Construction of Computer Experiment Designs from Marked Point Processes

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Abstract

This article presents a method for constructing computer experiment designs. This methodis based on the theory of stochastic processes, particularly two-type marked point processes. The designs obtained using the Monte Carlo Markov Chain (MCMC) method and the Metropolis-Hastings algorithm are highly adaptable and can, therefore, address various objectives. A detailed study on the convergence of the Markov chain has been conducted. A comparison between our approach and other existing Computer designs has been performed.

Keywords: Experiment Designs, Computer Experiment Designs, Point Processes, Marked Point Processes, Markov Chain Monte Carlo (MCMC) Method, Metropolis-Hastings algorithm.

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1. Introduction

In the context of digital simulation, simulated experiments are computationally expensive, making it crucial to employ experimental design methods to optimize their planning. Many phenomena are modeled using digital simulation codes as tools for optimization and prediction. These codes consist of digital models that connect descriptive variables of the system's state to a set of parameters. The simulator takes these parameters as input and generates responses to the state variables of the system. Despite advances in computing, the code for these calculations is complex and often time-consuming to execute. To address this issue, the idea is to replace the simulator with one or more approximation functions constructed using approximation or interpolation methods and based on computer experimental designs. To effectively cover the parameter space and obtain information throughout the experimental domain, we propose a method for constructing computer experiment designs in which experiments are evenly distributed in the unit hypercube. To achieve this, we employ a point process to simulate the points that make up the computer experimental design. This process is Markovian in the sense of Ripley-Kelly [1].

In 2008, Franco [2] first introduced a computer experiment design based on the Strauss pointProcess, which incorporates the concept of interaction between pairs of points. In 2020, Elmossaoui *etal*[3, 4] proposed a method for constructing computer experimental designs based on the use of the marked Strauss process. These planning methods can achieve two objectives: one related to the distribution of points and the other concerning the characterization of the marks on these points. In 2023, Elmossaoui *et al* introduced a newmethod for constructing computer experiment designs based on the use of connected interaction point processes [5]. Our approach expands upon this by using a marked point process with two distinct marks[6]. To generate these designs, we will employ Monte Carlo simulation techniques via MarkovChain (MCMC) and the Metropolis-Hastings algorithm [7].

2. Preliminaries

Let $(\Omega, \mathrm{A}, \mathrm{P})$ be a probability space. Consider χ as a non-empty set equipped with the Euclidean distance d, which makes it a complete separable metric space. If we assume that the model has p continuous factors of interest, where $p \geq 1$, then in most cases, χ will be equal to $[0,1]^p$ (a subset of $\mathbb{R}^p$).Let m denote the Lebesgue measure on this space, equipped with its Borel sigma-algebra A .

Definition 2.1. A configuration is defined as a countable set, unordered set of points $x = (x_1, x_2, ..., x_n)$, where $x_i \in (\chi, d)$, representing the points resulting from a random experiment. A configuration is said to be locally finite if it contains at most a finite number of points within any bounded Borel set A in (χ, d). We denote N^{lf} as the family of locally finite configurations.

Definition 2.2.A point process is a mapping X from a probability space (comprising a metric space χ equipped with a sigma-algebra A and a probability measure P) to the family of locally finite configurations of points in χ. This mapping satisfies the property that for any Borel set $A \subseteq \chi$, the number of points in A, denoted by $N_X(A)$, is a finite discrete random variable.

Definition 2.3.A marked point process is a random sequence $X = \{x_n, m_n\}$ consisting of a point process x_n defined on (χ, d) and corresponding marks m_n for each x_n in a mark space $M = (K, d')$.

Definition 2.4. Let $\sim$ be a symmetric and reflexive relation on χ. Two points x_i and $x_{i'}$ are neighbors if $x_i \sim x_{i'}$. The neighborhood of y is given by:

$$\partial x_i = \{x_i \in x \text{ et } x_i \notin y : \exists x_{i'} \in y \text{ such us } x_{i'} \sim x_i\}$$

Definition 2.5. A function $\pi : \Omega \to [0, +\infty[$ is called a Markov function in the sense of Ripley and Kelly with respect to the relation $\sim$, if for all $x \in \Omega$:

- $\pi(x) > 0$ Implies $\pi(y) > 0$ for all $y \subset x$.
- If $\pi(x) > 0$, then for any $x_i \in \chi$, the ratio $\dfrac{\pi(x \bigcup \{x_i\})}{\pi(x)}$ depends only on x_i and $\partial x_i \bigcap x$

3. Computer Experimental Design Using Marked Markovian Strauss Point Process

The main idea is to consider each experiment x_i as a point or particle defined within $[0,1]^p$, and each configuration x as a matrix of experiments. Each point in this configuration is characterized by two marks m_i and m_i' defined in the mark space M. The point and its marks form an object defined as (x_i, m_i, m_i'). Therefore, we equate the objects (experiment design) to realizations of the two-marked point process X. The marked process implies the possibility of interaction. These interactions correspond to neighborhood properties defined in the

Ripley-Kelly [1]Markov field. The most commonly used interaction potential is the interaction between pairs of objects. These object processes are crucial for modeling repulsive phenomena. The probability density of a two-marked point process for a configuration x of points is given by:

$\pi(x) = \alpha\beta_1^{m_1(x)}\beta_2^{m_2(x)}\gamma_{11}^{m_{11}(x)}\gamma_{12}^{m_{12}(x)}\gamma_{22}^{m_{22}(x)}$ (1.1)Where,

- α is the normalization constant,
- $0 < \gamma_{kl} \leq 1$, where $k \in \{1,2\}$ and $l \in \{1,2\}$ are interaction coefficients,
- β_k, where $k \in \{1,2\}$, is the intensity of the process,
- $m_k(x)$ is the number of points with mark k in x,
- $m_{kl}(x)$ is the number of pairs of $\sim_x$-neighbors of type (k,l) or (l,k) in x (both marked as k and l simultaneously).

3.1. Mark Selection

In this study, we characterize the points using two marks: the first one will be the value of the prediction error $\hat{y}_{x_i}$ at point x_i. Recall that this value is defined as [2]:

$$\text{var}\left(\hat{y}_{x_i}\right) = {}^t f(x_i)\left({}^t XX\right)^{-1} f(x_i)$$

Where,

- $X = {}^t\left[f(x_1), f(x_2), \ldots, f(x_n)\right]$ is the computation matrix, which depends on the chosen experimental points and the assumed model,
- $\left({}^t XX\right)^{-1}$ is the dispersion matrix,
- $f(x_i)$ is the modeled vector for point x_i.

In this case, we define $n_1(x)$ for a configuration x as follows:

$$m_1(x) = \sum_{i=1}^{n} 1_{\text{var}\left(\hat{y}_{x_i}\right) \leq \varepsilon}$$

As a second mark, we will take the average of the normal density distances between point x_i and the other points in configuration x. This mark will be given by:

$$m_2(x) = \sum_{i=1}^{n} 1_{\mu(x_i) \geq r}$$

Where,

- $\mu(x_i) = \frac{1}{n-1}\sum_{\substack{i=1 \\ j \neq i}}^{n} \delta(x_i, x_j)$ with $\delta(x_i, x_j) = \int_0^l \varphi(t)dt$,
- l is the usual distance between points x_i and x_j,
- φ represents the density of the normal distribution,
- where ε and r are fixed values.

4. Simulation of Point Processes using the MCMC Method and the Metropolis-Hastings Algorithm

This method involves constructing a chain $\{X_0, X_1, \ldots, X_N\}$ that converges to the desired distribution π. In fact, the Metropolis-Hastings (MH) algorithm can perform this construction using the π-reversible transition kernel. Recall that the algorithm goes through two steps.

- We propose a state change from x to y according to the probability distribution $Q(x,\cdot)$,
- We accept y with probability $a(x,y)$, otherwise, we stay in the state x (Where $a:\Omega\times\Omega\mapsto[0,1]$).

Let $q(x,y)$ be the density of $Q(x,\cdot)$, the MH transition is written as [8]:

$$P_{MH}(x,y)=a(x,y)q(x,y)+\left[1-\int_{\Omega}a(x,z)q(x,z)dz\right]\delta_x(y)$$

With $\delta_x(.)$ representing the point mass at x. To simplify calculations, we use the Dirac measure at x ($\delta_x(y)=1$ if $x=y$ and 0 otherwise).

The choice of (Q,a) will ensure the π-reversibility of P_{MH} if the following equilibrium equation is satisfied:

$$\forall x,y\in\Omega:\ \pi(x)\times q(x,y)\times a(x,y)=\pi(y)\times q(y,x)\times a(y,x)$$

The choice of the acceptance probability a is more constrained: it is essentially dictated by the goal of (asymptotically) simulating a given probability distribution π. This is the case in the usual choice, where:

$$a(x,y)=\frac{\pi(y)\times q(y,x)}{\pi(x)\times q(x,y)}$$

Two important points to note. Firstly, the calculation of $a(x,y)$ does not require any knowledge of the normalization constant in (1.2).Secondly, in this work, we consider the case where two configurations x and y differ by exactly one point. This is referred to as the 'spin flop dynamics,' and thus, the density q is symmetric:

$$q(y,x)=q(x,y)$$

In this case, the acceptance probability reduces to:

$$a(x,y)=\frac{\pi(y)}{\pi(x)}=\frac{\beta_1^{m_1(y)}\beta_2^{m_2(y)}\gamma_{11}^{m_{11}(y)}\gamma_{12}^{m_{12}(y)}\gamma_{22}^{m_{22}(y)}}{\beta_1^{m_1(x)}\beta_2^{m_2(x)}\gamma_{11}^{m_{11}(x)}\gamma_{12}^{m_{12}(x)}\gamma_{22}^{m_{22}(x)}}$$

4.1. The algorithm for constructing the proposed experiment designs

The computer experiment design proposed in this work [referred to as the two-type marked experiment design] is generated using the following algorithm:

Algorithm.

- **Initialization step**: Choose an initial configuration (experiment design) $\left(X_0 = x \text{ or } x = (x_1, x_2, \ldots, x_n) \text{ and } x \in [0,1]^k\right)$ according to a given probability distribution, for example, the uniform distribution**.**
- **Iteration step:**

For $N = 1, 2, \cdots, N_{MCMC}$

For each configuration x Sample y using the spin flop dynamic:

- Choose a spin s uniformly at random from $\{1, \cdots, n\}$.
- Simulate an experiment y_j according to the uniform distribution on $[0,1]^p$.
- We then take this as the new configuration: $y = \left(x_1, x_2, \ldots x_{s-1}, y_j, x_{s+1} \ldots, x_n\right)$.

End.

- Calculation of the acceptance probability :

$$a(x, y) = \min\left(1; \beta_1^{m_1(y)-m_1(x)} \beta_2^{m_2(y)-m_2(x)} \gamma_{11}^{m_{11}(y)-m_{11}(x)} \gamma_{12}^{m_{12}(y)-m_{12}(x)} \gamma_{22}^{m_{22}(y)-m_{22}(x)}\right).$$

- Take $x = \begin{cases} y & \text{with a probability :} \quad a \\ x & \text{with a probability :} \quad 1-a \end{cases}$

Repeat these last two steps n times for each iteration N.

Take $X_N = x$

End.

For $N = 1000$, Figure 1 shows the convergence towards a configuration that characterizes the realization of a two-marked Strauss point process from an initial configuration of 50 points chosen uniformly in $[0,1]^2$:

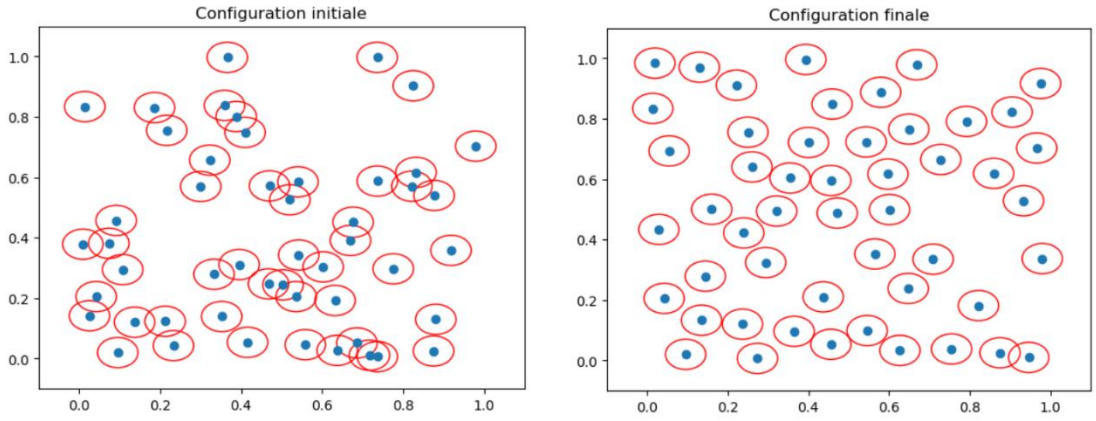


FIGURE 1.On the left, represents an initial configuration of 50 points, and on the right, a final configuration for $\gamma_{11} = 0.01$, $\gamma_{12} = 0.01$, $\gamma_{22} = 0.05$, $\beta_1 = 0.9$, $\beta_2 = 1.5$ and $r = 0.1$.

The interactions between the experiments will be represented in Figure 1 by drawing circles with a radius of $r/2$. When two circles intersect, it indicates a specific interaction between those experiments. If the radius r is too small, the distribution shows no interactions.

Conversely, if the radius is too large, the distribution exhibits clusters. Therefore, it is important to choose an appropriate radius to avoid such issues.

5. Convergence study

For each iteration N of the construction algorithm described above, we perform n basic transformations. Therefore, the chain of experimental designs $\left(X_N\right)_{N\geq 0}$ generated in this way is the realization of a Markov chain with the transition kernel:

$$P\left(x,y\right)=P_{MH}^{n}\left(x,y\right)$$

At this point, the fundamental question is whether the chain converges to the distribution $\pi(x)$ defined in (3.1).The chain converges to the invariant distribution π if: $P^t\left(x,A\right)\underset{t\to\infty}{\to}\pi\left(A\right)$ .Where A is a Borel set from A , and $P^t\left(x,A\right)=p(X_t=A/X_0=x)$ is a transition kernel at time t. Let's state the main result of interest here:

Proposition 5.1. On a finite space, the transition kernel P of the Markov chain $\left(X_N\right)_{N\geq 0}$ obtained from the construction algorithm is positive recurrent, π-stationary, aperiodic, and primitive (primitive Kernel).

Proof.

First, we proof three important properties for the kernel P_{MH} : π-reversibility, π-stationarity, and π-irreducibility.

- **The π-reversibility:**By definition, the transition P_{MH} is π-reversible if:

$$\forall x,y\in\Omega:\pi\left(x\right)P_{MH}\left(x,y\right)=\pi\left(y\right)P_{MH}\left(y,x\right)$$

Let $x\in\Omega$ and $B\in\mathrm{A}$, we have:

$$\int_{\Omega}1_{B(x,y)}\pi\left(x\right)P_{MH}\left(x,y\right)dx=\int_{\Omega}1_{B(x,y)}\pi\left(x\right)a\left(x,y\right)q\left(x,y\right)dx$$

$$+\int_{\Omega}1_{B(x,y)}\pi\left(x\right)\left[1-\int_{\Omega}a\left(x,z\right)q\left(x,z\right)dz\right]\delta_x\left(y\right)dx$$

$$=\int_{\Omega}1_{B(x,y)}\pi\left(x\right)a\left(x,y\right)q\left(x,y\right)dx$$

$$+\int_{\Omega}1_{B(x,y)}\delta_x\left(y\right)\pi\left(x\right)\left[1-\int_{\Omega}a\left(x,z\right)q\left(x,z\right)dz\right]dx$$

$$=\int_{\Omega}1_{B(x,y)}\pi\left(x\right)a\left(x,y\right)q\left(x,y\right)dx$$

$$+\int_{\Omega}1_{B(x,x)}\pi\left(x\right)\left[1-\int_{\Omega}a\left(x,z\right)q\left(x,z\right)dz\right]dx$$

And since:

$$\pi(x)a(x,y)q(x,y)=\alpha\beta_1^{m_1(x)}\beta_2^{m_2(x)}\gamma_{11}^{m_{11}(x)}\gamma_{12}^{m_{12}(x)}\gamma_{22}^{m_{22}(x)}$$

$$\times\min\left(1;\beta_1^{m_1(y)-m_1(x)}\beta_2^{m_2(y)-m_2(x)}\gamma_{11}^{m_{11}(y)-m_{11}(x)}\gamma_{12}^{m_{12}(y)-m_{12}(x)}\gamma_{22}^{m_{22}(y)-m_{22}(x)}\right)q(x,y)$$

$$=\alpha\min\left(\beta_1^{m_1(x)}\beta_2^{m_2(x)}\gamma_{11}^{m_{11}(x)}\gamma_{12}^{m_{12}(x)}\gamma_{22}^{m_{22}(x)},\beta_1^{m_1(y)}\beta_2^{m_2(y)}\gamma_{11}^{m_{11}(y)}\gamma_{12}^{m_{12}(y)}\gamma_{22}^{m_{22}(y)}\right)q(x,y)$$

$$=\alpha\beta_1^{m_1(y)}\beta_2^{m_2(y)}\gamma_{11}^{m_{11}(y)}\gamma_{12}^{m_{12}(y)}\gamma_{22}^{m_{22}(y)}$$

$$\times\min\left(\beta_1^{m_1(x)-m_1(y)}\beta_2^{m_2(x)-m_2(y)}\gamma_{11}^{m_{11}(x)-m_{11}(y)}\gamma_{12}^{m_{12}(x)-m_{12}(y)}\gamma_{22}^{m_{22}(x)-m_{22}(y)};1\right)\times q(x,y)$$

$$=\pi(y)\min\left(1;\beta_1^{m_1(x)-m_1(y)}\beta_2^{m_2(x)-m_2(y)}\gamma_{11}^{m_{11}(x)-m_{11}(y)}\gamma_{12}^{m_{12}(x)-m_{12}(y)}\gamma_{22}^{m_{22}(x)-m_{22}(y)}\right)q(x,y)$$

$$=\pi(y)a(y,x)q(x,y)$$

And since $q(x,y)=q(y,x)$, then:

$$\pi(x)a(x,y)q(x,y)=\pi(y)a(y,x)q(y,x),$$

We obtain:

$$\int_\Omega 1_{B(x,y)}\pi(x)P_{MH}(x,y)dx$$

$$=\int_\Omega 1_{B(x,y)}\pi(y)a(y,x)q(y,x)dx+\int_\Omega 1_{B(y,y)}\pi(y)\left[1-\int_\Omega a(y,z)q(y,z)dz\right]dy$$

$$=\int_\Omega 1_{B(x,y)}\pi(y)P_{MH}(y,x)dy$$

So $\pi(x)P_{MH}(x,y)=\pi(y)P_{MH}(y,x)$, and therefore, the chain is π-reversible.

- **The π-stationarity:** The transition P_{MH} is π-stationary if:

$$\forall x,y\in\Omega;A,B\in\mathrm{A}:\int_\Omega 1_{B(x,y)}\pi(x)P_{MH}(x,A)dx=\int_\Omega 1_{B(x,y)}\pi(x)dx$$

Let $x\in\Omega$ and $B\in\mathrm{A}$. We then have:

$$\int_\Omega 1_{B(x,y)}\pi(x)P_{MH}(x,y)dx=\int_\Omega 1_{B(x,y)}\pi(x)\left[\int_\Omega a(x,y)q(x,y)dy\right]dx$$

$$+\int_\Omega 1_{B(x,y)}\pi(x)\left[\int_\Omega 1-a(x,z)q(x,z)dz\right]\delta_x(y)dx$$

$$=\int_{\Omega}\int_{\Omega} 1_{B(x,y)}\pi(x)a(x,y)q(x,y)dydx+\int_{\Omega} 1_{B(x,x)}\pi(x)dx-\int_{\Omega}\int_{\Omega}\pi(x)a(x,z)q(x,z)dzdx$$

$$=\int_{\Omega} 1_{B(x,x)}\pi(x)dx$$

So, the chain admits π as a stationary distribution.

- **The π-irreducibility:** The transition P_{MH} is π-irreducible if:

$$\forall A\in \mathrm{A}, \pi(A)>0 \Rightarrow \exists t\ ,\ P_{MH}^{t}(x,A)>0$$

Let A be a Borel set from A, and for $t=1$ we have:

$$\int_{\Omega} 1_{B(x,A)}P_{MH}(x,A)dx=\int_{\Omega} 1_{B(x,A)}a(x,A)q(x,A)dx$$

$$+\int_{\Omega} 1_{B(x,A)}\left[1-\int_{\Omega} a(x,z)q(x,z)dz\right]\delta_x(A)dx$$

$$=\int_{\Omega} 1_{B(x,A)}a(x,A)q(x,A)dx+\int_{\Omega} 1_{B(x,x)}\left[1-\int_{\Omega} a(x,z)q(x,z)dz\right]dx$$

$$=\int_{\Omega} 1_{B(x,A)}a(x,A)q(x,A)dx+1-\int_{\Omega}\int_{\Omega} a(x,z)q(x,z)dzdx$$

Since: $a(x,A)=\min\left(1;\beta_1^{m_1(A)-m_1(x)}\beta_2^{m_2(A)-m_2(x)}\gamma_{11}^{m_{11}(A)-m_{11}(x)}\gamma_{12}^{m_{12}(A)-m_{12}(x)}\gamma_{22}^{m_{22}(A)-m_{22}(x)}\right)$ and $a(x,z)=\min\left(1;\beta_1^{m_1(z)-m_1(x)}\beta_2^{m_2(z)-m_2(x)}\gamma_{11}^{m_{11}(z)-m_{11}(x)}\gamma_{12}^{m_{12}(z)-m_{12}(x)}\gamma_{22}^{m_{22}(z)-m_{22}(x)}\right)$. Then we have four possible cases:

- If $a(x,A)=1$ and $a(x,z)=\beta_1^{m_1(z)-m_1(x)}\beta_2^{m_2(z)-m_2(x)}\gamma_{11}^{m_{11}(z)-m_{11}(x)}\gamma_{12}^{m_{12}(z)-m_{12}(x)}\gamma_{22}^{m_{22}(z)-m_{22}(x)}$ then:

$$\int_{\Omega} 1_{B(x,A)}P_{MH}(x,A)dx=\int_{\Omega} 1_{B(x,A)}q(x,A)dx+1$$

$$-\int_{\Omega}\int_{\Omega}\beta_1^{m_1(z)-m_1(x)}\beta_2^{m_2(z)-m_2(x)}\gamma_{11}^{m_{11}(z)-m_{11}(x)}\gamma_{12}^{m_{12}(z)-m_{12}(x)}\gamma_{22}^{m_{22}(z)-m_{22}(x)}q(x,z)dzdx$$

$$=\int_{\Omega} 1_{B(x,A)}q(x,A)dx+1$$

$$-\beta_1^{m_1(z)-m_1(x)}\beta_2^{m_2(z)-m_2(x)}\gamma_{11}^{m_{11}(z)-m_{11}(x)}\gamma_{12}^{m_{12}(z)-m_{12}(x)}\gamma_{22}^{m_{22}(z)-m_{12}(x)}>0$$

- If $a(x,z)=\beta_1^{m_1(A)-m_1(x)}\beta_2^{m_2(A)-m_2(x)}\gamma_{11}^{m_{11}(A)-m_{11}(x)}\gamma_{12}^{m_{12}(A)-m_{12}(x)}\gamma_{22}^{m_{22}(A)-m_{22}(x)}$ and $a(x,z)=1$ then:

$$\int_{\Omega} 1_{B(x,A)} P_{MH}(x,A)\,dx$$

$$= \int_{\Omega} 1_{B(x,A)} \beta_1^{m_1(A)-m_1(x)} \beta_2^{m_2(A)-m_2(x)} \gamma_{11}^{m_{11}(A)-m_{11}(x)} \gamma_{12}^{m_{12}(A)-m_{12}(x)} \gamma_{22}^{m_{22}(A)-m_{22}(x)} q(x,A)\,dx$$

$$+1 - \int_{\Omega}\int_{\Omega} q(x,z)\,dz dx$$

$$= \beta_1^{m_1(A)-m_1(x)} \beta_2^{m_2(A)-m_2(x)} \gamma_{11}^{m_{11}(A)-m_{11}(x)} \gamma_{12}^{m_{12}(A)-m_{12}(x)} \gamma_{22}^{m_{22}(A)-m_{22}(x)} \int_{\Omega} 1_{B(x,A)} q(x,A)\,dx > 0$$

– If $a(x,z) = \beta_1^{m_1(A)-m_1(x)} \beta_2^{m_2(A)-m_2(x)} \gamma_{11}^{m_{11}(A)-m_{11}(x)} \gamma_{12}^{m_{12}(A)-m_{12}(x)} \gamma_{22}^{m_{22}(A)-m_{22}(x)}$
And $a(x,z) = \beta_1^{m_1(z)-m_1(x)} \beta_2^{m_2(z)-m_2(x)} \gamma_{11}^{m_{11}(z)-m_{11}(x)} \gamma_{12}^{m_{12}(z)-m_{12}(x)} \gamma_{22}^{m_{22}(z)-m_{22}(x)}$ then:

$$\int_{\Omega} 1_{B(x,A)} P_{MH}(x,A)\,dx$$

$$= \int_{\Omega} 1_{B(x,A)} \beta_1^{m_1(A)-m_1(x)} \beta_2^{m_2(A)-m_2(x)} \gamma_{11}^{m_{11}(A)-m_{11}(x)} \gamma_{12}^{m_{12}(A)-m_{12}(x)} \gamma_{22}^{m_{22}(A)-m_{22}(x)} q(x,A)\,dx + 1$$

$$- \int_{\Omega}\int_{\Omega} \beta_1^{m_1(z)-m_1(x)} \beta_2^{m_2(z)-m_2(x)} \gamma_{11}^{m_{11}(z)-m_{11}(x)} \gamma_{12}^{m_{12}(z)-m_{12}(x)} \gamma_{22}^{m_{22}(z)-m_{22}(x)} q(x,z)\,dz dx$$

$$= \beta_1^{m_1(A)-m_1(x)} \beta_2^{m_2(A)-m_2(x)} \gamma_{11}^{m_{11}(A)-m_{11}(x)} \gamma_{12}^{m_{12}(A)-m_{12}(x)} \gamma_{22}^{m_{22}(A)-m_{22}(x)} \int_{\Omega} 1_{B(x,A)} q(x,A)\,dx + 1$$

$$- \beta_1^{m_1(z)-m_1(x)} \beta_2^{m_2(z)-m_2(x)} \gamma_{11}^{m_{11}(z)-m_{11}(x)} \gamma_{12}^{m_{12}(z)-m_{12}(x)} \gamma_{22}^{m_{22}(z)-m_{22}(x)} \int_{\Omega}\int_{\Omega} q(x,z)\,dz dx$$

$$= \beta_1^{m_1(A)-m_1(x)} \beta_2^{m_2(A)-m_2(x)} \gamma_{11}^{m_{11}(A)-m_{11}(x)} \gamma_{12}^{m_{12}(A)-m_{12}(x)} \gamma_{22}^{m_{22}(A)-m_{22}(x)} \int_{\Omega} 1_{B(x,A)} q(x,A)\,dx + 1$$

$$- \beta_1^{m_1(z)-m_1(x)} \beta_2^{m_2(z)-m_2(x)} \gamma_{11}^{m_{11}(z)-m_{11}(x)} \gamma_{12}^{m_{12}(z)-m_{12}(x)} \gamma_{22}^{m_{22}(z)-m_{22}(x)} > 0$$

So $\int_{\Omega} 1_{B(x,A)} P_{MH}{}^{t}(x,A)\,dx > 0 \ \forall t \geq 0$, then P_{MH} is π-irreducible.

Since π is the invariant distribution of P_{MH}, it is also an invariant distribution for P. Indeed, $\pi P_{MH} = \pi$, and by induction on the integer, $\pi P_{MH} = \pi$, we obtain:

$$\pi P_{MH} = \pi P_{MH}^2 = \pi P_{MH}^3 = \ldots = \pi P_{MH}^n = \pi$$

So, $\pi P = \pi$. By construction of $P = P_{MH}^n$, the π-irreducibility of P_{MH} implies the π-irreducibility of P. If P is π-irreducible and has an invariant distribution π, then P is positive recurrent, and π is the unique invariant distribution of P.

By construction of $P = P_{MH}^{n}$, we have $\pi P = \pi$. If P is π-irreducible and has an invariant distribution π, then P is positive recurrent, and π is the unique invariant distribution of P [8](see proposition 1).

Furthermore, the chain created by the construction algorithm will also be aperiodic as long as there exists at least one pair of configurations (x, y) such that $a(x, y) < 1$, because then we have $P(x, x) > 0$. It is quickly evident that the chain is aperiodic, as the event $X_{(N+1)} = X_{(N)}$ is possible practically at any time. Indeed, each state can be visited in two consecutive iterations, so $P^{1}(x, x) > 0$, making their period 1.

Since the chain generated by the algorithm is irreducible and aperiodic, its transition kernel P is primitive (a characterization of a primitive Markov Kernel more common in probability theory is to say that it is irreducible and aperiodic).

Theorem 5.1. The Markov chain $(X_N)_{N \geq 0}$ obtained from the proposed construction algorithm is geometrically ergodic, and its kernel P simulates a marked point process with two types of density: $\pi(x) = \alpha \beta_1^{m_1(x)} \beta_2^{m_2(x)} \gamma_{11}^{m_{11}(x)} \gamma_{12}^{m_{12}(x)} \gamma_{22}^{m_{22}(x)}$**.** In other words, vP^m converges to π as m tends to infinity, where v is the initial distribution, and we have: $\lim_{m \to \infty} \left\| vP^m - \pi \right\| = 0$

Proof.

Let v be an initial distribution, for any integer m and for all $x \in N^{lf}$, we have:

$$\left\| vP^m(x,.) - \pi \right\| = \left\| vP^m - \pi P^m \right\| \leq 2C(P^m) \leq 2\left(C(P)\right)^m$$

Where $C(P)$ is the Dobrushin contraction coefficient of P [9].

According to Proposition 1, the kernel P is primitive, so $0 \leq C(P) < 1$ [10]. (see lemma 4.2.3 p.72). Therefore, as m tends to infinity, $\left\| vP^m - \pi \right\| \underset{m \to \infty}{\to} 0$. Thus, the chain is uniformly ergodic and converges to the distribution defined in (3.1).

6. Numerical Results and Quality of the Proposed Designs

In this section, we will conduct a comparison of the point distributions in the suggested computer experiments design by employing established criteria. This evaluation aims to assess the extent to which the experimental space is effectively covered and the level of uniformity in the distribution of points.

- Minimum Distance Criterion (Mindist) [11]: aims to maximize the minimum distance between two points in the design. $Mindist = \min_{i} \min_{j \neq i} d(x_i, x_j)$

Where $d(x_i, x_j)$ is the Euclidean distance between point x_i and x_j. A higher value of Mindist should correspond to a more regular dispersion of the points in the design.

- Discrepancy criterion (Disc) [12]: The discrepancy measures the difference between the empirical distribution function of the points on the design and that of the uniform distribution. Unlike the previous two criteria, the discrepancy is not based on the distance between points. There are different measures of discrepancy. We retain the L_2-norm discrepancy.

$$Disc = \left(\frac{1}{3}\right)^p - \frac{2^{1-p}}{n}\sum_{i=1}^{n}\prod_{j=1}^{p}\left(1-\left(x_i^j\right)^2\right) + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{k=1}^{n}\prod_{j=1}^{p}\left(1-\max\left(x_i^j, x_k^j\right)\right)$$

- Coverage criterion (Cov) [13]: allows us to measure the difference between the points of the design and those of a regular grid. This criterion is zero for a regular grid. The objective is therefore to minimize it to approach a regular grid and thus ensure space-filling, without reaching it to respect a uniform distribution, particularly in projection onto the factorial axes:

$$Cov = \frac{1}{\bar{\delta}}\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\delta_i - \bar{\delta}\right)^2}$$

with $\delta_i = \min_{i\neq j}\left(d(x_i, x_j)\right)$ and $\bar{\delta} = \frac{1}{n}\sum_{i=1}^{n}\delta_i$.

- The R criterion is the ratio between the maximum and minimum distance between the points of the experimental design. For a regular grid, $R = 1$. Thus, the closer R is to 1, the closer the points are to those of a regular grid. $R = \frac{\max_{i\in\{1,..,n\}}\left(\delta_i\right)}{\min_{i\in\{1,..,n\}}\left(\delta_i\right)}$ where $\delta_i = \min_{i\neq j}\left(d(x_i, x_j)\right)$.

The table 1 presents a comparison based on the discrepancy criterion between the designs proposed in this work (denoted TMD: Two Mark Designs) and low-discrepancy sequences (Halton sequence [14], Sobol sequence [15], and Faure sequence [16], It is interesting to observe that the proposed designs have low discrepancy, comparable to that of low-discrepancy sequences.

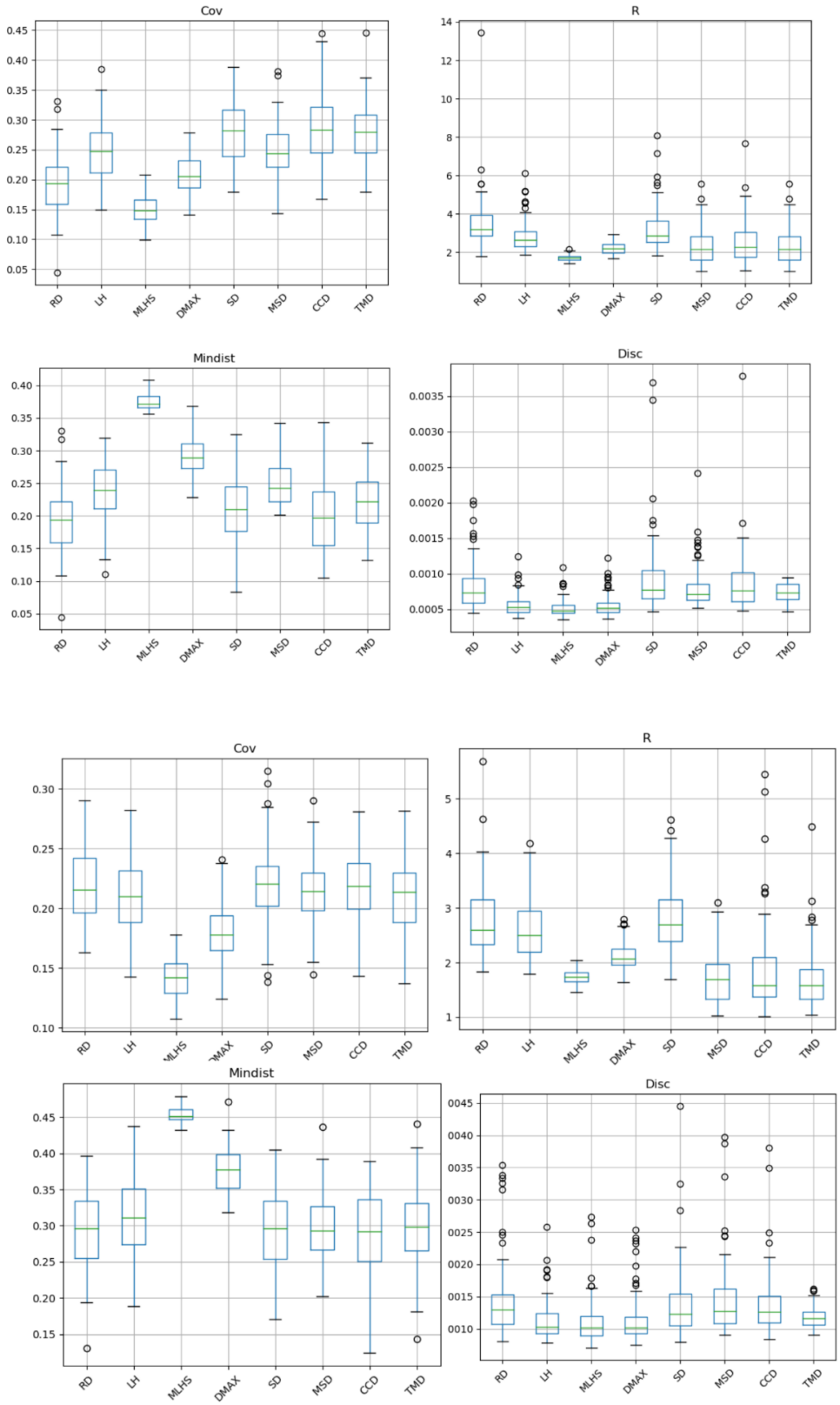
TABLE 1. The values of discrepancy for the proposed designs TMD, Halton sequences, Sobol sequences and faure sequence for different dimensions

Number of Factors	Number of Points	TMD	Halton Sequence	Sobol Sequence	Faure Sequence
4	32	0.00176	0.001779	0.000843	0.001641
7	64	0.0001207	0.00048	0.000224	0.000480
10	128	0.00000696	0.000109	0.0000605	0.000109

In this article, the constructed designs are also compared to commonly used designs incomputer experiments, with the exception of low-discrepancy sequences. In order to provide meaning to the results, the criteria were computed for 80 designs. The designs under scrutiny in this section are as follows:

- Random Designs (RD)
- Latin Hypercube Designs (LH) [17]
- Maximin Latin Hypercube Designs (mLHS) [18]
- Strauss Designs (SD) [2]
- Maximum Entropy Designs (Dmax) [19]
- Marked Strauss Designs [3]
- Connected Component Designs (CCD) [5]
- Proposed Designs (TMD).

The figures below represent the results of various criteria in the form of box plots for five and



seven dimensions:

FIGURE 2. Box plots of quality criteria calculated for 100 designs with 30 points in 5 Dimensions.

FIGURE3. Box plots of quality criteria calculated for 80 designs with 50 points in 7 dimensions.

Several remarks regarding the figures above are worth noting. Maximum entropy designs, Latin hypercube designs, maximin Latin hypercube sampling (LHS) designs, connected component designs, and two-level designs all achieved favorable results in terms of the discrepancy criterion. It is noteworthy that two-level designs are part of the aforementioned designs that also exhibit very good results according to the R-criterion.

7. Conclusion

The design of experiments method comprises a set of methods and reasoning ideas available to all experimenters seeking to plan their experiments. In this context, the use of two-type marked point processes and the Markov Chain Monte Carlo (MCMC) method allows for the construction of new computer experiment designs specified based on the law for a pairwise interaction model. This approach offers great flexibility, as one can easily manipulate this law through its representation to impose properties such as filling, for instance.

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