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Covariate Allocation in Completely Randomized Designs under Capsule–Based Cost Constraints

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SUMMARY

The incorporation of covariates into Completely Randomized Designs (CRDs) enhances inferential precision by accounting for systematic variation among experimental units, yet in practical contexts, structural and economic constraints often limit the freedom of covariate assignment. This paper presents a unified framework for optimal covariate allocation in CRDs under a capsule–based cost structure, where a *capsule* represents a subset of plots constrained to share identical covariate values. Such a formulation transforms the classical design problem into a discrete optimization setting that explicitly captures the trade–off between information gain and economic expenditure. For the single–covariate case, it is established that balanced two–capsule partitions achieve the theoretical upper bound on information while minimizing cost, thereby yielding a greedy allocation strategy that is provably D–optimal under the proposed cost model. For the multiple–covariate case, the same two–capsule allocation principle is adopted as far as possible, with higher capsule splits introduced only when necessary to maintain orthogonality or budget feasibility. If the available budget permits each treatment to employ its optimal capsule configuration, the resulting design achieves D–optimality for the covariate parameters; otherwise, partial implementation continues to yield near–optimal efficiency. The framework assumes capsule cost depends solely on its size, ensuring analytical tractability while realistically modelling cost escalation. The proposed methodology unifies theoretical optimality with practical feasibility and can be naturally extended to Randomized Block, Latin Square, and Balanced Incomplete Block Designs under similar capsule–based constraints.

Keywords: Completely Randomized Design; Covariate design; Capsule costs; Optimal allocation; Information matrix; D-optimality.

Prologue

There was a period of time, spanning over several decades, when I frequently visited the Indian Agricultural Statistics Research Institute (IASRI), Pusa, and met both established and emerging design theorists working there. To name a few, these included the late Aloke Dey, Arun K. Nigam, and A. C. Kulshreshtha among the seniors, and Vinod K. Gupta, Seema Jaggi, and Rajender Prasad among the juniors. On most occasions, I was introduced to the then director(s) of the institute, namely Dr. Daroga Singh (1973–1981), Dr. Prem Narayan (1981–1992), Dr. S. D. Sharma (1997–2008), and Dr. V. K. Bhatia (2008–2013).

My brief encounters with the directors invariably ended with warm smiles and exchanges of greetings. I found Dr. Prem Narayan to be a soft-spoken person, and he would often address me by my first name, Bikas. He was aware that I was a friend of G. M. Saha, who had been a first-rate doctoral student of the late Prof. M. N. Das at the Institute during the late 1960s.

I had more than one opportunity to interact with Dr. Prem Narayan during the 48th session of the International Statistical Institute (ISI), held in Cairo from September 9 to 17, 1991. Both Dr. Narayan and I were invited delegates to the conference, and I had the occasion to engage in academic discussions with him during a few technical sessions of mutual interest.

I also witnessed a lighter side of Dr. Narayan during a cruise on the river Nile that was organised for the delegates. We arrived in time for a lively and enjoyable evening, filled with music, dancing, and conviviality, followed by dinner. A group of accomplished dancers initiated the programme and

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soon invited participation from the delegates. To my surprise, Dr. Prem Narayan volunteered to join the dance, following the rhythm with ease, and continued smoothly for nearly ten to fifteen minutes. It was indeed a memorable and delightful sight.

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1. INTRODUCTION

The incorporation of covariates into experimental design has long been recognized as a powerful means of enhancing the efficiency of statistical inference by accounting for systematic sources of variation. Within this context, the Completely Randomized Design (CRD) provides a simple yet fundamental framework for treatment allocation, while the inclusion of covariates introduces an additional dimension of precision and control. When covariate values can be freely assigned, their optimal allocation becomes crucial for maximizing the efficiency of estimation. However, once practical constraints—such as grouping, availability, or cost—are introduced, the problem of determining an optimal allocation structure becomes considerably more intricate.

Early contributions by Troya (Troya 1982a, 1982b) established the notion of *Optimum Covariate Designs* (OCDs) within the framework of completely randomized designs (CRDs). These ideas were subsequently generalized to randomized block designs (RBDs) and balanced incomplete block designs (BIBDs) by Das, Mandal, and Sinha (Das *et al.* 2003).

Further developments by Rao, Rao, Saha, and Sinha (Rao *et al.* 2003), Dutta (Dutta 2004), Dey and Mukerjee (Dey and Mukerjee 2006), Dutta, Das, and Mandal (Dutta *et al.* 2009, 2010), Dutta and Das (Dutta and Das 2013), Dutta and Sinha (Dutta and Sinha 2017a, 2017b), and Saha Ray and Dutta (Saha Ray and Dutta 2019) considerably expanded the scope and applicability of covariate design theory.

In parallel, algorithmic approaches to optimal allocation have been explored in the broader design literature. Harville (Harville 1974) proposed a multistage allocation procedure in which experimental units are assigned sequentially, with iterative improvements achieved through local adjustments such as exchanges between treatments. Building on this framework, Cook and Nachtsheim (Cook and Nachtsheim 1989) incorporated block structures into the allocation process and developed procedures for obtaining nearly D-optimal designs. Hore, Dewanji, and Chatterjee (Hore *et al.* 2014) further extended these ideas to scenarios where covariate values are known in advance, proposing algorithms for generating near-optimal allocation schemes.

The breadth of contemporary research in this area is reflected in recent advances on covariate-adaptive designs balancing efficiency and ethical considerations (Atkinson *et al.* 2017), developments in optimality theory for multi-covariate regression models (Dette and Grigoriev 2022), and covariate-adjusted response-adaptive procedures (Biswas *et al.* 2016; Bhattacharya and Biswas 2023). A comprehensive exposition of these developments is provided in the monograph by Das, Dutta, Mandal, and Sinha (Das *et al.* 2015).

A common feature of the aforementioned works is the assumption that covariates can be assigned freely at the level of individual experimental units. From an applied perspective, however, such unrestricted allocation may be impractical or economically infeasible. To address this limitation, practitioners often adopt structured allocation schemes in which groups of units share common covariate values. This approach not only enhances operational feasibility but also reduces resource wastage and stabilizes treatment comparisons.

Recent contributions have begun to explore such structured frameworks. For instance, Sinha *et al.* (Sinha *et al.* 2014) investigated varietal treatment experiments, while Sinha and Rao (Sinha and Rao 2019) extended the methodology to factorial designs with set size two. Sapam *et al.* (Sapam *et al.* 2024, 2025) examined asymmetric and symmetric factorial designs involving two covariates, and Sarkar *et al.* (Sarkar *et al.* 2025) further advanced the framework to accommodate multiple covariates under the D-optimality criterion.

Nevertheless, the existing body of work largely assumes either unrestricted covariate allocation or ignores explicit cost considerations, thereby overlooking the budgetary trade–offs that naturally arise in practice. In most experimental contexts, resource limitations or implementation logistics necessitate that groups of plots share the same covariate value. Motivated

by this observation, we introduce the concept of *capsules*—subsets of plots within a treatment that must take identical covariate values. Each capsule incurs an associated cost depending on its size, generating a natural trade–off between maximizing information and minimizing resource expenditure. To our knowledge, such a cost–constrained, capsule–based framework for covariate design has not previously been investigated.

Our contribution is threefold. First, we formulate a transparent optimization framework that incorporates capsule costs directly into the covariate allocation process within each treatment, thereby quantifying the trade–off between attainable information for covariate parameters and associated experimental expenditure. The optimization is carried out under the D–optimality criterion. Second, we use sharp treatment–level information bounds for both single and multiple covariates under capsule constraints. Third, we employ two–capsule allocation strategies to develop simple yet general rules that determine how many treatments can be upgraded to informative capsule structures under a fixed total budget, and demonstrate that such allocations lead to globally D–optimal designs.

The remainder of the paper is organized as follows. Section 2 presents a motivating agricultural application. Section 3 introduces the CRD setup with a single covariate. Section 4 extends the analysis to multiple covariates. Section 5 concludes the paper and outlines potential directions for future research. Finally, in Appendix 6, we provide the corresponding R code for implementing the proposed methodology.

2. AGRICULTURAL MOTIVATION AND APPLICATION

While the theoretical framework developed in this paper is general, its motivation is strongly rooted in practical agricultural experimentation, particularly in small-plot farming systems where resource constraints, heterogeneity of soil conditions, and operational feasibility play a crucial role.

In many agricultural settings, especially in small and fragmented landholdings, experimental units are not always independent in terms of covariate assignment. Instead, groups of plots often receive identical treatment conditions due to logistical constraints such as irrigation layout, fertilizer application methods, or labour efficiency. This naturally leads to the concept of *capsules*, as introduced in the present work.

2.1 Small-Plot Nutrient Management as Capsule Structures

The use of fertilizers and manures in small agricultural plots provides a natural real-world interpretation of capsule-based covariate allocation. In such settings, nutrient application is often performed in grouped units rather than at the level of individual plants, leading to structured covariate assignment.

Organic nutrient sources such as compost, vermicompost, and farmyard manure are typically applied uniformly over a group of adjacent plots to improve soil structure and water retention. Similarly, green manures such as *Sesbania* and *Sunnhemp* are incorporated over contiguous areas rather than isolated units. These practices correspond directly to *larger capsule sizes* in our framework, where multiple experimental units share the same covariate value.

On the other hand, inorganic fertilizers such as urea, diammonium phosphate (DAP), and balanced NPK mixtures are often applied more selectively, particularly in high-value crops or controlled experiments. Techniques such as band placement, side dressing, and fertigation allow more precise application, effectively creating *smaller capsules* or even near unit-level variation.

2.2 Mapping Agricultural Practices to Capsule Design

The correspondence between agricultural practices and the proposed capsule model may be summarized as follows:

- **Large capsules (low cost, low variability):** Broadcast application of manure or basal incorporation over large areas.
- **Medium capsules:** Row-based fertilizer placement or grouped irrigation zones.
- **Small capsules (high cost, high information):** Targeted application such as side dressing or fertigation at fine spatial resolution.

Thus, the capsule size directly reflects the trade-off between operational cost and statistical information. Larger capsules reduce cost but limit covariate variability, whereas smaller capsules increase information at higher implementation cost—precisely the trade-off formalized in our optimization framework.

2.3 Illustrative Example: Small Plot Experiment

Consider an agricultural experiment involving v crop varieties grown on small plots with r replications per treatment. Suppose nutrient levels (e.g., nitrogen application) are treated as a covariate. Due to practical constraints, the researcher may choose to divide the plots of each treatment into two groups:

- One group receiving high nutrient input (+1),
- Another group receiving low nutrient input (–1).

This corresponds exactly to the *two-capsule partition* shown in Section 3, which is theoretically optimal under the proposed model. If resources permit more refined application (e.g., multiple nutrient gradients), additional capsules may be introduced, though at increased cost.

2.4 Practical Implications

The proposed framework provides a principled way to design agricultural experiments under realistic constraints:

- It formalizes the balance between cost and statistical efficiency.
- It aligns with existing agronomic practices such as integrated nutrient management.
- It offers implementable design strategies for field experiments involving fertilizers, irrigation, or soil amendments.

Consequently, the capsule-based design approach is not merely theoretical but directly applicable to modern agricultural experimentation, particularly in smallholder and resource-constrained environments.

3. CRD SETUP WITH SINGLE COVARIATE

3.1 Model and Optimality Condition

Consider a CRD with v treatments and r replications per treatment, so that the total number of experimental units is

$$N = vr.$$

Let y_{ij} denote the observed response from treatment $i\left(i=1,\ldots,v\right)$ in replication $j\left(j=1,\ldots,r\right)$. A linear model representation of the response is given by

$$y_{ij} = \mu + \tau_i + \gamma x_{ij} + \varepsilon_{ij},\ \ i=1,\ldots,v,\ j=1,\ldots,r, \qquad (1)$$

where

- μ is the overall mean,
- τ_i is the fixed effect of the i th treatment, subject to the constraint $\sum_{i=1}^{v}\tau_i = 0$,
- $x_{ij} \in [-1,1]$ is the value of the covariate associated with unit (i,j),
- γ is the regression coefficient corresponding to the covariate,
- ε_{ij} are independent random errors with mean 0 and variance σ^2.

In the CRD framework, we randomly allocate v treatments such that each treatment is replicated an equal number of times, say r. It is important to note that the optimality condition for estimating all treatment contrasts is achieved when replications are equal (or at least nearly equal). Hence, for clarity of exposition and analytical tractability, we confine our attention to the case of equal replication.

The design problem is to determine an allocation of covariate values $\{x_{ij}\}$ across the N experimental units so as to maximize the information available for estimating the regression parameter γ. This objective is pursued under capsule cost constraints, thereby linking statistical efficiency with practical feasibility. The resulting criterion defines the optimality condition for the design.

3.2 Capsule Constraints

In practice, plots within a replication cannot always be assigned independent covariate values. Instead, they are grouped into *capsules*, which are subsets of plots required to share a common covariate value. Formally, if a capsule $\mathcal{C}_k$ contains $|\mathcal{C}_k| = k$ plots, i.e. a capsule of size k, then

$$x_{ij} = a \ \text{ for all } (i,j) \in \mathcal{C}_k,$$

where $a \in [-1,1]$ is the covariate value assigned uniformly to every experimental unit within capsule $\mathcal{C}_k$.

Let $K_{\max} = |\mathcal{C}_{\max}|$ denote the size of the largest admissible capsule. We assume that capsules of sizes $1,2,\ldots,K_{\max}$ are feasible in the experimental setup, and let f_k denote the number of capsules of size k, i.e. of type $\mathcal{C}_k$, used with $f_k \geq 0$. Accordingly, the replication number r can be expressed as

$$r = \sum_{k=1}^{K_{\max}} k f_k.$$

For example, if $K_{\max} = 7$ and $r = 36$, one admissible decomposition is

$$f_1 = 9,\ f_3 = 5,\ f_6 = 2,$$

corresponding to 9 capsules of type $\mathcal{C}_1$ (single-unit), 5 capsules of type $\mathcal{C}_3$ (three-unit), and 2 capsules of type $\mathcal{C}_6$ (six-unit), together accounting for the total of $r = 36$ replications. It should be noted that such a decomposition is not unique, since different capsule configurations may yield the same replication number.

Each capsule of type $\mathcal{C}_k$ incurs a cost denoted by $C(k)$, representing the resources required to implement its covariate assignment. For analytical tractability, we assume that the cost of a capsule depends *only* on its size k and not on the actual covariate value a assigned. This simplification is natural in many experimental contexts, although in practice one may argue that certain covariate values could be more difficult or costly to implement even for capsules of the same size.

Following an economy-of-scale principle, the average cost per unit decreases with capsule size, i.e.

$$\frac{C(1)}{1} > \frac{C(2)}{2} > \frac{C(3)}{3} > \cdots > \frac{C(K_{\max})}{K_{\max}}.$$

A convenient parametric specification consistent with the assumed cost ordering may be expressed as

$$C(k) = k + c^{\alpha} = k + t, \text{ where } t = c^{\alpha}, c > 0, 0 < \alpha < 1.$$

This formulation reflects that each additional capsule contributes an incremental cost determined by the experimental conditions, without any corresponding gain in statistical information.

Remark 3.1. The exponent α $(0 < \alpha < 1)$ regulates the rate at which the cost escalates with capsule formation. Smaller values of α imply a sublinear or diminishing cost pattern, capturing scenarios where economies of scale or operational efficiencies reduce the marginal expense of introducing additional capsules. This flexible cost model therefore accommodates a wide range of experimental conditions while maintaining the D–optimality of the resulting design.

In this section we have restricted attention to the case of a single covariate x_{ij} under capsule constraints. The extension to multiple covariates, where capsule structures must be coordinated simultaneously across several dimensions, will be developed in subsequent sections under the general framework of *cost capsules*.

3.3 Optimization Problem

Let n_p denote the number of treatments allocated to partition type p. Each partition p specifies a decomposition of the r replications of a treatment into admissible capsule types $\mathcal{C}_k$ with $k \leq K_{\max}$. Such a partition may consist either of repeated capsules of the same type or a mixture of different capsule types.

For clarity, let

$$f_k^{(p)},\ k = 1,\ldots,K_{\max},$$

denote the number of capsules of size k, i.e. of type $\mathcal{C}_k$, used in partition p. By construction, every partition satisfies the consistency condition

$$\sum_{k=1}^{K_{\max}} k f_k^{(p)} = r.$$

For example, when $r = 10$ and $K_{\max} \geq 6$, admissible partitions include:

- $[2+2+2+2+2]$, corresponding to $f_2^{(p)} = 5$,
- $[4+6]$, corresponding to $f_4^{(p)} = 1$ and $f_6^{(p)} = 1$,
- $[3+3+4]$, corresponding to $f_3^{(p)} = 2$ and $f_4^{(p)} = 1$.

These examples illustrate both homogeneous partitions (all capsules of the same size) and heterogeneous partitions (mixtures of different capsule sizes). In general, any admissible partition of r into

capsule sizes not exceeding $K_{\max}$ corresponds to a feasible design configuration.

Within a given treatment i, let $a_{i,k,m} \in [-1,1]$ denote the covariate value assigned to the m-th capsule of type $\mathcal{C}_k$, where $m = 1,\ldots, f_k^{(p)}$. The within-treatment covariate mean is then defined as

$$\bar{x}_{i\cdot} = \frac{1}{r}\sum_{k=1}^{K_{\max}}\sum_{m=1}^{f_k^{(p)}} k\, a_{i,k,m}.$$

The within-treatment sum of squares for treatment i under partition p is

$$S_i(x) = \sum_{k=1}^{K_{\max}}\sum_{m=1}^{f_k^{(p)}} k\,(a_{i,k,m} - \bar{x}_{i\cdot})^2.$$

Hence, the information contribution of partition p for a single covariate is

$$\mathcal{I}_\gamma(p) = \frac{1}{\sigma^2}\sum_{i=1}^{v} S_i(x).$$

The total cost associated with partition p is

$$\text{Cost}(p) = \sum_{k=1}^{K_{\max}} f_k^{(p)}\, C(k).$$

The design optimization problem can now be formulated as

$$\begin{aligned} \max_{\{n_p\}} \quad & \sum_p n_p \cdot \mathcal{I}_\gamma(p) \\ \text{subject to} \quad & \sum_p n_p \cdot Cost(p) \le M, \\ & \sum_p n_p = v, \\ & n_p \in \mathbb{Z}_{\ge 0}, \end{aligned}$$

where M is the total budget.

This formulation highlights the central trade-off: larger capsules (e.g. $\mathcal{C}_k$ with large k) are more economical but restrict covariate variability across the r replications of each treatment, while smaller capsules enhance covariate variation and increase information, but at the expense of higher cost.

3.4 Information Maximization for a Single Treatment under Cost Constraint

For a treatment i under partition p, the within–treatment scatter is

$$S_i(x) = \sum_{k=1}^{K_{\max}}\sum_{m=1}^{f_k^{(p)}} k\,(a_{i,k,m} - \bar{x}_{i\cdot})^2, \quad \bar{x}_{i\cdot} = \frac{1}{r}\sum_{k=1}^{K_{\max}}\sum_{m=1}^{f_k^{(p)}} k\, a_{i,k,m}.$$

By Popoviciu's inequality on variances,

$$\frac{1}{r}S_i(x) = \text{Var}\underbrace{(a_{i,1,1},\ldots,a_{i,k,m},\ldots)}_{r \text{ terms}} \le \frac{(\max_{k,m} a_{i,k,m} - \min_{k,m} a_{i,k,m})^2}{4} \le 1,$$

so

$$S_i(x) \le r.$$

Equality occurs only when the capsule values $a_{i,k,m}$ take exactly the two extreme points $\{-1,+1\}$, with s replications at $+1$ and $r-s$ replications at -1. In this case,

$$\bar{x}_{i\cdot} = \frac{2s-r}{r}, \quad S_i(x) = \frac{4s(r-s)}{r}.$$

The quadratic $s(r-s)$ is maximized when s is as close as possible to $r/2$. Thus the extremal configuration always corresponds to a *balanced* or *near–balanced* split of the replications between $+1$ and -1:

$$\max_p S_i(x) = \begin{cases} r, & r \text{ even}, \\ r-1/r, & r \text{ odd}. \end{cases}$$

Such an extremal assignment can always be realized by a two–capsule partition $p = [r-s+s]$, with one capsule assigned to $+1$ and the other to -1. Any refinement of this configuration into more than two capsules, while preserving the same counts at $+1$ and -1, leaves $S_i(x)$ unchanged. Under the capsule cost model

$$C(k) = k + t,$$

each additional capsule increases the total cost by an amount governed by the experimental conditions, without contributing to any improvement in information. Therefore, among all partitions attaining the maximum information, the two–capsule configuration remains strictly cost–minimal.

The single–capsule partition $[r]$, although less expensive, yields $S_i(x) = 0$ and thus provides no information. Consequently, this case is excluded from consideration within the optimal design framework.

Illustrations

Suppose $K_{\max} \geq r$, so that all partitions of r are feasible. Then the extremal information is always attained by a two–capsule partition that balances the replications as evenly as possible.

Example 3.1: $r = 4$.

Admissible partitions are

$[4],\ [3+1],\ [2+2],\ [2+1+1],\ [1+1+1+1].$

The balanced two–capsule partition $[2+2]$, consisting of two capsules of type $\mathcal{C}_2$, attains

$$\max S_i(x) = 4,$$

at the minimal cost $4 + 2t$.

Example 3.2: $r = 5$.

Admissible partitions include

$[5],\ [4+1],\ [3+2],\ [3+1+1],\ [2+2+1],\ [2+1+1+1],\ [1+1+1+1+1].$

The extremal partition $[3+2]$, with one $\mathcal{C}_3$ and one $\mathcal{C}_2$, achieves

$$\max S_i(x) = 5 - 1/5 = 4.8,$$

at minimal cost $5 + 2t$.

Example 3.3: $r = 6$.

Admissible partitions include

$[6],\ [5+1],\ [4+2],\ [3+3],\ [2+2+2],\ [2+2+1+1],\ [1+1+1+1+1+1],\ldots$

The balanced two–capsule partition $[3+3]$, with two capsules of type $\mathcal{C}_3$, achieves

$$\max S_i(x) = 6,$$

again at the minimal cost $6 + 2t$.

Note 3.1. Since $\max_p S_i(x)$ is independent of the treatment i, the maximum total information is

$$\max_p \mathcal{I}_\gamma(p) = \begin{cases} \dfrac{vr}{\sigma^2}, & r \text{ even}, \\ \dfrac{v}{\sigma^2}(r - 1/r), & r \text{ odd}. \end{cases}$$

This bound is attained under a two–capsule balanced partition, which is strictly cost–minimal among all information–maximizing designs. If the corresponding total cost does not exceed the available budget, such an allocation can be adopted in practice.

4. CRD SETUP WITH MULTIPLE COVARIATES

Building on the single–covariate model (1), we now extend the framework to incorporate multiple quantitative covariates. Let $x_{ij}^{(\ell)} \in [-1,1]$ denote the value of the ℓ th covariate $(\ell = 1,\ldots,q)$ associated with unit (i,j), with corresponding regression parameter $\gamma^{(\ell)}$. The response model is

$$y_{ij} = \mu + \tau_i + \sum_{\ell=1}^{q} \gamma^{(\ell)} x_{ij}^{(\ell)} + \varepsilon_{ij}, \quad i = 1,\ldots,v,\ j = 1,\ldots,r,$$

where μ, τ_i, and ε_{ij} retain their interpretations from the single–covariate case.

After eliminating treatment effects, the information available for the regression parameters $\boldsymbol{\gamma} = (\gamma^{(1)},\ldots,\gamma^{(q)})^\top$ is determined by the scatter of covariates across all replications and treatments.

For treatment i, define the mean of covariate ℓ as

$$\bar{x}_i^{(\ell)} = \frac{1}{r}\sum_{j=1}^{r} x_{ij}^{(\ell)}, \quad \ell = 1,\ldots,q,$$

and the treatment–level scatter matrix as

$$\mathbf{S_i} = \sum_{j=1}^{r} \left(x_{ij} - \bar{x}_i\right)\left(x_{ij} - \bar{x}_i\right)^\top, \ \bar{x}_i = \frac{1}{r}\sum_{j=1}^{r} x_{ij},$$

where $x_{ij} = (x_{ij}^{(1)},\ldots,x_{ij}^{(q)})^\top$.

Ignoring the factor σ^2, the full information matrix for $\boldsymbol{\gamma}$ is

$$\mathrm{M} = \sum_{i=1}^{v} \mathrm{S}_i,$$

a $q \times q$ positive semi-definite matrix representing the total information under the CRD with multiple covariates.

The design objective is to maximize $\mathbf{M}$—in practice, its determinant under the D–optimality criterion—subject to the capsule cost constraints described earlier.

Before proceeding to the analysis of multiple covariates, we note two general principles: (i) under D–optimality, the maximum information is attained when covariates are placed at the extreme points $\{-1,+1\}$; (ii) the determinant of $\mathbf{M}$ is bounded above by an expression that depends only on r, v, and the capsule partition.

These principles form the basis for the subsequent development of D–optimal covariate designs.

Proposition 4.1. Let

$$\mathrm{M} = \sum_{i=1}^{v} \mathrm{S}_i$$

be the full information matrix for

$$\boldsymbol{\gamma} = (\gamma^{(1)},\ldots,\gamma^{(q)})^{\top},$$

where

$$\mathrm{S}_i = \sum_{j=1}^{r} \left(x_{ij} - \bar{x}_i\right)\left(x_{ij} - \bar{x}_i\right)^{\top},\ \bar{x}_i = \frac{1}{r}\sum_{j=1}^{r} x_{ij}.$$

If each covariate satisfies $x_{ij}^{(\ell)} \in [-1,1]$, then

Det($\mathbf{M}$) is maximized when $x_{ij}^{(\ell)} \in \{-1,+1\}$, $\ell = 1,\ldots,q,\ i = 1,\ldots,v.$

Proposition 4.2. Suppose each replication for treatment i carries a q–dimensional covariate vector

$$\boldsymbol{x}_{ij} = (x_{ij}^{(1)},\ldots,x_{ij}^{(q)})^{\top},\ x_{ij}^{(\ell)} \in \{-1,+1\}.$$

Then the full information matrix

$$\mathrm{M} = \sum_{i=1}^{v} \mathrm{S}_i$$

satisfies the inequality

$$\det(\mathbf{M}) \le \det\left((c-d)\mathbf{I}_q + d\,\mathbf{J}_q\right),$$

where $\boldsymbol{I}_q$ is the identity matrix of order q, $\boldsymbol{J}_q$ is the $q \times q$ matrix of ones, c denotes the maximal diagonal entry across all $\mathbf{S}_i$, and d is determined by the capsule partition and replication structure.

This inequality provides a benchmark: any feasible capsule–based allocation must respect it, and designs approaching the bound may be regarded as highly D–efficient.

Finally, since Proposition 4.1 shows that the determinant of the full information matrix $\mathbf{M}$ is maximized when covariate values are chosen at $\{-1,+1\}$, it follows that, under capsule constraints, only capsules formed with covariate assignments ± 1 need be considered. This principle holds uniformly across all treatments $i = 1,\ldots,v$, and will guide the constructions in the subsequent subsection. In particular, recall from Subsection 3.4 that the two–capsule partition is strictly cost–minimal among all information–maximizing allocations. Moreover, when r is even, equal–sized capsules yield the maximum information, while for odd r, nearly equal sizes attain the extremal value. Accordingly, for the case of multiple covariates, we adopt this strategy within each treatment as far as possible, employing balanced (or nearly balanced) two–capsule partitions whenever feasible, and thereby accommodating as many covariates as permitted under the D–optimality criterion.

4.1 Allocation Strategy for Multiple Covariates

In Subsection 3.4 we established that, under capsule constraints, balanced (or nearly balanced) two–capsule partitions provide maximal information for each treatment while remaining strictly cost–minimal. We now extend this reasoning to the case of multiple covariates, where the central question is how many covariates can be accommodated in a D–optimal manner under the same two–capsule strategy.

The following results show that the existence of Hadamard matrices provides a natural construction for achieving D–optimal covariate designs.

Theorem 4.1. If a Hadamard matrix $\mathbf{H}_v$ of order v exists and the replication number r is even, then it is possible to accommodate up to $q = v$ covariates optimally under a two–capsule partition within each treatment.

Proof. Let

$$\mathbf{u} = \begin{pmatrix} \mathbf{1}_{r/2} \\ -\mathbf{1}_{r/2} \end{pmatrix},$$

where $\mathbf{1}_m$ denotes the m–dimensional vector of ones. Thus $\mathbf{u}$ encodes the assignment in which each treatment is divided into two equal capsules of size $r/2$, with covariate values $+1$ and -1.

Let $\mathbf{H}_v = (h_{ij})$ be a Hadamard matrix of order v, with h_{ij} denoting its (i, j)th entry. Construct the covariate allocation matrix

$$\mathbf{X}^{N\times v} = \mathbf{H}_v \otimes \mathbf{u}, \quad N = vr,$$

where $\otimes$ is the Kronecker product. Equivalently, the j th column of $\mathbf{X}$, representing the allocation of the j th covariate, is

$$\mathbf{X}_j = \left(h_{1j}\mathbf{u}', h_{2j}\mathbf{u}', \ldots, h_{vj}\mathbf{u}'\right)', \quad j = 1, 2, \ldots, v.$$

The orthogonality of $\mathbf{H}_v$ ensures that the columns of $\mathbf{X}$ are mutually orthogonal and balanced across treatments. Consequently, the resulting information matrix is proportional to the identity matrix of order N, and hence its determinant attains the maximum possible value, thereby establishing the D–optimality of the design.

Example 4.1. Suppose $v = 4$ treatments and $r = 4$ replications per treatment. Since $v = 4$ and a Hadamard matrix H_4 exists, we can accommodate $q = 4$ covariates.

The basic two–capsule vector is

$$\boldsymbol{u} = \begin{pmatrix} \mathbf{1}_2 \\ -\mathbf{1}_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}.$$

corresponding to two capsules of size $r/2 = 2$ with covariate values $+1$ and -1.

Take the Hadamard matrix of order 4:

$$\mathbf{H}_4 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}.$$

The covariate allocation matrix is then constructed as

$$\mathbf{X}^{16\times 4} = \mathbf{H}_4 \otimes \mathbf{u}.$$

Explicitly,

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}.$$

Thus, each of the four columns of $\mathbf{X}$ represents the allocation of a distinct covariate, and the Kronecker construction guarantees that the covariates are mutually orthogonal and perfectly balanced across the $N = vr = 16$ experimental units. Hence the design achieves D–optimality under two–capsule partitions.

Remark 4.1. If the above conditions are satisfied, the v covariates can be estimated with the minimum possible variance, namely σ^2 / N. Consequently, this construction yields an OCD under the CRD setup (see (Das *et al.* 2015)).

Remark 4.2. When the replication number r is odd and a Hadamard matrix $\mathbf{H}_v$ of order v exists, a perfectly balanced two–capsule partition is not possible. In this case, each treatment is split into two capsules of sizes $(r+1)/2$ and $(r-1)/2$, with covariate values assigned as $+1$ and -1, respectively.

Formally, define

$$\boldsymbol{u} = \begin{pmatrix} \mathbf{1}_{(r+1)/2} \\ -\mathbf{1}_{(r-1)/2} \end{pmatrix},$$

so that $\boldsymbol{u}$ encodes the "almost balanced" partition. The covariate allocation matrix is then constructed as

$$\mathbf{X}^{N\times v} = \mathbf{H}_v \otimes \mathbf{u}, \quad N = vr.$$

Here the Hadamard structure guarantees orthogonality of the covariates across treatments, while the slight imbalance in capsule sizes introduces only a negligible efficiency loss of order $1/r$ for each treatment. By Propositions 4.1 and 4.2, the resulting allocation continues to satisfy the conditions for D–optimality.

Remark 4.3. When v is even but a Hadamard matrix of order v does not exist, it is still possible to construct a D–optimal covariate design in which two covariates can be accommodated optimally under a two–capsule partition. In this case, the allocation may be taken as

$$\mathbf{X} = \begin{pmatrix} \mathbf{1}_{v/2} & \mathbf{1}_{v/2} \\ \mathbf{1}_{v/2} & -\mathbf{1}_{v/2} \end{pmatrix} \otimes \mathbf{u},$$

where $\mathbf{u}$ is the capsule vector defined in Theorem 4.1 and Remark 4.2, depending on whether r is even or odd. These constructions retain mutual orthogonality and balance across treatments, thereby providing valid D–optimal covariate allocations even in the absence of a Hadamard matrix.

Remark 4.4. When v is odd, the allocation strategy can be adapted by treating the last treatment separately, while applying the even–v construction to the remaining $v-1$ treatments.

Let the overall covariate allocation vector be denoted as

$$\boldsymbol{w}^{N\times 1}=\begin{pmatrix}\boldsymbol{w}_1\\ \boldsymbol{w}_2\end{pmatrix},$$

where $N=vr$, $\boldsymbol{w}_1^{(v-1)r\times 1}$ represents the covariate allocation for the first $v-1$ treatments, and $\boldsymbol{w}_2^{r\times 1}$ corresponds to the allocation for the final (odd) treatment.

The construction of $\boldsymbol{w}_1$ follows directly from Theorem 4.1 and Remark 4.3, depending on whether a Hadamard matrix of order $v-1$ exists:

- When $v-1$ is even but a Hadamard matrix does not exist, two $\boldsymbol{w}_1$'s can be accommodated optimally under two–capsule partitions (see Remark 4.3).
- If a Hadamard matrix of order $v-1$ exists, then we can accommodate $v-1$ $\boldsymbol{w}_1$'s under two–capsule partitions (see Theorem 4.1).

The final (odd) treatment requires a modified allocation depending on the replication number r, and $\boldsymbol{w}_2$ is constructed as follows:

- **If** $r\equiv 0 \pmod 4$**:** A two–capsule split $(r/2, r/2)$ with values $+1$ and -1 provides one $\boldsymbol{w}_2$. Alternatively, a four–capsule allocation $(r/4, r/4, r/4, r/4)$ with alternating signs (e.g. $+1,-1,+1,-1$ or $+1,-1,-1,+1$) may be employed to obtain two additional $\boldsymbol{w}_2$'s, and it can be verified that these three $\boldsymbol{w}_2$'s are mutually orthogonal.
- **If** $r\equiv 1 \pmod 4$**:** For $r=2q+1$, a two–capsule partition $(q+1, q)$ with values $+1$ and -1 yields one $\boldsymbol{w}_2$. If $r=4q+1$, a nearly balanced four–capsule configuration $(q+1, q, q, q)$ with alternating signs (e.g. $+1,-1,+1,-1$ or $+1,-1,-1,+1$) can be used to generate two further $\boldsymbol{w}_2$'s.

If the total budget permits a four–capsule partition for constructing $\boldsymbol{w}_2$ in the last treatment, up to three covariates can be accommodated optimally by combining the allocations as follows:

1. When $v-1$ is even but no Hadamard matrix exists, this combination yields two $\boldsymbol{w}_1$'s from the first $v-1$ treatments and any two of the three possible $\boldsymbol{w}_2$'s from the last treatment. Combining these vectors produces two global $\boldsymbol{w}$'s, which together yield a D–optimal covariate design.
2. If a Hadamard matrix of order $v-1$ exists, any three $\boldsymbol{w}_1$'s from the first $v-1$ treatments, combined with the three $\boldsymbol{w}_2$'s from the final treatment, ensure D–optimality of the overall design.

Example 4.2: Consider $v=5$ treatments, each with $r=4$ replications. The first $v-1=4$ treatments follow the even–v construction based on the Hadamard matrix

$$\mathbf{H}_4=\begin{pmatrix}1 & 1 & 1 & 1\\ 1 & -1 & 1 & -1\\ 1 & 1 & -1 & -1\\ 1 & -1 & -1 & 1\end{pmatrix}.$$

With the capsule contrast vector

$$\mathbf{u}=\begin{pmatrix}1\\ 1\\ -1\\ -1\end{pmatrix},$$

corresponding to any treatment, the four covariate allocations for the first $v-1$ treatments are obtained as

$$\left(\boldsymbol{w}_1^{(1)}, \boldsymbol{w}_1^{(2)}, \boldsymbol{w}_1^{(3)}, \boldsymbol{w}_1^{(4)}\right)=\mathbf{H}_4\otimes\mathbf{u},$$

each of order 16×1 and mutually orthogonal across treatments.

For the fifth (odd) treatment, three allocation vectors are constructed, one using a two–capsule partition and the remaining two using four–capsule partitions:

$$\boldsymbol{w}_2^{(1)} = \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, \ \boldsymbol{w}_2^{(2)} = \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \ \boldsymbol{w}_2^{(3)} = \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix},$$

each orthogonal and mean–zero.

Finally, the global covariate allocations are constructed as

$$\boldsymbol{w}^{(i)} = \begin{pmatrix} \boldsymbol{w}_1^{(i)} \\ \boldsymbol{w}_2^{(i)} \end{pmatrix}, \ i = 1,2,3.$$

This allocation achieves D–optimality while maintaining near–minimal loss of efficiency, provided that the higher capsule cost is affordable within the experimental budget.

5. CONCLUSION

This paper has presented a unified framework for covariate allocation in CRDs under capsule–based cost constraints. By introducing the notion of *capsules*—groups of experimental units required to share identical covariate values—we have formalized the trade–off between statistical information and economic expenditure within a discrete optimization setting.

For the single–covariate case, it was shown that two–capsule partitions attain the maximal information bound at the lowest feasible cost increment, thereby yielding a greedy allocation strategy that is provably optimal under the given cost model. For the case of multiple covariates, we have adopted the same principle wherever feasible: the construction relies primarily on two–capsule allocations within each treatment, supplemented, when necessary and affordable, by higher capsule splits to preserve orthogonality across covariates. In particular, if the available budget permits all treatments to employ their corresponding optimal capsule configurations for the covariates, the resulting design achieves at least D–optimality for the covariate parameters within the proposed framework. Otherwise, partial implementation of the capsule structure still yields near–optimal performance with controlled efficiency loss.

For analytical tractability, it has been assumed that the cost of a capsule depends solely on its size k, and not on the actual covariate value assigned to it. However, this assumption may not hold universally, especially when covariate levels themselves influence experimental cost or logistical complexity. Future work may therefore explore models in which the cost function depends jointly on capsule size and covariate value, offering a richer and more realistic understanding of resource allocation in covariate–adjusted designs.

Further extensions may also consider the application of this capsule–based methodology to other classical designs such as Randomized Block Designs (RBDs), Latin Square Designs (LSDs), and Balanced Incomplete Block Designs (BIBDs), thereby broadening the practical scope of D–optimal covariate allocation under realistic cost constraints.

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A Computational Implementation in R

To enhance the practical usability of the proposed capsule-based covariate design methodology, we provide a complete R implementation covering construction, evaluation, optimization, and explicit generation of covariate designs. The code supports both single and multiple covariate settings under cost constraints and includes D-optimal constructions based on Hadamard matrices.

A.1 Core Functions

```
# Capsule cost
capsule_cost <- function(k, t) {
 k + t
}

# Generate partitions
generate_partitions <- function(r, Kmax) {
 partitions <- list()

 helper <- function(remain, max_k, current)
{
 if (remain == 0) {
  partitions[[length(partitions) + 1]] <-
current
 return()
 }
 for (k in seq(min(max_k, remain), 1)) {
 helper(remain - k, k, c(current, k))
 }
 }

 helper(r, Kmax, c())
 partitions
}

# Within-treatment information
compute_Si <- function(x) {
 xbar <- mean(x)
 sum((x - xbar)^2)
}

# Evaluate partition
evaluate_partition <- function(partition,
t) {
 cost <- sum(sapply(partition, capsule_cost,
t = t))
  signs <- rep(c(1, -1), length.out =
length(partition))
```

```
 x <- unlist(mapply(function(k, s) rep(s, k), partition, signs))
 Si <- compute_Si(x)
 list(Si = Si, cost = cost, x = x)
}

# Evaluate design
evaluate_design <- function(v, r, partition, t) {
 results <- lapply(1:v, function(i) evaluate_partition(partition, t))
 total_S <- sum(sapply(results, function(res) res$Si))
    total_cost    <-    sum(sapply(results, function(res) res$cost))
 list(I_gamma = total_S, cost = total_cost)
}

# Optimization
optimize_design <- function(v, r, Kmax, t, budget) {
 partitions <- generate_partitions(r, Kmax)
 best <- NULL
 best_info <- -Inf

 for (p in partitions) {
 res <- evaluate_design(v, r, p, t)
 if (res$cost <= budget && res$I_gamma > best_info) {
 best_info <- res$I_gamma
 best <- list(partition = p, result = res)
 }
 }
 best
}
```

A.2 Single Covariate Design Generation

```
generate_single_design <- function(v, r, partition) {
 design <- c()
 for (i in 1:v) {
  signs <- rep(c(1, -1), length.out = length(partition))
 xi <- unlist(mapply(function(k, s) rep(s, k), partition, signs))
 design <- c(design, xi)
 }

 matrix(design, ncol = 1)
}
```

A.3 Multiple Covariate Design

```
hadamard_matrix <- function(n) {
 if (n == 1) return(matrix(1, 1, 1))
 H <- hadamard_matrix(n/2)
 rbind(cbind(H, H), cbind(H, -H))
}

capsule_vector <- function(r) {
 if (r %% 2 == 0)
 c(rep(1, r/2), rep(-1, r/2))
 else
 c(rep(1, (r+1)/2), rep(-1, (r-1)/2))
}

generate_multi_design <- function(v, r) {
 H <- hadamard_matrix(v)
 u <- capsule_vector(r)
 kronecker(H, u)
}
```

A.4 Information Matrix and D-optimality

```
compute_information_matrix <- function(X, v, r) {
 q <- ncol(X)
 M <- matrix(0, q, q)

 for (i in 1:v) {
 rows <- ((i-1)*r + 1):(i*r)
 Xi <- X[rows, ]
 xbar <- colMeans(Xi)
```

```
 for (j in 1:r) {
 diff <- Xi[j, ] - xbar
 M <- M + tcrossprod(diff)
 }
 }
 M
}

check_d_optimality <- function(M) {
 det(M)
}
```

A.5 Illustrative Examples

Single Covariate: Example 1

```
v <- 4; r <- 6; t <- 0.5; Kmax <- 6; budget <- 100

opt <- optimize_design(v, r, Kmax, t, budget)
X1 <- generate_single_design(v, r, opt$partition)

print(opt$partition)
print(X1)
```

Interpretation: The optimal partition is typically (3,3), yielding a balanced two-capsule structure with maximum information.

Single Covariate: Example 2

```
v <- 3; r <- 5; t <- 0.5; Kmax <- 5; budget <- 100

opt <- optimize_design(v, r, Kmax, t, budget)
X2 <- generate_single_design(v, r, opt$partition)

print(opt$partition)
print(X2)
```

Interpretation: The near-balanced partition (3,2) is selected, consistent with theoretical results for odd r.

Multiple Covariates: Example 1

```
v <- 4; r <- 4

X <- generate_multi_design(v, r)
M <- compute_information_matrix(X, v, r)

print(X)
print(check_d_optimality(M))
```

Interpretation: The design achieves full orthogonality using a Hadamard matrix, ensuring D-optimality.

Multiple Covariates: Example 2

```
v <- 2; r <- 6

X <- generate_multi_design(v, r)
M <- compute_information_matrix(X, v, r)

print(X)
print(check_d_optimality(M))
```

Interpretation: Even with fewer treatments, the Kronecker construction preserves orthogonality and efficiency.

The above implementation provides a complete computational framework for generating and analysing capsule-based covariate designs. It explicitly constructs the covariate allocation matrices and verifies their optimality properties, thereby bridging theoretical development and practical application.