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A General Intuitive Design Pattern for Optimally Sequencing Treatment Combinations in 2^k Factorial Experiment and a Simple Estimation Algorithm

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Abstract

The number of model parameters of a 2^k factorial design grows exponentially. When the number of factors is large, numerous higher-order interactions constitute a vast majority of the model parameters while many of them do not exist or are insignificant. The classic methods of fractional factorial designs, Plackett-Burman designs, Taguchi designs etc. seek an already developed and often cataloged design that fits exactly the problem being tackled or select a design that fits it the most. Most, if not all, of these designs were developed in absence of convenient computation tools and enjoy computational simplicity. The necessary number of treatment combinations for unbiased estimation of significant parameters is often exceeded; undesirable confounding, i.e., biased estimation, is difficult to avoid. An opposite approach is to determine, for any set of model parameters considered as significant, a corresponding set of equal (and minimum) number of treatment combinations for unbiased parameter estimation. A companion feature of that approach is active avoidance of confounding. In addition, if the experimenter, particularly when unsure of the "borderline" significance of some parameters, can attempt to sequence model parameters in non-increasing order of magnitude (based on prior knowledge or subjective judgment), a corresponding sequence of treatment combinations can be numerically determined (with one treatment combination added for each additional possibly significant model parameter). Recently, a simple design pattern was proposed with which such a sequence of treatment combinations can be intuitively and easily obtained, without numerical computation. However, that pattern requires for the estimability of an interaction that all main effects and all lower-order interactions among all factors involved in the experiment have been estimated. For example, the interaction AB may not be estimable without main effect C having been estimated first. This paper relaxes that requirement and extends the use condition of the

approach to virtually all practical situations and presents a simple algorithm to estimate model parameters recursively. As sequential experimentation progresses, no experiments already conducted could be considered unnecessary for unbiased estimation of significant parameters, and hence "forward compatibility" in minimizing the number of treatment combinations is achieved. Therefore, such optimality may be referred to as *FC*-optimality.

Key Words: Design of Experiment; Two-level Factorial Design; Fractional Factorial Design; Run Minimization; Parameter Estimablility; Sequential Design

1. Introduction

When each of the *k* factors of a factorial experiment can be set at one of exactly two levels, the experiment is referred to as a *k*-factor two-level full factorial design or a 2^k full factorial design. Such a design has 2^k model parameters and 2^k treatment combinations. When all the 2^k parameters must be estimated, via unbiased estimators and without confounding, all 2^k treatment combinations must be experimented. When the number of factors is large, numerous higher-order interactions constitute a vast majority of the model parameters while many of them can be considered insignificant and do not require estimation. (This is often referred to the Effect Sparsity Principle.) As a result, to estimate those significant, i.e., non-zero, model parameters, only a subset of the 2^k treatment combinations is required. In such a situation, the classical methods of fractional factorial designs, Plackett-Burman designs, Taguchi designs etc. all seek a design already developed and often cataloged that fits exactly the problem being tackled or select a design that fits it the most. General methodologies can be found in Box et al.(1978), Montgomery(2009) and Taguchi and Konishi (1987). Examples for development of designs meeting more specific requirements include (Franklin, 1985; Hedayat and Pesotan 1997; He and Tang, 2003; and Mee, 2004).

The classical fractional factorial approach capitalizes on computational simplicity in estimation, resulting from orthogonality among columns of the "design matrix." But, adding a fraction for the purpose of estimating additional model parameters with less or without confounding doubles the number of treatment combinations. High experimentation cost, long experimentation duration and short product life-cycle of some industries have motivated research on minimizing the

number of treatment combinations in a statistically valid manner. In the semiconductor-fabrication industry, one complete experimental run of a new "recipe" for wafer fabrication may cost $20,000 and may take one month. In that and some other mature industries, much domain knowledge and past experience has accumulated regarding presence or absence of interactions among some of the experimental factors. However, the exact magnitudes of some existent interactions must still be estimated through experimentation.

The Plackett-Burman method basically focuses on all main effects, with their possible confounding with two-factor and higher-order interactions ignored. The column orthogonality associated with any of the design matrices enables simple arithmetic estimation in screening a superset of possible factors. It requires the minimum number of treatment combinations for estimating all main effects, including the grand effect, only if all interactions are indeed non-existent. In addition, confounding pattern is unclear or complicated at best. The Taguchi orthogonal-array method seeks to reduce the number of treatment combinations with domain knowledge about presence/absence of interactions between two factors while the orthogonality among columns of the design matrix and the resulting computational simplicity is kept. It is able to single out some two-factor interactions for their estimation and for avoiding their confounding with each other and with main effects. But, the discrete jump in the number of treatment combinations (typically of 4) does not minimize the number of treatment combinations. Also, confounding pattern with other model parameters is unclear or complicated at best.

Recently, Tsao and Wibowo (2005) emphasized that when only m of the 2^k effects/interactions may be non-zero, only m treatment combinations are required for their estimability, i.e., unbiased

estimation or estimation without confounding among themselves or with other parameters. With their estimation, one can build an adequate regression model. They developed a numerical method, based on the Phase-I Simplex Method for linear programming, to identify a minimal set of exactly *m* treatment combinations to estimate the *m* non-zero effects/interactions. The design matrix is "irregular" in the sense that the columns of the design matrix no longer enjoy orthogonality, and hence parameter estimation requires numerical inversion of the design matrix. (Although the computation involved in such inversion is a little more complex than the inner-product and division operations required for the classical fractional factorial, Taguchi, and Plackett-Burman methods, it is a trivial task in this computer era.) Such a method has been referred to as a least-treatment-combination method in Tsao and Patel (2013).

Confounding in parameter estimation is a major issue in reducing the number of treatment combinations. It occurs when the expected value of a parameter estimator is not exactly the parameter being estimated but is "contaminated" with some other parameters. In other words, it occurs when the estimator is biased. When an estimator exists whose expected value is exactly the parameter it is intended to estimate, the parameter is said to be estimable (and the estimator is said to be unbiased); an alternative expression is that the parameter can be estimated. In this paper, when we state that a parameter can be estimated, we mean its estimability. In addition, when all significant model parameters are estimable, we say that the model is adequate. When such an unbiased estimator does not exist, given the treatment combinations of an experiment, the parameter is said to be non-estimable. Estimability is the focus of this paper. Estimation accuracy, i.e., precision under assumption of estimability, hinges upon the number of replications for the selected treatment combinations and is beyond the scope of this paper.

The classical fractional factorial method uses the concepts of resolution level and aberration level as primary measures for non-estimability. These concepts treat a higher-order interaction as less important or smaller in magnitude than a lower-order interaction (or a main effect). For example, main effect A is always more important or larger (in magnitude) than interaction AB or BC. These concepts also treat any interaction of the same order as equally important as any other interaction of the same order. For example, the interaction between factors A and B is treated as equal in importance as the interaction between factors C and D. (This is often referred to as the Effect Hierarchy Principle.) In this approach, there are only three practical levels of resolution, namely, Resolution III, IV, and V, and such categorization could be quite coarse. These reflect the statistical purity of the method in the sense that domain knowledge about (a) possible larger magnitude (or importance) of a two-factor interaction than a main effect or (b) larger relative importance (or magnitude) of one two-factor interaction than another cannot be incorporated, at least not easily. As mentioned earlier, the confounding patterns of Taguchi and Plackett-Burman methods are complicated if not unclear.

Rather than passively selecting from alternatives the design that incurs least amount of confounding, Tsao and Patel (2011, 2013) defined the concept of "active confounding avoidance": identifying those model parameters that should be estimated without confounding among themselves. These parameters can be those considered non-zero, based on domain knowledge or prior knowledge, and hence their accurate estimation is important; confounding of any of them with any of the parameters considered as zero should not pose significant problems.

Tsao and Patel (2013) proved active confounding avoidance for the least-treatment combination methods proposed in Tsao and Wibowo (2005) and Tsao and Liu (2008).

In the larger context of experimentation planning, Montgomery (2009) suggested that experimentation should be conducted iteratively and sequentially, and the initial design, which is often intended for gaining experience and learning, should not consume more than 25% to 30% of the budget. This is consistent with the sequential nature of model building and parameter estimation commonly practiced in the real world. When one more fraction is added to a current fractional factorial design of an experiment, all the experiments already conducted and their results remain useful. This concept was defined as "forward compatibility" in Tsao and Patel (2013). But, in the Taguchi and Plackett-Burman methods, a design enabling estimation of a larger number of model parameters may not contain all the treatment combinations of the current design; therefore, forward compatibility may not hold. Extending the work of Tsao and Wibowo (2005), Tsao and Liu (2008) considered the situation where the experimenter has domain or prior knowledge such that he/she can sequence parameters or blocks of them approximately in non-increasing magnitude. They treated the most complicated case where all model parameters can be sequenced this way and proposed, for any first m parameters in the sequence, a numerical algorithm for generating a corresponding sequence of m treatment combinations with which the m parameters are estimable. With these two corresponding sequences, estimability of one additional model parameter is ensured by adding the corresponding treatment combination. This obviously ensures least treatment combination for estimating any set of first m parameters, hence achieving forward compatibility. Tsao and Patel (2013) proved that this algorithm also achieves active confounding avoidance. Experimentation can be stopped once the current model is

deemed adequate, e.g., when the estimation residuals cannot be distinguished statistically from realizations of a white noise and the newest parameter in the current model cannot be distinguished statistically from 0. To the experimenter, the sequential expansion proposed in Tsao and Liu (2008) and Tsao and Patel (2013) is optimal in the sense that the experimentation can stop whenever the current model is deemed adequate and no experiments already conducted could be considered unnecessary, hence achieving "forward compatibility" in minimizing the number of treatment combinations. Therefore, such optimality may be referred to as *FC*-optimality.

Early on, Box et al. (1978), in their commentaries on the examples given in the chapter More Applications of Fractional Factorial Designs, recognized the necessity for experimenters to use judgment for efficiency, with a calculated risk. This sequencing of effects/interactions and the corresponding sequencing of treatment combinations proposed in Tsao and Liu (2008), Tsao and Patel (2013) and this paper provide experimenters new ways to formulate judgment and improve efficiency. We refer to these two sequencing concepts as parameter-sequencing and treatment-combination sequencing and these two types of sequences as a parameter sequence and a treatment-combination sequence, respectively.

Tsao and Patel (2013) defined for all i, $0 \le i \le n$, the concept of i-th degree reduced factorial model $2^{k,i}$, which is the full-factorial model with all model parameters involving i+1 or more factors removed from the model. They also proposed a simple and intuitive design pattern that produces, without any computation, for all i, $0 \le i \le n$, a set of treatment combinations whose experimentation ensures estimability of all the parameters of $2^{k,i}$, all with least treatment

combinations, active confounding avoidance and forward compatibility. In addition, if the experimenter, in expanding $2^{k,i}$ to $2^{k,i+1}$, can sequence the parameters newly added to the model in non-increasing order of magnitude or importance, the simple and intuitive design pattern produces a corresponding sequence of treatment combinations, without numerical computation. As in Tsao and Liu (2008), exactly one additional treatment combination is added for one additional model parameter that needs to be estimated. The model building process can be stopped at any time when the current model is deemed adequate.

Note, however, that the intuitive design pattern proposed in Tsao and Patel (2013) requires for the estimability of any parameter (of the parameter sequence) that all lower-order parameters among all factors involved in the experiment can be estimated . For example, the interaction AB may not be estimable without main effect C having been estimated first. This paper relaxes that requirement and extends the use condition of the approach to virtually all practical situations. The use condition is that when one additional parameter is added to the model, all lower-order parameters must have already been included in the model. For example, when AB is added to the model, the grand effect G, the main effects A and B must have already been included in the model. (The main effect C needs not be included in the model already, however.) This requirement is similar to but stronger than the so-called Effect Heredity Principle, which states that in order for an interaction to be significant, at least one of its "parent factors" should be significant. Therefore, this requirement may be referred to as the Full Heredity Assumption. To the experimenter, the sequential expansion proposed in this paper is optimal, as the more restrictive sequential expansion proposed in Tsao and Patel (2013) and as the less restrictive but much more computation-intensive sequential expansion proposed in Tsao and Liu (2008), in the

sense that the experimentation can stop whenever the current model is deemed adequate and no experiments already conducted could be considered unnecessary. As one new parameter is added to the model and one corresponding treatment combination is added to the experiment, the new parameter needs to be estimated and the estimates for the existing parameters may change. We provide a simple estimator for the former and a simple updating formula for the latter. With these, estimating parameters requires no matrix inversion throughout the model building process, thus keeping the computation simplicity enjoyed by fractional factorial design, Plackett-Burman design and Taguchi orthogonal-array design.

This type of optimality can be considered sequential optimality; it has not received much attention until Tsao and Liu (2008). Other optimality criteria have been studied, e.g., *D*-optimality (e.g., Kiefer and Wolfowitz, 1959; Box and Draper, 1971; St. John and Draper, 1975; Evans, 1979; Bulutoglu and Ryan, 2009). Given a model, a set of candidate runs and a prescribed number of runs, *D*-optimality seeks a design, i.e., a subset of the candidate runs, that has exactly the prescribed number of runs and produces the smallest possible variances for the parameter estimators. *D*-optimality is attempted through numerical search. Due to the non-convex nature of the optimization problem, no existing algorithms can guarantee achievement of *D*-optimality. If candidate runs involve no replications or the number of replications is the same for all treatment combinations, then *D*-optimality reduces to a problem of selecting a set of treatment combinations that has a prescribed number of treatment combinations and produces minimum variances for the parameter estimators. Moreover, if the row rank of the matrix relating all the treatment combinations to the mean responses is equal to the number of model parameters, then all the model parameters are estimable. Under these conditions, *D*-optimality seeks estimability

and minimum variance. We, in this paper, deal primarily with the model building process through which an adequate or correct model is built and significant parameters are estimable, while an adequate or correct model is usually assumed as given in the theory of *D*-optimality. "Conditional *D*-optimality" has been studied so that, given a set of runs, the most *D*-efficient additional runs can be identified (e.g., Mitchell, 1974; Welch, 1982; Verotta, 1988). However, the achievability of overall *D*-optimality of the final model cannot be guaranteed at all when additional parameters are added to a current model sequentially during the model building process, with the corresponding treatment combinations of "conditional *D*-optimality" sequentially added to the design. In short, *D*-optimality is particularly useful when the model is already adequately built; conditional *D*-optimality attempted in individual steps of the model building process ensures no global *D*-optimality or even anywhere close to it when the exploratory stage ends and an adequate model has been built.

These sequencing proposals have been intended for cost minimization without sacrificing statistical validity. Statistical tests that should be conducted to ensure such validity have been addressed in detail in Tsao and Liu (2008), including a thorough diagnostic check after experimenting for each additional treatment combination to estimate one more effect/interaction. They were also summarized in Tsao and Patel (2013). As discussed in detail in Tsao and Liu (2008), the sequential experimentation can be implemented block by block, where a block represents a set of effects/interactions of indistinguishable magnitudes or significance levels. The focus of this paper is on findings beyond the work of Tsao and Patel (2013),

This paper is organized as follows. Section 2 focuses on the 2^4 factorial design and use it to illustrate the main contributions of this paper beyond the work of Tsao and Patel (2013). Section 3 defines the problem in the general context of 2^k full factorial design, states the general design pattern and provides the simple parameter-estimation algorithms. Section 4 provides all the proofs. Concluding remarks are given in Section 5.

2. Motivation, Problem Description and Main Contributions, via the 2^4 Factorial Design

As in Tsao and Patel (2013), we use the 2^4 factorial design to motivate the problem and to illustrate the solution. We focus on the value added by this paper, particularly (a) the general intuitive design pattern and the general and practical use conditions under which the pattern expands a sequence of treatment combinations one at a time for estimating one additional model parameter of a parameter sequence, (b) why the pattern works and how to estimate the newly added model parameter (as a simple inner product) and how to update the estimates (as simple modifications) already obtained for the existing but inadequate model parameters to become estimates for the expanded model. Discussions on the advantages possessed by the general intuitive design pattern to be proposed in this paper but also enjoyed by the intuitive design pattern proposed in Tsao and Patel (2013) are omitted. Such advantages include least treatment combinations, active confounding avoidance, and forward compatibility. For similar reasons, comparisons with other existing methods are also omitted.

2.1 Problem Description

We first describe the full 2^4 factorial design. The four factors are denoted as Factors A, B, C and

D. Sixteen, i.e., 2^4, treatment combinations are required in the full factorial design. We use a vector of four "–" or "+" signs to represent the low or high levels of the four factors of a treatment combination, respectively. We refer to such a representation as a level-vector representation. When convenient, we also use another common representation of a treatment combination (Montgomery, 2009), where presence of a lower case letter *a*, *b*, *c* or *d* in such a representation signifies that the treatment of the corresponding upper-case factor is set at the high level "+" while absence of such a lower case letter signifies that the treatment is set at the low level "-". For example, a treatment combination *ac* represents the treatment combination where Factors A and C are set at their respective high levels "+" while Factors B and D are set at their respective low levels "-". (In the level-vector representation, this treatment combination is represented as (+,-,+,-).) When all factor treatments are set at their respective low levels "-", the treatment combination is represented by a period ".". We use this alternative presentation also for denoting the mean responses. For example, the mean responses appearing in the last column of Table 2 below are indexed with respect to this alternative representation.

To define a full regression model for a 2^4 full factorial design, we use the following conventional notation, which is also used in Tsao and Patel (2013). G denotes the grand effect; A, B, C, and D denote the four main effects; AB, AC, AD, BC, BD and CD denote the six two-factor interactions; ABC, ABD, ACD and BCD denote the four three-factor interactions; ABCD denotes the four-factor interaction. In the notation just defined, the full regression model for the 2^4 factorial design is:

$$Y_{x_A x_B x_C x_D} = \mu_{x_A x_B x_C x_D} + \varepsilon_{x_A x_B x_C x_D} \quad (1)$$

where $\mu_{x_A x_B x_C x_D} = G + \frac{A}{2}x_A + \frac{B}{2}x_B + \frac{C}{2}x_C + \frac{D}{2}x_D$

$$+ \frac{AB}{2}x_A x_B + \frac{AC}{2}x_A x_C + \frac{AD}{2}x_A x_D + \frac{BC}{2}x_B x_C + \frac{BD}{2}x_B x_D + \frac{CD}{2}x_C x_D$$

$$+ \frac{ABC}{2}x_A x_B x_C + \frac{ABD}{2}x_A x_B x_D + \frac{ACD}{2}x_A x_C x_D + \frac{BCD}{2}x_B x_C x_D + \frac{ABCD}{2}x_A x_B x_C x_D \quad , \quad (2)$$

$x_i = \pm 1$ for *i*=A, B ,C and D, *r* = 1, 2,…,*n*, and *n* is the number of replications. As commonly practiced in the literature and for discussion convenience, we use A, B, C and D to denote the Factors A, B, C and D as well as the main effects of Factors A, B, C and D. When distinction among the grand effect, the main effects and interactions is not important, we refer to all of them as model parameters or simply as parameters. Note that in this regression model, the unknown coefficients are actually G, A/2, B/2, C/2, D/2, AB/2, AC/2, AD/2, BC/2, BD/2, CD/2, ABC/2, ABD/2, ACD/2, BCD/2 and ABCD/2. They, except for the grand effect G, are half of the corresponding model parameters. We will refer to them as the regression coefficients of the regression model or simply the regression coefficients. These regression coefficients are sequenced in an identical manner as their corresponding model parameters. For convenience in discussing the mathematical crux of the proposed method, we deal primarily with the regression coefficients in presenting the numerical examples in this Section 2 and proving the main theorems in Section 4. However, the main contributions of this paper will also be expressed in terms of the model parameters.

As in Tsao and Patel (2013), this paper focuses mainly on the relationship between the 2^k parameters (i.e., effects/interactions) and the 2^k mean responses and how the latter, or some of them, can be used to estimate the former, particularly those whose magnitudes are significantly

and statistically different from zero. A common modeling principle is parsimony, i.e., use of as few model parameters as possible to represent the relationship. Another common practice is sequential modeling. Guided by the parameter estimates of a current model and the resulting residuals, the experimenter conducts statistical tests to determine whether the current model is adequate or not, and, if not, may explore further parameters and treatment combinations to better represent the relationship. (Such exploration may be conducted for the ultimate purpose of identifying treatment combinations that can eventually produce responses close to either optimality or a pre-determined target.) Because of the focus on mean responses and their relationships with the parameters, Eq. (2), without the random-error term, plays a pivotal role in this special case. It is clear from Eq. (2) that all 16 model parameters can be solved explicitly as 16 linear functions of the 16 mean responses once these 16 mean responses have been obtained. Because of the orthogonality between any two columns of the matrix associated with the right-hand side of Eq. (2), the 16 model parameters can be easily solved.

As in Tsao and Liu (2008) and Tsao and Patel (2013), we seek, for any given sequence of model parameters of non-increasing magnitude or importance, a corresponding treatment-combination sequence so that the first m, $1 \le m \le 2^4$, model parameters in the parameter sequence can be estimated with the first m treatment combinations of the treatment-combination sequence.

In other words, throughout the sequential experimental process, one additional model parameter is estimable with the addition of the corresponding treatment combination.

2.2 Main Contributions – The General, Simple and Intuitive Design Pattern and Its Use Condition

To illustrate the main contribution of this paper, we consider a particular sequence of model

parameters (i.e., effects/interactions) in non-increasing order of magnitude. This particular parameter sequence is G, A, B, AB, C, AC, BC, ABC, D, AD, BD, CD, ABD, ACD, BCD and ABCD, as shown as the column headers of Table 1. Note that interaction AB is considered as more important than main effect C; interaction ABC is considered as more important than main effect D and three two-factor interactions, namely AD, BD and CD, out of the six possible two-factor interactions. Note also that this parameter sequence is beyond the scope of Tsao and Patel (2013), which requires that (i) main effect C be ahead of interaction AB in the parameter sequence, (ii) main effect D be ahead of all two-factor interactions among Factors A, B and C, (not to mention interaction ABC), (iii) interaction AD be ahead of interaction ABC. This is a main contribution of this paper.

We seek to sequence the 16 treatment combinations so that (a) they can be experimented in the sequence until no more statistically non-zero model parameters need to be estimated, and (b) the first m parameters of the parameter sequence, $1 \le m \le 2^4$, can be estimated with the first m treatment combinations of this treatment-combination sequence, with no confounding among the m parameters. The general intuitive design pattern to be proposed and proved later in this paper produces the following sequence of treatment combinations: ".", *a*, *b*, *ab*, *c*, *ac*, *bc*, *abc*, *d*, *ad*, *bd*, *cd*, *abd*, *acd*, *bcd*, and *abcd*. These treatment combinations are the row headers of Table 1. Note that each of these treatment combinations is defined by the four elements (of 1 or –1) of the same row corresponding to the low "-" or high "+" levels of the four Factor A, B, C and D. The correspondence between this parameter sequence and the treatment-combination sequence produced according to the general intuitive design pattern proposed in this paper is detailed in Table 2. For visual clarity, the treatment combinations are also defined in the clearer contrast

between "-" and "+" symbols, i.e., in their level-vector representation; their position numbers *x's*, in order of their appearance in a conventional full design matrix, are also provided and are denoted as TC*x*'s

Note that the treatment-combination sequence is exactly the same as the model-parameter sequence, except that the former is in lower case while the latter is in upper case. The general intuitive design pattern proposed in this paper exhibits such exact correspondence between the model-parameter sequence and the treatment-combination sequence. The only condition required for the new proposed general intuitive design pattern to work is that the new additional parameter to be estimated completes a "parameter factorial" associated with all the factors relevant to the new parameter. We explain and illustrate this condition with this particular example as follows. At the beginning, none of the factors is considered insignificant, not to mention the interactions among the factors, and hence the only parameter to be estimated is G. Although any treatment combination would suffice for the estimation, we choose "." as the base treatment combination, i.e., the treatment combination (-,-,-,-). (In fact, labeling of low vs. high levels can be arbitrary. Any existing labeling scheme can be easily altered so that the base treatment combination can be relabeled as (-,-,-,-).) For the next parameter (of the parameter sequence), i.e., A, one treatment combination is selected; the treatment combination is "*a*". Note that A together with the grand effect G constitute a full parameter factorial {G,A}of Factor A. Similarly, the treatment combination "*a*" together with the base treatment combination "." constitute a full "treatment-combination factorial" for Factor A. A full treatment-combination factorial or simply a treatment-combination factorial of a subset of all the factors is defined to be a subset of all the treatment combinations of the 2^k factorial design whose treatment levels of the

factors of the subset span the full factorial design for the factors, as if they are the only factors considered in an experiment.

Similarly to the discussion about parameter A and the corresponding treatment combination "*a*", the same can be said about the following parameter *B* of the parameter-sequence and the following treatment combination "*b*" of the corresponding treatment-combination sequence. The next model parameter in the parameter-sequence is AB, and the next corresponding treatment combination is "*ab*". With the grant effect G, and the main effects A and B already considered in the model, the interaction AB completes the full "parameter factorial" associated with the Factors A and B; the full "parameter factorial" associated with Factors A and B is {G,A,B,AB}. In addition, the treatment combinations "*ab*" completes the full treatment-combination factorial for Factors A and B. The same can be said about the main effect C, interactions AC and BC and the corresponding treatment combinations "*c*", "*ac*" and "*bc*". Now all parameters associated with Factors A, B and C have been estimated, except for the interaction ABC, and all treatment combinations associated with the full treatment-combination factorial for Factors A, B and C have been selected and experimented, except for the treatment combination "*abc*". Therefore, interaction ABC completes the full parameter factorial of parameters for Factors A, B and C; the full parameter factorial associated with Factors A, B and C is {G,A,B,C,AB,AC,BC,ABC}. In addition, treatment combination "*abc*" completes the full treatment-combination factorial for Factors A, B and C. The same logic establishes the fact that inclusion of each new model parameter in the parameter sequence completes the parameter factorial associated with all the factors relevant to the new parameter. In addition, the inclusion of the corresponding treatment combination completes a full treatment-combination factorial associated with the same factors.

For ease of discussion, we refer to such completions as "parameter-factorial completion" and "treatment-combinaion-factorial completion", and refer to the model parameter and treatment combination that lead to the corresponding completion as "parameter-factorial completing" and "treatment-combination-factorial completing," respectively. It may be informative to give an example for which the proposed general intuitive design pattern does not work. The proposed design pattern would not work for any sequence starting with G, A, B, C, D, AB, AC, and ABC, for example. This is because the three-factor interaction ABC does not complete the parameter factorial for Factors A, B and C, i.e., the three factors involved in this interaction; the two-factor interactions BC is necessary for the completion but has not been included in the model for unbiased estimation yet.

Another example not satisfying the use condition of Tsao and Patel (2013), but satisfying the use condition of the general intuitive design pattern proposed in this paper, is the parameter sequence G, A, B, C, D, AB, AC, BC, ABC, AD, BD, CD, ABD, ACD, BCD and ABCD and the corresponding treatment-combination sequence ".", *a*, *b*, *c*, *d*, *ab*, *ac*, *bc*, *abc*, *ad*, *bd*, *cd*, *abd*, *acd*, *bcd*, and *abcd*. In terms of the labeling used in conventional design matrix, these treatment combinations are numbered as 1, 2, 3, 5, 9, 4, 6, 7, 8, 10, 11, 13, 12, 14, 15 and 16.

As in Tsao and Patel (2013), invertibility of any of the m leading principal submatrix, $1 \le m \le 2^4$, delineated in Table 1 plays a key role in parameter estimability. All such submatrices are invertible. The proof will be by mathematical induction, and it will be shown in Section 4 that invertibility of any such an $m \times m$ leading principal submatrix guarantees the invertibility of the next $(m+1) \times (m+1)$ leading principal submatrix.

2.3 Why the Design Pattern Works and How to Estimate the Parameters

Let T' be an $(m+1)\times(m+1)$ matrix and T be its $m\times m$ leading principal submatrix. In other words, T' is obtained by expanding T with one row and one column. Suppose that T is invertible. To obtain T^{-1}, we can perform elementary operations on T such that T | I becomes I | T^{-1}, where I is the $m\times m$ identity matrix. T^{-1} can be used to help determine the invertibility of T' and, if so, the inverse of T'. In our case, T represents a square design matrix, and we expand a given design matrix with one parameter and the corresponding treatment combination at a time. We use the step of adding interaction AD to the current model consisting of parameters G, A, B, AB, C, AC, BC, ABC and D. In the rest of this section, we assume the knowledge of the inverse matrix T^{-1} for ease of illustration only. This knowledge is not required to show the invertibility of T'; it is not required to motivate an unbiased estimator for the new parameter AD or the formulae for updating the current parameter estimates to become the new estimates. (It is required, however, for obtaining recursively the inverse matrices of the leading principal submatrices of the full design matrix, as to be discussed later.) For ease of illustration, the true parameter values are assumed to be G=100, A=90, B=80, AB=70, C=60, AC=50, BC=40, ABC=30, D=20, AD=10, with all other parameters assumed to be 0 or non-existent. The 10 resulting mean responses are 45, 35, 45, 115, 45, 75, 65, 295, 55, 65. Note again that regression coefficients of the regression model, as opposed to the parameters of the 2^k full factorial experiment, are G=100, A/2=45, B/2=40, AB/2=35, C/2=30, AC/2=25, BC/2=20, ABC/2=15, D/2=10, and AD/2=5, with all other regression coefficients assumed to be 0 or non-existent.

To illustrate how to estimate the new parameter AD and how to update the current estimates of the current parameters, we use the elementary row operations needed to transform the 10×10 matrix on the left-hand side of the vertical line in Table 3 into the 10×10 identity matrix. The main idea of this illustration is that pre-multiplying the 10×10 design matrix (associated with the first 10 parameters) by the 10×10 matrix to the right-hand side of the vertical line produces the 10×10 matrix to the left of the vertical line. Transforming the 10×10 matrix to the left of the vertical line to the 10×10 identity matrix and performing the same elementary row operations on the 10×10 matrix to the right of the vertical line produces the inverse matrix of the 10×10 design matrix, to the right of the vertical line. We now briefly explain the composition of the two 10×10 matrices.

The 9×9 inverse of the design matrix with nine model parameters (G, A, B, AB, C, AC, BC, ABC, D) and the nine corresponding treatment combinations is seen on the right-hand side of the solid vertical line in Table 3; it consists of the first nine columns and the top nine rows. The rest of the elements, i.e., the last row and the last column, in the matrix on the right-hand side are all zero except the (10,10) element, which is set to 1. (They are the last row and column of the 10×10 identity matrix.) We now focus on the left-hand side of the vertical line. The counterpart to the 9×9 inverse matrix is the 9×9 identity matrix. We add interaction AD and its corresponding treatment combination *ad* to the design matrix. In this case, the last row is the *ad* row of the 10×10 design matrix associated with the first 10 model parameters (G, A, B, AB, C, AC, BC, ABC, D, AD) appended with the mean response of the treatment combination *ad*. The first 9 rows of the RHS column are the estimates of G, A/2, B/2, AB/2, C/2, AC/2, BC/2, ABC/2, and D/2, respectively, obtained in the previous iteration based on (i) the incomplete model of

only the first nine parameters of the parameter sequence and (ii) the corresponding nine (true) mean responses calculated based on 10 parameters and the assumed parameter values. The column to the left of the RHS column is the updated first nine elements of the AD column, which can be obtained by pre-multiplying the first nine elements of the AD column of the 10×10 design matrix by the inverse of the 9×9 design matrix of (G, A, B, AB, C, AC, BC, ABC, D). These updated first nine elements turn out to be $(-1, -1, 0, 0, 0, 0, 0, 0, -1)^T$. The reason is as follows. Let us focus on the first nine rows of the 10×10 design matrix. The invertibility of the 9×9 design matrix of the nine-parameter model implies that the AD column, i.e., the last column, is linearly dependent on the first nine, and the linear combination is unique. Note that the updated first nine elements of the AD column just mentioned constitute the nine multipliers of this linear combination. For the moment, focus on those columns associated with the effects G, A, D and AD. For each of the nine rows, two of the four constant multipliers are +1 and the other two are -1. (In general, for each treatment combination of a full 2^k factorial design, except for the one with all factors set to the high level, the number of the +1 constant multipliers in the corresponding regression equation and that of the -1 coefficients are equal.) This implies that the four columns G, A, D and AD sum to a zero vector or, equivalently, the AD column can be obtained by multiplying the sum of the G, A and D columns by -1. This implies the three -1's of (-1, -1, 0, 0, 0, 0, 0, 0, -1). Uniqueness of the linear combination further implies that the first nine elements of the AD column are (-1, -1, 0, 0, 0, 0, 0, 0, -1).

Performing elementary row operations in Table 3 to convert the first ten elements of the last row to the left of the vertical line to (0, 0, 0, 0, 0, 0, 0, 0, 0, 1) and then make the column of AD $(0, 0, 0, 0, 0, 0, 0, 0, 0, 1)^T$ (to the left of the vertical line) produces the inverse of the 10×10 design

matrix, as exhibited on the right-hand side of the vertical line in Table 4. Two quick observations provide hints for a general phenomenon. First, the last row of the inverse matrix reveals that the regression coefficient AD/2 can be estimated the way they should be as if only the four treatment combinations constituting a treatment-combination of Factors A and D are available, with all other factors set to their low levels. In general, the newly added parameter should be estimated as if only the treatment combinations constituting the treatment-combination factorial of all the relevant factors, with all other factors set at their level levels; this will be proved in Section 4. To the left of the vertical line is the 10×10 identity matrix and the RHS column, which contains the updated regression coefficients G, A/2, B/2, AB/2, C/2, AC/2, BC/2, ABC/2, and D/2, and the value for the new regression coefficient AD/2, respectively. Note that only the estimates of regression coefficients G, A/2, and D/2 have changed. All other old estimates have remained the same. In fact, the new G is the previous G plus AD/2. Similarly, the new A/2 and D/2 are, respectively, previous A/2 plus AD/2 and previous D/2 plus AD/2. These amount to the change of model parameters from G to G+AD/2, from A to A+AD, and from D to D+AD. In general, the current grand effect G will be updated to become G plus half of the estimate of the newly added parameter while any of all the other parameters constituting the parameter factorial will be updated to become itself plus the estimate of the newly added parameter. Finally, it can be seen that the RHS column exhibits the correct regression coefficients.

3. Problem Definition, Notation and Main Results

We first define the general problem and then describe the main results. To facilitate the discussion, we adopt a set of notation that is more amenable for addressing the general case of

2^k factorial design. It is the same set of notation used in Tsao and Patel (2013); it is essentially the same set of notation used in Tsao and Liu (2008) and Tsao and Patel (2011) except that the index for the factors used in this paper is *j*, instead of *i*. Let *j* be the index for the factors, *j* = 1, 2, …,*k*. Denote the grand effect as e_G and the effect of factor *j* as e_j , *j* = 1, 2, …, *k*. Let j_l , *l* = 1, …, *k*, denote a factor 1, 2, …, or *k*, and when *L* arbitrary factors appear in a subscript, the subscript is denoted as $j_1 j_2 \cdots j_l \cdots j_L$ and the factors appear in ascending order of their indices, i.e., $j_1 < j_2 < \ldots < j_l < \ldots < j_L$. Denote the interaction among factors $1 \le j_1 < j_2 < \ldots < j_l < \ldots < j_L \le k$ as $e_{j_1 j_2 \cdots j_l \cdots j_L}$, with a subscript encompassing all the factors involved and with the involved factors placed in an ascending order of factor indices. For convenience of discussion, we refer to any of the grand effect, main effects of the *k* factors, and all the interactions as a *model parameter* or, simply, a parameter. As usual, x_j = +1 or -1, *j* = 1, 2, …, *k*. Let *r* = 1, 2, …, *n*, denote the number of replications. With this notation, the full regression model for a 2^k factorial design can be stated as

$$y_{x_1 x_2 \ldots x_k ; r} = \mu_{x_1 x_2 \ldots x_k} + \varepsilon_{x_1 x_2 \ldots x_k ; r} \tag{3}$$

where $\mu_{x_1 x_2 \ldots x_k} = e_G + \sum_{1 \le j_1 \le k} \frac{e_{j_1}}{2} x_{j_1} + \sum_{1 \le j_1 < j_2 \le k} \frac{e_{j_1 j_2}}{2} x_{j_1} x_{j_2} + \sum_{1 \le j_1 < j_2 < j_3 \le k} \frac{e_{j_1 j_2 j_3}}{2} x_{j_1} x_{j_2} x_{j_3}$

$$+ \sum_{1 \le j_1 < j_2 < j_3 < j_4 \le k} \frac{e_{j_1 j_2 j_3 j_4}}{2} x_{j_1} x_{j_2} x_{j_3} x_{j_4} + \ldots\ldots$$

$$+ \sum_{1 \le j_1 < j_2 < j_3 < \ldots < j_{k-1} < j_k \le k} \frac{e_{j_1 j_2 j_3 j_4 \ldots . j_{k-1} j_k}}{2} x_{j_1} x_{j_2} x_{j_3} x_{j_4} \ldots . x_{j_{k-1}} x_{j_k} . \tag{4}$$

Note that the last term of Eq. (4) is simply $\frac{e_{1234..k}}{2} x_1 x_2 x_3 x_4 \ldots . . x_k$. Eq. (4) has 2^k equations and 2^k model parameters, which consist of the grand effect, *k* main (factor) effects and $2^k - k - 1$

interactions. A regression model involving only *m* non-zero parameters will be referred to an *m*-parameter model.

This paper focuses on estimability of model parameters and deals with the issue of identifying treatment combinations through whose experimentation significant model parameters can be estimated with an unbiased estimator, without confounding. Although the estimation process includes estimation of the mean responses based on experimental results, we focus only on the remainder of the estimation process and concern ourselves only with the relationship between the mean responses $\mu_{x_1 x_2 \ldots x_k}$ and all the model parameters. Therefore, our focus is on Eq. (4) and the random error term $\varepsilon_{x_1 x_2 \ldots x_k ; r}$ of Eq. (3) and possible replications are ignored. With the error terms ignored, we are not really dealing with estimation of the model parameters; we are actually solving the model parameters in terms of the mean responses. However, to distinguish a model parameter from its solution in terms of the mean responses and to be consistent with the larger context of estimation, we denote the solution of a model parameter in terms of the mean responses with a "hat". For example, such a solution for $e_{j_1 j_2 \ldots j_l \ldots j_L}$ is denoted as $\hat{e}_{j_1 j_2 \ldots j_l \ldots j_L}$.

A treatment combination $(x_1, x_2, x_3, \ldots\ldots, x_{k-1}, x_k)$ of a 2^k full factorial design, where x_j = + or - , j = 1, 2, …, k, is alternatively represented as a set of those of the k factors that are set at the high level (+). To distinguish such a treatment-combination representation from a set of factors, the factor indices of such a representation will be delimited with a pair of angle brackets "$\langle\ \rangle$", instead of the curly bracket "$\{\ \}$"commonly used to delimit a set of elements. This notation will be used whether the factors are expressed explicitly as an integer from 1 through k or implicitly

as a set of symbols for the *k* factors. When all factors are set at the low level (-), the treatment combination is represented, for convenience, as ".", i.e., as a dot. (This is consistent with the convention.) For example, the treatment combination (- , + , +, -) of 2^4 full factorial design is alternatively represented as $\langle 2,3 \rangle$. Also, a treatment combination of 2^4 full factorial design where factors j_1 and j_2 are set at the high level (+) is represented as $\langle j_1, j_2 \rangle$. Similarly, we adopt a corresponding alternative representation for the mean responses according to this alternative treatment-combination representation. More precisely, we use this alternative treatment-combination representation as the subscript of the corresponding mean response. Since there is little chance for confusion, the pair of angular brackets may be omitted for notational convenience. We continue the above examples. When all factors are set at the low level (-), the mean response is represented as $\mu_{\langle \cdot \rangle}$ or simply $\mu_{\cdot}$. The mean response of the treatment combination $\langle 2,3 \rangle$ of any full 2^k factorial design is alternatively represented as $\mu_{2,3}$, regardless of the number *k* of factors involved. Also, the mean response of the treatment combination $\langle j_1, j_2 \rangle$ of any full 2^k factorial design is represented as μ_{j_1, j_2}.

Definition: The parameter factorial of *L* factors { j_1, j_2, ….., j_L } is the set of model parameters consisting of the grand effect, the main effects of all these factors and all possible interactions among these factors. (The parameter factorial of one factor consists of the grand effect and the main effect of the factor.)

Definition: Consider any parameter $e_{j_1 j_2 \cdots j_l \cdots j_L}$ in any parameter sequence of a 2^k full factorial in which the grand effect is the leading parameter. Suppose the preceding parameters include all

the parameters of the parameter factorial of factors $\{ j_1, j_2, \ldots, j_L \}$, except $e_{j_1 j_2 \ldots j_l \ldots j_L}$. Then, addition of this parameter to the preceding parameters is said to complete the parameter factorial of the L factors $\{ j_1, j_2, \ldots, j_L \}$. Also, for ease of discussion, this parameter is said to be parameter-factorial completing, with the context of the L factors $\{ j_1, j_2, \ldots, j_L \}$ implicitly assumed and omitted. (When the parameter is a main effect e_{j_1}, it always completes the parameter factorial of Factor j_1, because the leading parameter is the grand effect.)

Definition: A parameter sequence of a 2^k full factorial design is parameter-factorial completing if and only if each of its parameter is parameter-factorial completing.

With the notation and terminology just defined, we first discuss the four main contributions of this paper and then capture them in two separate algorithms. It is clear that any such parameter-factorial-completing parameter sequence must start with the grand effect, as the leading parameter of the sequence. With the grand effect being the leading parameter of a parameter-completing parameter sequence, a main contribution of this paper is about sequencing the treatment combinations of a 2^k full factorial design according to the given parameter sequence, ordered in non-increasing importance or magnitude. Note that each parameter is indexed by the factors involved. More precisely, each main effect e_j, $j = 1, 2, \ldots, k$, is indexed by the factor j; each of the L-factor interaction $e_{j_1 j_2 \ldots j_l \ldots j_L}$ is indexed by the L factors involved, namely $j_1, j_2, \ldots, j_L$. The factors specified in such an index are referred to in this paper as the relevant factors of the parameter or, equivalently, parameters relevant to the parameter. For each of these parameters, a corresponding treatment combination can be obtained in the following simple

manner. The treatment combination corresponding to the grand effect e_G is set to the treatment combination ".", i.e., the treatment combination with all factors set to the low level (-). For all other parameters, simply place the factor index (i.e., the subscript) of the parameter in an angle bracket. (e_G involves no factors, and hence the correspondence can be considered as being obtained with no factor indices set to the high level (+).) Given the sequence of parameters, the sequence of treatment combinations is nothing but the sequence of the corresponding treatment combinations so obtained. We refer to such a correspondence as a *factor-to-high-level correspondence*. Note that this correspondence is unique. The general intuitive design pattern proposed in this paper is this unique and simple correspondence. This design pattern is the first major contribution of this paper.

When the equations of Eq. (4) are written according to the given parameter sequence and the corresponding factor-to-high-level treatment combination sequence, the theory can be succinctly developed. First, switch the sides of the mean-response terms and the linear combinations of model parameters so that the latter appear on the left-hand side of the equations. Next, rearrange the order of the summands of the linear combinations according to the exact order of the given model-parameter sequence. Finally, rearrange the treatment combinations and the companion model equations according to the corresponding factor-to-high-level treatment-combination sequence. This process has been illustrated in Section 2 with the process leading to Table 1. With this particular manifestation of the full 2^k design matrix, the $m \times m$ leading principal submatrix, for each m such that $1 \le m \le 2^k$, together with the m corresponding mean responses constitute an m-parameter model. In the rest of this paper, such an $m \times m$ leading principal submatrix of this manifestation of the full 2^k design matrix will be denoted as $D_{m\times m}$ and will be

referred to as the *m*-th "design matrix" or simply as a design matrix, when the number *m* of parameters is not important. In such an *m*-parameter model, only these *m* parameters are considered as significant or non-zero. The second main contribution of this paper is that, for each *m* such that $1 \le m \le 2^k$, the *m*-th design matrix $D_{m\times m}$ is invertible, and, therefore, the *m* parameters can be uniquely solved with the *m* corresponding mean responses. The third main contribution of this paper is that the inverse matrix $D_{m\times m}^{-1}$ of each $D_{m\times m}$ can be obtained recursively with simple closed-form formulae, and the fourth main contribution is that the values of the *m* parameters of the *m*-parameter model can also be obtained recursively with simple closed-form formulae.

The first and the fourth major contributions constitute all what an end-user needs to know. They are captured below in an algorithm. The second major contribution lays the foundation of all the other contributions and will be stated as Theorem 1 in Section 4, together with its proof. The third major contribution is useful for calculating the variances of the individual parameter estimators or the covariance structure of the estimators, among other uses, and is captured below in another algorithm. The rationales for the two algorithms have been illustrated in Section 2. We now state the two algorithms and leave the proofs for their validity to the next section. The first algorithm generates for any given parameter-factorial-completing parameter sequence a corresponding treatment-combination sequence according to the one-to-one factor-to-high-level correspondence and generates recursively the parameter estimators for all the *m*-parameter models. We refer to it as "The Sequentially and Optimally Estimating Parameters (SOEP) Algorithm for 2^k DOE" or simply as "The SOEP Algorithm".

The Sequentially and Optimally Estimating Parameters (SOEP) Algorithm for 2^k DOE

Initialization:

Let S_P any parameter-factorial-completing sequence of the parameters of a 2^k factorial design starting with the grand effect as the leading parameter. Let S_{TC} denote the treatment-combination sequence to be constructed by this algorithm. Set $m = 1$. Set S_{TC} to be the base treatment combination "." (where all factors are set at the low level).

Iteration:

Step 1: Set $m = m + 1$. Let the m-th parameter of S_P be denoted as $e_{j_1 j_2 \cdots j_l \cdots j_L}$, where j_1, j_2, ….., j_L are the factors involved.

Step 2: Augment sequence S_{TC} with the treatment combination $\langle j_1 j_2 \cdots j_l \cdots j_L \rangle$. (In other words, select the treatment combination where factors j_1, j_2, ….., j_L are set to the high level while all other factors are set to the low level.)

Step 3: Set the estimate $\hat{e}_{j_1 j_2 \cdots j_l \cdots j_L}$ of $e_{j_1 j_2 \cdots j_l \cdots j_L}$ to be

$$\frac{1}{2^{L-1}}\left[\sum_{\{j_1',j_2',\ldots\ldots,j_{N-1}',j_N'\}\subseteq\{j_1,j_2,\ldots\ldots,j_{L-1},j_L\};\,L-N\,being\,even} \mu_{j_1',j_2',\ldots\ldots,j_{N-1}',j_N'}\right]$$

$$-\frac{1}{2^{L-1}}\left[\sum_{\{j_1',j_2',\ldots\ldots,j_{N-1}',j_N'\}\subseteq\{j_1,j_2,\ldots\ldots,j_{L-1},j_L\};\,L-N\,being\,odd} \mu_{j_1',j_2',\ldots\ldots,j_{N-1}',j_N'}\right],$$

where $\{j_1', j_2', \ldots\ldots, j_{N-1}', j_N'\}$ denotes the set of factors of a treatment combination that are set at the high level and the N denotes the number of such factors. (In other words, estimate $e_{j_1 j_2 \cdots j_l \cdots j_L}$ the same

way as if one is to estimate it with only an *L*-factor full factorial design and with all other *k*-*L* factors set to the low level.)

Step 4: Set $\hat{e}_G$ to $\hat{e}_G + \frac{1}{2}\hat{e}_{j_1 j_2 \cdots j_l \cdots j_L}$ (In other words, update the estimate of the grand effect by adding half of the $\hat{e}_{j_1 j_2 \cdots j_l \cdots j_L}$ obtained in Step 3.) Set all other $\hat{e}_{j_1^{'}, j_2^{'}, \ldots\ldots, j_{N-1}^{'}, j_N^{'}}$ such that $\{j_1^{'}, j_2^{'}, \ldots\ldots, j_{N-1}^{'}, j_N^{'}\} \subseteq \{j_1, j_2, \ldots\ldots, j_{L-1}, j_L\}$ to $\hat{e}_{j_1^{'}, j_2^{'}, \ldots\ldots, j_{N-1}^{'}, j_N^{'}} + \hat{e}_{j_1 j_2 \cdots j_l \cdots j_L}$. (In other words, update estimates of all other parameters constituting the parameter-factorial of a 2^L full factorial design by adding the estimate $\hat{e}_{j_1 j_2 \cdots j_l \cdots j_L}$ of $e_{j_1 j_2 \cdots j_l \cdots j_L}$ obtained in Step 3.) Also, leave all the other parameter estimates intact. Go to Step 1.

The recursive parameter-solution process of SOEP is equivalent to inverting recursively the design matrix of the *m*-parameter model for all *m* such that $1 \le m \le 2^k$. We state this recursive design-matrix inversion as the "Inverting Matrix for Sequentially and Optimally Estimating Parameters (IM-SOEP) Algorithm for 2^k DOE" and as "The IM-SOEP Algorithm" for short. We state the algorithm here and prove it in Section 4 in terms of regression coefficients exclusively and not translating it in terms of the model parameters, because of the nature of matrix operation. Recall that, in Eq. (4), the regression coefficient associated with the grand effect is identical to the grand effect itself while the regression coefficient associated with any other model parameter is half the corresponding model parameter.

The "Inverting Matrix for Sequentially and Optimally Estimating Parameters (IM-SOEP) Algorithm for 2^k DOE" (The IM-SOEP Algorithm)

Initialization:

Let S_P any parameter-factorial-completing sequence of the parameters of a 2^k factorial design starting with the grand effect as the leading parameter. Let S_{TC} denote the treatment-combination sequence constructed by the SOEP Algorithm. The design matrix $D_{2^k \times 2^k}$ is formed with respect to these two corresponding sequences, with the *j*-th column associated with the *j*-th parameter (or regression coefficient) of the given parameter sequence and with the *i*-th row associated with the *i*-th treatment combination of the corresponding treatment-combination sequence. So are the the *m*-th design matrix $D_{m \times m}$ (i.e., the $m \times m$ leading principal submatrix of $D_{2^k \times 2^k}$) and the matrix $D_{m \times m}^{INV}$ produced by this algorithm. Set $m = 1$. Set $D_{m \times m}^{INV}$ to be the 1×1 matrix $D_{1 \times 1}$ with 1 as the single (1,1) element.

Iteration:

Step 1: Set $m = m + 1$. Let the *m*-th parameter of S_P be denoted as $e_{j_1 j_2 \ldots j_l \ldots j_L}$, where j_1, j_2, ….., j_L are the factors involved.

Step 2: Augment $D_{(m-1) \times (m-1)}^{INV}$ by appending the following $m \times 1$ row vector to form the *m*-th row of $D_{m \times m}^{INV}$. For any set of $N \le L$ factors $\{j_1', j_2', \ldots\ldots, j_{N-1}', j_N'\}$ such that $\{j_1', j_2', \ldots\ldots, j_{N-1}', j_N'\} \subseteq \{j_1, j_2, \ldots\ldots, j_{L-1}, j_L\}$, set the element corresponding to $e_{j_1', j_2', \ldots\ldots, j_{N-1}', j_N'}$ to $\frac{(-1)^{L-N}}{2^L}$. Set the rest of the elements to 0.

Step 3: Augment the $D_{(m-1) \times (m-1)}^{INV}$ to form the first *m*-1 rows of $D_{m \times m}^{INV}$ in the following three sub-steps.

Sub-step 3.1:

Augment each row of $D_{(m-1) \times (m-1)}^{INV}$ by appending 0 as the *m*-th element of the row.

Sub-step 3.2: For any row whose corresponding treatment combination $\left\langle j_1^{'}, j_2^{'}, \ldots\ldots, j_{N-1}^{'}, j_N^{'} \right\rangle$ is such that $\{j_1^{'}, j_2^{'}, \ldots\ldots, j_{N-1}^{'}, j_N^{'}\} \subseteq \{j_1, j_2, \ldots\ldots, j_{L-1}, j_L\}$, add the row obtained in Step 2 (i.e., the *m*-th and last row of $D_{m\times m}^{INV}$) to the corresponding row just obtained in Step 3.1.

Sub-step 3.3: Go to Step 1.

4. Theorems and Proofs

We first show, in Theorem 1, the invertibility of $D_{m\times m}$; the proof is by mathematical induction. The validity of the recursive estimation of the *m*+1 parameters of the (*m*+1)-parameter model based on (a) the *m* estimators of the *m*-parameter model and (b) the (*m*+1)-st regression equation, as stated in the SOEP Algorithm, is proved in three theorems – Theorems 2, 3 and 4. Theorem 2 is about how to estimate the new and (*m*+1)-st parameter, involving neither recursion nor mathematical induction. Given this estimator, Theorem 3 is about how to recursively update the estimators of the first *m* parameters of the *m*-parameter model to obtain the estimators of the first *m* parameters of the (*m*+1)-parameter model. Integrating Theorem 2 and Theorem 3 via mathematical induction, Theorem 4 completes the validity of the recursive estimation of model parameters and hence the validity of the SOEP Algorithm. Theorem 5 establishes that the recursive estimation process of Theorems 2, 3 and 4, i.e., that of the SOEP Algorithm, is equivalent to calculating recursively the inverse matrix $D_{(m+1)\times(m+1)}^{INV}$ based on the inverse matrix $D_{m\times m}^{INV}$ and the new information contained in the (*m*+1)-parameter model. In other words, the recursive parameter-estimation process of the SOEP Algorithm is equivalent to the recursive design-matrix-inversion process of IM-SOEP Algorithm.

The proof of Theorem 1 and Theorem 3 can be facilitated by recognizing a general phenomenon of a full $2^{k'}$ factorial design involving $k' \le k$ factors, as stated in the following Lemma 1. Since this phenomenon holds for any 2^k full factorial design, we state the lemma and prove it in the general context of a general full 2^k factorial design, instead of the present context of a full $2^{k'}$ factorial design.

Lemma 1: In each of the 2^k rows of any 2^k full factorial design of k factors, the number of "-" (i.e., "-1") signs is always equal to the number of "+" signs (i.e., "+1"), except for the row corresponding to the treatment combination with all factors set at the high level (+).

Proof: The 2^k signs of the 2^k model parameters in each row of the 2^k design matrix (or in each equation of Eq. (4)) are exactly the 2^k terms of the sum-of-product expression of $\prod_{j=1}^{k}(1+x_j)$, where the sum-of-product expression is simply $1 + x_1 + ... + x_k + x_1x_2 + ... + x_{k-1}x_k + ... + x_1x_2.....x_{k-1}x_k$. Therefore, the sum of the coefficients in each of the rows is simply $\prod_{j=1}^{k}(1+x_j)$. As a result, the sum is 0 as long as one of the x_j's is -1 or, equivalently, as long as one of the factors is set at low level (-), with the only exception being the case of all factors set to their high levels. This completes the proof.

Lemma 1 means that, in each of the 2^k model equations, there are equal number of negative signs and positive signs in front of the 2^k model parameters, with only one exception. The

exception is the model equation corresponding to the treatment combination with all factors set at their high levels (+).

Theorem 1: Let a parameter-factorial-completing parameter sequence of a 2^k full factorial experiment be given and the treatment-combination sequence be generated by the factor-to-high-level correspondence in Step 2 of the SOEP Algorithm. Then, for any given m such that $1 \le m \le 2^k$, the $m \times m$ design matrix $D_{m\times m}$ is invertible, and the m-parameter model has a unique solution.

Proof: We use the method of mathematical induction. The case of m=1 is trivial. Now suppose, as the induction hypothesis, that the $m \times m$ design matrix $D_{m\times m}$ is invertible. Denote its inverse matrix as $D_{m\times m}^{-1}$, as usual. We seek an $(m+1)\times(m+1)$ matrix such that pre-multiplying it to the $(m+1)\times(m+1)$ design matrix $D_{(m+1)\times(m+1)}$ produces the $(m+1)\times(m+1)$ identity matrix $I_{(m+1)\times(m+1)}$. We use a linear-algebra technique to determine the invertibility of $D_{(m+1)\times(m+1)}$ and, in case of invertibility, to calculate the inverse matrix $D_{(m+1)\times(m+1)}^{-1}$ based on $D_{m\times m}^{-1}$. We define, as the left-hand side of Eq. (5), an $(m+1)\times(m+1)$ matrix in terms of $D_{m\times m}^{-1}$ and $D_{(m+1)\times(m+1)}$ with a goal to transform it into $I_{(m+1)\times(m+1)}$ through a set of elementary row operations (EROs) and to transform simultaneously the bracketed matrix on the right-hand side of Eq. (5) into the inverse matrix $D_{(m+1)\times(m+1)}^{-1}$ of $D_{(m+1)\times(m+1)}$ through the same set of EROs.

$$\begin{bmatrix} I_{m\times m} & C_{m\times 1} \\ R_{1\times m} & 1 \end{bmatrix} = \begin{bmatrix} D_{mxm}^{-1} & 0_{m\times 1} \\ 0_{1\times m} & 1 \end{bmatrix} D_{(m+1)\times(m+1)} \tag{5}$$

where $I_{m\times m}$ is the *m*-dimensional identity matrix, $C_{m\times 1}$ is an *m*-dimensional column vector, $R_{1\times m}$ is an *m*-dimensional row vector, $0_{m\times 1}$ is the *m*-dimensional column vector of 0's, and $0_{1\times m}$ is the *m*-dimensional row vector of 0's. It is clear that the (*m*+1)-dimensional row vector $[R_{1\times m}\ 1]$ is simply the (*m*+1)-st row of $D_{(m+1)\times(m+1)}$. We now relate $C_{m\times 1}$ to $D^{-1}_{m\times m}$ and $D_{(m+1)\times(m+1)}$ as follows. The first *m* rows of $D_{(m+1)\times(m+1)}$ is simply $[D_{m\times m}\ C'_{m\times 1}]$, where $C'_{m\times 1}$ denotes the last column of the first *m* rows of $D_{(m+1)\times(m+1)}$. Since $D_{m\times m}$ is invertible, by the induction hypothesis, $C'_{m\times 1}$ is linearly dependent on the *m* columns of $D_{m\times m}$. Note that the unique set of multipliers of the linear combination, when expressed as a column vector, is simply $D^{-1}_{m\times m}C'_{m\times 1}$. By Eq. (5), we have $D^{-1}_{m\times m}C'_{m\times 1} = C_{m\times 1}$. We now show that $C_{m\times 1}$ consists of -1's and 0's as follows. Let the (*m*+1)-st parameter be denoted as $e_{j_1 j_2 \cdots j_l \cdots j_L}$, where j_1, j_2, ..., j_L denote the *L* factors involved. Narrow the focus on those columns associated with all 2^L parameters of the parameter factorial of these factors. By Lemma 1, there are an equal number of "+" signs (i.e. +1's) and "–" signs (i.e., -1 's). This implies that all the 2^L columns (limited to the first *m* rows of $D_{(m+1)\times(m+1)}$, i.e., $[D_{m\times m}\ C'_{m\times 1}]$) sum to the *m*-dimensional 0 vector. This further implies that the element of $C_{m\times 1}$ corresponding to any parameter of the parameter factorial of the *L* factors is -1. By the uniqueness of the linear combination, all the other elements of $C_{m\times 1}$ are 0. We now turn our attention to identification of a set of EROs that, when applied to both sides of Eq. (5), transforms the left-hand side to $I_{(m+1)\times(m+1)}$ and hence transforms the bracketed matrix of the right-hand side to $D^{-1}_{(m+1)\times(m+1)}$. Consider two subsets of EROs. The first subset is used to transform the *m*-dimensional row vector $R_{1\times m}$ to the *m*-dimensional 0 vector $0_{1\times m}$. Because $R_{1\times m}$ consists of +1's

and -1's, this subset involves multiplying each of the rows of $[I_{m\times m}\ C_{m\times 1}]$ by either +1 or -1 and adding the resulting row to the last row of the left-hand-side matrix. Note that all the elements of $R_{1\times m}$ in the columns corresponding to the parameter factorial of factors j_1, j_2, ..., j_L are 1. Therefore, the corresponding rows of $[I_{m\times m}\ C_{m\times 1}]$ are multiplied by -1 and then added to the last row $[\,R_{1\times m}\ 1\,]$. For these rows, the corresponding element of $C_{m\times 1}$ *is* -1. Since there are 2^L-1 such rows and all other elements of $C_{m\times 1}$ are 0's, the last element of this last row becomes 2^L Finally, the last row is divided by 2^L. Therefore, the first subset of EROs transforms the last row $[\,R_{1\times m}\ 1\,]$ of the left-hand-side matrix of Eq. (5) to the last row of $I_{(m+1)\times(m+1)}$. Adding this last row to any of those rows with -1 as the last and (m+1)-st element constitutes the second subset of EROs. These two subsets of EROs transform the left-hand-side matrix of Eq. (5) to $I_{(m+1)\times(m+1)}$ and the bracketed matrix of the right-hand side of Eq. (5) to $D^{-1}_{(m+1)\times(m+1)}$. The existence of these two subsets of EROs ensures the invertibility of $D_{(m+1)\times(m+1)}$, which in turn implies uniqueness of the solution to the corresponding parameter model. By mathematical induction, the proof is compete.

We have proved the invertibility of $D_{m\times m}$ for all m such that $1\le m\le 2^k$. This invertibility implies the existence of a unique solution to the m unknown parameters of an m-parameter model. As will be shown below, the SOEP Algorithm produces a solution to these m unknown parameters; hence it produces the unique solution. In the context of statistical estimability, this invertibility implies the existence of a unique set of unbiased estimators; we are content with discussing existence of a set of unbiased estimators, without explicitly referring to the uniqueness. We now prove that, for all m such that $1\le m\le 2^k$, the SOEP Algorithm indeed produces recursively all m

parameter estimates of the *m*-parameter model, all done without any numerical matrix inversion. Let us focus on any model parameter in the given parameter-factorial-completing parameter sequence other than the leading parameter e_G, i.e., the grand effect. More precisely, focus on $e_{j_1 j_2 \ldots j_l \ldots j_L}$.

Due to the construction of the treatment-combination sequence according to the factor-to-high-level correspondence, the treatment combination corresponding to this focal model parameter $e_{j_1 j_2 \ldots j_l \ldots j_L}$ can be expressed in general as $-1,\ldots..,-1,x_{j_1}=1,-1,\ldots..,-1,x_{j_L}=1,-1,\ldots..-1$. This treatment combination together with some preceding ones in the treatment-combination sequence constitute a full treatment-combination factorial for Factors j_1, j_2, ….., j_L, with the treatment levels of all the other factors set at low level (-). Now, focus on exclusively the rows in the current design matrix corresponding to these treatment combinations and the companion mean responses. Obtain the coefficients of $e_{j_1 j_2 \ldots\ldots j_{L-1} j_L}$ associated with all these treatment combinations (corresponding to the full parameter-factorial for the *L* factors). Set the estimator of this parameter $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{i-1} j_L}$ to be the inner product of the coefficients of $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ just obtained and the corresponding mean responses, divided by the divisor 2^{L-1}. More precisely, the linear-combination estimator of the focal parameter $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ can be obtained as follows:

$$f_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L} \equiv f'_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L} \Big/ 2^{L-1} \qquad (6)$$

where 2^{L-1} is the usual divisor and

$$f'_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L} \equiv (-1)^{L-0} \mu_{-1,-1,\ldots..,-1,-1} + (-1)^{L-1} \sum_{u_1 \subset \{j_1, j_2, \ldots\ldots j_{L-1}, j_L\}} \mu_{-1,\ldots..,-1,x_{u_1}=1,-1,\ldots..,-1}$$

$$+(-1)^{L-2}\sum_{\{u_1,u_2|u_1<u_2\}\subset\{j_1,j_2,.....j_{L-1},j_L\}}\mu_{-1,.....,-1,x_{u_1}=1,-1,.....,-1,x_{u_2}=1,-1,....-1} \quad (7)$$

+…..

$$+(-1)^{L-(L-1)}\sum_{\{u_1,u_2,.....u_{L-1}|u_1<u_2<....<u_{L-1}\}\subset\{j_1,j_2,.....j_{L-1},j_L\}}\mu_{-1,.....,-1,x_{u_1}=1,-1,.....,-1,x_{u_{L-1}}=1,-1,....-1}$$

$$+(-1)^{L-(L)}\mu_{-1,.....,-1,x_{j1}=1,-1,.....,-1,x_{jL}=1,-1,....-1}$$

Note that this linear function $f'_{j_1j_2j_3j_4.....j_{L-1}j_L}$ does not involve any treatment combination in which at least one factor not belonging to the set of factors $j_1, j_2, \ldots, j_{L-1}$ and j_L is set to the high level (+). Note again that all the treatment combinations involved constitute a treatment-combination factorial design for the L factors $j_1, j_2, \ldots, j_L$ and that the levels for all the other factors are set at their corresponding low levels (i.e., "-").

Theorem 2: Let a parameter-factorial-completing parameter sequence of a 2^k full factorial experiment be given and the treatment-combination sequence be generated by the factor-to-high-level correspondence accordingly. Let $e_{j_1j_2j_3j_4.....j_{L-1}j_L}$ be any arbitrary and (m+1)-st parameter of the sequence. Then, the estimator defined in Equation (6) is an unbiased estimator of $e_{j_1j_2j_3j_4.....j_{L-1}j_L}$ for the (m+1)-parameter model.

Proof: Denote the number of parameters preceding $e_{j_1j_2j_3j_4.....j_{L-1}j_L}$ in the given parameter sequence as m; $e_{j_1j_2j_3j_4.....j_{L-1}j_L}$ is the (m+1)-st parameter. Each of the mean responses in Eq. (7) can be replaced with a linear combination of the parameters of the (m+1)-parameter model. To show that $f_{j_1j_2j_3j_4.....j_{L-1}j_L}$ produces exactly $e_{j_1j_2j_3j_4.....j_{L-1}j_L}$, we replace each of the mean responses in

Eq. (7) with the corresponding linear combination. We show first that, after the replacements, the coefficient of the new parameter $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ in Eq. (7) is 2^L and then that the coefficients for all the other m parameters are 0. Recall that the treatment combinations involved in calculating $f_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ constitute a full treatment-combination factorial for the L factors, with the levels of all other factors set at the low ("-"); no other treatment combinations are involved. In the rest of this proof, we will limit our attention exclusively to only these treatment combinations. For ease of discussion, when we refer to a column, we actually address only those entries of these treatment combinations in this column. Similarly, when we refer to a full design matrix, we actually address only those rows of these treatment combinations of this design matrix. For ease of discussion, we will drop the qualifier "with the levels of all other factors set at the low ("-")" and will refer to these treatment combinations as "L-factor (full) treatment-combination factorial." Note again that the coefficients of the mean responses in Eq. (7) are exactly the corresponding entries in the $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ column of the full 2^k design matrix. Therefore, Eq. (7) is nothing but the inner product of the $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ column and the mean response column, with the scope limited to only L-factor (full) treatment-combination factorial. This implies that the coefficient of $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ in Eq. (7) is 2^L. We now show that the coefficients for all the other m parameters are 0.

The other m parameters can be partitioned into two groups. Group 1 is the set of all the parameters of the parameter factorial of the L factors $j_1, j_2, \ldots, j_{L-1}$ and j_L, except $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$; these parameters include all main effects of the L factors $j_1, j_2, \ldots, j_{L-1}$ and j_L, all interactions between any two of these L factors, and up to all interactions among any L-1 factors of these L

factors. Group 2 consists of all the other parameters. We deal with group 1 first and then group 2. The orthogonality among all columns of this full design matrix (limited to the L-factor (full) treatment-combination factorial of the L factors $j_1, j_2, \ldots, j_{L-1}$ and j_L) implies that in Eq. (7), the coefficients for all the parameters of group 1 is 0. Group 2 parameters can be further partitioned into two sub-groups: those involving at least one of the L factors $j_1, j_2, \ldots, j_{L-1}$ and j_L and those involving no such factors at all. The column associated with any parameter of the first sub-group is obtained by multiplying the levels of those factors (expressed as either +1 or -1) belonging to the set of factors $j_1, j_2, \ldots, j_{L-1}$ and j_L by a constant -1 or 1 depending on whether there are an odd or even number of other factors involved in the parameter. (Note that the first sub-group of parameters does not contain $e_{j_1 j_2 j_3 j_4 \ldots j_{L-1} j_L}$ because it appears as the (m+1)-st parameter in the given parameter sequence, beyond the range of its m preceding parameters being considered for the two groups.) As a result, the orthogonality among the columns associated with the parameter factorial of $j_1, j_2, \ldots, j_{L-1}$ and j_L ensures the orthogonality between any of those columns associated with the parameters of the first sub-group and the column associated with $e_{j_1 j_2 j_3 j_4 \ldots j_{L-1} j_L}$. The orthogonality between the column associated with any parameter of the second sub-group and the $e_{j_1 j_2 j_3 j_4 \ldots j_{i-1} j_i}$ column results from the fact that the coefficients of the latter column sum up to 0 and the fact that the coefficients of the former column are identically -1 or 1, depending on whether there are an odd or even number of other factors involved in the parameter. This completes the proof.

We have just shown how to estimate the newly added model parameter $e_{j_1 j_2 \ldots j_l \ldots j_L}$. We now show how to update the estimators of the preceding parameters in the parameter sequence in light of the newly added model parameter, the corresponding treatment combination, and its mean

response. The proof can be facilitated by recognizing two general phenomena of a full $2^{k'}$ factorial design involving $k' \leq k$ factors; one of them being Lemma 1 and the other one being stated in the following Lemma 2. As mentioned earlier, since these facts hold for any 2^k full factorial design, the two lemmas are stated and proved in the general context of a general full 2^k factorial design, instead of the present context of a full $2^{k'}$ factorial design.

Lemma 2: Consider the model equations in Eq. (4). Denote the 2^k parameters as $v_1, v_2, ..., v_{2^k-1}$ and v_{2^k}. Let v_1 be the grand effect e_G and v_{2^k} be the *k*-factor interaction and the last model parameter; let treatment combination 2^k be the last treatment combination and the one in which all factor levels are set to the high level (+). Consider any generic model equation associated with any of the first 2^k -1 treatment combination. Let $c_1, c_2, ..., c_{2^k-1}$ denote the coefficients of the first 2^k-1 parameters $v_1, v_2, ..., v_{2^k-1}$ and let μ denote the mean response. Suppose that the first 2^k -1 parameters $v_1, v_2, ..., v_{2^k-1}$ can be solved with the first 2^k-1 model equations, with the last parameter v_{2^k} excluded from the equations; let $v_1^*, v_2^*, ..., v_{2^k-1}^*$ denote the solutions, respectively. Then, for any real number α, $\sum_{i=1}^{2^k-1} c_i (v_i^* + \alpha) + (-1)^N \alpha = \mu$, where *N* is the number of factors set at their low levels. Moreover, if the *k*-factor interaction v_{2^k} is included in the full 2^k model and can be solved and if its solution is denoted as $v_{2^k}^*$, then $v_i^* + v_{2^k}^*$, *i*=1,….., 2^k-1 and $v_{2^k}^*$ satisfy the corresponding expanded generic model equation, expanded with one more term $(-1)^N v_{2^k}$.

Proof: None of the 2^k-1 treatment combination is the one with all factor levels set to their high levels. In particular, the arbitrarily chosen treatment combination is not this one. By Lemma 1, we have $\sum_{i=1}^{2^k} c_i = 0$ and hence $\sum_{i=1}^{2^k-1} c_i + (-1)^N = 0$, where N is the number of factors set at low levels. Multiplying both sides by a real number α produces $\sum_{i=1}^{2^k-1} c_i\alpha + (-1)^N\alpha = 0$. Since the first 2^k -1 parameters $v_1, v_2, ..., v_{2^k-1}$ can be solved with the first 2^k-1 model equations and model equation associated with this arbitrarily chosen treatment combination can be any one of the 2^k-1 model equations, we also have $\sum_{i=1}^{2^k-1} c_i v_i^* = \mu$. Summing these two equations produces $\sum_{i=1}^{2^k-1} c_i(v_i^* + \alpha) + (-1)^N\alpha = \mu$. This proves the first part of the Lemma. With α substituted by $v_{2^k}^*$, it is clear that $\sum_{i=1}^{2^k} c_i v_i' = \mu$ where $v_i' \equiv v_i^* + v_{2^k}^*$, i=1,….., 2^k-1, $c_{2^k} = (-1)^N$ and $v_{2^k}' \equiv v_{2^k}^*$. This completes the proof.

As mentioned earlier, estimating the new (m+1)-st model parameter, according to Step 3 of the SOEP Algorithm, involves no recursion and hence requires no mathematical induction for the proof. However, updating the old parameter estimates of the m parameters of the m-parameter model, according to Step 4 of the SOEP Algorithm, involves recursion and requires mathematical induction for the proof. Theorem 3 below establishes the validity of the updating recursion after experimenting the (m+1)-st treatment combination, based on hypothesized validity of the updating recursion after experimenting the first m treatment combinations. This

induction validity will be integrated, in Theorem 4, with the corresponding induction hypothesis and Theorem 2 to establish the validity of the SOEP Algorithm.

Theorem 3: Suppose that the m parameters of the m-parameter model can be estimated with the m corresponding factor-to-high-level treatment combinations. Suppose also that the (m+1)-st model parameter is $e_{j_1 j_2 j_3 j_4 \cdots j_{L-1} j_L}$ and is estimated with the estimator defined in Eq. (6). Then, the m+1 parameters of the parameter sequence of the (m+1)-parameter model can be estimated with the m+1 treatment combinations of the corresponding factor-to-high-level treatment-combination sequence. The new estimate of the grand effect e_G is the old estimate plus half of the estimate for $e_{j_1 j_2 j_3 j_4 \cdots j_{L-1} j_L}$. Moreover, the new estimate of any other of the first m model parameters being part of the parameter factorial of Factors $j_1, j_2, \ldots, j_{L\text{-}1}, j_L$ is simply the old estimate plus the estimate for $e_{j_1 j_2 j_3 j_4 \cdots j_{L-1} j_L}$; the value of any other model parameter remains unchanged.

Proof: Let us focus on any of the m equations of the m-parameter model. We show that the new estimates specified in the theorem statement satisfy the corresponding equation of the (m+1)-parameter model. Since the estimates for all the model parameters not part of the parameter factorial of L factors $j_1, j_2, \ldots, j_{L\text{-}1}$ and j_L remain unchanged, as specified at the end of Step 4 of the SOEP Algorithm, they do not play a role in continued satisfaction of the equation of the (m+1)-parameter model corresponding to the focal equation. Therefore, it suffices to focus on only those model parameters that are part of the parameter factorial of L factors $j_1, j_2, \ldots, j_{L\text{-}1}$ and j_L. This portion of the equation matches the corresponding regression equation associated with a full-factorial model of only the L factors $j_1, j_2, \ldots, j_{L\text{-}1}$ and j_L (without any model parameters involving any of the other factors) except the absence of the focal parameter $e_{j_1 j_2 j_3 j_4 \cdots j_{L-1} j_L}$.

(Here, the correspondence refers to the factor levels.) By Lemma 2, replacing each of the old parameter estimates obtained from the m design equations (associated with the m-parameter model) with the new estimate will produce the new corresponding equation for the (m+1)-parameter model. Note that the new estimates for all the parameters constituting the parameter factorial of L factors $j_1, j_2, \ldots, j_{L-1}$ and j_L. are their old estimates plus the estimate of $e_{j_1 j_2 j_3 j_4 \ldots j_{L-1} j_L}$, except the grand effect e_G. This is because the regression coefficient associated with e_G is the parameter e_G itself while any of the other 2^k regression coefficients is defined to be half of the corresponding model parameter. Since this is true for any of the m equations of the m-parameter model, we have shown that the new estimates satisfy the first m of the m+1 equations of the (m+1)-parameter model. Theorem 1 has established that the $(m+1)\times(m+1)$ design matrix $D_{(m+1)\times(m+1)}$ is invertible. This implies that the solution for the (m+1)-st parameter $e_{j_1 j_2 j_3 j_4 \ldots j_{L-1} j_L}$ specified in Eq. (6) together with the solutions to the first m parameters of any m of the m+1 equations of an (m+1)-parameter model constitute solutions to the m+1 parameters of the (m+1)-parameter model. The theorem follows immediately because the new estimates satisfy the first m of the m+1 equations. The proof is complete.

Theorem 4: Let a parameter-factorial-completing parameter sequence of a 2^k full factorial experiment be given and the treatment-combination sequence be generated by the factor-to-high-level correspondence in Step 2 of the SOEP Algorithm. The first m, for each m such that $1 \le m \le 2^k$, model parameters of the given model-parameter sequence are estimable if the first m treatment combinations of the corresponding treatment-combination sequence are experimented. Moreover, the formulae specified in Theorem 2 and Theorem 3, or, equivalently, in Steps 3 and 4 of the SOEP Algorithm, provide recursively unbiased estimators of the m model parameters.

Proof: The proof is by mathematical induction. When $m = 1$, only e_G appears in the model. The treatment combination "." produces a single equation equating e_G to the mean response of this treatment combination. Now, suppose, as the induction hypothesis, that the first m model parameters of the given model parameter sequence, for any given m such that $1 \le m \le 2^k$, are estimable with the first m treatment combinations of the corresponding treatment-combination sequence. We need to show that the $(m+1)$-st parameter of the sequence, which completes the parameter factorial of its constituent factors with some of the preceding model parameters and is denoted as $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$, as well as all the preceding model parameters are estimable with the first $m+1$ treatment combinations of the corresponding treatment-combination sequence. By Theorem 2, we know that the expected value of the estimator for $e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ as specified in Eq. (6) is the parameter itself and hence that the parameter is indeed estimable. This and the induction hypothesis together constitute the condition of Theorem 3. Therefore, this theorem follows immediately from Theorem 3.

We have established the validity of the SOEP Algorithm. We now prove that, for all m such that $1 \le m \le 2^k$, the IM-SOEP Algorithm produces recursively the inverse of the design matrix $D_{m \times m}$, all done without any numerical matrix inversion. In a nutshell, the proof establishes the equivalence between the recursive parameter-estimation process of the SOEP Algorithm and the recursive design-matrix-inversion process of the IM-SOEP Algorithm.

Theorem 5: Let a parameter-factorial-completing parameter sequence of a 2^k full factorial experiment be given and the treatment-combination sequence be generated by the factor-to-high-

level correspondence in Step 2 of the SOEP Algorithm. The matrix $D_{m\times m}^{INV}$ generated by the IM-SOEP Algorithm recursively for all *m* such that $1 \le m \le 2^k$ is indeed the inverse matrix $D_{m\times m}^{-1}$ of the design matrix $D_{m\times m}$ of the *m*-parameter model.

Proof: Let *m* be any integer such that $1 \le m \le 2^k$, and let the *m*-th parameter of S_P be denoted as $e_{j_1 j_2 \ldots j_l \ldots j_L}$, where j_1, j_2, ….., j_L are the factors involved. We prove the theorem in two parts. We first prove that Step 2 of the IM-SOEP Algorithm produces the *m*-th row of $D_{m\times m}^{-1}$. We then prove that Step 3 of the IM-SOEP Algorithm produces the first *m*-1 rows of $D_{m\times m}^{-1}$. (Part 1) The mean responses involved in Step 2 of the IM-SOEP Algorithm are identical to those involved in Eq. (7), although the indexing of the former is more compact than that of the latter. In Eq. (7), the multipliers applied to the mean responses involved are $(-1)^{L-0}$, $(-1)^{L-1}$, $(-1)^{L-2}$,….., $(-1)^{L-(L-1)}$ and $(-1)^{L-L}$, and this pattern matches exactly the $(-1)^{L-N}$ appearing as the numerator of $\frac{(-1)^{L-N}}{2^L}$ defined in the Step 2 of the IM-SOEP Algorithm, where *N* ranges from 0 to *L*. While the divisor used in Eq. (6) for estimating the model parameter is 2^{L-1}, the divisor used in Step 2 of the IM-SOEP algorithm, as appearing in the denominator of $\frac{(-1)^{L-N}}{2^L}$, is 2^L. These two divisors are consistent because the estimator $f_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ of Eq. (6) is defined to estimate the model parameter $e_{j_1 j_2 \ldots\ldots j_{L-1} j_L}$ while multiplication of the last row of $D_{m\times m}^{INV}$ by the mean responses of the corresponding treatment combinations taking place in Step 2 of the IM-SOEP Algorithm produces the regression coefficient $\frac{e_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}}{2}$. Therefore, the definition of $f'_{j_1 j_2 j_3 j_4 \ldots\ldots j_{L-1} j_L}$ as

specified in Eq.(7) is exactly the result of multiplying the *m*-th row of $D^{INV}_{m\times m}$ by the mean responses of the corresponding treatment combinations. Note that multiplying the *m*-th (and last) row of $D^{INV}_{m\times m}$ by the $m\times 1$ column vector of the mean responses (of the *m*-parameter model) is simply multiplying the same row by the product of design matrix $D_{m\times m}$ multiplied by the $m\times 1$ column vector of the *m* model parameters. (The reason is that this product and the $m\times 1$ column vector of mean responses are simply the two sides of the equations relating model parameters to mean responses of an *m*-parameter model.) Recall in proof of Theorem 1 that, in Eq. (7), only the multiplier of $e_{j_1 j_2 \cdots j_{L-1} j_L}$ is not zero, and that multiplier is 1. This implies that multiplying the *m*-th row of $D^{INV}_{m\times m}$ obtained in Step 2 by the design matrix $D_{m\times m}$ of the *m*-parameter model produces the *m*-th row of $I_{m\times m}$. We have established that Step 2 of the IM-SOEP Algorithm does produce the *m*-th row of $D^{-1}_{m\times m}$. (Part 2) We now prove that Step 3 of the IM-SOEP Algorithm produces the first *m*-1 rows of $D^{-1}_{m\times m}$. Let *i* be any integer such that $1\le i<m$. We consider the *i*-th model parameter (of the parameter sequence). The new estimates established in Theorem 3 and 4 are expressed in terms of the old estimate and the estimate of the new regression coefficient $\frac{e_{j_1 j_2 j_3 j_4 \cdots j_{L-1} j_L}}{2}$. Any such old estimate and the estimate of the new regression coefficient in turn result from multiplying a $1\times m$ row vector by the $m\times 1$ vector of mean responses. Let the *i*-th row of $D^{INV}_{m\times m}$ be the row vector that, when multiplied by the $m\times 1$ column vector of the *m* model parameters, produces the new estimate for the *i*-th model parameter. We consider two cases for *i*. In case 1, the *i*-th model parameter (of the parameter sequence) belongs to the parameter factorial of Factors $j_1, j_2, \ldots, j_{L-1}, j_L$; case 2 applies to all the other model parameters. Theorem 3 establishes for case 1 that the new estimate of the *i*-th regression coefficient is simply the old

estimate plus the estimate for the (m-th) regression coefficient $\frac{e_{j_1 j_2 j_3 j_4 \ldots . j_{L-1} j_L}}{2}$. Note, as discussed in Part 1 for the m-th row of $D_{m\times m}^{-1}$, that multiplying the i-th row of any $m \times m$ matrix by the $m \times 1$ column vector of the mean responses (of the m-parameter model) is simply multiplying the same row by the design matrix $D_{m\times m}$ first and then by the $m \times 1$ column vector of the m model parameters. This simply implies for case 1 that the product of pre-multiplying the design matrix $D_{m\times m}$ by the sum of (a) the i-th row of the $D_{(m-1)\times(m-1)}^{-1}$ augmented with 0 as the m-th element of the augmented row and (b) the m-th (and last row) of $D_{m\times m}^{INV}$ is the i-th row of $I_{m\times m}$. Note that (a) is exactly what Step 3.1 of the IM-SOEP Algorithm produces and (b) is exactly what Step 3.2 of the same Algorithm produces. We now turn our attention to case 2, which is simpler. Theorem 3 establishes for case 2 that the new estimate of the i-th regression coefficient is simply the old estimate itself. Similarly to case 1 (and actually more simply), the product of pre-multiplying the design matrix $D_{m\times m}$ by the i-th row of the matrix $D_{(m-1)\times(m-1)}^{-1}$ augmented with 0 as the m-th element of the augmented row is the i-th row of $I_{m\times m}$. We have now established that Step 3 of the IM-SOEP Algorithm produces the first m-1 rows of $D_{m\times m}^{-1}$. In fact, the Steps 2 and 3 together produce the inverse matrix $D_{m\times m}^{-1}$. The proof for this theorem is complete.

5. Concluding Remarks

Minimization of the number of treatment combinations and unbiased estimation for significant model parameters, i.e., without confounding, are critically important performance goals for 2^k factorial design. Rather than passively choosing from available designs that perform differently

in these and other criteria as a multi-criteria decision-making, Tsao and Liu (2008) and Tsao and Patel (2013) proposed ways to actively achieve both goals simultaneously. Given a set of important model parameters (i.e., factor effects and interactions), their methods achieve the minimum number of treatment combinations for unbiased estimation of these parameters. In the conventional language of design of experiment, these parameters are estimated without confounding among themselves. Tsao and Patel (2013) defined this concept as "active confounding avoidance." Achieving these goals during the stage of identification of significant model parameters, i.e., model building, is more difficult but more important than when these parameters have been identified. Experimentation conducted during this stage is inevitably sequential of some sort. If the sequencing is not done appropriately, experimentation already done earlier in the stage may turn out to be irrelevant or redundant in the end. In such a case, minimization of treatment combinations is not achieved. Tsao and Patel (2013) defined the concept of "forward compatibility" where no treatment combinations already experimented turn out to be unnecessary at the end of the model building process. The methods of Tsao and Liu (2008) and Tsao and Patel (2013) dealt with the most fundamental case where the model parameters of a 2^k design are sequenced in non-increasing order of importance or significance. Their methods produce a corresponding sequence of treatment combinations that achieve minimum treatment combinations, active confounding avoidance and forward compatibility simultaneously.

While the method proposed in Tsao and Liu (2008) is a numerical algorithm, the method of Tsao and Patel (2013) is a design pattern that can be used to generate the treatment-combination sequence intuitively and with ease. (Although that generation process requires no computation

at all, actual estimation of the model parameters requires matrix inversion.) Although the former method requires numerical computation, it requires no use condition at all. In other words, given any parameter sequence, the former method can produce a treatment-combination sequence that achieves the three goals. On the other hand, although the latter method requires no computation at all for the sequencing, it works only for a parameter sequence with a special structure. The required structure is that the sequence be partitioned into blocks of parameters, with the block of grand and main factor effects followed by the block of two-factor interactions, followed by the block of three-factor interactions, and so on until the single-parameter block of the k-factor interaction. (The sequence of the parameters within each block can be arbitrary.) This paper relaxes this structure requirement on the parameter sequence and requires only that, for any parameter of the sequence, all lower-order parameters associated with the factors involved in this parameter have already appeared in the sequence. For example, the interaction between factors A and B must be preceded in the sequence by the grand effect, the main effect of factor A and the main effect of factor B. This condition is stronger than the Effect Heredity Principle, and we refer to it as the Full Heredity Assumption. We believe that this is a very reasonable assumption in practice. Moreover, the method of recursive parameter estimation, as stated in the SOEP Algorithm, and the method of recursive design matrix inversion, as stated in the IM-SOEP Algorithm, not only eliminate the need for matrix inversion throughout the model building process but also provide insights into the process. Therefore, we believe that the intuitive and simple design pattern proposed in this paper achieves not only least treatment combinations, active confounding avoidance and forward compatibility but also high applicability and low complexity.

This paper continues the general approach first proposed in Tsao and Patel (2013) and proposes a significantly improved method along the same approach. Details about this general approach and comparisons between this general approach and other major approaches and methods can be found in Tsao and Patel (2013). Some such details, e.g., what statistical tests are needed to determine when no more experimentation is needed for model building, can also be found in Tsao and Liu (2008).

Worthy subjects of future work include extension of these methods or the underlying approach to more complex real-world restrictions or requirements. Such restrictions or requirements include the situations where nuisance factors exist and blocking is necessary or where unknown factors may exist and randomization is necessary. Some preliminary work on the blocking necessity has been reported (Tsao and Patel, 2012).

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Table 1: Full Design Matrix Facilitating Parameter Estimation

T.C. \ P	G	**A**	**B**	AB	**C**	AC	BC	ABC	**D**	AD	BD	CD	ABD	ACD	BCD	ABCD	M.R.
.	1	**-1**	**-1**	1	**-1**	1	1	-1	**-1**	1	1	1	-1	-1	-1	1	μ_1
a	1	**1**	**-1**	-1	**-1**	-1	1	1	**-1**	-1	1	1	1	1	-1	-1	μ_2
b	1	**-1**	**1**	-1	**-1**	1	-1	1	**-1**	1	-1	1	1	-1	1	-1	μ_3
ab	1	**1**	**1**	1	**-1**	-1	-1	-1	**-1**	-1	-1	1	-1	1	1	1	μ_4
c	1	**-1**	**-1**	1	**1**	-1	-1	1	**-1**	1	1	-1	-1	1	1	-1	μ_5
ac	1	**1**	**-1**	-1	**1**	1	-1	-1	**-1**	-1	1	-1	1	-1	1	1	μ_6
bc	1	**-1**	**1**	-1	**1**	-1	1	-1	**-1**	1	-1	-1	1	1	-1	1	μ_7
abc	1	**1**	**1**	1	**1**	1	1	1	**-1**	-1	-1	-1	-1	-1	-1	-1	μ_8
d	1	**-1**	**-1**	1	**-1**	1	1	-1	**1**	-1	-1	-1	1	1	1	-1	μ_9
ad	1	**1**	**-1**	-1	**-1**	-1	1	1	**1**	1	-1	-1	-1	-1	1	1	μ_{10}
bd	1	**-1**	**1**	-1	**-1**	1	-1	1	**1**	-1	1	-1	-1	1	-1	1	μ_{11}
cd	1	**-1**	**-1**	1	**1**	-1	-1	1	**1**	-1	-1	1	1	-1	-1	1	μ_{13}
abd	1	**1**	**1**	1	**-1**	-1	-1	-1	**1**	1	1	-1	1	-1	-1	-1	μ_{12}
acd	1	**1**	**-1**	-1	**1**	1	-1	-1	**1**	1	-1	1	-1	1	-1	-1	μ_{14}
bcd	1	**-1**	**1**	-1	**1**	-1	1	-1	**1**	-1	1	1	-1	-1	1	-1	μ_{15}
abcd	1	**1**	**1**	1	**1**	1	1	1	**1**	1	1	1	1	1	1	1	μ_{16}
Divisor	16	8	8	8	8	8	8	8	**8**	8	8	8	8	8	8	8	

Table 2: Correspondence Between the Example Parameter Sequence and Its Treatment-Combination Sequence According to the General Intuitive Design Pattern

Parameter Sequence	Corresponding Treatment Combination Sequence – Factors at High Levels	Treatment Combination Sequence – Level Vector	Treatment Combination Sequence - Standard Numbering	Corresponding Mean Response with respect to Equation (2)
G	.	−−−−	TC1	$\mu_{.}$
A	a	+−−−	TC2	μ_{a}
B	b	−+−−	TC3	μ_{b}
AB	ab	++−−	TC4	μ_{ab}
C	c	−−+−	TC5	μ_{c}
AC	ac	+−+−	TC6	μ_{ac}
BC	bc	−++−	TC7	μ_{bc}
ABC	abc	+++−	TC8	μ_{abc}
D	d	−−−+	TC9	μ_{d}
AD	ad	+−−+	TC10	μ_{ad}
BD	bd	−+−+	TC11	μ_{bd}
CD	cd	−−++	TC13	μ_{cd}
ABD	abd	++−+	TC12	μ_{abd}
ACD	acd	+−++	TC14	μ_{acd}
BCD	bcd	−+++	TC15	μ_{bcd}
ABCD	abcd	++++	TC16	μ_{abcd}

Table 3: Set-up for Use of Elementary Row Operations to Calculate Inverse of the 10×10 Design Matrix

	G	A	B	AB	C	AC	BC	ABC	D	AD	RHS	G	A	B	AB	C	AC	BC	ABC	D	AD
G	1	0	0	0	0	0	0	0	0	-1	95	-0.375	0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.5	0
A	0	1	0	0	0	0	0	0	0	-1	40	-0.125	0.125	-0.125	0.125	-0.125	0.125	-0.125	0.125	0	0
B	0	0	1	0	0	0	0	0	0	0	40	-0.125	-0.125	0.125	0.125	-0.125	-0.125	0.125	0.125	0	0
AB	0	0	0	1	0	0	0	0	0	0	35	0.125	-0.125	-0.125	0.125	0.125	-0.125	-0.125	0.125	0	0
C	0	0	0	0	1	0	0	0	0	0	30	-0.125	-0.125	-0.125	-0.125	0.125	0.125	0.125	0.125	0	0
AC	0	0	0	0	0	1	0	0	0	0	25	0.125	-0.125	0.125	-0.125	-0.125	0.125	-0.125	0.125	0	0
BC	0	0	0	0	0	0	1	0	0	0	20	0.125	0.125	-0.125	-0.125	-0.125	-0.125	0.125	0.125	0	0
ABC	0	0	0	0	0	0	0	1	0	0	15	-0.125	0.125	0.125	-0.125	0.125	-0.125	-0.125	0.125	0	0
D	0	0	0	0	0	0	0	0	1	-1	5	-0.5	0	0	0	0	0	0	0	0.5	0
AD	1	1	-1	-1	-1	-1	1	1	1	1	65	0	0	0	0	0	0	0	0	0	1

Table 4: Inverse of the 10×10 Design Matrix

	G	A	B	AB	C	AC	BC	ABC	D	AD	RHS	G	A	B	AB	C	AC	BC	ABC	D	AD
G	1	0	0	0	0	0	0	0	0	0	100	-0.125	-0.125	0.125	0.125	0.125	0.125	0.125	0.125	0.25	0.25
A	0	1	0	0	0	0	0	0	0	0	45	0.125	-0.125	-0.125	0.125	-0.125	0.125	-0.125	0.125	-0.25	0.25
B	0	0	1	0	0	0	0	0	0	0	40	-0.125	-0.125	0.125	0.125	-0.125	-0.125	0.125	0.125	0	0
AB	0	0	0	1	0	0	0	0	0	0	35	0.125	-0.125	-0.125	0.125	0.125	-0.125	-0.125	0.125	0	0
C	0	0	0	0	1	0	0	0	0	0	30	-0.125	-0.125	-0.125	-0.125	0.125	0.125	0.125	0.125	0	0
AC	0	0	0	0	0	1	0	0	0	0	25	0.125	-0.125	0.125	-0.125	-0.125	0.125	-0.125	0.125	0	0
BC	0	0	0	0	0	0	1	0	0	0	20	0.125	0.125	-0.125	-0.125	-0.125	-0.125	0.125	0.125	0	0
ABC	0	0	0	0	0	0	0	1	0	0	15	-0.125	0.125	0.125	-0.125	0.125	-0.125	-0.125	0.125	0	0
D	0	0	0	0	0	0	0	0	1	0	10	-0.25	-0.25	0	0	0	0	0	0	0.25	0.25
AD	0	0	0	0	0	0	0	0	0	1	5	0.25	-0.25	0	0	0	0	0	0	-0.25	0.25