorithm.

6 An Application Example

The durability y of an engine component has to be investigated with respect to 3 potential influence factors. Thus, a discrete D-optimal design should be found for the linear model $y = g'(\mathbf{x})\boldsymbol{\theta}_{\mathbf{x}} + \varepsilon$ with an intercept, $m_0 = 3$ quantitative factors, and all two-factor-interactions. The restrictions for the factors are:

I: $-x_1 \qquad + x_3 \leq 1$

II: $\frac{4}{3}x_1 - 4x_2 + x_3 \leq \frac{5}{3}$

Factors x_1 and x_3 can take only values from the standardized set $\{-1, -1/2, 0, 1/2, 1\}$, factor x_2 is continuously adjustable between its standardized bounds $[-1; 1]$. This will be approximated by a mesh density of 25 points equally distributed on $[-1; 1]$.

The final design should contain $n = 15$ experiments, four of them mandatory with factor settings listed in Table 5. In addition, four experiments should be considered with fixed settings for the factors x_1 and x_2 but free for x_3 within the design space. Table 6 contains the corresponding settings.

Module 1 of the DDoE algorithm provides the candidate set $\Xi_{\mathbf{x}}$ with the alternative vector $\boldsymbol{\xi}_A$ and the status vector $\boldsymbol{\xi}_S$ as shown in Table 7.

Table 5: Fixed experiments.

Exp.	ID in Fig. 3	x_1	x_2	x_3
1	▲	1	4/5	1
2	▲	1	1	4/5
3	▲	1	1	−1
4	▲	0	1	−1

Table 6: Partly fixed experiments.

Exp.	ID in Fig. 3	x_1	x_2	x_3
5	◇	−1	−1/2	?
6	▽	−1	1	?
7	□	1	1	?
8	○	1	1/2	?

Table 7: Consideration of the partly fixed and fixed experiments in the candidate set.

j	ξ_{Sj}	ξ_{Aj}	ID in Fig. 3	Int.	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3
1	0	1		1	−1	−1	−1	1	1	1
2	0	2		1	−1	−11/12	−1	11/12	1	11/12
⋮	⋮	⋮		⋮	⋮	⋮	⋮	⋮	⋮	⋮
389	0	389		1	1	1	1	1	1	1
390	1	390	◇	1	−1	−1/2	−1	1/2	1	1/2
391	1	390	◇	1	−1	−1/2	−1/2	1/2	1/2	1/4
392	1	390	◇	1	−1	−1/2	0	1/2	0	0
393	1	391	▽	1	−1	1	−1	−1	1	−1
394	1	391	▽	1	−1	1	−1/2	−1	1/2	−1/2
395	1	391	▽	1	−1	1	0	−1	0	0
396	1	392	□	1	1	1	−1	1	−1	−1
397	1	392	□	1	1	1	−1/2	1	−1/2	−1/2
398	1	392	□	1	1	1	0	1	0	0
399	1	392	□	1	1	1	1/2	1	1/2	1/2
400	1	392	□	1	1	1	1	1	1	1
401	1	393	○	1	1	1/2	−1	1/2	−1	−1/2
402	1	393	○	1	1	1/2	−1/2	1/2	−1/2	−1/4
403	1	393	○	1	1	1/2	0	1/2	0	0
404	1	393	○	1	1	1/2	1/2	1/2	1/2	1/4
405	1	393	○	1	1	1/2	1	1/2	1	1/2
406	1	394	▲	1	1	4/5	1	4/5	1	4/5
407	1	395	▲	1	1	1	4/5	1	4/5	4/5
408	1	396	▲	1	1	1	−1	1	−1	−1
409	1	397	▲	1	0	1	−1	0	0	−1

After $n_{\text{sim}} = 1,000$ trials with modules 2 and 3 of the DDoE algorithm, the results contain designs with five different values of the determinant criterion, i.e. at least four pseudo D-optimal designs. Figure 3 summarizes the results and shows that all designs declared as optimal are of similar quality concerning D. The coefficient of variation is ≈ 0.003. The presented solutions have to be interpreted as *D-optimized* designs even the best performing out of n_{sim} designs will be called *discrete D-optimal regarding the given candidate set.* Table 8 lists the factor settings of the design with $D \approx 1.977$. The corresponding continuous optimal design with $D \approx 1.7347$ provided by R AlgDesign does not consider the partly fixed and fixed experiments. Thus, the comparability is limited.

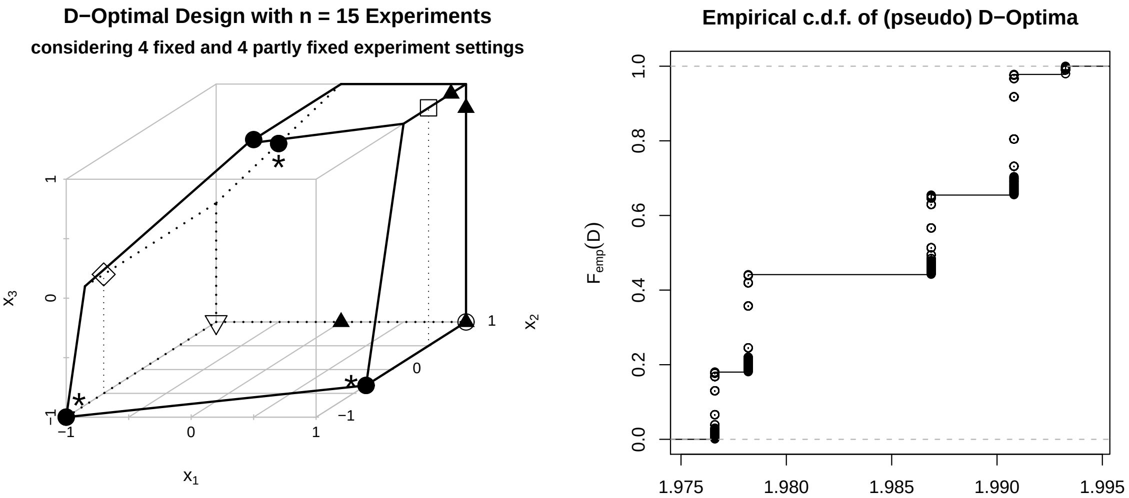

Figure 3: The left panel shows the D-optimal design, reached in approximately 20% of the trials, as indicated in the right panel. The points marked with an asterisk represent two experiments. The selected experiments of the alternative groups as well as the fixed experiments are marked accordingly.

If $y = \tau(t)$ there may occur life time terminating events during experimentation. The capacity reserved for a planned duration t_r of the experiments should be used with maximum efficiency, even after the occurrence of a life time terminating event. The first four experiments (Exp. 1, 2, 3, 4) have been carried out already in the past. The remaining 11 experiments run in the study and may be terminated by a corresponding event before the planned duration t_r will be reached. If such an event occurs, the task is to extend the design D-optimally. Module 4 provides this feature.

Table 9 contains the life time experiments terminated by an event occurring before t_r (in the following denoted shortly as *failed* experiments). Experiment 9 fails at first and will be replaced by experiment 16 with new, different settings. Then, experiment 8 fails which has partly fixed settings of the factors x_1 and x_2. I.e., the new experiment 17 should have the same settings for x_1 and x_2 etc. This procedure will be continued until the planned experiment duration t_r is reached or if the required precision of the parameter estimators is obtained.

If the failed experiment has partly fixed factor settings, the candidate set for the design extension may include only members of the corresponding alternative group.

The analysis of the data showed that the durability of the investigated component is significantly influenced by factor x_2. Corresponding modifications of the component led to a satisfactory performance in the series production.

Our DDoE algorithm has been applied successfully to various tasks in the automotive industry. In particular, we solved problems connected with the development of innovative power-trains (engine, transmission, exhaust gas aftertreatment).

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Table 8: Factor settings of the D-optimized design ($D \approx 1.977$) provided by the DDoE algorithm. The non-fixed experiments 9 to 15 are listed in randomized order.

Exp.	x_1	x_2	x_3	Remark
1	1	4/5	1	fixed
2	1	1	4/5	fixed
3	1	1	-1	fixed
4	0	1	-1	fixed
5	-1	$-1/2$	0	partly fixed
6	-1	1	-1	partly fixed
7	1	1	-1	partly fixed
8	1	1/2	1	partly fixed
9	$-1/2$	1	1/2	
10	0	$-1/6$	1	
11	-1	-1	-1	
12	$-1/2$	1	1/2	
13	-1	-1	-1	
14	1	$-1/3$	-1	
15	1	$-1/3$	-1	

Table 9: After the occurrence of a life time terminating event, the experiment will be restarted with a new object realization and new, D-optimal factor settings with respect to the candidates set depending on the experiment failed.

Failed Exp.	x_1	x_2	x_3	New Exp.	x_1	x_2	x_3	D
9	$-1/2$	1	$1/2$	16	-1	1	-1	1.8175
8	1	$1/2$	1	17	1	$1/2$	1	1.7340
17	1	$1/2$	1	18	1	$1/2$	1	1.6738
6	-1	1	-1	19	-1	1	-1	1.5903
7	1	1	-1	20	1	1	-1	1.5108
19	-1	1	-1	21	-1	1	0	1.4416
16	-1	1	-1	22	0	$-1/6$	1	1.3387
22	0	$-1/6$	1	23	1	$-1/3$	-1	1.2755

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