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Abstract	Efficient algorithms for available. They maxin design. Nevertheless, random design and fin general, be different. A algorithm again in sea discovery probability SAS has been develop	or searching for optimal saturated designs for sampling experiments are widely nize a given efficiency measure (such as D-optimality) and provide an optimum they do not guarantee a <i>global</i> optimal design. Indeed, they start from an initial d a local optimal design. If the initial design is changed the optimum found will, in A natural question arises. Should we stop at the design found or should we run the rch of a better design? This paper uses very recent methods and software for to support the decision to continue or stop the sampling. A software tool written in red.					
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ORIGINAL PAPER

Optimal design generation: an approach based on discovery probability

Roberto Fontana

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Abstract Efficient algorithms for searching for optimal saturated designs for sam-1 pling experiments are widely available. They maximize a given efficiency measure 2 (such as D-optimality) and provide an optimum design. Nevertheless, they do not з guarantee a *global* optimal design. Indeed, they start from an initial random design 4 and find a local optimal design. If the initial design is changed the optimum found 5 will, in general, be different. A natural question arises. Should we stop at the design 6 found or should we run the algorithm again in search of a better design? This paper 7 uses very recent methods and software for discovery probability to support the deci-8 sion to continue or stop the sampling. A software tool written in SAS has been 9 developed. 10

11 Keywords Design of experiments · Optimal designs · Unobserved species ·

12 Discovery probability

13 **1 Introduction**

¹⁴ In the design of experiments, optimal designs, or optimum designs, are a class of ¹⁵ experimental designs that are optimal with respect to a given statistical criterion.

In this paper we focus on saturated optimum designs for sampling experiments even if the methodology can also be applied to non-saturated designs without any modification. Saturated designs contain a number of points that is equal to the number of parameters of the model. It follows that saturated optimum designs are often used

²⁰ in place of standard designs, such as orthogonal fractional factorial designs, when

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the cost of each experimental run is high. Main references to optimal designs include
Atkinson et al. (2007), Goos and Jones (2011), Pukelsheim (2006), Rasch et al. (2011),
Shah and Sinha (1989) and Wynn (1970).

The optimality of a design depends on the statistical model that is assumed and is assessed with respect to a statistical criterion, which, for information-based criteria, is related to the variance-matrix of the model parameter estimators. Well-known and commonly used criteria are A-optimality and D-optimality.

Widely used statistical systems like SAS and R have procedures for finding an optimal design according to the user's specifications. In this paper we will refer to Proc Optex of SAS/QC (SAS Institute, Inc. 2010), but the approach can be adopted for other software.

The Optex procedure searches for optimal experimental designs. The user specifies an efficiency criterion, a set of candidate design points, a model and the size of the design to be found and the procedure generates a subset of the candidate set so that the terms in the model can be estimated as efficiently as possible. By default, the standard output of the procedure is a list of 10 designs that are found as the result of 10 runs of the exchange search algorithm (Mitchell and Miller 1970) starting each time from an initial completely randomly chosen design.

The number of times that we decide to run the search algorithm is crucial. Obviously, if we increase it, in general we will explore different local optima with the possibility to find better designs. On the other hand, sometimes, the extra time that we use to explore other possibilities is wasted because new optima do not exist. This work aims at developing a methodology based on a Bayesian updating methodology that could support the user in making the decision whether to stop or continue the search.

Let us consider an example that will be described in more detail in Sect. 4.1. An 45 experimenter wants to study the influence on a response Y (e.g. the fuel consumption 46 of a given engine) of 7 factors (the type of fuel, the age of the engine, etc.) where 47 each factor has 2 levels. The full factorial design has $2^7 = 128$ runs. Let us suppose 48 that both the size of the full factorial design is too high with respect to the available 49 budget and the experimenter believes that a model with only the main effects and 50 2-factor interactions would be sufficiently rich to describe with a good accuracy the 51 phenomenon under study. A minimum size orthogonal fractional factorial design for 52 this case requires 64 runs, which is still a high value (Fontana 2013). The experimenter 53 decides to use a saturated D-optimal design (29 runs). The experimenter runs the Proc 54 Optex procedure of SAS/QC with the default settings and gets a saturated D-optimal 55 design with D-efficiency equal to 82.32. With the methodology described in this paper 56 the experimenter would have been able to find both a better design (D-efficiency equal 57 to 85.63) and a list of 103 D-optimal designs that could be further analysed with respect 58 to different criteria like space filling. 59

The paper is organized as follows. In Sect. 2 we state the problem of finding new optimal designs as the problem of finding new species in a population. Then, in Sect. 3 we describe how our methodology, which is based on the estimator of the discovery probability, could be used for optimal design generation. We also provide a detailed description of the algorithm. In Sect. 4 we describe the results of a computational study in which we ran our algorithm in different cases. Concluding remarks are made in Sect. 5.

The software code that has been developed is written in SAS, is available on request and can be used for any choice of factors, levels and model. It is worth noting that the algorithm, being based on the Proc Optex procedure, can manage not only classical linear model but also nonstandard linear or nonlinear models, (SAS Institute, Inc. 2010).

72 2 Optimal designs vs richness of species

⁷³ We consider the following setting that is quite common in optimal design problems. ⁷⁴ We have *d* factors, A_1, \ldots, A_d . The factor A_i has s_i levels coded with the integer ⁷⁵ $0, \ldots, s_i - 1, i = 1, \ldots, d$. The full factorial design is $\mathcal{D} = \{0, \ldots, s_1 - 1\} \times \ldots \times$ ⁷⁶ $\{0, \ldots, s_d - 1\}$. For each point $\zeta = (\zeta_1, \ldots, \zeta_d)$ of \mathcal{D} we consider a real-valued ⁷⁷ random variable $Y_{\zeta_1, \ldots, \zeta_d}$. We make the hypothesis that the means of the responses, ⁷⁸ E[Y] where Y is the column vector $[Y_{\zeta}; \zeta \in \mathcal{D}]$ can be modeled as

$$E[Y] = X_{\mathcal{D}}\beta, \qquad (1)$$

where X_D is the non-overparametrized design matrix, as it will be defined in Sect. 2.1, and β is the subset of all the effects (constant effect, main effects and interactions) that are supposed to affect the response Y. There is no restriction to the order of the interactions; polynomial effects (linear, quadratic, etc) can also be considered.

Given an efficiency criterion ϕ , a saturated optimal design is a subset of the full factorial design $\mathcal{D} = \{0, \ldots, s_1 - 1\} \times \ldots \times \{0, \ldots, s_d - 1\}$, whose size is equal to the number of degrees of freedom of the model (1) and that maximizes this criterion ϕ . In this paper we focus on information-based criteria and, in particular, on *D*-optimality but other criteria can be chosen (like *A*-optimality and *G*-optimality). We denote this type of problem with the triple ($\mathcal{D}, \mathcal{M}, \phi$) where \mathcal{D} is the full design, \mathcal{M} is the hypothesized model (see Eq. 1) and ϕ is the optimality criterion.

Given a subset \mathcal{F} of \mathcal{D} , the information matrix is defined as $X'_{\mathcal{F}}X_{\mathcal{F}}$ where $X_{\mathcal{F}}$ is the design matrix corresponding to \mathcal{F} and X' is the transpose of X. *D*-optimality aims at maximizing $D_{\mathcal{F}}$, the determinant of the information matrix

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$$D_{\mathcal{F}} = \det(X'_{\mathcal{F}}X_{\mathcal{F}}).$$
⁽²⁾

There are several algorithms for searching for *D*-optimal designs. They have a common structure. They start from an initial design, randomly generated or user specified, and move, in a finite number of steps, to a better design. In general, if a different initial design is chosen, a different optimal design is found.

It follows that, given an algorithm α , a population \mathcal{A}^{D}_{α} of *D*-optimal designs can be defined. This population is made up of all the saturated designs that are the result of the execution of the algorithm α and is a subset of all the subsets of \mathcal{D} of size equal to the number of degrees of freedom of the model.

The elements of \mathcal{A}^{D}_{α} can be classified into species, according to the criterion for which $\mathcal{F}_{1} \in \mathcal{A}^{D}_{\alpha}$ and $\mathcal{F}_{2} \in \mathcal{A}^{D}_{\alpha}$ are of the same species if and only if they have the same value in terms of the *D* criterion, $D_{\mathcal{F}_{1}} = D_{\mathcal{F}_{2}}$.

Studying the species of \mathcal{A}^{D}_{α} or, in general, of $\mathcal{A}^{\phi}_{\alpha}$ where ϕ is an optimal criterion, 106 is interesting for optimal design generation. Let us consider the problem $(\mathcal{D}, \mathcal{M}, \phi)$ 107 and let us choose an algorithm α to search for ϕ -optimal saturated designs. If we run 108 this algorithm *n* times, each time starting from a completely random initial design, 109 we will get a sample of *n* elements of $\mathcal{A}^{\phi}_{\alpha}$. Such elements can be classified in $k_n \leq 1$ 110 *n* different species according to the value of the criterion ϕ . Recent methods for 111 discovery probability estimation, Favaro et al. (2012), can be applied to the vector 112 $(\ell_1, \ell_2, \ldots, \ell_n)$ where ℓ_r is the number of species in the sample with frequency r, 113 $r = 1, \ldots, n$. In particular, based on a sample of size n, for any additional unobserved 114 sample size $m \ge 0$ and for any frequency k = 0, ..., n + m, these methods provide, 115 an explicit estimator for the probability $U_{n+m}(k)$ that the (n+m+1)-th observation 116 coincides with a species whose frequency, within the sample size n + m, is exactly k. 117 The case m = k = 0 corresponds to assessing the probability of finding a new species 118 in the subsequent observation, that in the context of optimal designs, is the probability 119 of finding a saturated design with a different value of the criterion ϕ in the subsequent 120 run of the algorithm. If this probability $U_{n+0}(0)$ is sufficiently high (let us say greater 121 than 0.1 or even 0.05) it would be convenient to run the algorithm again because it 122 is quite likely that we could find a new optimal design. If we found a new design, it 123 could have a greater value of ϕ and this obviously represents an improvement to our 124 optimization process. Even if this new design did not have an higher value of ϕ than 125 the existing ones, this would give the possibility to increase the known part of $\mathcal{A}^{\phi}_{\alpha}$. 126 It is quite common, in practical applications, to choose a design where the optimal 127 criterion has a slightly smaller value than the maximum obtained but which has other 128 better characteristics, such as space filling properties. 129

In particular, for *D*-optimal designs, we know that designs with different values of $D_{\mathcal{F}}$ are non-isomorphic designs. Indeed we observe that, as proved in Proposition 1, see Angelopoulos et al. (2007), isomorphic designs belong to the same species. In general, the opposite is not true because there are designs with the same value of the *D* criterion but that are not isomorphic. As is known two designs are isomorphic if one can be obtained from the other by relabeling the factors, reordering the runs, and switching the levels of factors, e.g. Clark and Dean (2001).

Proposition 1 Let us consider $\mathcal{F}_1 \subseteq \mathcal{D}$ and $\mathcal{F}_2 \subseteq \mathcal{D}$. If \mathcal{F}_1 and \mathcal{F}_2 are isomorphic then $D_{\mathcal{F}_1} = D_{\mathcal{F}_2}$.

Proof We separately analyse row/column permutations and the switching of the levels of some factors. If \mathcal{F}_2 is obtained permuting the rows and/or the columns of \mathcal{F}_1 it follows that

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$$X_{\mathcal{F}_2} = R X_{\mathcal{F}_1} C$$

where R and C are permutation matrices. Then

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$$D_{\mathcal{F}_2} = \det((X'_{\mathcal{F}_2}X_{\mathcal{F}_2}))$$

$$= (\det(R))^2 \det((X'_{\mathcal{F}_1}X_{\mathcal{F}_1}))(\det(C))^2$$
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$$= D_{\mathcal{F}_1}$$

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being det(R) = det(C) = 1. A similar argument holds for switching the levels of some factors.

The knowledge of a set of non-isomorphic designs can also be used for non parametric testing procedures, Giancristofaro et al. (2012) and Basso et al. (2004).

In Sect. 2.1 and 2.2 we provide some details on how the design matrix is built and on how to compute the estimates of the discovery probabilities.

153 2.1 The design matrix

The design matrix $X_{\mathcal{D}}$ in Eq. 1 is built as follows.

The first column is equal to 1 and corresponds to the constant effect, denoted by μ . The constant effect is always considered as a term of the model.

If the main effect of the factor A_i is to be considered in the model, the corresponding $s_i - 1$ columns are computed as follows. For a design point with A_i at its *k*-th level if $1 \le k \le s_i - 1$ the columns are all 0 except for the *k*-th column that is 1; if $k = s_i$ the columns are all -1.

If an interaction $A_{i_1} \star \ldots \star A_{i_k}$ is to be considered in the model, the corresponding $(s_{i_1} - 1) \cdot \ldots \cdot (s_{i_k} - 1)$ columns are computed by taking the horizontal direct product of the columns corresponding to the main effects of A_{i_1}, \ldots, A_{i_k} .

This coding corresponds to modeling without over parametrization and X_D is full rank.

For a subset \mathcal{F} of \mathcal{D} , the design matrix $X_{\mathcal{F}}$ is simply built deleting from $X_{\mathcal{D}}$ the rows that correspond to the points of \mathcal{D} that are not in \mathcal{F} .

168 2.2 Discovery probability

We briefly summarize the main results that are used in this work, as in Favaro et al. (2012). The interested reader should refer to the original paper for a detailed description of the methodology. We observe that the results in Favaro et al. (2012) are an improvement of those in Lijoi et al. (2007) concerning the evaluation of the probability that further sampling reveals new species.

Given a sample of size *n*, the vector (ℓ_1, \ldots, ℓ_n) is built, where ℓ_r is the frequency of species that have been observed *r*-times in the sample, $r = 1, \ldots, n$. We have $\sum_{i=1}^{n} i\ell_i = n$. We denote the number of different species that have been observed in the sample by *j*. We get $\sum_{i=1}^{n} \ell_i = j$.

Based on a sample of size n, for an additional unobserved sample size $m \ge 0$ and for any frequency k = 0, ..., n + m, using a non parametric Bayesian approach, Favaro et al. (2012) provide an estimator for the probability $U_{n+m}(k)$ that the (n + m + 1)-th observation coincides with a species whose frequency, within the sample of size n+m, is exactly k.

We are interested in discovering new species, that correspond to the case k = 0.

From Sect. 2, p.1,190 of Favaro et al. (2012) we obtain

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$$U_{n+0}(0) = \frac{V_{n+1,j+1}}{V_{n,j}}$$

where, for the two-parameter Poisson-Dirichlet process, we have $V_{n,j} = \prod_{i=1}^{j-1} (\theta + i\sigma)/(\theta + 1)_{n-1}, \sigma \in (0, 1), \theta > -\sigma$. The symbol $(a)_n$ denotes the *n*-th ascending factorial of $a, (a)_n = a(a+1) \dots (a+n-1), (a)_0 \equiv 1$. It follows that

$$U_{n+0}(0) = \frac{\theta + j\sigma}{\theta + n}$$

and, for m > 0, we obtain

 $U_{n+m}(0) = \frac{\theta + j\sigma}{\theta + n} \frac{(\theta + n + \sigma)_m}{(\theta + n + 1)_m} \,.$

¹⁹² The estimates $\hat{\sigma}$, $\hat{\theta}$ of σ , θ are obtained as

$$\arg\max_{(\sigma,\theta)} \frac{\prod_{i=1}^{j-1} (\theta+i\sigma)}{(\theta+1)_{n-1}} n! \prod_{i=1}^{n} \left\{ \frac{(1-\sigma)_{i-1}}{i!} \right\}^{\ell_i} \frac{1}{\ell_i!}.$$
(3)

Using $(\hat{\theta}, \hat{\sigma})$ we finally obtain the estimates of the discovery probability at the (n + 1)-th observation

$$\hat{U}_{n+0}(0) = \frac{\theta + j\hat{\sigma}}{\hat{\theta} + n} \tag{4}$$

and at the (n + m + 1)-th observation, m > 0,

$$\hat{U}_{n+m}(0) = \frac{\hat{\theta} + j\hat{\sigma}}{\hat{\theta} + n} \frac{(\hat{\theta} + n + \hat{\sigma})_m}{(\hat{\theta} + n + 1)_m}$$
(5)

199 3 Methodology

²⁰⁰ We repeat the search for optimal designs to analyse the population \mathcal{A}^{D}_{α} of *D*-optimal ²⁰¹ designs that can be found for a given problem using a predefined algorithm α . Each ²⁰² time the algorithm starts from a randomly chosen initial design. We set a maximum ²⁰³ (minimum) number of iterations equal to M_{\star} (m_{\star}). We continue the process until the ²⁰⁴ minimum number m_{\star} of iterations is performed and the estimate of the discovery ²⁰⁵ probability at the subsequent observation goes under a given threshold p_{\star} , or until the ²⁰⁶ maximum number M_{\star} of iterations is reached.

The procedure can be described as follows. A problem $(\mathcal{D}, \mathcal{M}, \phi)$, with $\phi = D$ in our examples, is defined and an algorithm α for ϕ -optimal design generation is chosen. For each iteration $s, s = 1, ..., M_{\star}$,

- 1. using the algorithm α , a ϕ -optimal saturated design \mathcal{F}_s is obtained;
- 211 2. the value of the ϕ -criterion of \mathcal{F}_s is computed;
- 3. the vector (ℓ_1, \dots, ℓ_s) is built, where ℓ_r is the number of species with frequency $r, r = 1, \dots, s;$
- 4. an estimate $(\hat{\sigma}_s, \hat{\theta}_s)$ is obtained, see Eq. 3;
- 5. an estimate of $\hat{U}_{s+0}(0)$ is computed using Eq. 4;

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6. if $\hat{U}_{s+0}(0) < p_{\star}$ and $s \ge m_{\star}$ the algorithm stops, otherwise the next iteration s+1is performed (if $s+1 > M_{\star}$ the algorithm stops).

The main output of the algorithm is a set of designs, where each design belongs to a different species, i.e. has a different value of the ϕ -criterion.

We now provide a detailed description of each step of the algorithm.

221 3.1 Steps 1 and 2

At iteration *s*, with the chosen algorithm α , the Proc Optex procedure is used to generate a *D*-optimal design, \mathcal{F}_s . The species of \mathcal{F}_s is the value of its *D*-efficiency, $E_{\mathcal{F}_s}^D$. The *D*-efficiency of a \mathcal{F} , is defined as

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$$E_{\mathcal{F}}^{D} = 100 \times \left(\frac{1}{\#\mathcal{F}} D_{\mathcal{F}}^{\frac{1}{\#\mathcal{F}}}\right)$$

where $\#\mathcal{F}$ is the number of runs of \mathcal{F} that coincides with the degrees of freedom of the model for saturated designs and $D_{\mathcal{F}}$ is the determinant of the information matrix. The value of the efficiency is rounded to four decimal digits to avoid creating different species from numerical effects.

Using all the designs $\mathcal{F}_1, \ldots, \mathcal{F}_s$ with their corresponding *D*-efficiencies, $E_{\mathcal{F}_1}^D, \ldots, E_{\mathcal{F}_s}^D$ the vector (ℓ_1, \ldots, ℓ_s) is built, where ℓ_r is the number of species with frequency $r, r = 1, \ldots, s$.

234 3.3 Step 4

An estimate $(\hat{\sigma}_s, \hat{\theta}_s)$ must be obtained searching for $(\sigma, \theta), \sigma \in (0, 1), \theta > -\sigma$ that maximizes $f(\sigma, \theta)$, (see Eq. 3),

$$\mathbf{f}(\sigma,\theta) = \frac{\prod_{i=1}^{J-1}(\theta+i\sigma)}{(\theta+1)_{n-1}} n! \prod_{i=1}^{n} \left\{ \frac{(1-\sigma)_{i-1}}{i!} \right\}^{\ell_i} \frac{1}{\ell_i!}$$

The Genetic Algorithm module of SAS/IML has been used. In order to manage the constraints $\sigma \in (0, 1)$, $\theta > -\sigma$ the search has been performed in the region $\mathcal{R} = [\delta, 1 - \delta] \times [-(1 - \delta), T_M]$ with $\delta = 0.01$ and $T_M = 1,000$. This region contains the non-feasible region made by the points inside the simplex $\mathcal{S} = \mathcal{R} \cap \{(\sigma, \theta) : \theta \le -\sigma\}$ whose vertices are $(\delta, -(1 - \delta)), (\delta, -\delta)$ and $(1 - \delta, -(1 - \delta))$. We observe that the edges of \mathcal{S} contain non-feasible points.

We decided to manage this constraint with the penalty method, because this method usually works well when most of the points in the solution space do not violate the constraints, as in our problem. The way in which the penalty in the objective function for unsatisfied constraints has been imposed is described here.

From the point of view of the search of the point $(\sigma_{\star}, \theta_{\star})$ that maximizes $f(\sigma, \theta)$, 248 it is equivalent to consider log $f(\sigma, \theta)$ instead of $f(\sigma, \theta)$ 249

$$\log f(\sigma, \theta) = \log \left(\prod_{i=1}^{j-1} (\theta + i\sigma) \right) + \log(n!) - \log((\theta + 1)_{n-1}) + \log \left(\prod_{i=1}^{n} \left\{ \frac{(1-\sigma)_{i-1}}{i!} \right\}^{\ell_i} \right) - \log(\ell_i!).$$

Omitting the terms that do not depend on σ and θ and as $(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}$ where Γ is 252 the gamma function, the previous equation becomes the function $f_{\star}(\sigma, \theta)$ here 253

$$f_{\star}(\sigma,\theta) = f_{\star}^{(1)}(\sigma,\theta) + f_{\star}^{(2)}(\sigma,\theta),$$

where 255

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$$\mathbf{f}_{\star}^{(1)}(\sigma,\theta) = \sum_{i=1}^{k} \mathbf{f}_{\star}^{(1,i)}(\sigma,\theta)$$

$$f_{\star}^{(2)}(\sigma,\theta) = -\log \Gamma(\theta+n) + \log \Gamma(\theta+1) + \sum_{i=1}^{n} \ell_i \log \Gamma(i-\sigma) - j \log \Gamma(1-\sigma).$$

with $f^{(1,i)}(\sigma,\theta) = \log(\theta + i\sigma)$ and

We observe that, when the point $(\sigma, \theta) \in \mathcal{R}$ does not satisfy the constraint $\theta > -\sigma$ 260 only $f^{(1)}_{\star}(\sigma,\theta)$ becomes not defined. We apply a penalty value to $f^{(1)}_{\star}(\sigma,\theta)$ and to 26 $f^{(2)}_{\star}(\sigma, \theta)$ as described below. 262

Given a point P_1 in the non-feasible region, $P_1 = (\sigma, \theta) \in S$, \tilde{P}_1 , the closest 263 point to P_1 with respect to the Euclidean distance that lies in the feasible region, is 264 determined 265

$$\tilde{P}_1 = (\tilde{\sigma}, \tilde{\theta}) = \left(\frac{1}{2}(\sigma - \theta + \epsilon), \frac{1}{2}(\theta - \sigma + \epsilon)\right)$$

where ϵ is a very small number to ensure that \tilde{P}_1 is feasible, i.e. $\tilde{P}_1 \in \mathcal{R} \cap \overline{\mathcal{S}}$. We used $\epsilon = 0.001$. The value of the function $f_{\star}^{(1,1)}$ is computed in \tilde{P}_1 getting $\tilde{Y}_1 = f_{\star}^{(1,1)}(\tilde{\sigma}, \tilde{\theta}) = \log \epsilon$. Then the value Y_1 of $f_{\star}^{(1,1)}$ in P_1 is defined as $f_{\star}^{(1,1)}(\sigma, \theta) = (1 + \epsilon)$. 267 268 269 $b_1)\tilde{Y}_1$ where b_1 is the Euclidean distance between P_1 and \tilde{P}_1 , $b_1 = \sqrt{\frac{1}{2}(\sigma + \theta - \epsilon)^2}$. 270 In an analogous way, we apply this penalty method to all $P_i = (i\sigma, \theta)$ that even-271 tually fall in the non-feasible region S getting $f_{\star,P}^{(1)}(\sigma,\theta)$, the penalized version of 272 $f^{(1)}_{\star}(\sigma,\theta)$. 273

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$$\mathbf{f}_{\star,P}^{(1)}(\sigma,\theta) = \sum_{i=1}^{j-1} \mathbf{f}_{\star,P}^{(1,i)}(\sigma,\theta)$$

where 275

$$\mathbf{f}_{\star,P}^{(1,i)} = \begin{cases} \log(\theta + i\sigma) & \text{if } \theta + i\sigma > 0\\ (1+b_i)\log(\epsilon) & \text{if } \theta + i\sigma \le 0 \end{cases}, \ i = 1, \dots, j-1,$$

and b_i is the Euclidean distance between $P_i = (i\sigma, \theta)$ and $\tilde{P}_i = (\frac{1}{2}(i\sigma - \theta + \epsilon), \frac{1}{2}(\theta - \theta + \epsilon))$ 277 $(i\sigma + \epsilon)$) determined as described above. The penalized version $f_{\star,P}^{(2)}(\sigma,\theta)$ of $f_{\star}^{(2)}(\sigma,\theta)$ 278 is simply defined as 279

$$\mathbf{f}_{\star,P}^{(2)}(\sigma,\theta) = \begin{cases} \mathbf{f}_{\star}^{(2)}(\sigma,\theta) & \text{if } \theta + \sigma > 0\\ (1+b_1)\mathbf{f}_{\star}^{(2)}(\sigma,\theta) & \text{if } \theta + \sigma \le 0\\ & \text{and } \mathbf{f}_{\star}^{(2)}(\sigma,\theta) \le 0 \\ (1-b_1)\mathbf{f}_{\star}^{(2)}(\sigma,\theta) & \text{if } \theta + \sigma \le 0\\ & \text{and } \mathbf{f}_{\star}^{(2)}(\sigma,\theta) > 0 \end{cases}$$

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$$\begin{cases} p < q \Rightarrow b_p > b_q \ p, q = 1, \dots, j-1; \\ b_1 \le \frac{\sqrt{2}}{2}(1 + \epsilon - 2\delta). \end{cases}$$

For $\delta = 0.01$ and $\epsilon = .001$ we get $b_1 < 0.694$.

Using the penalty method, an estimate $(\hat{\sigma}_s, \hat{\theta}_s)$ is obtained finding the maximum of 284 $f_{\star,P}(\sigma,\theta) = f_{\star,P}^{(1)}(\sigma,\theta) + f_{\star,P}^{(2)}(\sigma,\theta).$ 285

Finally we point out that if n = 1 then $f_{\star}(\sigma, \theta) = 0 \ \forall \sigma, \theta$. It follows that n must be 286 greater than 1 to obtain the estimates of σ and θ . If j = 1 then $\ell_1 = \ldots = \ell_{n-1} = 0$, 287 $\ell_n = 1, f_{\star}(\sigma, \theta) \equiv f_{\star}^{(2)}(\sigma, \theta)$ and 288

$$f_{\star}^{(2)}(\sigma,\theta) = -\log\Gamma(\theta+n) + \log\Gamma(\theta+1) + \log\Gamma(n-\sigma) - \log\Gamma(1-\sigma).$$

In this case we get $\hat{\sigma} = \delta$ and $\hat{\theta} = -\delta + \epsilon$. 29

3.4 Steps 5 and 6 292

The estimate of the discovery probability at the next iteration, $\hat{U}_{s+0}(0)$, is computed 293 as described in Sect. 2, Eq 4. If its value is lower than p_{\star} and $s \geq m_{\star}$ the algorithm 294 stops, otherwise the next iteration s + 1 is performed (if $s + 1 > M_{\star}$ the algorithm 295 stops). The algorithm takes a decision only if $s \ge m_{\star}$ because we want to avoid that 296 the estimates $(\hat{\sigma}_s, \hat{\theta}_s)$ and consequently $\hat{U}_{s+0}(0)$ be based on too small sample sizes. 297 We suggest using m_{\star} at least equal to 50. 298

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Table 1 Test cases description; ID is the test case number, *d* is the number of factors, *p* is the number of levels of each factor, \mathcal{M} is the model and Method is the algorithm that is used for *D*-optimal design generation. The notation $x_1 | \ldots | x_d @h$ means that all the *k*-factor interactions, $k \le h$, are included in the model \mathcal{M} ; k = 1 refers to main effects

ID	d	р	\mathcal{M}	Method
1	7	2	$ \begin{array}{c} x_1 \dots x_7 @ 2 \\ x_1 \dots x_7 @ 2 \\ x_1 \dots x_6 @ 1 \\ x_1 \dots x_6 @ 1 \\ x_1 \dots x_5 @ 2 \end{array} $	Exchange
2	7	2		Fedorov
3	6	2		Exchange
4	6	2		Fedorov
5	5	3		Exchange

Table 2 Number ℓ_r of D optimal designs that have found r times, r = 1, ..., 487; only $\ell_r \neq 0$ are shown

r	1	2	3	4	5	6	9	10	11	12	14	15	16	17	20	35	39	40	45	Т
ℓ_r	48	17	8	10	1	4	1	1	1	1	2	2	1	1	1	1	1	1	1	103

299 4 Computational study

We show how the methodology works using the test cases summarized in Table 1. We point out that all the test cases consider the problem of finding saturated D-optimal designs.

³⁰³ 4.1 Test cases 1 and 2

Let us consider 7 factors, each with 2 levels, and the model that contains the overall mean, the main effects and all the 2-factor interactions for a total of 1 + 7 + 21 = 29degrees of freedom. We search for *saturated D*-optimal designs, that is, *D*-optimal designs that contain 29 points.

In test case 1, we use Proc Optex SAS Institute, Inc. (2010) with the exchange method, which is its default search method. With the default setting, the algorithm starts from 10 initial randomly chosen designs providing 10 *D*-optimal designs. We consider the design with the highest value of the *D*-efficiency of the 10 optimal designs as the optimal design found by the algorithm.

Setting the seed that is used for the random generation of the initial designs at 6789, the best of the 10 optimal designs, that we denote by \mathcal{F}_1 , has $D_{\mathcal{F}_1} = 9.0911E39$ and $E_{\mathcal{F}_1}^D = 82.3162$.

Now we run the procedure above with $M_{\star} = 1,000, m_{\star} = 50$ and $p_{\star} = 0.10$. After 316 487 runs, the estimate of the discovery probability at the next observation becomes 317 lower than $p_{\star} = 0.10$ and the algorithm stops ($\hat{U}_{487\pm0}(0) \approx 0.099$). We find 103 dif-318 ferent species of local D-optimal designs. All these designs are not isomorphic (Propo-319 sition 1). The maximum (minimum) value of D-efficiency is 85.6265 (78.9605) and it 320 has been found 9 times (1 time). The statistics ℓ_r , $r = 1, \dots, 487$ are shown in Table 2. 321 The estimates of the discovery probability at the next iteration $\hat{U}_{s+0}(0)$ as a function 322 of the iteration s are plotted in Figure 1. The increase of the sample size seems clearly 323 to stabilize the discovery probability estimates. 324

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Fig. 1 Estimate of the discovery probability at the next iteration $\hat{U}_{s+0}(0)$ as a function of the iteration s. Test case 1, $M_{\star} = 1,000$, $m_{\star} = 50$ and $p_{\star} = 0.10$

We decide to continue the search for new species choosing $p_{\star} = 0.05$ and $M_{\star} = 2,000$. The latter value is chosen taking into account that using Eq. 5 we get $\hat{U}_{487+1000}(0) = 0.048$ and $\hat{U}_{487+2000}(0) = 0.034$. These supplementary runs are added to the previous ones.

After 1,252 supplementary runs the estimate of the discovery probability at the next observation becomes lower than 0.05, $\hat{U}_{1739+0}(0) \approx 0.0499$. After 1,252 + 487 = 1,739 simulations we observe 191 different species of *D*-optimal designs. The maximum value of *D*-efficiency is still 85.6265, while the minimum is 78.1134.

In test case 2 we use the Fedorov algorithm, Fedorov (1972), that is considered more reliable, even if slower, than the exchange algorithm. We keep the standard setting for which, at each iteration, 10 local *D*-optimal designs are generated and the one among them that has the highest *D*-efficiency value is taken as the optimal design.

We choose 3456 as the initial seed. The first iteration provides an optimal design 337 \mathcal{F}_1 with $E_{\mathcal{F}_1}^D = 82.7079$. Now we repeat the procedure with $M_{\star} = 1,000$ and $p_{\star} =$ 338 0.10. After only 18 iterations the estimate of the discovery probability at the next 339 observation becomes less than 0.10, $\hat{U}_{18+0}(0) \approx 0.097$. But being $m_{\star} = 50$ the 340 algorithm continues to iterate. It stops after 50 iterations, with the discovery probability 341 approximately equal to 2% and with 4 designs. The maximum (minimum) value of 342 D-efficiency is 83.9844 (82.4212). Thus we have empirical evidence that the Fedorov 343 algorithm is more stable than the exchange algorithm. We observe that the best design 344 found with the exchange algorithm, that has D-efficiency equal to 85.6265, is not 345 found in this first sample. We were able to find it running the algorithm again with 346 $M_{\star} = 1,000$ and $p_{\star} = 0.01$. In this case after 47 supplementary runs, 97 in total, we 347

find 5 designs and $\hat{U}_{97+0}(0) = 0.0099$. The maximum value of *D*-efficiency becomes 85.6265. If we run the algorithm again with $M_{\star} = 2,000$ and $p_{\star} = 0.001$ after 1,009 supplementary runs, 1,106 in total we find 8 designs and $\hat{U}_{1106+0}(0) = 0.00099$. The maximum (minimum) value of *D*-efficiency is 85.6265 (82.3622).

352 4.2 Test cases 3 and 4

Let us consider 6 factors, each with 2 levels, and the model that contains the overall mean and the main effects for a total of 1 + 6 = 7 degrees of freedom. We search for *D*-optimal designs that contains 7 points.

In test case 3 we use the same *D*-optimal design generation method of test case 1 (i.e. at each iteration the optimal design is the best design among ten optimal designs found using the exchange method starting from ten initial randomly chosen designs). We run our algorithm setting the initial seed to 6116 and with $M_{\star} = 1,000, m_{\star} = 50$ and $p_{\star} = 0.10$. After 50 iterations the algorithm stops with $\hat{U}_{50+0}(0) \approx 0.005$ and has found two classes of designs with *D*-efficiency equal to 84.91 and 87.92.

After 50 iterations the estimate of the discovery probability at the next iteration is already quite small, around 0.5% but we decide to run a maximum of $M_{\star} = 1,000$ supplementary runs setting $p_{\star} = 0.0001$. After a total of 1,050 runs the algorithm stops. No designs with different *D*-optimal efficiency are found. The estimate of the discovery probability at the next iteration is $\hat{U}_{1050+0}(0) \approx 0.00014$.

In test case 4 we replace the exchange algorithm with the Fedorov method. After 50 iterations we find only one class of optimal designs with *D*-efficiency equal to 87.92. The estimate of the discovery probability at the next iteration is $\hat{U}_{51+0}(0) \approx 0.00002$.

370 4.3 Test case 5

Let us now consider 5 factors, each with 3 levels, and the model that contains the overall mean, the main effects and all the 2-factor interactions for a total of $1+5\cdot 2+10\cdot 4=51$ degrees of freedom. We search for *D*-optimal designs that contain 51 points.

If we run the algorithm with the setting of test case 1 or 3 ($M_{\star} = 1,000, m_{\star} = 50$, $p_{\star} = 0.10$, method=exchange) after 1,000 iterations we find $\hat{U}_{1000+0}(0) \approx 95\%$ and 978 different *D*-optimal designs with efficiencies ranging between 25.4333 and 28.6677.

In this case it can be appropriate to round the efficiency values not to four decimal digits (as in all the previous test cases) but to one decimal digit. If we adopt this rounding, after 3,600 iterations we get 33 different designs with *D*-efficiencies ranging between a minimum of 25.2 to a maximum of 28.7. The estimate of the discovery probability at the next iteration is $\hat{U}_{3600+0}(0) \approx 0.0014$ ($\hat{U}_{3600+1000}(0) \approx 0.0011$).

383 4.4 Practical considerations and guidelines

After *s* iterations the algorithm provides $\hat{U}_{s+0}(0)$, an estimate of the probability of discovery of a new value of efficiency at the next iteration. This value is useful to assess how far the set of optimal designs that has been collected up to the iteration *s* is repre-

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³⁸⁷ sentative of *all* the optimal designs $\mathcal{A}^{\phi}_{\alpha}$. $1 - \hat{U}_{s+0}(0)$ estimates the *sample coverage*, that ³⁸⁸ is the proportion of distinct species present in the sample observed with respect to the ³⁸⁹ total population. If the probability of discovery is judged to be still too high or, equiv-³⁹⁰ alently, the sample coverage too low, the user can decide to run the algorithm again.

From a practical point of view, the ideal situation is when the computational budget 301 of the user, M_{\star} , is large enough to reach a very high coverage, let us say of around 392 99.9% (i.e. $\hat{U}_{s+0}(0) \approx 0.1\%$). In practice, in this ideal case, the algorithm can be run 393 for the first time with $p_{\star} = 0.001$, $M_{\star} = 1,000$ and $m_{\star} = 50$. If after the first 1,000 304 iterations the estimate of the discovery probability at the next iteration has not gone 395 under p_{\star} the algorithm can be run again to obtain supplementary observations. The 306 value of M_{\star} can be chosen computing the estimates of the discovery probability at 397 the (1000 + m + 1)-th observation with different values m of the size of an additional 398 unobserved sample size. 399

In any case, even if M_{\star} is not large enough to make the estimate of the discovery probability at the next iteration as small as desired, the user has valuable information about the sample coverage that has been reached so far. Again, an estimate of the discovery probability at the next (n + m + 1)-th observation can be computed. It is useful to consider this estimate for some values of m, let us say m = 1,000 and m = 2,000, to make the decision to continue or stop the sampling.

It is important that the number of simulations is not too small to make the estimates of the discovery probabilities sufficiently stable. We chose to work with $m_{\star} = 50$. To support the choice of m_{\star} the plot of the estimate of the discovery probability $\hat{U}_{s+0}(0)$ as function of the iteration *s* is useful (see Fig. 1).

The values of the efficiency must be rounded to avoid creating different species from 410 numerical effects. Different values of rounding allow us to reduce or to enlarge the 411 number of species of the population under study. This reflects the user's opinion regard-412 ing the difference between efficiency values that must be considered significant from a 413 practical point of view. For example, at the initial stage of our exploration we can round 414 the values of the efficiency to one decimal digit just to know their approximate range. 415 Then in the next stages we can decide to run the algorithm with more decimal digits. 416 We ran the simulation study on a standard laptop (CPU Intel Core i7-2620M CPU 417

2.70 GHz 2.70 GHz, RAM 8 Gb). To give an idea of the computational times required
we report that the first stage of test case 1 (487 iterations, exchange method) needed
around 387 seconds (1.26 second per iteration) while the the first stage of test case 2
(50 iterations, Fedorov method) needed around 27 seconds (1.85 second per iteration).

422 5 Conclusion

Given an optimality criterion ϕ , the problem of ϕ -optimal design generation has been addressed. A methodology to support the decision whether to continue or stop the search for optimal designs has been developed. It combines recent advances on discovery probability estimation, based on a Bayesian non parametric approach, Favaro et al. (2012), with well known methods for optimal design generation.

In principle, this methodology could be applied to any discrete optimisation problem. This topic will be part of future research.

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A software code, written in SAS, that makes use of the Proc Optex procedure, has been developed.

It should also be pointed out that the innovative side of this work lies in using 432 sampling stopping rules to improve the generation process of optimal designs. In this 433 paper we used the Bayesian updating of the discovery probability as proposed by 434 Favaro et al. (2012) but other approaches could be adopted. For example Christen and 435 Nakamura (2003) developed an algorithm based on backward induction. It makes use 436 of a utility function based on the number of new species to be observed and the effort 437 saved from the maximum horizon for accumulation. It could be part of future research 438 using this algorithm in the context of optimal designs generation. 439

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445 References

- Angelopoulos P, Evangelaras H, Koukouvinos C, Lappas E (2007) An effective step-down algorithm for
 the construction and the identification of nonisomorphic orthogonal arrays. Metrika 66(2):139–149
- Atkinson AC, Donev AN, Tobias RD (2007) Optimum experimental designs, with SAS. Oxford University
 Press, New York
- Basso D, Salmaso L, Evangelaras H, Koukouvinos C (2004) Nonparametric testing for main effects
 on inequivalent designs. In: Bucchianico A, Luter H, Wynn H (eds) mODa 7 advances in model oriented design and analysis contributions to statistics. Physica-Verlag, HD, pp 33–40. doi:10.1007/
 978-3-7908-2693-7_4
- Christen JA, Nakamura M (2003) Sequential stopping rules for species accumulation. J Agric Biol Environ
 Stat 8(2):184–195
- 456 Clark JB, Dean A (2001) Equivalence of fractional factorial designs. Stat Sin 11(2):537–548
- Favaro S, Lijoi A, Prunster I (2012) A new estimator of the discovery probability. Biometrics 68(4):1188–
 1196. doi:10.1111/j.1541-0420.2012.01793.x
- 459 Fedorov VV (1972) Theory of optimal experiments. Access Online via Elsevier
- Fontana R (2013) Algebraic generation of minimum size orthogonal fractional factorial designs: an approach
 based on integer linear programming. Comput Stat 28(1):241–253
- 462 Gasparini M (2012) Mixtures and limits of symmetric random integer partitions. Metron LXX(2–3):1–11
- Giancristofaro RA, Fontana R, Ragazzi S (2012) Construction and nonparametric testing of orthogonal
 arrays through algebraic strata and inequivalent permutation matrices. Commun Stat Theory Methods
 41(16–17):3162–3178. doi:10.1080/03610926.2011.579380
- 466 Goos P, Jones B (2011) Optimal design of experiments: a case study approach. Wiley. com
- Lijoi A, Mena RH, Prünster I (2007) Bayesian nonparametric estimation of the probability of discovering
 new species. Biometrika 94(4):769–786
- Mitchell TJ, Miller Jr F (1970) Use of design repair to construct designs for special linear models. Math
 Div Ann Progr Rept(ORNL-4661) pp 130–131
- 471 Pukelsheim F (2006) Optimal design of experiments, vol 50. Society for Industrial Mathematics,
 472 New York
- 473 Rasch D, Pilz J, Verdooren L, Gebhardt A (2011) Optimal experimental design with R. Taylor & Francis,
 474 US
- 475 SAS Institute, Inc (2010) SAS/QC 9.2 User's Guide, 2nd edn. SAS Institute Inc, Cary
- 476 Shah KR, Sinha BK (1989) Theory of optimal designs, vol 582. Springer-Verlag, New York
- Wynn HP (1970) The sequential generation of *d*-optimum experimental designs. Ann Math Stat 41(5):1655–
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